



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2016 – 11:40 PM EDT

PDB ID : 5LEY
Title : Human 20S proteasome complex with Oprozomib at 1.9 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 : 1.90 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

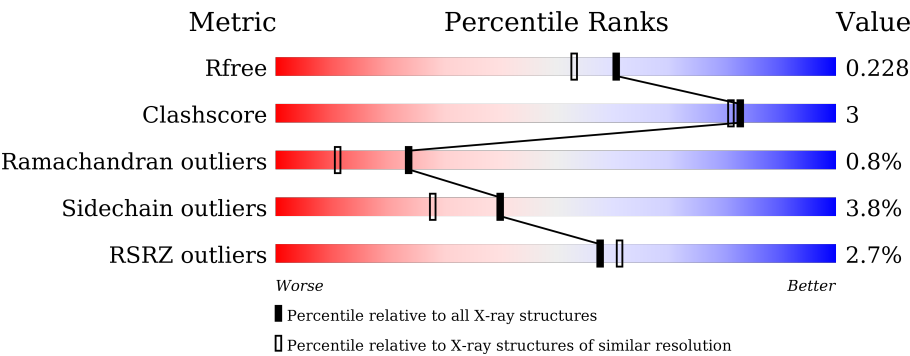
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	234	<div><div>2%</div><div>84%11%...</div></div>
1	O	234	<div><div>7%</div><div>87%8%..</div></div>
2	B	261	<div><div>3%</div><div>85%8%5%</div></div>
2	P	261	<div><div>7%</div><div>81%11%5%</div></div>
3	C	248	<div><div>6%</div><div>81%11%..</div></div>
3	Q	248	<div><div>11%</div><div>81%13%..</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	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CL	B	302	-	-	X	-
16	CL	M	301	-	-	-	X
16	CL	S	301	-	-	-	X
16	CL	b	302	-	-	-	X
19	1PE	H	306	-	-	-	X
19	1PE	I	303	-	-	-	X
19	1PE	I	304	-	-	-	X
19	1PE	L	301	-	-	-	X
19	1PE	M	305	-	-	-	X
19	1PE	W	303	-	-	-	X
7	YCM	U	137	-	-	X	-
7	6V1	U	47	X	-	-	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 51947 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	240	Total	C	N	O	S	0	0	0
			1825	1139	321	360	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	236	Total	C	N	O	S	0	3	0
			1853	1160	335	347	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
			1545	974	269	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			

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	P	1	Total Cl 1 1	0	0
16	K	4	Total Cl 4 4	0	0
16	B	2	Total Cl 2 2	0	0
16	W	1	Total Cl 1 1	0	0
16	N	3	Total Cl 3 3	0	0
16	S	3	Total Cl 3 3	0	0
16	E	3	Total Cl 3 3	0	0
16	b	4	Total Cl 4 4	0	0
16	V	2	Total Cl 2 2	0	0
16	A	4	Total Cl 4 4	0	0
16	R	2	Total Cl 2 2	0	0
16	M	4	Total Cl 4 4	0	0
16	D	2	Total Cl 2 2	0	0
16	I	1	Total Cl 1 1	0	0
16	a	3	Total Cl 3 3	0	0
16	U	1	Total Cl 1 1	0	0
16	G	2	Total Cl 2 2	0	0
16	Q	2	Total Cl 2 2	0	0
16	H	2	Total Cl 2 2	0	0
16	C	2	Total Cl 2 2	0	0
16	O	4	Total Cl 4 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	Y	5	Total 5	Cl 5	0	0
16	F	1	Total 1	Cl 1	0	0

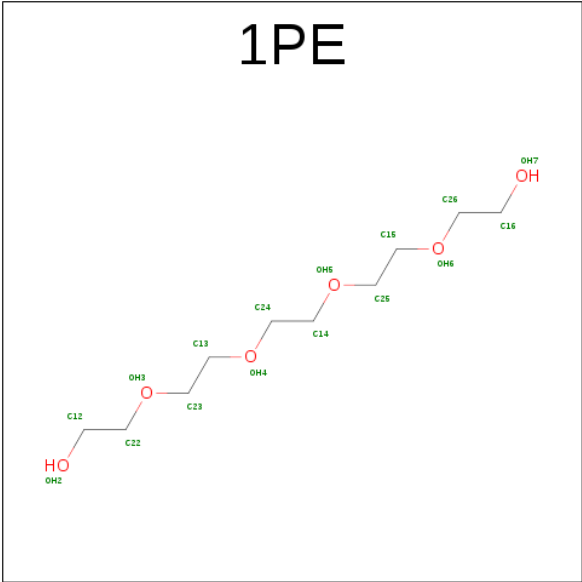
- Molecule 17 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 19 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	H	1	Total	C	O	0	0
			16	10	6		
19	H	1	Total	C	O	0	0
			16	10	6		
19	I	1	Total	C	O	0	0
			16	10	6		
19	I	1	Total	C	O	0	0
			16	10	6		
19	L	1	Total	C	O	0	0
			16	10	6		
19	M	1	Total	C	O	0	0
			16	10	6		
19	V	1	Total	C	O	0	0
			16	10	6		
19	W	1	Total	C	O	0	0
			16	10	6		
19	Z	1	Total	C	O	0	0
			16	10	6		

