



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:48 PM UTC

PDB ID : 5LEZ / pdb_00005lez
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 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

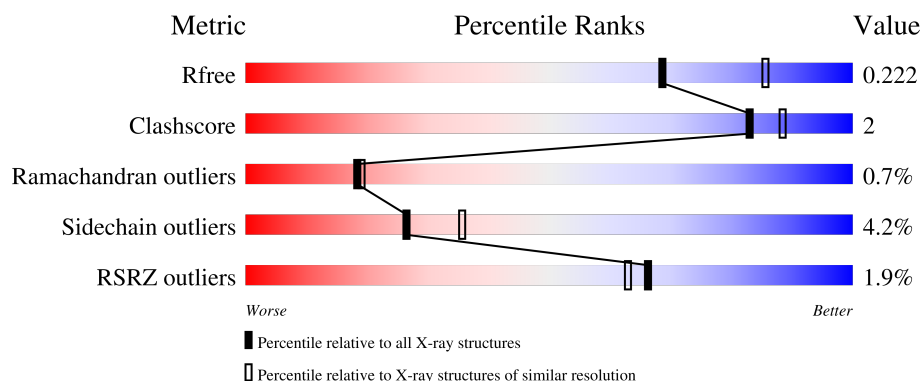
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	2% 85% 11% ..
1	O	234	3% 86% 10% ..
2	B	261	2% 89% 5% 5%
2	P	261	3% 85% 9% 5%
3	C	248	2% 82% 12% ..

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Mol	Chain	Length	Quality of chain
3	Q	248	
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	

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Mol	Chain	Length	Quality of chain
15	e	4	
15	f	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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	6V9	d	1	-	X	-	-
15	6V9	f	1	-	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			

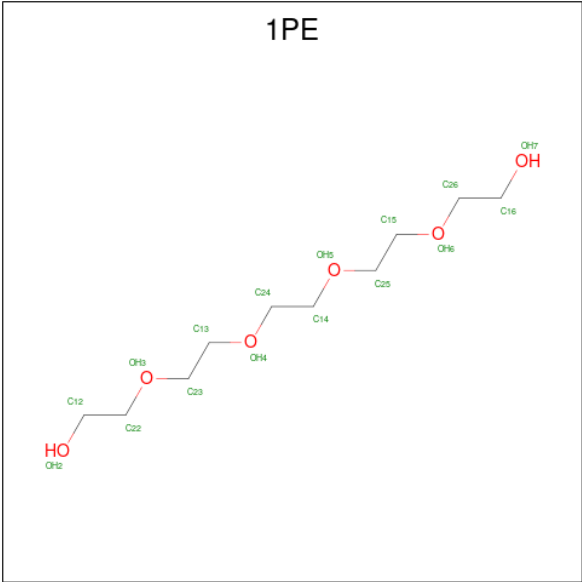
- Molecule 16 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

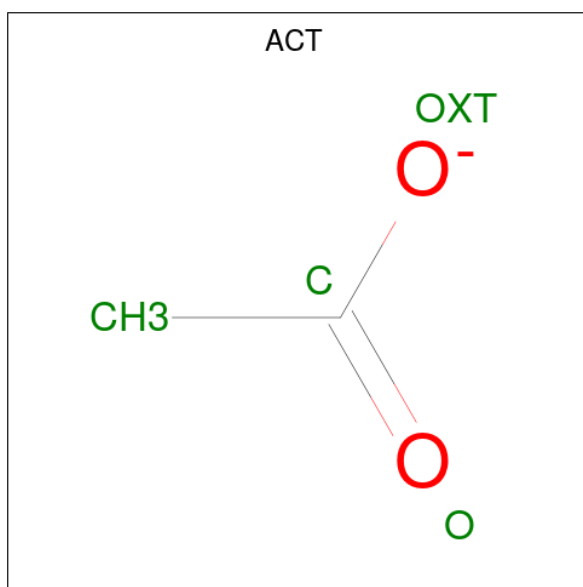
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	H	2	Total	Mg	0	0
			2	2		
17	I	2	Total	Mg	0	0
			2	2		
17	J	1	Total	Mg	0	0
			1	1		
17	K	1	Total	Mg	0	0
			1	1		
17	L	1	Total	Mg	0	0
			1	1		
17	V	1	Total	Mg	0	0
			1	1		
17	W	1	Total	Mg	0	0
			1	1		
17	X	1	Total	Mg	0	0
			1	1		

- Molecule 18 is PENTAETHYLENE GLYCOL (CCD ID: 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 (CCD ID: 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 O 161 161	0	0
20	J	136	Total O 136 136	0	0
20	K	106	Total O 106 106	0	0
20	L	127	Total O 127 127	0	0
20	M	155	Total O 155 155	0	0
20	N	160	Total O 160 160	0	0
20	O	94	Total O 94 94	0	0
20	P	127	Total O 127 127	0	0
20	Q	77	Total O 77 77	0	0
20	R	133	Total O 133 133	0	0
20	S	132	Total O 132 132	0	0
20	T	95	Total O 95 95	0	0
20	U	116	Total O 116 116	0	0
20	V	114	Total O 114 114	0	0
20	W	120	Total O 120 120	0	0
20	X	129	Total O 129 129	0	0
20	Y	149	Total O 149 149	0	0
20	Z	168	Total O 168 168	0	0
20	a	179	Total O 179 179	0	0
20	b	118	Total O 118 118	0	0
20	c	2	Total O 2 2	0	0

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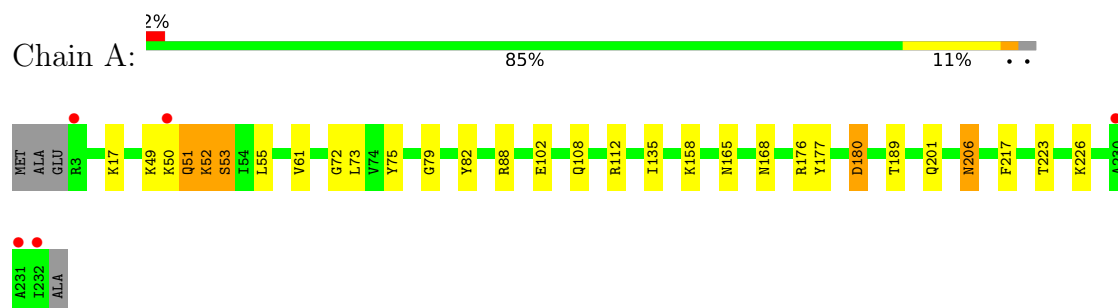
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	d	2	Total 2	O 2	0	0
20	e	3	Total 3	O 3	0	0
20	f	1	Total 1	O 1	0	0

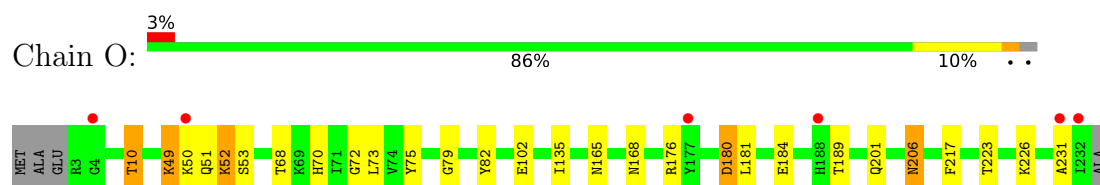
3 Residue-property plots [i](#)

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

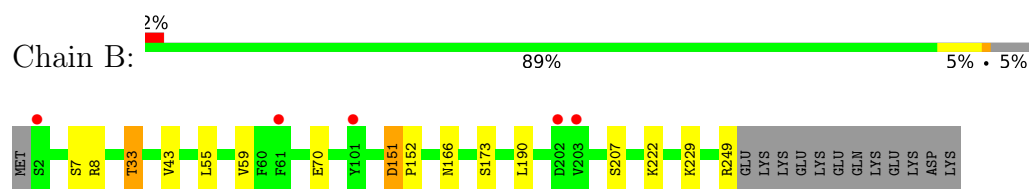
- Molecule 1: Proteasome subunit alpha type-2



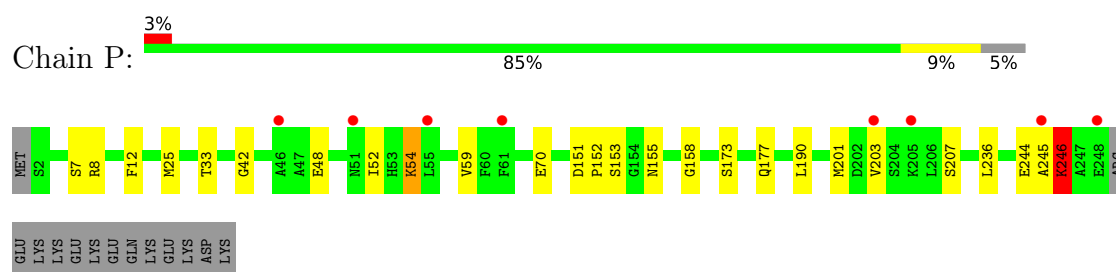
- Molecule 1: Proteasome subunit alpha type-2



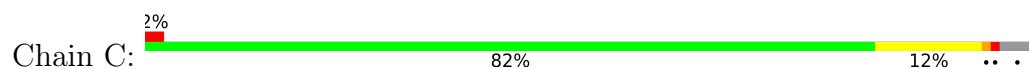
- Molecule 2: Proteasome subunit alpha type-4

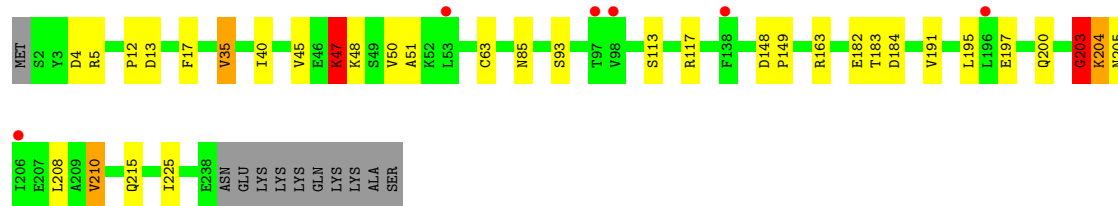


- Molecule 2: Proteasome subunit alpha type-4

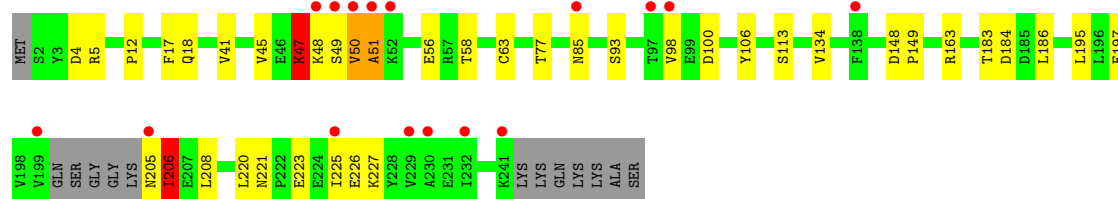
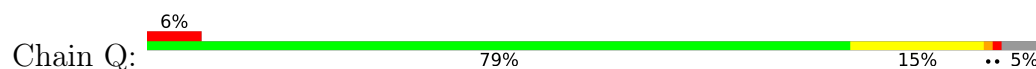


- Molecule 3: Proteasome subunit alpha type-7

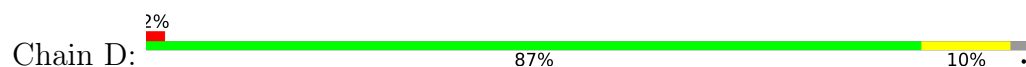




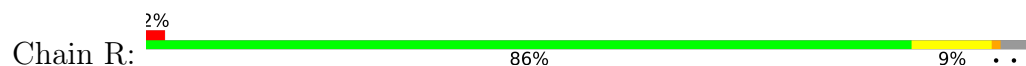
• Molecule 3: Proteasome subunit alpha type-7



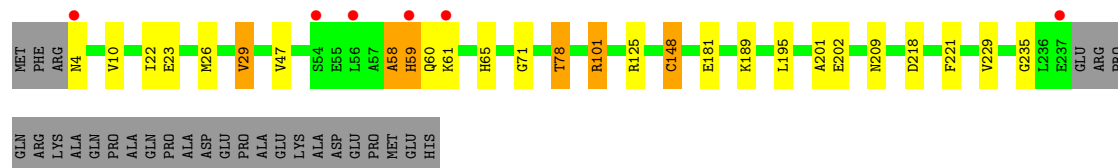
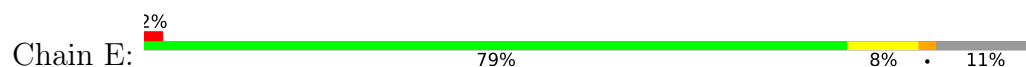
• Molecule 4: Proteasome subunit alpha type-5



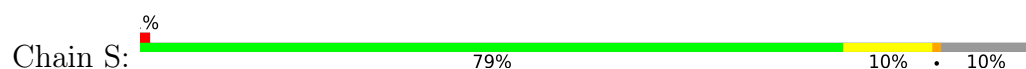
• Molecule 4: Proteasome subunit alpha type-5



• Molecule 5: Proteasome subunit alpha type-1



• Molecule 5: Proteasome subunit alpha type-1



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

• Molecule 6: Proteasome subunit alpha type-3

Chain F:  86% 6% • 6%

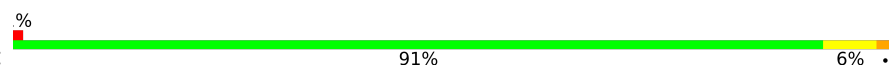
MET SER SER ILE GLY THR G6 D17 K28 G44 K51 L52 V53 S62 N63 L81 L87 F131 N143 R169 R187 V190 D206 K207 V227 R232 K240 K244 GLU GLU ASP GLU SER ASP ASP ASN MET

• Molecule 6: Proteasome subunit alpha type-3

Chain T:  85% 6% • 6%

MET SER SER ILE GLY THR G6 D17 K28 K51 L52 V53 L54 S62 N63 L81 L87 F131 N143 D152 V190 D202 E203 V204 K205 D206 K207 A208 I226 K240 K244 GLU ASP GLU SER ASP ASP ASN MET

• Molecule 7: Proteasome subunit alpha type-6

Chain G:  91% 6% • •

MET S2 R11 I32 V42 C47 C78 R88 N100 R117 Y125 E130 C137 L140 C161 V183 F187 D188 W189 T190 L206 S207 I208 D209 P212 K226 E232 R245 ASP

• Molecule 7: Proteasome subunit alpha type-6

Chain U:  87% 8% • •

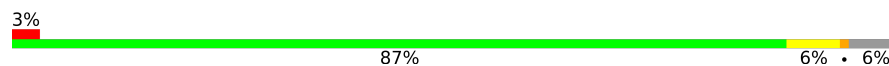
MET S2 V42 C47 D58 K59 C78 N100 I118 Y125 M131 C137 M138 I139 L140 V151 C161 K185 K186 PHE ASP THR PHE GLU Q193 T194 V195 E196 I199 L206 S207 I208 D209 P212 E232 L239 E244 R245 ASP

• Molecule 8: Proteasome subunit beta type-7

Chain H:  87% 7% 6%

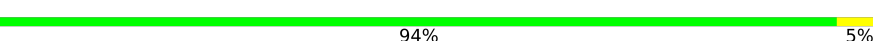
T1 V6 I12 T55 L65 L68 V77 K84 Q85 M86 S131 L132 R143 M153 L183 T197 R198 L199 C204 K215 E220 ILE GLU VAL LEU GLU THR VAL GLN THR MET ASP THR SER

• Molecule 8: Proteasome subunit beta type-7

Chain V:  87% 6% • 6%

T1 V6 I12 K33 M54 T55 L65 L68 V76 M86 D104 L132 R143 L183 T197 R198 L199 R200 Y202 R203 C204 T213 E214 K215 E220 ILE GLU VAL LEU GLU THR VAL GLN THR MET ASP THR SER

• Molecule 9: Proteasome subunit beta type-3

Chain I:  94% 5%



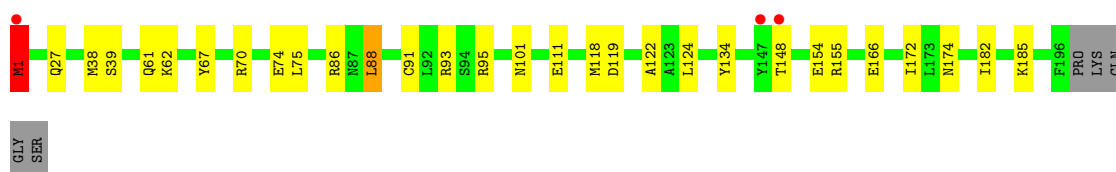
- Molecule 9: Proteasome subunit beta type-3

Chain W: 95%



- Molecule 10: Proteasome subunit beta type-2

Chain J: 83% 14%



- Molecule 10: Proteasome subunit beta type-2

Chain X: 85% 11%



- Molecule 11: Proteasome subunit beta type-5

Chain K: 87% 10%



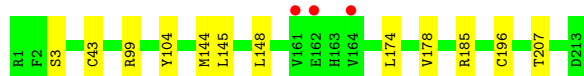
- Molecule 11: Proteasome subunit beta type-5

Chain Y: 87% 10%



- Molecule 12: Proteasome subunit beta type-1

Chain L: 94% 6%

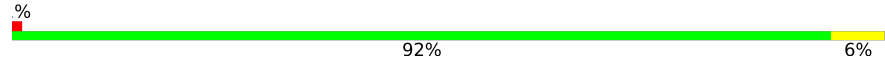


- Molecule 12: Proteasome subunit beta type-1

Chain Z:  95% 5%

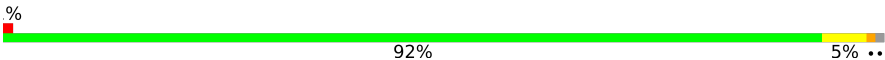


- Molecule 13: Proteasome subunit beta type-4

Chain M:  92% 6% .

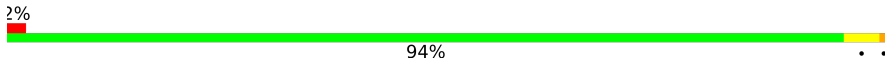


- Molecule 13: Proteasome subunit beta type-4

Chain a:  92% 5% ..

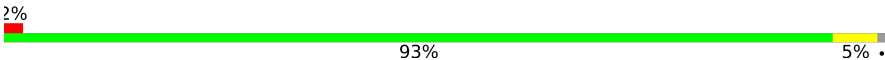


- Molecule 14: Proteasome subunit beta type-6

Chain N:  94% . .



- Molecule 14: Proteasome subunit beta type-6

Chain b:  93% 5% .



- Molecule 15: bound Oprozomib

Chain c:  50% 50%



- Molecule 15: bound Oprozomib

Chain d:  75% 25%



- Molecule 15: bound Oprozomib

Chain e:  50% 50%

6V91	S2	S3	6VA4
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- Molecule 15: bound Oprozomib

Chain f:  50% 50%

6V91	S2	S3	6VA4
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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 – 2.19 170.81 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.4 (170.81-2.19) 99.4 (170.81-2.19)	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 (4.94%)	wwPDB-VP
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 , 45.9	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.91	0/1833	1.00	2/2489 (0.1%)
1	O	0.82	0/1778	0.98	2/2419 (0.1%)
2	B	0.96	1/1958 (0.1%)	1.02	1/2645 (0.0%)
2	P	0.86	0/1934	1.01	2/2617 (0.1%)
3	C	1.01	1/1818 (0.1%)	1.14	8/2469 (0.3%)
3	Q	0.98	1/1814 (0.1%)	1.08	6/2462 (0.2%)
4	D	0.93	0/1789	0.99	2/2424 (0.1%)
4	R	1.06	0/1780	1.07	5/2408 (0.2%)
5	E	0.97	1/1842 (0.1%)	1.01	2/2493 (0.1%)
5	S	0.96	1/1901 (0.1%)	1.05	2/2571 (0.1%)
6	F	1.00	1/1935 (0.1%)	1.09	4/2605 (0.2%)
6	T	1.02	2/1894 (0.1%)	1.11	8/2556 (0.3%)
7	G	1.02	2/1909 (0.1%)	1.05	3/2579 (0.1%)
7	U	0.94	2/1804 (0.1%)	1.00	2/2441 (0.1%)
8	H	1.07	0/1697	1.05	1/2299 (0.0%)
8	V	0.88	0/1655	0.97	0/2251
9	I	0.98	0/1648	1.07	4/2219 (0.2%)
9	W	0.82	0/1630	0.95	4/2197 (0.2%)
10	J	1.10	4/1613 (0.2%)	1.06	1/2180 (0.0%)
10	X	0.98	3/1599 (0.2%)	1.01	2/2163 (0.1%)
11	K	0.93	0/1582	1.05	1/2138 (0.0%)
11	Y	1.05	0/1610	1.04	1/2172 (0.0%)
12	L	0.88	0/1672	0.94	0/2257
12	Z	1.05	1/1675 (0.1%)	0.99	1/2257 (0.0%)
13	M	1.02	0/1728	1.01	3/2339 (0.1%)
13	a	1.09	0/1724	1.02	2/2336 (0.1%)
14	N	1.13	1/1548 (0.1%)	1.09	1/2095 (0.0%)
14	b	1.07	1/1554 (0.1%)	1.08	2/2104 (0.1%)
All	All	0.98	22/48924 (0.0%)	1.04	72/66185 (0.1%)