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	109	Total	O	0	0
			109	109		
20	B	120	Total	O	0	0
			120	120		
20	C	76	Total	O	0	0
			76	76		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	D	93	Total 93	O 93	0	0
20	E	137	Total 137	O 137	0	0
20	F	180	Total 180	O 180	0	0
20	G	187	Total 187	O 187	0	0
20	H	157	Total 157	O 157	0	0
20	I	155	Total 155	O 155	0	0
20	J	133	Total 133	O 133	0	0
20	K	98	Total 98	O 98	0	0
20	L	124	Total 124	O 124	0	0
20	M	148	Total 148	O 148	0	0
20	N	168	Total 168	O 168	0	0
20	O	89	Total 89	O 89	0	0
20	P	117	Total 117	O 117	0	0
20	Q	74	Total 74	O 74	0	0
20	R	122	Total 122	O 122	0	0
20	S	118	Total 118	O 118	0	0
20	T	92	Total 92	O 92	0	0
20	U	102	Total 102	O 102	0	0
20	V	112	Total 112	O 112	0	0
20	W	111	Total 111	O 111	0	0
20	X	124	Total 124	O 124	0	0

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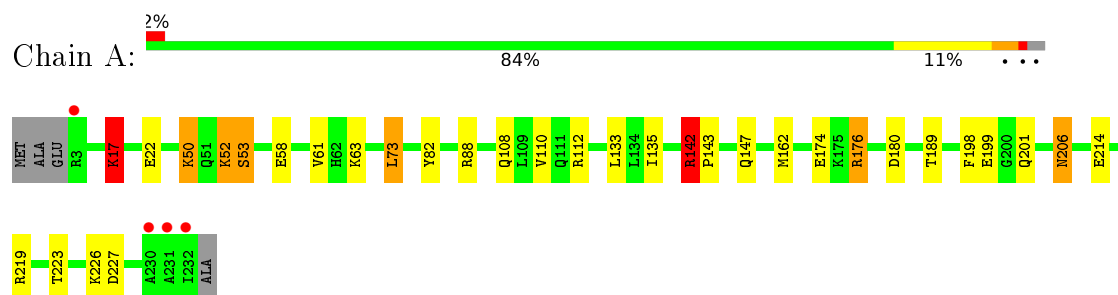
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	Y	137	Total 137	O 137	0	0
20	Z	164	Total 164	O 164	0	0
20	a	167	Total 167	O 167	0	0
20	b	126	Total 126	O 126	0	0
20	c	1	Total 1	O 1	0	0
20	d	1	Total 1	O 1	0	0

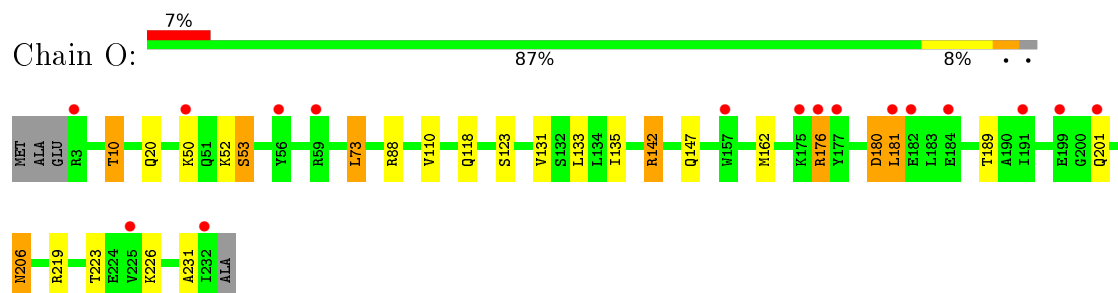
3 Residue-property plots [i](#)

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.

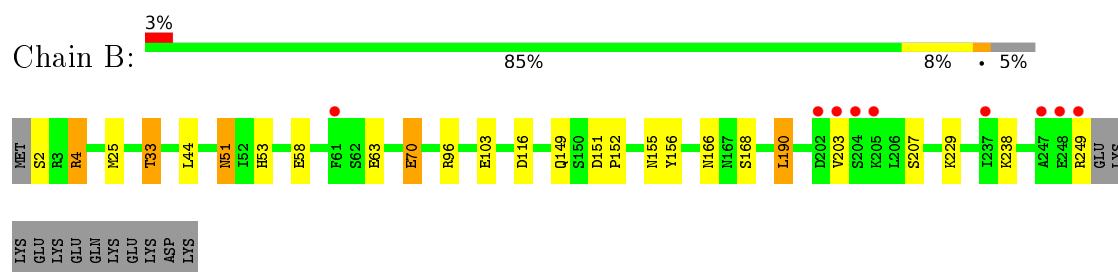
- Molecule 1: Proteasome subunit alpha type-2



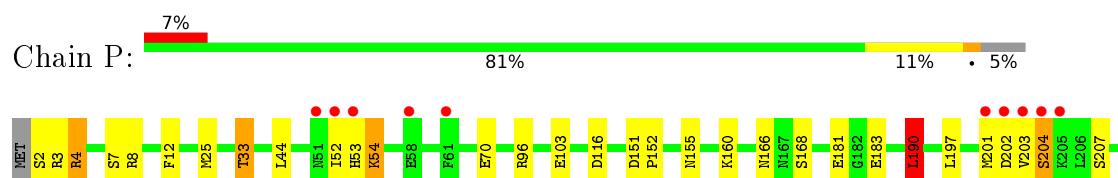
- Molecule 1: Proteasome subunit alpha type-2



- Molecule 2: Proteasome subunit alpha type-4



- Molecule 2: Proteasome subunit alpha type-4





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

• Molecule 5: Proteasome subunit alpha type-1

Chain S: 3% 79% 10% 10%

MET PHE ARG N4 D7 R18 R19 E23 V45 L46 V47 A48 L49 K50 R51 A52 Q53 S54 E55 L56 A57 A58 H59 K62 H65 D100 R101 S114 R122 Y123 S150 A151 N152 Y153 F154 R174 M180 L187 L195 R196 E234 E237 E238 R239

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

• Molecule 6: Proteasome subunit alpha type-3

Chain F: 78% 12% 6%

MET SER SER ILE GLY THR G6 D17 V30 E31 S34 R40 D43 V53 R65 D70 G74 L81 A82 D83 A84 R85 S86 L87 R89 Y104 R114 M117 C133 I151 D152 V156 R169 Q170 T174 R187 V190 V204