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

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	X	154	GLU	C-O	10.76	1.36	1.24
6	T	7	TYR	N-CA	6.64	1.58	1.46
10	J	148	THR	CA-CB	6.56	1.62	1.54
10	X	154	GLU	CA-C	6.02	1.60	1.52
10	J	148	THR	C-O	-5.84	1.18	1.24
6	F	44	GLY	N-CA	5.81	1.50	1.45
5	E	4	ASN	N-CA	5.80	1.57	1.46
3	Q	206	ILE	CA-C	5.58	1.59	1.52
10	J	154	GLU	C-O	-5.54	1.17	1.24
7	G	125	TYR	C-O	-5.39	1.17	1.24
14	b	162	LEU	CA-C	5.26	1.59	1.52
7	G	130	GLU	CA-C	5.25	1.60	1.52
14	N	201	THR	N-CA	5.18	1.53	1.45
10	J	154	GLU	CA-CB	5.17	1.61	1.53
7	U	125	TYR	C-O	-5.17	1.17	1.24
10	X	24	ASN	CA-C	5.17	1.57	1.52
7	U	131	MET	C-O	-5.14	1.17	1.23
6	T	152	ASP	C-O	5.13	1.28	1.24
12	Z	100	ARG	C-O	-5.12	1.18	1.24
2	B	151	ASP	CA-C	5.12	1.57	1.52
3	C	182	GLU	CD-OE2	5.05	1.34	1.25
5	S	123	TYR	N-CA	-5.05	1.39	1.46

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	X	154	GLU	O-C-N	10.51	132.89	122.07
6	F	190	VAL	CB-CA-C	-10.00	98.94	112.04
9	I	16[A]	LYS	CA-C-N	9.68	135.91	122.07
9	I	16[A]	LYS	C-N-CA	9.68	135.91	122.07
9	I	16[B]	LYS	CA-C-N	9.68	135.91	122.07
9	I	16[B]	LYS	C-N-CA	9.68	135.91	122.07
6	T	190	VAL	CB-CA-C	-9.18	100.02	112.04
6	T	6	GLY	CA-C-N	8.31	136.66	121.70
6	T	6	GLY	C-N-CA	8.31	136.66	121.70
14	b	1	THR	N-CA-CB	7.79	124.75	111.50
5	E	58	ALA	N-CA-C	7.49	119.09	111.07
3	C	200	GLN	N-CA-C	7.46	119.06	111.07
2	P	246	LYS	N-CA-C	7.43	121.61	112.54
4	D	128	ALA	N-CA-C	7.43	120.60	110.35
10	X	154	GLU	CA-C-O	-7.22	113.24	120.82
6	F	143	ASN	N-CA-C	7.22	118.79	111.07
6	F	190	VAL	N-CA-CB	6.97	119.19	110.47
11	K	1	THR	N-CA-CB	6.92	123.27	111.50
4	R	120[A]	ALA	N-CA-C	-6.92	98.75	109.76
4	R	120[B]	ALA	N-CA-C	-6.92	98.75	109.76
4	D	120	ALA	N-CA-C	6.83	119.31	111.11
7	G	183	VAL	CB-CA-C	-6.78	101.28	112.26
3	C	47	LYS	N-CA-C	6.74	125.15	110.80
4	R	128	ALA	N-CA-C	6.57	124.80	110.80
6	T	143	ASN	N-CA-C	6.55	118.08	111.07
3	C	17	PHE	N-CA-C	6.46	118.32	111.28
7	G	183	VAL	N-CA-C	6.44	119.14	111.09
6	T	190	VAL	N-CA-CB	6.32	118.37	110.47
7	U	199	ILE	CB-CA-C	6.30	120.69	112.24
6	T	7	TYR	N-CA-CB	6.29	121.20	110.50
13	a	71	VAL	N-CA-CB	6.22	119.92	110.58
9	W	16[A]	LYS	CA-C-N	6.13	134.37	123.34
9	W	16[A]	LYS	C-N-CA	6.13	134.37	123.34
9	W	16[B]	LYS	CA-C-N	6.13	134.37	123.34
9	W	16[B]	LYS	C-N-CA	6.13	134.37	123.34
11	Y	1	THR	N-CA-CB	6.13	121.92	111.50
7	G	208	ILE	N-CA-C	6.07	116.78	111.56
14	b	35	THR	CB-CA-C	6.01	116.57	109.47
13	a	10	SER	N-CA-C	6.00	118.05	110.24
3	Q	220	LEU	CA-C-N	5.99	132.48	121.70
3	Q	220	LEU	C-N-CA	5.99	132.48	121.70
2	B	55	LEU	N-CA-C	5.98	120.31	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	102	GLU	CA-C-N	-5.90	113.86	119.76
1	O	102	GLU	C-N-CA	-5.90	113.86	119.76
13	M	10	SER	N-CA-C	5.81	117.80	110.24
7	U	208	ILE	N-CA-C	5.71	116.47	111.56
3	C	197	GLU	N-CA-C	5.68	117.55	111.36
6	F	207	LYS	N-CA-C	5.63	117.28	111.03
13	M	133	GLU	CB-CA-C	5.61	120.39	109.33
1	A	102	GLU	CA-C-N	-5.53	114.06	119.76
1	A	102	GLU	C-N-CA	-5.53	114.06	119.76
3	Q	17	PHE	N-CA-C	5.44	117.21	111.28
6	T	226	ILE	CB-CA-C	-5.44	103.08	111.08
8	H	77	VAL	CB-CA-C	-5.43	103.74	112.16
4	R	127	ASP	CA-C-N	5.35	131.76	121.54
4	R	127	ASP	C-N-CA	5.35	131.76	121.54
3	Q	220	LEU	CA-C-O	-5.32	115.07	120.71
3	C	203	GLY	CA-C-N	5.31	131.26	121.70
3	C	203	GLY	C-N-CA	5.31	131.26	121.70
12	Z	99	ARG	NE-CZ-NH2	-5.26	114.46	119.20
5	S	3	ARG	N-CA-C	5.26	122.00	110.80
3	Q	47	LYS	N-CA-C	5.25	121.97	110.80
10	J	154	GLU	O-C-N	5.18	127.62	122.12
3	C	12	PRO	N-CA-C	-5.17	103.07	111.14
3	C	117	ARG	CG-CD-NE	5.10	123.22	112.00
2	P	42	GLY	N-CA-C	5.09	117.46	110.69
5	E	209	ASN	N-CA-C	5.08	119.63	113.38
5	S	4	ASN	N-CA-C	5.06	116.79	111.28
3	Q	12	PRO	N-CA-C	5.04	120.39	113.84
13	M	19	GLY	N-CA-C	5.04	117.39	110.69
14	N	116	MET	CG-SD-CE	-5.04	89.82	100.90
6	T	53	VAL	CB-CA-C	5.03	118.70	111.81

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

All (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

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Mol	Chain	Res	Type	Group
6	F	206	ASP	Peptide
9	I	78	GLY	Peptide
10	J	1[A]	MET	Peptide
10	J	1[B]	MET	Peptide
2	P	244	GLU	Peptide
2	P	245	ALA	Peptide
2	P	54	LYS	Peptide
3	Q	47	LYS	Peptide
3	Q	49	SER	Peptide
4	R	130	PRO	Peptide
9	W	78	GLY	Peptide
10	X	1	MET	Peptide
10	X	148	THR	Mainchain
13	a	215	ILE	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	13	0
1	O	1741	0	1683	10	0
2	B	1922	0	1913	4	0
2	P	1898	0	1861	9	0
3	C	1798	0	1718	14	0
3	Q	1801	0	1735	15	0
4	D	1762	0	1709	10	0
4	R	1753	0	1726	12	0
5	E	1822	0	1779	11	0
5	S	1875	0	1818	16	0
6	F	1888	0	1882	5	0
6	T	1856	0	1816	6	0
7	G	1912	0	1882	7	0
7	U	1815	0	1748	8	0
8	H	1664	0	1681	8	0
8	V	1622	0	1595	8	0
9	I	1613	0	1646	6	0
9	W	1599	0	1621	6	0
10	J	1590	0	1581	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	X	1576	0	1561	18	0
11	K	1551	0	1506	9	0
11	Y	1570	0	1547	12	0
12	L	1636	0	1625	6	0
12	Z	1642	0	1635	6	0
13	M	1692	0	1670	6	0
13	a	1688	0	1658	6	0
14	N	1519	0	1493	8	0
14	b	1524	0	1493	8	0
15	c	37	0	6	0	0
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	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
20	M	155	0	0	0	0
20	N	160	0	0	1	0
20	O	94	0	0	1	0
20	P	127	0	0	1	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	0	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	232	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.

All (232) 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)
12:L:144:MET:HE1	12:L:185:ARG:HB2	1.54	0.89
5:E:23:GLU:HA	5:E:26:MET:HE3	1.58	0.83
10:J:1[A]:MET:HE1	10:J:134:TYR:H	1.43	0.81

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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
13:a:86:ARG:NH1	13:a:133:GLU:OE1	2.18	0.76
10:X:1:MET:HE1	10:X:134:TYR:H	1.51	0.74
2:P:12:PHE:H	3:Q:18:GLN:HE22	1.35	0.74
5:S:65[A]:HIS:CE1	20:S:304:HOH:O	2.39	0.74
2:P:25[B]:MET:HE3	2:P:25[B]:MET:HA	1.69	0.73
5:S:152[B]:ASN:ND2	20:S:301:HOH:O	2.22	0.73
6:T:202:ASP:O	6:T:205:LYS:O	2.05	0.73
11:Y:35:ILE:HD11	11:Y:45:MET:SD	2.29	0.72
11:K:35:ILE:HD11	11:K:45:MET:SD	2.29	0.72
8:V:1:THR:HB	8:V:33:LYS:HZ3	1.55	0.70
9:I:64:GLN:OE1	10:J:86:ARG:NH2	2.26	0.69
3:C:47:LYS:CB	3:C:48:LYS:O	2.41	0.68
10:J:1[A]:MET:HE1	10:J:134:TYR:N	2.08	0.68
7:U:138:MET:HE3	7:U:140:LEU:HD11	1.77	0.67
7:U:118:ILE:HG13	7:U:138:MET:HE1	1.76	0.66
5:E:58:ALA:O	5:E:59:HIS:CB	2.43	0.66
6:F:169[A]:ARG:NH1	20:F:302:HOH:O	2.30	0.65
20:H:542:HOH:O	12:Z:160:ASN:CB	2.44	0.64
7:U:199:ILE:HD11	7:U:239:LEU:HD23	1.81	0.63
10:X:1:MET:HE1	10:X:134:TYR:N	2.14	0.63
9:I:35:THR:HG21	20:I:437:HOH:O	1.98	0.63
5:S:86:ASN:ND2	20:S:302:HOH:O	2.33	0.62
4:R:20:ARG:HD2	4:R:25:GLU:CD	2.26	0.61
5:S:238:GLU:CB	5:S:239:ARG:C	2.74	0.61
5:S:101:ARG:NH1	20:S:303:HOH:O	2.34	0.60
4:D:20:ARG:HD2	4:D:25:GLU:CD	2.27	0.60
4:R:129:ASP:CB	4:R:130:PRO:CD	2.80	0.59
8:V:54:MET:HE1	20:W:448:HOH:O	2.01	0.59
4:D:96:THR:OG1	20:D:301:HOH:O	2.17	0.59
11:K:141:ARG:NH1	10:X:166:GLU:OE2	2.35	0.59
13:a:5:MET:HE2	14:b:116:MET:HB3	1.84	0.59
8:V:1:THR:HB	8:V:33:LYS:NZ	2.18	0.58
13:a:96:MET:HE3	13:a:127:MET:HA	1.85	0.58
5:E:22:ILE:HG22	5:E:26:MET:HE2	1.86	0.57
7:U:195:VAL:O	7:U:199:ILE:HG23	2.05	0.57
3:Q:41:VAL:HG11	3:Q:134:VAL:HB	1.87	0.57
4:R:49:ALA:HB2	4:R:217:LEU:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:96:MET:HE3	13:M:127:MET:HA	1.86	0.56
4:R:78:MET:HG3	4:R:82:ILE:HD12	1.87	0.56
9:I:13[A]:MET:HE3	9:I:162:LEU:HD12	1.88	0.56
10:J:101:ASN:HD22	10:J:119:ASP:HA	1.71	0.55
10:J:166:GLU:OE2	11:Y:141[A]:ARG:NH1	2.40	0.55
12:L:144:MET:CE	12:L:185:ARG:HB2	2.32	0.55
9:W:64:GLN:OE1	10:X:86:ARG:NH2	2.40	0.55
13:M:5:MET:HE2	14:N:116:MET:HB3	1.88	0.54
4:D:49:ALA:HB2	4:D:217:LEU:HD12	1.88	0.54
11:Y:40:TYR:CD2	11:Y:73:ARG:CZ	2.90	0.54
9:W:13:MET:HE3	9:W:162:LEU:HD12	1.91	0.53
10:J:118:MET:HE2	10:J:124:LEU:HD13	1.90	0.53
3:C:203:GLY:CA	3:C:204:LYS:CB	2.87	0.53
7:G:11:ARG:HG2	7:G:11:ARG:HH11	1.74	0.53
1:O:10:THR:HG23	20:O:301:HOH:O	2.09	0.53
7:U:78:CYS:HB2	7:U:140:LEU:HD23	1.90	0.53
3:C:47:LYS:CB	3:C:48:LYS:C	2.82	0.52
4:D:78:MET:HG3	4:D:82:ILE:HD12	1.91	0.52
8:H:204:CYS:SG	12:Z:158:MET:CE	2.97	0.52
6:F:51:LYS:NZ	6:F:62:SER:O	2.28	0.52
1:A:108:GLN:HE21	1:A:112:ARG:HH12	1.57	0.52
12:L:148:LEU:HD23	12:L:178:VAL:CG1	2.39	0.52
3:Q:4:ASP:O	4:R:125:GLU:HB2	2.10	0.52
7:G:78:CYS:HB2	7:G:140:LEU:HD23	1.90	0.52
11:Y:158:ARG:HE	11:Y:162:GLN:HE21	1.56	0.51
3:C:4:ASP:O	4:D:125:GLU:HB2	2.11	0.51
10:X:28:MET:HE3	20:Y:487:HOH:O	2.10	0.51
10:X:118:MET:HE2	10:X:124:LEU:HD13	1.91	0.51
11:Y:35:ILE:CD1	11:Y:45:MET:SD	2.98	0.51
8:H:132:LEU:HD22	14:N:25:TYR:CE2	2.46	0.51
6:T:87:LEU:HD13	6:T:131:PHE:CE1	2.46	0.51
6:T:6:GLY:HA3	6:T:7:TYR:CD2	2.47	0.50
11:K:35:ILE:CD1	11:K:45:MET:SD	2.99	0.50
12:Z:148:LEU:HD23	12:Z:178:VAL:CG1	2.41	0.50
8:H:204:CYS:SG	12:Z:158:MET:HE2	2.52	0.50
2:P:155:ASN:OD1	3:Q:77:THR:OG1	2.25	0.50
12:L:43[B]:CYS:HG	12:L:196:CYS:HG	1.57	0.50
9:I:13[A]:MET:HE2	9:I:166:ILE:HB	1.92	0.50
13:a:5:MET:HE2	14:b:116:MET:CB	2.42	0.49
10:X:88:LEU:HB3	10:X:122:ALA:HB2	1.94	0.49
1:A:180:ASP:OD1	1:A:180:ASP:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:40:TYR:CD2	11:K:73:ARG:CZ	2.95	0.49
2:P:8:ARG:NH2	3:Q:5:ARG:HD2	2.27	0.49
3:C:35:VAL:HG13	3:C:191:VAL:CG2	2.42	0.49
9:W:13:MET:HE2	9:W:166:ILE:HB	1.95	0.49
9:W:13:MET:HE1	9:W:166:ILE:N	2.27	0.49
10:X:46[B]:CYS:SG	10:X:102:LEU:HD22	2.52	0.49
5:S:60:GLN:HE22	5:S:78:THR:HG21	1.78	0.49
11:K:36:GLU:HG2	11:K:184:TRP:CZ2	2.48	0.49
12:Z:145:LEU:HD22	12:Z:178:VAL:HB	1.94	0.48
3:C:183:THR:OG1	3:C:184:ASP:N	2.45	0.48
5:E:101[A]:ARG:NH1	20:E:304:HOH:O	2.46	0.48
7:G:32:ILE:HD13	7:G:137:YCM:HD2	1.95	0.48
7:G:190:THR:HG23	20:G:421:HOH:O	2.12	0.48
3:C:203:GLY:HA2	3:C:204:LYS:CB	2.44	0.48
5:E:71:GLY:HA3	5:E:221:PHE:CZ	2.48	0.48
2:P:155:ASN:ND2	20:P:301:HOH:O	2.43	0.48
13:a:92:LEU:HD12	13:a:112:ILE:HD11	1.96	0.48
1:O:180:ASP:N	1:O:180:ASP:OD1	2.46	0.47
2:P:48:GLU:HB2	2:P:201:MET:HE2	1.96	0.47
4:D:59:MET:SD	4:D:64:ILE:HD11	2.54	0.47
2:P:246:LYS:HE3	2:P:246:LYS:N	2.29	0.47
1:A:52:LYS:CB	20:A:402:HOH:O	2.62	0.47
4:R:132:ALA:HB1	20:R:306:HOH:O	2.14	0.47
8:H:55:THR:HG23	8:H:86:MET:HE1	1.96	0.47
12:L:145:LEU:HD22	12:L:178:VAL:HB	1.96	0.47
8:V:76:VAL:HG23	8:V:104[A]:ASP:OD2	2.15	0.47
8:H:132:LEU:HD22	14:N:25:TYR:CZ	2.49	0.47
10:J:67:TYR:CD1	10:J:75:LEU:HG	2.50	0.47
8:V:213:THR:HB	9:W:198:THR:OG1	2.14	0.47
10:X:95:ARG:HH11	10:X:95:ARG:HB2	1.79	0.47
8:V:132:LEU:HD22	14:b:25:TYR:CZ	2.50	0.47
1:A:79:GLY:O	1:A:82:TYR:HB3	2.15	0.46
5:E:60:GLN:NE2	5:E:78:THR:HG21	2.30	0.46
10:J:88:LEU:HB3	10:J:122:ALA:HB2	1.97	0.46
4:R:59:MET:SD	4:R:64:ILE:HD11	2.55	0.46
14:b:14:LEU:HD23	14:b:44:CYS:SG	2.54	0.46
12:Z:99:ARG:HG3	12:Z:104:TYR:CE2	2.50	0.46
14:b:35:THR:HG21	14:b:45:ARG:NE	2.30	0.46
1:O:79:GLY:O	1:O:82:TYR:HB3	2.16	0.46
13:M:86:ARG:NH1	13:M:133:GLU:OE2	2.49	0.46
11:Y:36:GLU:HG2	11:Y:184:TRP:CZ2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:ARG:NH2	3:C:5:ARG:HD2	2.31	0.46
13:M:5:MET:HE2	14:N:116:MET:CB	2.46	0.46
1:A:51:GLN:C	1:A:52:LYS:O	2.58	0.46
9:I:13[A]:MET:HE1	9:I:166:ILE:N	2.30	0.46
10:J:27[B]:GLN:NE2	10:J:174:ASN:O	2.49	0.46
3:Q:50:VAL:O	3:Q:51:ALA:HB3	2.15	0.46
3:C:215:GLN:CB	20:C:375:HOH:O	2.64	0.46
1:O:51:GLN:C	1:O:52:LYS:O	2.59	0.45
14:N:14:LEU:HD23	14:N:44:CYS:SG	2.56	0.45
5:E:29:VAL:HG22	5:E:148:6V1:C3	2.47	0.45
7:G:212:PRO:HB2	7:G:232:GLU:HG3	1.99	0.45
10:J:1[A]:MET:HE2	10:J:1[A]:MET:HB3	1.79	0.45
10:J:185:LYS:NZ	20:J:405:HOH:O	2.50	0.45
4:R:129:ASP:CB	4:R:130:PRO:HD2	2.46	0.45
11:Y:2:THR:OG1	11:Y:131:GLY:HA3	2.17	0.45
8:V:55:THR:HG23	8:V:86:MET:HE1	1.97	0.45
1:A:88[B]:ARG:NH2	20:A:302:HOH:O	2.50	0.45
1:A:158:LYS:HB3	1:A:177:TYR:CE1	2.51	0.45
10:X:1:MET:HE3	10:X:1:MET:C	2.42	0.45
10:X:44:LEU:HG	10:X:46[B]:CYS:SG	2.57	0.45
3:C:85[B]:ASN:OD1	10:J:70:ARG:NH1	2.50	0.45
3:Q:183:THR:CG2	3:Q:186:LEU:HD13	2.47	0.45
5:S:65[A]:HIS:ND1	20:S:304:HOH:O	2.36	0.45
1:O:72:GLY:HA3	1:O:217:PHE:CE1	2.52	0.45
5:S:154:PHE:HD2	6:T:63:ASN:HD21	1.65	0.45
1:A:55:LEU:HD23	7:G:183:VAL:HG21	1.99	0.44
1:O:75:TYR:HB3	1:O:82:TYR:CD2	2.52	0.44
10:X:1:MET:HE2	10:X:1:MET:HB3	1.81	0.44
1:A:72:GLY:HA3	1:A:217:PHE:CE1	2.52	0.44
11:K:133:VAL:HG21	10:X:137:PHE:HB3	1.99	0.44
13:M:112:ILE:HD12	13:M:112:ILE:N	2.32	0.44
13:a:112:ILE:HD12	13:a:112:ILE:N	2.32	0.44
2:P:151:ASP:HB2	2:P:152:PRO:CD	2.48	0.44
3:Q:183:THR:OG1	3:Q:184:ASP:N	2.50	0.44
6:T:51:LYS:NZ	6:T:62:SER:O	2.32	0.44
3:C:85[B]:ASN:OD1	10:J:70:ARG:CZ	2.65	0.44
5:E:65:HIS:HB2	20:E:376:HOH:O	2.18	0.44
9:I:52:LEU:HB2	9:I:59:VAL:HG13	2.00	0.44
3:C:40:ILE:HD11	3:C:210:VAL:HG13	1.99	0.44
8:H:84:LYS:NZ	14:N:53:GLN:OE1	2.46	0.43
11:K:2:THR:OG1	11:K:131:GLY:HA3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ASN:C	1:A:206:ASN:HD22	2.26	0.43
5:E:201:ALA:O	20:E:301:HOH:O	2.21	0.43
7:G:117:ARG:NH2	20:G:403:HOH:O	2.47	0.43
3:Q:47:LYS:HA	3:Q:205:ASN:HA	1.99	0.43
11:K:73:ARG:HG3	20:K:489:HOH:O	2.19	0.43
6:T:205:LYS:O	6:T:206:ASP:CG	2.61	0.43
1:O:206:ASN:C	1:O:206:ASN:HD22	2.27	0.43
3:Q:148:ASP:HB2	3:Q:149:PRO:CD	2.48	0.43
3:C:148:ASP:HB2	3:C:149:PRO:CD	2.48	0.43
1:O:165:ASN:OD1	1:O:168:ASN:HB2	2.18	0.43
5:S:237:GLU:O	5:S:238:GLU:CB	2.66	0.43
10:J:93:ARG:HD2	20:J:508:HOH:O	2.17	0.43
10:X:182:ILE:HG13	10:X:183:ILE:N	2.34	0.43
10:X:38:MET:HE1	10:X:61:GLN:HB2	2.01	0.43
7:U:58:ASP:O	7:U:59:LYS:CB	2.66	0.42
6:F:62:SER:O	6:F:63:ASN:C	2.62	0.42
1:A:165:ASN:OD1	1:A:168:ASN:HB2	2.19	0.42
14:b:35:THR:HG21	14:b:45:ARG:HE	1.84	0.42
2:B:151:ASP:HB2	2:B:152:PRO:CD	2.49	0.42
12:L:99:ARG:HG3	12:L:104:TYR:CE2	2.54	0.42
11:Y:4:LEU:C	11:Y:4:LEU:HD12	2.44	0.42
11:Y:12:VAL:HG13	11:Y:179:VAL:HB	2.01	0.42
11:K:12:VAL:HG13	11:K:179:VAL:HB	2.01	0.42
7:U:212:PRO:HB2	7:U:232:GLU:HG3	2.02	0.42
3:Q:106:TYR:CD1	3:Q:106:TYR:C	2.98	0.42
4:R:157:ASP:HB2	4:R:158:PRO:CD	2.50	0.42
5:S:71:GLY:HA3	5:S:221:PHE:CZ	2.54	0.42
4:D:91:LYS:HG2	4:D:119:LEU:HD11	2.00	0.42
3:Q:100:ASP:OD1	11:Y:107:ARG:NH2	2.52	0.42
4:R:91:LYS:HG2	4:R:119:LEU:HD11	2.00	0.42
1:A:52:LYS:O	1:A:53:SER:C	2.63	0.42
10:J:38:MET:HE1	10:J:61:GLN:HB2	2.02	0.42
14:b:35:THR:CG2	14:b:45:ARG:HE	2.33	0.42
1:O:49:LYS:O	1:O:51:GLN:N	2.53	0.42
11:Y:186[A]:ARG:HE	11:Y:186[A]:ARG:HB2	1.69	0.41
2:B:33:THR:HB	2:B:166:ASN:O	2.20	0.41
4:D:157:ASP:HB2	4:D:158:PRO:CD	2.50	0.41
20:N:521:HOH:O	19:d:101:ACT:H2	2.19	0.41
14:N:143:TYR:CE1	14:b:200:ALA:HB1	2.56	0.41
9:W:35:THR:HG21	20:W:417:HOH:O	2.20	0.41
3:C:5:ARG:HD3	4:D:125:GLU:OE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:158:GLY:HA3	3:Q:58:THR:HG21	2.03	0.41
3:Q:85:ASN:OD1	10:X:70:ARG:CZ	2.69	0.41
8:V:143:ARG:HE	8:V:143:ARG:HB2	1.67	0.41
11:Y:40:TYR:CD2	11:Y:73:ARG:NH1	2.89	0.41
6:F:87:LEU:HD13	6:F:131:PHE:CE2	2.55	0.41
1:A:75:TYR:HB3	1:A:82:TYR:CD2	2.56	0.41
8:H:143:ARG:HE	8:H:143:ARG:HB2	1.67	0.41
13:M:166:ARG:NH2	13:M:200:GLU:OE2	2.53	0.41
10:J:39:SER:HB2	10:J:74:GLU:CD	2.46	0.41
1:O:68:THR:HG1	1:O:70:HIS:CE1	2.39	0.41
4:R:228:MET:HE2	4:R:228:MET:HB2	1.98	0.40
4:D:127:ASP:HB3	5:E:125:ARG:HD3	2.03	0.40
3:Q:85:ASN:OD1	10:X:70:ARG:NH1	2.55	0.40
5:S:171:TYR:CD1	5:S:171:TYR:C	2.98	0.40
7:U:244:GLU:O	7:U:245:ARG:C	2.64	0.40
10:X:12:TYR:HB2	10:X:182:ILE:HD11	2.03	0.40
14:N:201:THR:HG22	14:N:202:LEU:N	2.37	0.40
4:R:225:ASN:O	4:R:226:PHE:C	2.65	0.40
5:S:18[B]:ARG:HG3	5:S:19:ILE:N	2.30	0.40
2:B:222:LYS:NZ	20:B:303:HOH:O	2.51	0.40