K205 D206 W215 E218 L219 R221 H224 V227 R232 K240 L243 K244 GLU ASP ASP ASN MET

• Molecule 6: Proteasome subunit alpha type-3

Chain T: 4% 77% 14% 6%

MET SER SER ILE GLY T5 G6 Y7 D17 V25 K26 K27 V30 E31 R32 S33 D43 V53 L54 H63 D70 G74 L81 R85 S86 L87 Y104 R110 D113 R114 M117 C133 I151 D152 V156 R169 Q170 K173 T174 Q190

V190 K191 D202 E203 V204 K205 K207 A208 F209 W215 R223 H224 D230 Y238 A239 K240 F244 GLU ASP ASP SER ASP ASP ASN MET

• Molecule 7: Proteasome subunit alpha type-6

Chain G: 2% 91% 6% ..

MET S2 R3 V42 R43 I72 C78 D86 S87 R88 E108 L114 R117 D120 E145 V151 V183 F187 D188 H189 T190 F191 E192 A198 L206 R245 ASP

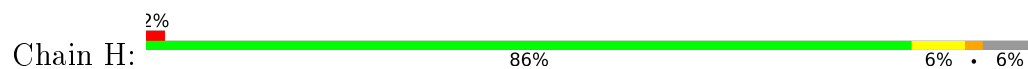
• Molecule 7: Proteasome subunit alpha type-6

Chain U: 5% 85% 9% ..

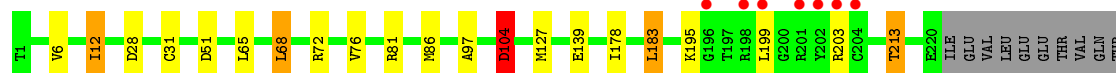
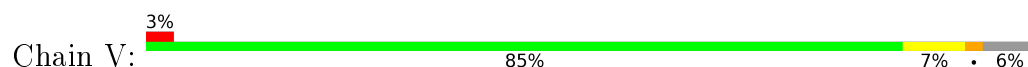
MET S2 R3 R11 V42 R43 V56 P57 D58 K59 I72 C78 V79 M80 T81 R88 V91 E108 L114 R117 D120 C137 M138 I139 L140 V151 A168 K166 PHE ASP TRP THR PHE GLU Q193 T194 V195 E196 T197 A198 I199 L206 S207 I208

P212 L239 V240 A241 L242 A243 E244 ASP

- Molecule 8: Proteasome subunit beta type-7



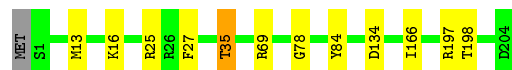
- Molecule 8: Proteasome subunit beta type-7



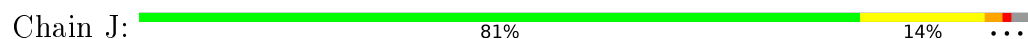
- Molecule 9: Proteasome subunit beta type-3



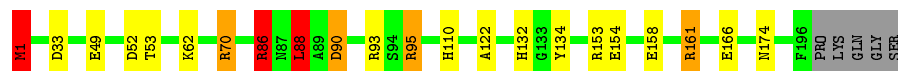
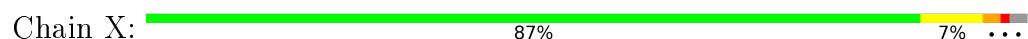
- Molecule 9: Proteasome subunit beta type-3




- Molecule 10: Proteasome subunit beta type-2



- Molecule 10: Proteasome subunit beta type-2



- Molecule 11: Proteasome subunit beta type-5

Chain K:  85% 11% ..



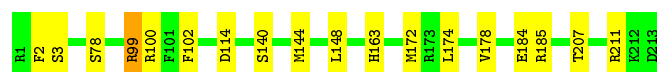
- Molecule 11: Proteasome subunit beta type-5

Chain Y:  85% 11% ..



- Molecule 12: Proteasome subunit beta type-1

Chain L:  92% 8%



- Molecule 12: Proteasome subunit beta type-1

Chain Z:  93% 7%




- Molecule 13: Proteasome subunit beta type-4

Chain M:  89% 9% .



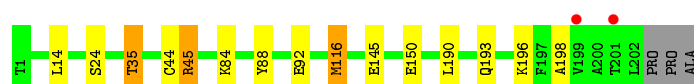
- Molecule 13: Proteasome subunit beta type-4

Chain a:  91% 7% .



- Molecule 14: Proteasome subunit beta type-6

Chain N:  91% 6% ..



- Molecule 14: Proteasome subunit beta type-6

Chain b:  94% 5% •



- 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.

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.39Å 202.65Å 315.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	170.45 – 1.90 106.69 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.8 (170.45-1.90) 97.8 (106.69-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.188 , 0.225 0.195 , 0.228	Depositor DCC
R_{free} test set	27607 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	51947	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% 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, CL, K, 6V1, 1PE, OAS, YCM, 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	0.92	2/1833 (0.1%)	0.94	5/2489 (0.2%)
1	O	0.81	1/1778 (0.1%)	0.92	7/2419 (0.3%)
2	B	0.99	4/1958 (0.2%)	1.01	6/2645 (0.2%)
2	P	0.89	2/1934 (0.1%)	0.96	7/2617 (0.3%)
3	C	0.95	2/1818 (0.1%)	1.05	8/2469 (0.3%)
3	Q	0.91	1/1839 (0.1%)	1.01	6/2497 (0.2%)
4	D	0.95	3/1789 (0.2%)	0.97	5/2424 (0.2%)
4	R	1.06	2/1780 (0.1%)	1.05	6/2408 (0.2%)
5	E	0.94	2/1842 (0.1%)	1.00	7/2493 (0.3%)
5	S	0.92	1/1878 (0.1%)	0.97	5/2541 (0.2%)
6	F	1.09	5/1935 (0.3%)	1.16	26/2605 (1.0%)
6	T	1.00	3/1894 (0.2%)	1.11	16/2556 (0.6%)
7	G	1.09	2/1909 (0.1%)	0.98	7/2579 (0.3%)
7	U	0.92	2/1804 (0.1%)	0.95	7/2441 (0.3%)
8	H	1.05	1/1697 (0.1%)	1.17	11/2299 (0.5%)
8	V	0.88	2/1655 (0.1%)	1.01	8/2251 (0.4%)
9	I	1.03	2/1648 (0.1%)	1.24	14/2219 (0.6%)
9	W	0.84	1/1630 (0.1%)	1.11	12/2197 (0.5%)
10	J	1.06	1/1613 (0.1%)	1.28	14/2180 (0.6%)
10	X	0.97	2/1599 (0.1%)	1.24	13/2163 (0.6%)
11	K	1.01	2/1576 (0.1%)	1.11	12/2131 (0.6%)
11	Y	1.10	4/1610 (0.2%)	1.20	14/2172 (0.6%)
12	L	0.93	3/1672 (0.2%)	1.05	6/2257 (0.3%)
12	Z	1.09	4/1675 (0.2%)	1.11	6/2257 (0.3%)
13	M	1.04	2/1728 (0.1%)	1.06	7/2339 (0.3%)
13	a	1.09	3/1724 (0.2%)	1.07	8/2336 (0.3%)
14	N	1.13	4/1548 (0.3%)	1.00	4/2095 (0.2%)
14	b	1.08	3/1554 (0.2%)	1.00	5/2104 (0.2%)
All	All	0.99	66/48920 (0.1%)	1.06	252/66183 (0.4%)

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	5
3	C	0	1
3	Q	0	2
4	D	0	5
4	R	0	2
5	E	0	1
6	T	0	1
7	U	1	0
9	I	0	1
9	W	0	1
10	J	0	2
10	X	0	2
12	L	0	1
12	Z	0	1
13	a	0	1
All	All	1	26

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	108	GLU	CD-OE1	13.81	1.40	1.25
14	N	150	GLU	CG-CD	11.07	1.68	1.51
12	Z	3	SER	CB-OG	10.22	1.55	1.42
13	a	75	GLU	CD-OE1	10.04	1.36	1.25
14	b	150	GLU	CG-CD	9.59	1.66	1.51

The worst 5 of 252 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	X	86	ARG	NE-CZ-NH2	-21.50	109.55	120.30
10	J	86	ARG	NE-CZ-NH2	-21.33	109.63	120.30
10	J	86	ARG	NE-CZ-NH1	20.61	130.60	120.30
10	X	86	ARG	NE-CZ-NH1	18.78	129.69	120.30
9	I	69	ARG	NE-CZ-NH1	17.32	128.96	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

5 of 26 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	237	GLU	Peptide
4	D	127	ASP	Peptide
4	D	175[A]	GLU	Peptide
4	D	175[B]	GLU	Mainchain,Peptide
4	D	223	GLY	Peptide

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	1788	0	1761	16	0
1	O	1741	0	1683	8	0
2	B	1922	0	1913	9	0
2	P	1898	0	1861	15	0
3	C	1798	0	1718	20	0
3	Q	1825	0	1751	17	0
4	D	1762	0	1709	9	0
4	R	1753	0	1726	12	0
5	E	1822	0	1779	12	0
5	S	1853	0	1796	24	0
6	F	1888	0	1882	12	0
6	T	1856	0	1816	14	0
7	G	1912	0	1882	7	0
7	U	1815	0	1748	20	0
8	H	1664	0	1681	8	0
8	V	1622	0	1595	6	0
9	I	1613	0	1646	10	0
9	W	1599	0	1621	4	0
10	J	1590	0	1581	19	0
10	X	1576	0	1561	12	0
11	K	1545	0	1495	7	0
11	Y	1570	0	1547	12	0
12	L	1636	0	1625	5	0
12	Z	1642	0	1635	5	0
13	M	1692	0	1670	8	0
13	a	1688	0	1658	0	0
14	N	1519	0	1496	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	b	1524	0	1496	0	0
15	c	37	0	6	0	0
15	d	37	0	6	0	0
16	A	4	0	0	1	0
16	B	2	0	0	2	0
16	C	2	0	0	1	0
16	D	2	0	0	0	0
16	E	3	0	0	0	0
16	F	1	0	0	0	0
16	G	2	0	0	0	0
16	H	2	0	0	1	0
16	I	1	0	0	0	0
16	K	4	0	0	0	0
16	M	4	0	0	1	0
16	N	3	0	0	0	0
16	O	4	0	0	0	0
16	P	1	0	0	0	0
16	Q	2	0	0	1	0
16	R	2	0	0	1	0
16	S	3	0	0	0	0
16	U	1	0	0	0	0
16	V	2	0	0	0	0
16	W	1	0	0	0	0
16	Y	5	0	0	0	0
16	a	3	0	0	0	0
16	b	4	0	0	0	0
17	G	1	0	0	0	0
17	L	1	0	0	0	0
17	N	1	0	0	0	0
17	U	1	0	0	0	0
17	Z	1	0	0	0	0
17	b	1	0	0	0	0
18	H	2	0	0	0	0
18	I	2	0	0	0	0
18	J	1	0	0	0	0
18	K	1	0	0	0	0
18	L	1	0	0	0	0
18	V	1	0	0	0	0
18	W	1	0	0	0	0
18	X	1	0	0	0	0
19	H	32	0	44	0	0
19	I	32	0	44	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	L	16	0	22	0	0
19	M	16	0	22	1	0
19	V	16	0	22	1	0
19	W	16	0	22	0	0
19	Z	16	0	22	0	0
20	A	109	0	0	4	0
20	B	120	0	0	0	0
20	C	76	0	0	1	0
20	D	93	0	0	3	0
20	E	137	0	0	2	0
20	F	180	0	0	4	0
20	G	187	0	0	4	0
20	H	157	0	0	4	0
20	I	155	0	0	1	0
20	J	133	0	0	2	0
20	K	98	0	0	0	0
20	L	124	0	0	0	0
20	M	148	0	0	1	0
20	N	168	0	0	0	0
20	O	89	0	0	1	0
20	P	117	0	0	2	0
20	Q	74	0	0	1	0
20	R	122	0	0	2	0
20	S	118	0	0	4	0
20	T	92	0	0	2	0
20	U	102	0	0	1	0
20	V	112	0	0	2	0
20	W	111	0	0	1	0
20	X	124	0	0	3	0
20	Y	137	0	0	0	0
20	Z	164	0	0	0	0
20	a	167	0	0	0	0
20	b	126	0	0	0	0
20	c	1	0	0	0	0
20	d	1	0	0	0	0
All	All	51947	0	47542	279	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 3.