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 [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%)	222 (96%)	4 (2%)	5 (2%)	5 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	228/234 (97%)	218 (96%)	4 (2%)	6 (3%)	4	2
2	B	248/261 (95%)	240 (97%)	8 (3%)	0	100	100
2	P	247/261 (95%)	233 (94%)	11 (4%)	3 (1%)	10	8
3	C	236/248 (95%)	217 (92%)	14 (6%)	5 (2%)	5	3
3	Q	230/248 (93%)	216 (94%)	8 (4%)	6 (3%)	4	2
4	D	232/241 (96%)	224 (97%)	5 (2%)	3 (1%)	9	8
4	R	232/241 (96%)	224 (97%)	4 (2%)	4 (2%)	7	5
5	E	232/263 (88%)	226 (97%)	5 (2%)	1 (0%)	30	34
5	S	238/263 (90%)	232 (98%)	4 (2%)	2 (1%)	16	16
6	F	241/255 (94%)	235 (98%)	5 (2%)	1 (0%)	30	34
6	T	239/255 (94%)	229 (96%)	6 (2%)	4 (2%)	7	5
7	G	241/246 (98%)	237 (98%)	4 (2%)	0	100	100
7	U	232/246 (94%)	227 (98%)	4 (2%)	1 (0%)	30	34
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%)	12	11
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
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%)	18	19

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	LYS

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Mol	Chain	Res	Type
1	A	53	SER
3	C	47	LYS
3	C	204	LYS
4	D	176	GLY
6	F	62	SER
1	O	50	LYS
1	O	52	LYS
1	O	53	SER
2	P	54	LYS
3	Q	47	LYS
3	Q	206	ILE
4	R	128	ALA
4	R	129	ASP
4	R	130	PRO
5	S	238	GLU
6	T	7	TYR
6	T	62	SER
6	T	208	ALA
1	A	52	LYS
4	D	175[A]	GLU
4	D	175[B]	GLU
5	E	59	HIS
1	O	231	ALA
2	P	52	ILE
3	Q	48	LYS
3	Q	221	ASN
1	A	176	ARG
1	O	176	ARG
7	U	58	ASP
3	C	50	VAL
3	Q	50	VAL
9	W	16[A]	LYS
9	W	16[B]	LYS
3	C	51	ALA
1	O	201	GLN
3	Q	51	ALA
4	R	126	GLU
5	S	236	LEU
1	A	201	GLN
2	P	203	VAL
3	C	203	GLY
6	T	204	VAL

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%)	18	22
1	O	176/191 (92%)	165 (94%)	11 (6%)	16	19
2	B	199/221 (90%)	189 (95%)	10 (5%)	22	28
2	P	196/221 (89%)	184 (94%)	12 (6%)	17	20
3	C	179/210 (85%)	168 (94%)	11 (6%)	17	20
3	Q	183/210 (87%)	169 (92%)	14 (8%)	12	13
4	D	189/203 (93%)	184 (97%)	5 (3%)	40	55
4	R	187/203 (92%)	185 (99%)	2 (1%)	65	79
5	E	192/223 (86%)	181 (94%)	11 (6%)	18	23
5	S	197/223 (88%)	189 (96%)	8 (4%)	27	37
6	F	199/212 (94%)	189 (95%)	10 (5%)	22	28
6	T	192/212 (91%)	183 (95%)	9 (5%)	23	31
7	G	202/207 (98%)	191 (95%)	11 (5%)	20	25
7	U	186/207 (90%)	178 (96%)	8 (4%)	26	35
8	H	181/195 (93%)	171 (94%)	10 (6%)	19	24
8	V	172/195 (88%)	162 (94%)	10 (6%)	18	22
9	I	176/174 (101%)	173 (98%)	3 (2%)	53	69
9	W	173/174 (99%)	171 (99%)	2 (1%)	63	78
10	J	166/170 (98%)	157 (95%)	9 (5%)	20	25
10	X	165/170 (97%)	159 (96%)	6 (4%)	31	42
11	K	155/159 (98%)	145 (94%)	10 (6%)	15	18
11	Y	158/159 (99%)	152 (96%)	6 (4%)	29	40
12	L	175/178 (98%)	171 (98%)	4 (2%)	44	59
12	Z	175/178 (98%)	172 (98%)	3 (2%)	53	69
13	M	180/181 (99%)	175 (97%)	5 (3%)	38	52
13	a	178/181 (98%)	172 (97%)	6 (3%)	32	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	158/159 (99%)	156 (99%)	2 (1%)	61	76
14	b	158/159 (99%)	154 (98%)	4 (2%)	42	56
All	All	5032/5366 (94%)	4819 (96%)	213 (4%)	26	36

All (213) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	49	LYS
1	A	51	GLN
1	A	61	VAL
1	A	73	LEU
1	A	135	ILE
1	A	180	ASP
1	A	189	THR
1	A	206	ASN
1	A	223	THR
1	A	226	LYS
2	B	7	SER
2	B	33	THR
2	B	43	VAL
2	B	59	VAL
2	B	70	GLU
2	B	173	SER
2	B	190	LEU
2	B	207	SER
2	B	229	LYS
2	B	249	ARG
3	C	13	ASP
3	C	35	VAL
3	C	45	VAL
3	C	93	SER
3	C	113	SER
3	C	163	ARG
3	C	195	LEU
3	C	205	ASN
3	C	208	LEU
3	C	210	VAL
3	C	225	ILE
4	D	46	VAL
4	D	126	GLU

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Mol	Chain	Res	Type
4	D	139	VAL
4	D	199	LEU
4	D	231	LYS
5	E	10	VAL
5	E	29	VAL
5	E	61	LYS
5	E	78	THR
5	E	101[A]	ARG
5	E	101[B]	ARG
5	E	181	GLU
5	E	189	LYS
5	E	202	GLU
5	E	218	ASP
5	E	229	VAL
6	F	17	ASP
6	F	28	LYS
6	F	51	LYS
6	F	53	VAL
6	F	81	LEU
6	F	87	LEU
6	F	187	ARG
6	F	190	VAL
6	F	240	LYS
6	F	244	LYS
7	G	11	ARG
7	G	42	VAL
7	G	78	CYS
7	G	88	ARG
7	G	100	ASN
7	G	183	VAL
7	G	190	THR
7	G	206	LEU
7	G	209	ASP
7	G	226	LYS
7	G	232	GLU
8	H	6	VAL
8	H	12	ILE
8	H	65	LEU
8	H	68	LEU
8	H	132	LEU
8	H	153	ASN
8	H	183	LEU