The worst 5 of 279 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)
10:J:1[A]:MET:HE1	10:J:134:TYR:H	1.25	0.99
10:X:1:MET:HE1	10:X:134:TYR:H	1.30	0.96
5:S:65[A]:HIS:CE1	20:S:404:HOH:O	2.27	0.87
16:R:301:CL:CL	20:R:506:HOH:O	2.29	0.86
5:E:47:VAL:HG12	5:E:195:LEU:HD22	1.60	0.84

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	231/234 (99%)	219 (95%)	7 (3%)	5 (2%)	8	1
1	O	228/234 (97%)	217 (95%)	5 (2%)	6 (3%)	7	1
2	B	248/261 (95%)	238 (96%)	8 (3%)	2 (1%)	24	11
2	P	247/261 (95%)	232 (94%)	12 (5%)	3 (1%)	16	5
3	C	236/248 (95%)	220 (93%)	9 (4%)	7 (3%)	5	1
3	Q	237/248 (96%)	221 (93%)	6 (2%)	10 (4%)	3	0
4	D	232/241 (96%)	223 (96%)	6 (3%)	3 (1%)	15	4
4	R	232/241 (96%)	221 (95%)	7 (3%)	4 (2%)	11	2
5	E	232/263 (88%)	225 (97%)	6 (3%)	1 (0%)	39	27
5	S	236/263 (90%)	228 (97%)	7 (3%)	1 (0%)	39	27
6	F	241/255 (94%)	239 (99%)	2 (1%)	0	100	100
6	T	239/255 (94%)	232 (97%)	4 (2%)	3 (1%)	15	4
7	G	241/246 (98%)	237 (98%)	4 (2%)	0	100	100
7	U	232/246 (94%)	227 (98%)	4 (2%)	1 (0%)	39	27
8	H	220/234 (94%)	217 (99%)	3 (1%)	0	100	100
8	V	220/234 (94%)	216 (98%)	3 (1%)	1 (0%)	34	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	205/205 (100%)	201 (98%)	4 (2%)	0	100	100
9	W	204/205 (100%)	198 (97%)	6 (3%)	0	100	100
10	J	195/201 (97%)	193 (99%)	2 (1%)	0	100	100
10	X	195/201 (97%)	193 (99%)	2 (1%)	0	100	100
11	K	198/204 (97%)	195 (98%)	3 (2%)	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%)	209 (97%)	6 (3%)	0	100	100
13	a	216/219 (99%)	208 (96%)	8 (4%)	0	100	100
14	N	201/205 (98%)	198 (98%)	2 (1%)	1 (0%)	34	21
14	b	202/205 (98%)	200 (99%)	1 (0%)	1 (0%)	34	21
All	All	6208/6458 (96%)	6025 (97%)	134 (2%)	49 (1%)	24	11

5 of 49 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	LYS
1	A	52	LYS
1	A	53	SER
3	C	50	VAL
3	C	216	SER

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%)	173 (94%)	12 (6%)	21	10
1	O	176/191 (92%)	164 (93%)	12 (7%)	20	9
2	B	199/221 (90%)	190 (96%)	9 (4%)	34	21
2	P	196/221 (89%)	183 (93%)	13 (7%)	21	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	179/210 (85%)	169 (94%)	10 (6%)	26	14
3	Q	184/210 (88%)	175 (95%)	9 (5%)	31	18
4	D	189/203 (93%)	182 (96%)	7 (4%)	41	29
4	R	187/203 (92%)	184 (98%)	3 (2%)	70	66
5	E	192/223 (86%)	183 (95%)	9 (5%)	32	20
5	S	195/223 (87%)	191 (98%)	4 (2%)	61	55
6	F	199/212 (94%)	188 (94%)	11 (6%)	27	14
6	T	192/212 (91%)	181 (94%)	11 (6%)	25	13
7	G	202/207 (98%)	196 (97%)	6 (3%)	48	38
7	U	186/207 (90%)	182 (98%)	4 (2%)	60	53
8	H	181/195 (93%)	174 (96%)	7 (4%)	39	27
8	V	172/195 (88%)	162 (94%)	10 (6%)	25	13
9	I	176/174 (101%)	174 (99%)	2 (1%)	80	79
9	W	173/174 (99%)	172 (99%)	1 (1%)	90	90
10	J	166/170 (98%)	158 (95%)	8 (5%)	31	19
10	X	165/170 (97%)	159 (96%)	6 (4%)	42	30
11	K	154/159 (97%)	143 (93%)	11 (7%)	18	8
11	Y	158/159 (99%)	150 (95%)	8 (5%)	29	17
12	L	175/178 (98%)	169 (97%)	6 (3%)	44	33
12	Z	175/178 (98%)	172 (98%)	3 (2%)	68	64
13	M	180/181 (99%)	177 (98%)	3 (2%)	68	64
13	a	178/181 (98%)	173 (97%)	5 (3%)	51	41
14	N	158/159 (99%)	154 (98%)	4 (2%)	55	47
14	b	158/159 (99%)	155 (98%)	3 (2%)	65	59
All	All	5030/5366 (94%)	4833 (96%)	197 (4%)	40	27