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Mol	Chain	Res	Type
8	H	197	THR
8	H	199	LEU
8	H	215	LYS
9	I	35	THR
9	I	69	ARG
9	I	115	THR
10	J	1[A]	MET
10	J	1[B]	MET
10	J	62	LYS
10	J	88	LEU
10	J	95	ARG
10	J	111	GLU
10	J	155	ARG
10	J	172	ILE
10	J	182	ILE
11	K	12	VAL
11	K	42	LEU
11	K	72	GLU
11	K	81	LYS
11	K	138	VAL
11	K	147	LEU
11	K	158	ARG
11	K	174	VAL
11	K	187	VAL
11	K	192	VAL
12	L	3[A]	SER
12	L	3[B]	SER
12	L	174	LEU
12	L	207	THR
13	M	119	GLU
13	M	154	LEU
13	M	156	LYS
13	M	204	SER
13	M	206	GLU
14	N	22	THR
14	N	68	ILE
1	O	10	THR
1	O	49	LYS
1	O	73	LEU
1	O	135	ILE
1	O	180	ASP
1	O	181	LEU

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Mol	Chain	Res	Type
1	O	184	GLU
1	O	189	THR
1	O	206	ASN
1	O	223	THR
1	O	226	LYS
2	P	7[A]	SER
2	P	7[B]	SER
2	P	33	THR
2	P	59	VAL
2	P	70	GLU
2	P	153	SER
2	P	173	SER
2	P	177	GLN
2	P	190	LEU
2	P	207	SER
2	P	236	LEU
2	P	246	LYS
3	Q	45	VAL
3	Q	56	GLU
3	Q	93	SER
3	Q	98	VAL
3	Q	113	SER
3	Q	163	ARG
3	Q	195	LEU
3	Q	197	GLU
3	Q	206	ILE
3	Q	208	LEU
3	Q	223	GLU
3	Q	225	ILE
3	Q	226	GLU
3	Q	227	LYS
4	R	46	VAL
4	R	139	VAL
5	S	10	VAL
5	S	29	VAL
5	S	45	VAL
5	S	78	THR
5	S	101	ARG
5	S	181	GLU
5	S	204	ASP
5	S	229	VAL
6	T	17	ASP

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Mol	Chain	Res	Type
6	T	28	LYS
6	T	51	LYS
6	T	53	VAL
6	T	54	LEU
6	T	81	LEU
6	T	87	LEU
6	T	190	VAL
6	T	240	LYS
7	U	42	VAL
7	U	78	CYS
7	U	100	ASN
7	U	151	VAL
7	U	196	GLU
7	U	199	ILE
7	U	206	LEU
7	U	232	GLU
8	V	1	THR
8	V	6	VAL
8	V	12	ILE
8	V	65	LEU
8	V	68	LEU
8	V	132	LEU
8	V	183	LEU
8	V	199	LEU
8	V	213	THR
8	V	215	LYS
9	W	35	THR
9	W	69	ARG
10	X	1	MET
10	X	27	GLN
10	X	62	LYS
10	X	88	LEU
10	X	95	ARG
10	X	182	ILE
11	Y	12	VAL
11	Y	41	LEU
11	Y	72	GLU
11	Y	138	VAL
11	Y	147	LEU
11	Y	192	VAL
12	Z	174	LEU
12	Z	207	THR

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Mol	Chain	Res	Type
12	Z	208	VAL
13	a	71	VAL
13	a	92	LEU
13	a	119	GLU
13	a	154	LEU
13	a	204	SER
13	a	216	SER
14	b	22	THR
14	b	29	ARG
14	b	35	THR
14	b	92	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	108	GLN
1	A	206	ASN
2	B	40	ASN
2	B	100	GLN
2	B	102	GLN
2	B	109	GLN
2	B	142	HIS
2	B	149	GLN
3	C	92	GLN
4	D	152	GLN
4	D	155	HIS
5	E	8	ASN
5	E	60	GLN
5	E	65	HIS
5	E	175	HIS
5	E	185	ASN
6	F	143	ASN
7	G	128	ASN
9	I	32	GLN
9	I	161	HIS
10	J	63	ASN
10	J	87	ASN
10	J	101	ASN
10	J	132	HIS
11	K	62	GLN
11	K	119	ASN

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Mol	Chain	Res	Type
11	K	162	GLN
12	L	77	HIS
12	L	131	GLN
12	L	157	ASN
13	M	47	ASN
13	M	65	GLN
13	M	162	GLN
13	M	188	GLN
14	N	66	HIS
14	N	77	HIS
14	N	110	GLN
1	O	118	GLN
1	O	206	ASN
2	P	40	ASN
2	P	88	ASN
2	P	102	GLN
2	P	109	GLN
2	P	142	HIS
2	P	149	GLN
3	Q	18	GLN
3	Q	92	GLN
4	R	97	GLN
4	R	152	GLN
4	R	186	HIS
5	S	8	ASN
5	S	60	GLN
5	S	175	HIS
6	T	63	ASN
6	T	68	ASN
7	U	128	ASN
8	V	57	GLN
9	W	32	GLN
9	W	172	ASN
10	X	24	ASN
10	X	63	ASN
10	X	174	ASN
11	Y	62	GLN
11	Y	119	ASN
11	Y	162	GLN
12	Z	79	ASN
12	Z	131	GLN
13	a	47	ASN

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Mol	Chain	Res	Type
13	a	65	GLN
13	a	89	HIS
13	a	162	GLN
13	a	188	GLN
14	b	110	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
15	OAS	c	2	15	5,6,9	0.69	0	2,6,11	2.54	2 (100%)
15	OAS	f	3	15	5,6,9	1.03	0	2,6,11	1.21	0
15	OAS	e	2	15	5,6,9	1.09	1 (20%)	2,6,11	2.00	1 (50%)
5	6V1	S	148	5	13,15,16	1.68	5 (38%)	10,20,22	2.63	5 (50%)
15	OAS	f	2	15	5,6,9	0.57	0	2,6,11	1.57	1 (50%)
10	6V1	J	91	10	13,15,16	1.74	4 (30%)	10,20,22	4.25	6 (60%)
15	6V9	e	1	15	7,8,9	1.56	1 (14%)	7,10,12	3.92	4 (57%)
15	OAS	e	3	15	5,6,9	0.51	0	2,6,11	0.77	0
3	YCM	Q	63	3	7,9,10	1.33	1 (14%)	5,10,12	2.52	2 (40%)
7	6V1	U	47	7	13,15,16	1.70	3 (23%)	10,20,22	1.98	2 (20%)
7	YCM	U	137	7	7,9,10	1.03	0	5,10,12	2.76	1 (20%)
3	YCM	C	63	3	7,9,10	1.06	1 (14%)	5,10,12	1.28	1 (20%)
15	OAS	d	2	15	5,6,9	0.57	0	2,6,11	1.67	0
15	6V9	f	1	15	7,8,9	1.70	2 (28%)	7,10,12	4.11	6 (85%)
5	6V1	E	148	5	13,15,16	1.72	4 (30%)	10,20,22	2.52	4 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	6V1	G	47	7	13,15,16	1.84	2 (15%)	10,20,22	1.97	3 (30%)
7	YCM	G	137	7	7,9,10	1.72	2 (28%)	5,10,12	2.39	2 (40%)
15	OAS	d	3	15	5,6,9	0.93	0	2,6,11	0.93	0
15	6V9	d	1	15	7,8,9	1.66	2 (28%)	7,10,12	4.43	7 (100%)
7	6V1	U	161	7	13,15,16	2.34	3 (23%)	10,20,22	2.84	5 (50%)
10	6V1	X	91	10	13,15,16	1.63	4 (30%)	10,20,22	4.09	6 (60%)
15	OAS	c	3	15	5,6,9	0.62	0	2,6,11	0.75	0
15	6V9	c	1	15	7,8,9	1.44	1 (14%)	7,10,12	4.99	5 (71%)
7	6V1	G	161	7	13,15,16	1.58	4 (30%)	10,20,22	1.98	4 (40%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	6V1	G	161	7	-	0/6/25/27	0/1/1/1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	U	161	6V1	C1-SG	-5.16	1.77	1.83
7	U	161	6V1	CB-SG	-5.12	1.77	1.82
7	G	47	6V1	CB-SG	-4.78	1.77	1.82
7	U	47	6V1	CB-SG	-4.41	1.77	1.82
10	J	91	6V1	C4-N3	-3.98	1.32	1.38
5	E	148	6V1	CB-SG	-3.97	1.78	1.82
15	e	1	6V9	C-C3	3.60	1.50	1.45
15	f	1	6V9	C-C3	3.33	1.49	1.45
5	S	148	6V1	CB-SG	-3.28	1.78	1.82
10	X	91	6V1	C4-N3	-3.20	1.33	1.38
3	Q	63	YCM	CD-SG	-3.11	1.73	1.81
15	c	1	6V9	C-C3	3.10	1.49	1.45
10	J	91	6V1	C1-SG	-3.06	1.79	1.83
5	S	148	6V1	C2-N3	-3.05	1.34	1.38
7	G	161	6V1	C1-SG	-3.03	1.80	1.83
15	d	1	6V9	C-C3	2.88	1.49	1.45
7	U	161	6V1	C2-N3	-2.82	1.34	1.38
7	U	47	6V1	C4-N3	-2.75	1.34	1.38
7	G	47	6V1	C2-N3	-2.74	1.35	1.38
7	G	137	YCM	CD-SG	2.67	1.88	1.81
5	E	148	6V1	C2-N3	-2.60	1.35	1.38
7	G	161	6V1	CB-SG	-2.59	1.79	1.82
7	G	137	YCM	CE-NZ2	2.56	1.41	1.32
10	X	91	6V1	C1-SG	-2.54	1.80	1.83
15	d	1	6V9	C1-N	2.44	1.38	1.31
5	S	148	6V1	C5-C4	2.44	1.54	1.50
10	X	91	6V1	CB-SG	-2.41	1.79	1.82
7	G	161	6V1	C4-N3	-2.36	1.35	1.38
5	E	148	6V1	C4-N3	-2.36	1.35	1.38
7	G	161	6V1	C2-N3	-2.32	1.35	1.38
15	f	1	6V9	C1-N	2.30	1.38	1.31
10	J	91	6V1	CB-SG	-2.27	1.79	1.82
3	C	63	YCM	CD-SG	-2.26	1.75	1.81
10	X	91	6V1	O7-C2	2.25	1.26	1.22
15	e	2	OAS	CA-N	-2.21	1.41	1.48
7	U	47	6V1	C2-N3	-2.16	1.35	1.38
10	J	91	6V1	O7-C2	2.10	1.26	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	148	6V1	C5-C4	2.07	1.54	1.50
5	S	148	6V1	C1-SG	-2.06	1.81	1.83
5	S	148	6V1	C4-N3	-2.04	1.35	1.38