5 of 197 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	187	VAL
1	O	176	ARG
11	Y	141[A]	ARG
11	K	200	SER
13	M	216	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	162	GLN
2	P	40	ASN
12	Z	79	ASN
14	N	193	GLN
1	O	62	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

18 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	1.04	0	5,10,12	1.65	1 (20%)
5	6V1	E	148	5	11,15,16	1.22	2 (18%)	11,20,22	1.76	4 (36%)
7	YCM	G	137	7	7,9,10	3.06	4 (57%)	5,10,12	4.08	2 (40%)
7	6V1	G	161	7	11,15,16	1.44	3 (27%)	11,20,22	3.20	8 (72%)
7	6V1	G	47	7	11,15,16	1.97	4 (36%)	11,20,22	3.61	4 (36%)
10	6V1	J	91	10	11,15,16	1.85	2 (18%)	11,20,22	4.92	7 (63%)
3	YCM	Q	63	3	7,9,10	1.86	2 (28%)	5,10,12	2.88	3 (60%)
5	6V1	S	148	5	11,15,16	1.62	4 (36%)	11,20,22	1.83	3 (27%)
7	YCM	U	137	7	7,9,10	2.63	2 (28%)	5,10,12	5.29	3 (60%)
7	6V1	U	161	7	11,15,16	1.33	2 (18%)	11,20,22	2.86	7 (63%)
7	6V1	U	47	7	11,15,16	1.36	2 (18%)	11,20,22	3.52	4 (36%)
10	6V1	X	91	10	11,15,16	1.95	4 (36%)	11,20,22	5.34	6 (54%)
15	6V9	c	1	15	6,8,9	0.76	0	2,10,12	3.34	1 (50%)
15	OAS	c	2	15	4,6,9	0.55	0	2,6,11	1.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	OAS	c	3	15	4,6,9	0.85	0	2,6,11	1.32	0
15	6V9	d	1	15	6,8,9	0.65	0	2,10,12	4.75	1 (50%)
15	OAS	d	2	15	4,6,9	1.03	0	2,6,11	3.37	1 (50%)
15	OAS	d	3	15	4,6,9	0.76	0	2,6,11	1.46	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

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	137	YCM	CB-SG	-5.76	1.70	1.81
7	U	137	YCM	CB-SG	-5.60	1.70	1.81
10	J	91	6V1	C1-SG	-4.63	1.77	1.83
3	Q	63	YCM	CD-SG	-4.16	1.72	1.81
7	G	47	6V1	C2-N3	-3.97	1.33	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	47	6V1	C5-C1-C2	-9.84	96.49	103.98
15	d	1	6V9	O1-C4-C3	-6.66	118.90	124.47
10	X	91	6V1	C6-N3-C4	-5.76	117.11	123.24
7	G	161	6V1	C5-C1-C2	-5.65	99.68	103.98
10	J	91	6V1	C6-N3-C4	-5.57	117.31	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.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	U	137	YCM	6	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 83 ligands modelled in this entry, 74 are monoatomic - leaving 9 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	$\# Z > 2$
19	1PE	H	305	-	15,15,15	0.60	0	14,14,14	0.67	0
19	1PE	H	306	-	15,15,15	0.61	0	14,14,14	0.50	0
19	1PE	I	303	-	15,15,15	0.57	0	14,14,14	1.02	1 (7%)
19	1PE	I	304	-	15,15,15	0.57	0	14,14,14	0.93	1 (7%)
19	1PE	L	301	-	15,15,15	0.64	0	14,14,14	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	1PE	M	305	-	15,15,15	0.58	0	14,14,14	0.38	0
19	1PE	V	304	-	15,15,15	0.78	0	14,14,14	0.84	1 (7%)
19	1PE	W	303	-	15,15,15	0.67	0	14,14,14	0.46	0
19	1PE	Z	301	-	15,15,15	0.66	0	14,14,14	0.59	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
19	1PE	H	305	-	-	0/13/13/13	0/0/0/0
19	1PE	H	306	-	-	0/13/13/13	0/0/0/0
19	1PE	I	303	-	-	0/13/13/13	0/0/0/0
19	1PE	I	304	-	-	0/13/13/13	0/0/0/0
19	1PE	L	301	-	-	0/13/13/13	0/0/0/0
19	1PE	M	305	-	-	0/13/13/13	0/0/0/0
19	1PE	V	304	-	-	0/13/13/13	0/0/0/0
19	1PE	W	303	-	-	0/13/13/13	0/0/0/0
19	1PE	Z	301	-	-	0/13/13/13	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	I	304	1PE	OH6-C15-C25	-2.30	100.20	110.40
19	V	304	1PE	OH5-C25-C15	2.03	119.42	110.40
19	I	303	1PE	C25-OH5-C14	2.46	123.82	113.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	I	303	1PE	1	0
19	M	305	1PE	1	0
19	V	304	1PE	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	230/234 (98%)	-0.01	4 (1%) 73 76	30, 47, 80, 96	0
1	O	230/234 (98%)	0.39	16 (6%) 19 21	40, 62, 100, 123	0
2	B	248/261 (95%)	0.07	9 (3%) 46 50	34, 49, 89, 136	0
2	P	247/261 (94%)	0.30	17 (6%) 20 22	39, 58, 99, 134	0
3	C	236/248 (95%)	0.41	14 (5%) 26 29	34, 59, 102, 140	0
3	Q	239/248 (96%)	0.67	28 (11%) 6 7	35, 63, 118, 149	0
4	D	233/241 (96%)	0.29	10 (4%) 39 42	36, 56, 86, 121	0
4	R	233/241 (96%)	-0.00	5 (2%) 67 70	33, 44, 67, 92	0
5	E	233/263 (88%)	0.16	11 (4%) 35 38	29, 42, 87, 105	0
5	S	235/263 (89%)	0.10	7 (2%) 54 57	34, 48, 81, 106	0
6	F	239/255 (93%)	-0.02	0 100 100	26, 36, 57, 75	0
6	T	240/255 (94%)	0.27	9 (3%) 44 48	35, 51, 85, 110	0
7	G	241/246 (97%)	0.05	4 (1%) 73 76	27, 40, 74, 106	0
7	U	235/246 (95%)	0.37	13 (5%) 29 32	41, 59, 93, 129	0
8	H	220/234 (94%)	0.07	4 (1%) 71 74	28, 37, 68, 100	0
8	V	220/234 (94%)	0.05	7 (3%) 51 54	38, 49, 81, 103	0
9	I	204/205 (99%)	-0.08	0 100 100	29, 37, 58, 73	0
9	W	204/205 (99%)	-0.06	0 100 100	37, 49, 71, 78	0
10	J	195/201 (97%)	-0.11	1 (0%) 91 92	29, 40, 57, 70	0
10	X	195/201 (97%)	-0.13	0 100 100	33, 42, 56, 69	0
11	K	200/204 (98%)	-0.03	1 (0%) 91 92	33, 44, 68, 83	0
11	Y	199/204 (97%)	-0.08	1 (0%) 91 92	27, 36, 58, 69	0
12	L	213/213 (100%)	-0.00	0 100 100	33, 48, 70, 85	0
12	Z	213/213 (100%)	-0.06	0 100 100	28, 38, 60, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	216/219 (98%)	0.02	1 (0%) 91 92	27, 39, 61, 89	0
13	a	216/219 (98%)	-0.06	1 (0%) 91 92	29, 40, 61, 81	0
14	N	202/205 (98%)	-0.02	2 (0%) 84 86	27, 35, 55, 87	0
14	b	203/205 (99%)	-0.07	1 (0%) 91 92	32, 40, 66, 96	0
15	c	0/4	-	-	-	-
15	d	0/4	-	-	-	-
All	All	6219/6466 (96%)	0.10	166 (2%) 58 61	26, 45, 84, 149	0

The worst 5 of 166 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	204	SER	15.2
1	O	232	ILE	10.8
4	D	241	ILE	10.0
3	Q	232	ILE	8.3
5	E	54	SER	8.2

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

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	6V9	d	1	8/9	0.99	0.09	-	33,33,35,36	0
10	6V1	J	91	15/16	0.93	0.19	-	33,51,56,57	0
5	6V1	S	148	15/16	0.94	0.16	-	37,61,67,67	0
3	YCM	C	63	10/11	0.90	0.10	-	52,53,61,61	0
7	6V1	U	47	15/16	0.83	0.28	-	73,107,113,116	0
7	6V1	G	47	15/16	0.95	0.16	-	38,57,61,61	0
15	OAS	d	3	7/10	0.98	0.10	-	27,28,29,30	0
5	6V1	E	148	15/16	0.93	0.14	-	33,49,59,60	0
7	YCM	U	137	10/11	0.85	0.24	-	51,60,74,76	0
7	YCM	G	137	10/11	0.92	0.10	-	31,40,53,56	0
7	6V1	U	161	15/16	0.93	0.13	-	53,71,79,80	0
7	6V1	G	161	15/16	0.96	0.12	-	33,51,58,61	0
15	OAS	c	2	7/10	0.96	0.12	-	34,37,41,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	YCM	Q	63	10/11	0.92	0.10	-	52,54,64,65	0
10	6V1	X	91	15/16	0.91	0.20	-	35,54,58,65	0
15	6V9	c	1	8/9	0.98	0.08	-	38,39,41,42	0
15	OAS	d	2	7/10	0.97	0.13	-	27,30,37,40	0
15	OAS	c	3	7/10	0.98	0.12	-	35,35,38,38	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
16	CL	S	301	1/1	0.96	0.29	9.71	65,65,65,65	0
19	1PE	I	304	16/16	0.82	0.22	9.46	53,62,77,81	0
19	1PE	M	305	16/16	0.79	0.24	9.17	70,73,87,90	0
16	CL	M	301	1/1	0.96	0.21	8.91	57,57,57,57	0
19	1PE	H	306	16/16	0.87	0.24	5.83	55,66,88,88	0
16	CL	b	302	1/1	0.96	0.14	3.26	62,62,62,62	0
19	1PE	L	301	16/16	0.84	0.13	3.06	53,64,70,71	0
19	1PE	I	303	16/16	0.89	0.14	2.67	50,55,61,67	0
19	1PE	W	303	16/16	0.87	0.12	2.01	52,61,70,71	0
19	1PE	Z	301	16/16	0.89	0.12	1.36	53,61,66,66	0
19	1PE	H	305	16/16	0.92	0.13	1.07	39,53,62,62	0
18	MG	H	302	1/1	0.99	0.11	1.03	34,34,34,34	0
19	1PE	V	304	16/16	0.90	0.12	0.91	44,54,78,83	0
16	CL	a	301	1/1	0.96	0.12	0.89	60,60,60,60	0
16	CL	D	301	1/1	0.92	0.15	0.67	66,66,66,66	0
18	MG	I	301	1/1	0.96	0.10	0.60	34,34,34,34	0
16	CL	Q	302	1/1	0.93	0.14	0.50	63,63,63,63	0
16	CL	U	301	1/1	0.98	0.11	-0.15	54,54,54,54	0
16	CL	M	302	1/1	0.94	0.11	-0.19	61,61,61,61	0
16	CL	E	301	1/1	0.99	0.11	-0.28	57,57,57,57	0
16	CL	N	301	1/1	0.97	0.10	-0.47	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
16	CL	G	301	1/1	0.98	0.10	-0.60	46,46,46,46	0
16	CL	B	302	1/1	0.97	0.10	-0.61	57,57,57,57	0
16	CL	S	302	1/1	0.96	0.08	-0.94	62,62,62,62	0
16	CL	b	304	1/1	0.97	0.08	-1.11	51,51,51,51	0
16	CL	b	303	1/1	0.97	0.09	-1.23	51,51,51,51	0
16	CL	A	304	1/1	0.98	0.09	-1.26	56,56,56,56	0
16	CL	E	303	1/1	0.98	0.07	-1.42	57,57,57,57	0