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	c	1	6V9	S-C1-N	-10.17	107.72	114.63
15	e	1	6V9	S-C1-N	-7.68	109.41	114.63
15	d	1	6V9	S-C1-N	-7.36	109.62	114.63
10	J	91	6V1	C6-N3-C2	7.14	131.74	123.37
10	X	91	6V1	C6-N3-C2	6.99	131.56	123.37
15	f	1	6V9	S-C1-N	-6.67	110.10	114.63
10	J	91	6V1	O7-C2-N3	6.27	131.74	124.14
5	E	148	6V1	C2-N3-C4	-6.07	109.52	113.07
7	U	161	6V1	C5-C4-N3	6.04	111.87	108.07
10	X	91	6V1	O7-C2-N3	5.95	131.36	124.14
10	J	91	6V1	C5-C4-N3	5.58	111.58	108.07
15	c	1	6V9	C1-S-C3	5.57	92.87	89.63
7	U	137	YCM	CE-CD-SG	5.51	131.20	113.81
15	f	1	6V9	O-C-C3	-5.25	115.72	124.98
15	d	1	6V9	O-C-C3	-5.09	116.00	124.98
10	X	91	6V1	C2-N3-C4	-5.03	110.12	113.07
10	J	91	6V1	C2-N3-C4	-4.93	110.18	113.07
10	X	91	6V1	C5-C4-N3	4.73	111.05	108.07
7	U	47	6V1	C2-N3-C4	-4.64	110.35	113.07
3	Q	63	YCM	CE-CD-SG	-4.60	99.30	113.81
7	U	161	6V1	C2-N3-C4	-4.45	110.47	113.07
15	d	1	6V9	C2-C1-N	4.31	132.77	123.75
10	X	91	6V1	C6-N3-C4	-4.25	117.50	122.52
15	e	1	6V9	C21-C3-C	4.23	132.04	127.15
7	G	137	YCM	CE-CD-SG	4.23	127.17	113.81
10	J	91	6V1	C6-N3-C4	-4.22	117.53	122.52
15	c	1	6V9	C21-C3-C	4.20	132.01	127.15
7	G	47	6V1	C2-N3-C4	-4.20	110.61	113.07
5	S	148	6V1	C2-N3-C4	-4.18	110.62	113.07
15	e	1	6V9	C1-S-C3	4.03	91.97	89.63
5	S	148	6V1	C6-N3-C4	3.99	127.24	122.52
7	G	161	6V1	O8-C4-N3	3.80	128.01	123.94
5	S	148	6V1	C5-C4-N3	3.77	110.44	108.07
7	U	161	6V1	O8-C4-C5	-3.71	121.85	127.28
15	f	1	6V9	C2-C1-N	3.67	131.44	123.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	d	1	6V9	C21-C3-C	3.64	131.36	127.15
10	X	91	6V1	O7-C2-C1	-3.45	117.01	124.52
15	f	1	6V9	C21-C3-C	3.43	131.11	127.15
5	E	148	6V1	C5-C4-N3	3.40	110.21	108.07
10	J	91	6V1	O7-C2-C1	-3.38	117.16	124.52
15	c	1	6V9	C2-C1-N	3.36	130.78	123.75
7	G	47	6V1	C5-C4-N3	3.32	110.16	108.07
5	S	148	6V1	O7-C2-N3	-3.28	120.16	124.14
15	d	1	6V9	C1-S-C3	3.19	91.49	89.63
7	G	161	6V1	O8-C4-C5	-3.16	122.65	127.28
15	d	1	6V9	C-C3-S	-3.12	117.51	121.31
15	f	1	6V9	C-C3-S	-3.10	117.53	121.31
15	c	2	OAS	OG-CB-CA	2.77	116.78	109.25
15	f	1	6V9	C1-S-C3	2.75	91.23	89.63
15	c	1	6V9	O-C-C3	-2.74	120.14	124.98
15	e	2	OAS	OG-CB-CA	2.70	116.60	109.25
15	e	1	6V9	O-C-C3	-2.66	120.28	124.98
5	S	148	6V1	CB-CA-C	-2.39	104.32	110.80
5	E	148	6V1	C6-N3-C4	2.38	125.34	122.52
5	E	148	6V1	CB-CA-C	-2.31	104.53	110.80
7	U	47	6V1	C5-C4-N3	2.30	109.52	108.07
3	C	63	YCM	CE-CD-SG	-2.29	106.59	113.81
15	d	1	6V9	C2-C1-S	-2.29	117.61	122.51
15	c	2	OAS	C1A-OG-CB	2.28	121.53	112.37
7	U	161	6V1	C6-N3-C4	2.24	125.17	122.52
7	U	161	6V1	O8-C4-N3	2.18	126.28	123.94
3	Q	63	YCM	CA-CB-SG	-2.18	105.48	113.51
15	f	2	OAS	OG-CB-CA	-2.17	103.33	109.25
7	G	47	6V1	C6-N3-C4	2.17	125.08	122.52
7	G	137	YCM	OZ1-CE-NZ2	-2.06	117.04	122.53
7	G	161	6V1	C5-C4-N3	2.01	109.33	108.07
7	G	161	6V1	O7-C2-N3	2.00	126.57	124.14

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	137	YCM	SG-CD-CE-NZ2

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Mol	Chain	Res	Type	Atoms
10	J	91	6V1	C3-C6-N3-C2
10	J	91	6V1	C3-C6-N3-C4
3	Q	63	YCM	SG-CD-CE-OZ1
3	Q	63	YCM	SG-CD-CE-NZ2
10	X	91	6V1	C3-C6-N3-C2
10	X	91	6V1	C3-C6-N3-C4
15	f	1	6V9	O-C-C3-C21
15	c	2	OAS	N-CA-CB-OG
15	c	2	OAS	C-CA-CB-OG
15	e	2	OAS	N-CA-CB-OG
15	e	2	OAS	C-CA-CB-OG
5	E	148	6V1	C3-C6-N3-C4
5	E	148	6V1	C3-C6-N3-C2
15	c	2	OAS	CA-CB-OG-C1A
15	d	1	6V9	O-C-C3-S
15	d	1	6V9	O-C-C3-C21
15	e	1	6V9	O-C-C3-C21
15	f	1	6V9	O-C-C3-S
15	f	3	OAS	CA-CB-OG-C1A
7	G	137	YCM	CE-CD-SG-CB
15	e	1	6V9	O-C-C3-S
7	U	47	6V1	C3-C6-N3-C4
7	U	161	6V1	N-CA-CB-SG
3	Q	63	YCM	CE-CD-SG-CB
7	U	137	YCM	CE-CD-SG-CB
15	e	3	OAS	CA-CB-OG-C1A
15	e	2	OAS	CA-CB-OG-C1A
15	c	3	OAS	CA-CB-OG-C1A

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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	N	301	-	15,15,15	0.57	0	14,14,14	0.50	0
18	1PE	Y	301	-	15,15,15	0.63	0	14,14,14	0.62	0
18	1PE	L	301	-	15,15,15	0.60	0	14,14,14	0.46	0
18	1PE	U	301	-	15,15,15	0.65	0	14,14,14	0.68	0
18	1PE	a	301	-	15,15,15	0.60	0	14,14,14	0.38	0
19	ACT	d	101	-	3,3,3	0.72	0	3,3,3	0.88	0
19	ACT	c	101	-	3,3,3	0.79	0	3,3,3	0.98	0
19	ACT	f	101	-	3,3,3	1.01	0	3,3,3	0.69	0
18	1PE	I	302	-	15,15,15	0.73	0	14,14,14	0.84	0
19	ACT	e	101	-	3,3,3	0.87	0	3,3,3	0.43	0
18	1PE	H	303	-	15,15,15	0.64	0	14,14,14	0.75	0
18	1PE	W	302	-	15,15,15	0.69	0	14,14,14	0.33	0
18	1PE	K	302	-	15,15,15	0.70	0	14,14,14	0.75	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
18	1PE	N	301	-	-	5/13/13/13	-
18	1PE	Y	301	-	-	7/13/13/13	-
18	1PE	L	301	-	-	5/13/13/13	-
18	1PE	U	301	-	-	6/13/13/13	-
18	1PE	a	301	-	-	6/13/13/13	-
18	1PE	I	302	-	-	8/13/13/13	-
18	1PE	H	303	-	-	7/13/13/13	-
18	1PE	W	302	-	-	5/13/13/13	-
18	1PE	K	302	-	-	7/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	I	302	1PE	C15-C25-OH5-C14
18	H	303	1PE	C24-C14-OH5-C25
18	K	302	1PE	C16-C26-OH6-C15
18	Y	301	1PE	C16-C26-OH6-C15
18	H	303	1PE	OH4-C13-C23-OH3
18	K	302	1PE	OH5-C14-C24-OH4
18	L	301	1PE	OH4-C13-C23-OH3
18	U	301	1PE	OH4-C13-C23-OH3
18	Y	301	1PE	OH6-C15-C25-OH5
18	W	302	1PE	OH6-C15-C25-OH5
18	K	302	1PE	OH6-C15-C25-OH5
18	H	303	1PE	OH5-C14-C24-OH4
18	U	301	1PE	OH6-C15-C25-OH5
18	a	301	1PE	OH5-C14-C24-OH4
18	a	301	1PE	OH4-C13-C23-OH3
18	L	301	1PE	OH5-C14-C24-OH4
18	N	301	1PE	OH4-C13-C23-OH3
18	H	303	1PE	OH7-C16-C26-OH6
18	I	302	1PE	OH2-C12-C22-OH3
18	U	301	1PE	C24-C14-OH5-C25
18	K	302	1PE	OH2-C12-C22-OH3
18	N	301	1PE	OH2-C12-C22-OH3
18	W	302	1PE	OH2-C12-C22-OH3
18	a	301	1PE	OH7-C16-C26-OH6
18	L	301	1PE	OH6-C15-C25-OH5
18	N	301	1PE	OH7-C16-C26-OH6
18	L	301	1PE	OH2-C12-C22-OH3
18	I	302	1PE	OH6-C15-C25-OH5
18	K	302	1PE	C25-C15-OH6-C26
18	L	301	1PE	C14-C24-OH4-C13
18	Y	301	1PE	C15-C25-OH5-C14
18	Y	301	1PE	C23-C13-OH4-C24
18	a	301	1PE	C25-C15-OH6-C26
18	a	301	1PE	OH6-C15-C25-OH5
18	I	302	1PE	C24-C14-OH5-C25
18	W	302	1PE	C14-C24-OH4-C13
18	a	301	1PE	C14-C24-OH4-C13

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Mol	Chain	Res	Type	Atoms
18	Y	301	1PE	OH2-C12-C22-OH3
18	U	301	1PE	OH7-C16-C26-OH6
18	Y	301	1PE	OH7-C16-C26-OH6
18	H	303	1PE	C16-C26-OH6-C15
18	U	301	1PE	C13-C23-OH3-C22
18	I	302	1PE	C14-C24-OH4-C13
18	H	303	1PE	C15-C25-OH5-C14
18	Y	301	1PE	C12-C22-OH3-C23
18	K	302	1PE	C13-C23-OH3-C22
18	K	302	1PE	C12-C22-OH3-C23
18	N	301	1PE	C13-C23-OH3-C22
18	W	302	1PE	C24-C14-OH5-C25
18	I	302	1PE	OH7-C16-C26-OH6
18	U	301	1PE	OH5-C14-C24-OH4
18	I	302	1PE	C13-C23-OH3-C22
18	I	302	1PE	OH4-C13-C23-OH3
18	H	303	1PE	OH6-C15-C25-OH5
18	W	302	1PE	C23-C13-OH4-C24
18	N	301	1PE	C16-C26-OH6-C15