16	CL	A	301	1/1	0.97	0.06	-1.59	48,48,48,48	0
16	CL	F	301	1/1	0.98	0.06	-1.99	51,51,51,51	0
16	CL	O	301	1/1	0.95	0.07	-2.09	55,55,55,55	0
17	K	b	305	1/1	0.96	0.06	-2.32	46,46,46,46	0
18	MG	L	303	1/1	0.97	0.07	-2.35	39,39,39,39	0
16	CL	Y	303	1/1	0.95	0.04	-2.42	67,67,67,67	0
17	K	N	304	1/1	0.99	0.06	-2.80	41,41,41,41	0
16	CL	K	303	1/1	0.97	0.04	-2.81	69,69,69,69	0
18	MG	K	301	1/1	0.98	0.05	-3.31	35,35,35,35	0
16	CL	Y	304	1/1	0.95	0.06	-3.33	56,56,56,56	0
17	K	Z	302	1/1	0.99	0.06	-3.33	42,42,42,42	0
18	MG	W	301	1/1	0.93	0.07	-3.89	38,38,38,38	0
16	CL	S	303	1/1	0.97	0.05	-4.20	53,53,53,53	0
17	K	L	302	1/1	0.97	0.05	-4.59	50,50,50,50	0
16	CL	N	303	1/1	0.96	0.06	-4.69	47,47,47,47	0
18	MG	I	305	1/1	0.97	0.07	-4.76	30,30,30,30	0
17	K	U	302	1/1	0.97	0.04	-5.32	42,42,42,42	0
17	K	G	303	1/1	0.99	0.06	-9.45	35,35,35,35	0
16	CL	C	301	1/1	0.92	0.12	-	60,60,60,60	0
16	CL	P	301	1/1	0.96	0.06	-	52,52,52,52	0
16	CL	K	304	1/1	0.95	0.18	-	60,60,60,60	0
16	CL	I	302	1/1	0.97	0.08	-	44,44,44,44	0
16	CL	V	303	1/1	0.90	0.07	-	59,59,59,59	0
16	CL	C	302	1/1	0.96	0.12	-	62,62,62,62	0
16	CL	K	302	1/1	0.97	0.08	-	38,38,38,38	0
16	CL	D	302	1/1	0.95	0.14	-	61,61,61,61	0
18	MG	X	301	1/1	0.97	0.03	-	53,53,53,53	0
16	CL	B	301	1/1	0.96	0.08	-	41,41,41,41	0
18	MG	H	301	1/1	0.96	0.04	-	45,45,45,45	0
16	CL	N	302	1/1	0.98	0.07	-	47,47,47,47	0
18	MG	V	301	1/1	0.95	0.07	-	53,53,53,53	0
18	MG	J	301	1/1	0.96	0.04	-	51,51,51,51	0
16	CL	E	302	1/1	0.97	0.07	-	51,51,51,51	0
16	CL	a	302	1/1	0.97	0.08	-	47,47,47,47	0
16	CL	Y	305	1/1	0.95	0.17	-	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	CL	b	301	1/1	0.95	0.07	-	48,48,48,48	0
16	CL	V	302	1/1	0.88	0.08	-	56,56,56,56	0
16	CL	M	304	1/1	0.98	0.10	-	54,54,54,54	0
16	CL	Y	302	1/1	0.98	0.12	-	59,59,59,59	0
16	CL	O	304	1/1	0.94	0.11	-	62,62,62,62	0
16	CL	K	305	1/1	0.91	0.14	-	59,59,59,59	0
16	CL	A	303	1/1	0.98	0.06	-	49,49,49,49	0
16	CL	G	302	1/1	0.98	0.05	-	61,61,61,61	0
16	CL	O	302	1/1	0.94	0.06	-	59,59,59,59	0
16	CL	H	303	1/1	0.91	0.07	-	53,53,53,53	0
16	CL	Y	301	1/1	0.99	0.13	-	35,35,35,35	0
16	CL	R	301	1/1	0.93	0.10	-	57,57,57,57	0
16	CL	W	302	1/1	0.97	0.05	-	50,50,50,50	0
16	CL	a	303	1/1	0.94	0.09	-	56,56,56,56	0
16	CL	M	303	1/1	0.99	0.05	-	44,44,44,44	0
16	CL	O	303	1/1	0.84	0.18	-	85,85,85,85	0
16	CL	H	304	1/1	0.98	0.05	-	49,49,49,49	0
16	CL	Q	301	1/1	0.92	0.19	-	67,67,67,67	0
16	CL	A	302	1/1	0.88	0.09	-	65,65,65,65	0
16	CL	R	302	1/1	0.97	0.12	-	53,53,53,53	0

6.5 Other polymers

There are no such residues in this entry.