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	d	101	ACT	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%)	-0.05	5 (2%) 62 59	32, 62, 99, 120	3 (1%)
1	O	230/234 (98%)	0.34	6 (2%) 57 54	55, 82, 127, 151	0
2	B	248/261 (95%)	0.12	5 (2%) 65 62	30, 67, 118, 170	2 (0%)
2	P	247/261 (94%)	0.25	8 (3%) 50 47	39, 80, 137, 171	2 (0%)
3	C	236/248 (95%)	0.43	6 (2%) 58 55	36, 78, 130, 180	2 (0%)
3	Q	234/248 (94%)	0.45	16 (6%) 23 20	44, 81, 152, 204	0
4	D	233/241 (96%)	0.27	6 (2%) 57 54	40, 75, 109, 141	1 (0%)
4	R	233/241 (96%)	-0.10	5 (2%) 63 60	21, 55, 84, 118	1 (0%)
5	E	233/263 (88%)	-0.09	6 (2%) 57 54	31, 56, 99, 130	1 (0%)
5	S	237/263 (90%)	-0.13	3 (1%) 75 73	27, 58, 94, 125	3 (1%)
6	F	239/255 (93%)	-0.23	2 (0%) 82 80	28, 50, 77, 98	4 (1%)
6	T	240/255 (94%)	0.17	6 (2%) 58 55	34, 63, 105, 134	1 (0%)
7	G	241/246 (97%)	-0.21	3 (1%) 76 74	27, 54, 99, 148	2 (0%)
7	U	235/246 (95%)	0.25	6 (2%) 57 54	37, 74, 111, 148	1 (0%)
8	H	220/234 (94%)	-0.34	0 100 100	26, 47, 82, 112	2 (0%)
8	V	220/234 (94%)	0.11	8 (3%) 46 43	33, 62, 106, 126	2 (0%)
9	I	204/205 (99%)	-0.37	0 100 100	29, 49, 76, 96	3 (1%)
9	W	204/205 (99%)	0.06	0 100 100	39, 66, 97, 109	2 (0%)
10	J	195/201 (97%)	-0.19	3 (1%) 72 69	22, 53, 74, 91	3 (1%)
10	X	195/201 (97%)	-0.15	2 (1%) 79 77	26, 56, 77, 95	2 (1%)
11	K	200/204 (98%)	-0.05	2 (1%) 79 77	46, 60, 90, 109	0
11	Y	199/204 (97%)	-0.41	1 (0%) 87 85	26, 46, 72, 83	3 (1%)
12	L	213/213 (100%)	0.03	3 (1%) 73 71	31, 65, 91, 114	2 (0%)
12	Z	213/213 (100%)	-0.38	0 100 100	33, 48, 78, 99	1 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	216/219 (98%)	-0.28	2 (0%) 81 79	35, 51, 77, 115	1 (0%)
13	a	216/219 (98%)	-0.37	2 (0%) 81 79	30, 47, 73, 107	2 (0%)
14	N	202/205 (98%)	-0.41	5 (2%) 58 55	29, 44, 70, 117	1 (0%)
14	b	203/205 (99%)	-0.30	5 (2%) 58 55	37, 50, 81, 131	1 (0%)
15	c	0/4	-	-	-	-
15	d	0/4	-	-	-	-
15	e	0/4	-	-	-	-
15	f	0/4	-	-	-	-
All	All	6216/6474 (96%)	-0.05	116 (1%) 66 63	21, 59, 107, 204	48 (0%)

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	S	2	PHE	4.4
7	U	186	LYS	4.3
14	N	202	LEU	4.2
13	a	215	ILE	4.1
8	V	220	GLU	4.1
11	Y	40	TYR	4.0
2	P	61	PHE	4.0
3	Q	50	VAL	4.0
10	X	147	TYR	3.9
3	Q	232	ILE	3.7
10	J	147	TYR	3.6
8	V	204	CYS	3.6
6	T	5	THR	3.5
5	E	59	HIS	3.4
11	K	40	TYR	3.4
4	R	241	ILE	3.4
3	Q	229	VAL	3.4
6	T	6	GLY	3.4
6	T	208	ALA	3.4
3	C	138	PHE	3.4
13	a	216	SER	3.3
13	M	215	ILE	3.3
5	S	239	ARG	3.2
4	R	130	PRO	3.2
3	C	53	LEU	3.2
8	V	1	THR	3.1
14	N	201	THR	3.1
7	U	185	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	O	188	HIS	3.1
3	Q	225	ILE	3.1
3	C	97	THR	3.0
12	L	161	VAL	2.9
3	Q	51	ALA	2.9
1	O	50	LYS	2.9
7	U	193	GLN	2.9
3	Q	241	LYS	2.9
2	P	203	VAL	2.9
14	N	198	ALA	2.9
1	A	3	ARG	2.8
14	b	202	LEU	2.8
1	O	231	ALA	2.8
2	P	46	ALA	2.8
7	G	189	TRP	2.8
14	b	203	PRO	2.8
7	G	245	ARG	2.8
7	U	245	ARG	2.8
2	B	61	PHE	2.8
2	B	101	TYR	2.7
3	Q	48	LYS	2.7
14	b	199	VAL	2.7
14	N	200	ALA	2.7
2	P	55	LEU	2.7
1	O	177	TYR	2.7
3	Q	85	ASN	2.7
5	S	18[A]	ARG	2.7
7	G	187	PHE	2.6
3	Q	199	VAL	2.6
6	T	204	VAL	2.5
5	E	4	ASN	2.5
3	Q	49	SER	2.5
8	V	199	LEU	2.5
1	O	232	ILE	2.5
8	V	202	TYR	2.5
4	D	131	GLY	2.5
6	F	6	GLY	2.5
3	C	206	ILE	2.5
2	P	205	LYS	2.5
3	Q	138	PHE	2.5
2	B	2	SER	2.4
1	O	4	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	203	VAL	2.4
11	K	200	SER	2.4
13	M	216	SER	2.4
3	Q	97	THR	2.4
6	T	207	LYS	2.4
5	E	54	SER	2.4
2	P	51	ASN	2.4
4	D	241	ILE	2.4
14	b	198	ALA	2.3
2	B	202	ASP	2.3
10	J	1[A]	MET	2.3
14	N	199	VAL	2.3
10	J	148	THR	2.3
2	P	245	ALA	2.3
8	V	203	ARG	2.3
12	L	164	VAL	2.3
14	b	201	THR	2.2
4	R	127	ASP	2.2
1	A	230	ALA	2.2
1	A	231	ALA	2.2
2	P	248	GLU	2.2
4	D	175[A]	GLU	2.2
7	U	194	THR	2.2
3	Q	205	ASN	2.2
5	E	237	GLU	2.2
4	R	131	GLY	2.1
3	Q	230	ALA	2.1
3	C	196	LEU	2.1
4	D	172	SER	2.1
10	X	196	PHE	2.1
6	T	63	ASN	2.1
7	U	209	ASP	2.1
1	A	232	ILE	2.1
3	Q	52	LYS	2.1
6	F	244	LYS	2.1
3	Q	98	VAL	2.1
4	D	132	ALA	2.1
4	R	120[A]	ALA	2.1
12	L	162	GLU	2.0
8	V	201	ARG	2.0
1	A	50	LYS	2.0
5	E	61	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
3	C	98	VAL	2.0
5	E	56	LEU	2.0
4	D	9	ASP	2.0
8	V	197	THR	2.0

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. 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	B-factors(Å ²)	Q<0.9
7	6V1	U	47	15/16	0.84	0.14	94,131,141,141	0
7	YCM	U	137	10/11	0.86	0.14	60,70,87,87	0
5	6V1	E	148	15/16	0.90	0.12	47,68,74,76	0
7	YCM	G	137	10/11	0.90	0.12	46,53,68,69	0
7	6V1	U	161	15/16	0.90	0.11	70,89,97,99	0
5	6V1	S	148	15/16	0.91	0.13	44,74,82,83	0
3	YCM	C	63	10/11	0.91	0.10	63,69,85,89	0
15	6V9	f	1	8/9	0.92	0.10	61,63,68,68	0
3	YCM	Q	63	10/11	0.93	0.09	67,72,78,79	0
7	6V1	G	47	15/16	0.93	0.13	53,79,84,85	0
10	6V1	X	91	15/16	0.94	0.12	48,69,76,76	0
10	6V1	J	91	15/16	0.95	0.11	43,64,69,69	0
15	6V9	d	1	8/9	0.95	0.09	52,55,61,63	0
7	6V1	G	161	15/16	0.95	0.11	46,69,77,78	0
15	OAS	f	3	7/10	0.95	0.08	52,53,58,60	0
15	OAS	e	2	7/10	0.96	0.08	34,37,43,48	0
15	6V9	c	1	8/9	0.96	0.09	51,52,53,53	0
15	OAS	c	2	7/10	0.97	0.06	49,50,52,54	0
15	OAS	f	2	7/10	0.97	0.06	53,56,58,60	0
15	OAS	c	3	7/10	0.97	0.06	47,48,48,48	0
15	OAS	e	3	7/10	0.97	0.05	35,35,38,39	0
15	OAS	d	2	7/10	0.97	0.06	45,46,47,49	0
15	6V9	e	1	8/9	0.98	0.05	41,42,44,45	0
15	OAS	d	3	7/10	0.98	0.05	42,45,51,52	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
18	1PE	H	303	16/16	0.80	0.15	71,82,101,107	0
18	1PE	W	302	16/16	0.81	0.14	75,93,100,103	0
18	1PE	I	302	16/16	0.82	0.14	76,88,94,95	0
18	1PE	K	302	16/16	0.84	0.14	78,86,93,94	0
18	1PE	a	301	16/16	0.85	0.17	77,82,114,116	0
18	1PE	L	301	16/16	0.86	0.18	80,89,117,117	0
18	1PE	Y	301	16/16	0.88	0.14	64,80,88,91	0
19	ACT	f	101	4/4	0.88	0.14	59,60,63,67	0
18	1PE	U	301	16/16	0.89	0.12	57,66,87,89	0
18	1PE	N	301	16/16	0.90	0.11	51,64,78,79	0
19	ACT	d	101	4/4	0.91	0.12	54,60,61,65	0
16	K	Z	301	1/1	0.91	0.16	67,67,67,67	0
17	MG	K	301	1/1	0.93	0.14	50,50,50,50	0
19	ACT	c	101	4/4	0.93	0.12	63,65,65,66	0
16	K	U	302	1/1	0.93	0.21	62,62,62,62	0
16	K	L	302	1/1	0.93	0.14	77,77,77,77	0
16	K	b	301	1/1	0.95	0.14	60,60,60,60	0
17	MG	I	303	1/1	0.95	0.10	40,40,40,40	0
19	ACT	e	101	4/4	0.95	0.12	47,48,49,49	0
16	K	G	301	1/1	0.95	0.15	59,59,59,59	0
17	MG	H	302	1/1	0.96	0.16	45,45,45,45	0
17	MG	H	301	1/1	0.96	0.07	59,59,59,59	0
17	MG	I	301	1/1	0.97	0.06	43,43,43,43	0
17	MG	L	303	1/1	0.97	0.14	49,49,49,49	0
16	K	N	302	1/1	0.97	0.11	56,56,56,56	0
17	MG	V	301	1/1	0.98	0.07	64,64,64,64	0
17	MG	W	301	1/1	0.98	0.09	50,50,50,50	0
17	MG	J	301	1/1	0.98	0.05	61,61,61,61	0
17	MG	X	301	1/1	0.99	0.03	65,65,65,65	0

6.5 Other polymers ⓘ

There are no such residues in this entry.