



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 07:52 am BST

PDB ID : 5LAJ
Title : Ligand-induced Lys33-Thr1 crosslinking at the yeast proteasomal subunit beta5 by sulfonate esters
Authors : Groll, M.; Dubiella, C.; Cui, H.
Deposited on : 2016-06-14
Resolution : 2.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

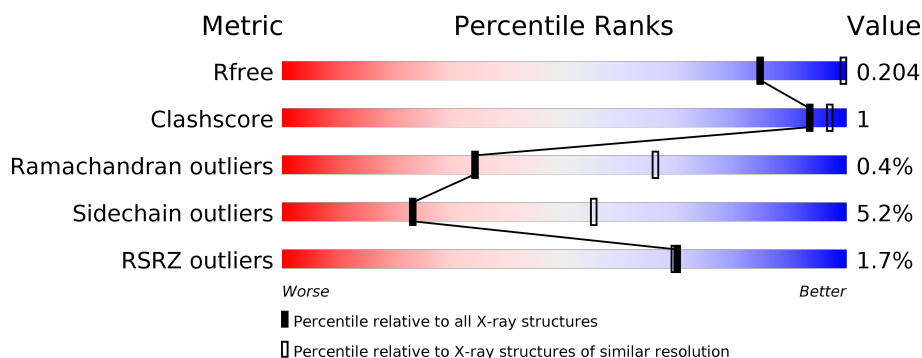
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.







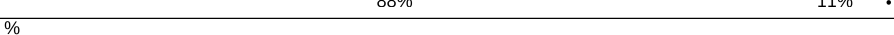
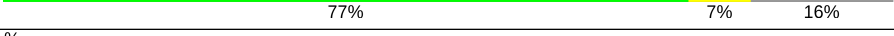



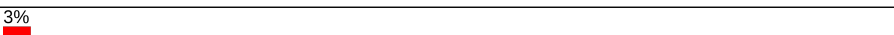
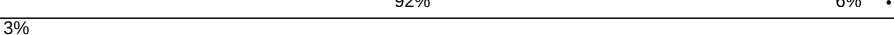

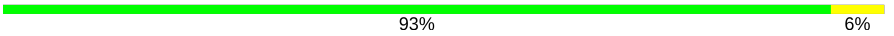








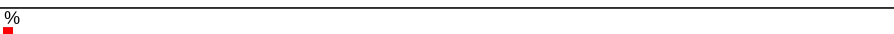
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 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	250	<div> <div>2%</div> <div> <div></div> <div>97%</div> <div></div> </div> <div></div> </div>
1	O	250	<div> <div>3%</div> <div> <div></div> <div>97%</div> <div></div> </div> <div></div> </div>
2	B	258	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>5%</div> </div> <div></div> </div>
2	P	258	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>5%</div> </div> <div></div> </div>
3	C	254	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>6%</div> </div> <div></div> </div>
3	Q	254	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>6%</div> </div> <div></div> </div>

Continued on next page...

Continued from previous page...

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

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 49524 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome subunit alpha type-2.

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

- Molecule 2 is a protein called Proteasome subunit alpha type-3.

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

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

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

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

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

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

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

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

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

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

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

- Molecule 8 is a protein called Proteasome subunit beta type-2.

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

- Molecule 9 is a protein called Proteasome subunit beta type-3.

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

- Molecule 10 is a protein called Proteasome subunit beta type-4.

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

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1643	1045	280	311	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1643	1045	280	311	7			

- Molecule 12 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

- Molecule 13 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	228	Total	C	N	O	S	0	0	0
			1786	1131	305	343	7			
13	a	231	Total	C	N	O	S	0	0	0
			1806	1142	309	348	7			

- Molecule 14 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	b	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Mg	0	0
			1	1		
15	J	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	K	2	Total 2	Mg 2	0	0
15	I	3	Total 3	Mg 3	0	0
15	Z	1	Total 1	Mg 1	0	0
15	N	2	Total 2	Mg 2	0	0
15	L	1	Total 1	Mg 1	0	0

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	8	Total 8	O 8	0	0
16	B	7	Total 7	O 7	0	0
16	C	7	Total 7	O 7	0	0
16	D	7	Total 7	O 7	0	0
16	E	6	Total 6	O 6	0	0
16	F	6	Total 6	O 6	0	0
16	G	7	Total 7	O 7	0	0
16	H	14	Total 14	O 14	0	0
16	I	5	Total 5	O 5	0	0
16	J	10	Total 10	O 10	0	0
16	K	9	Total 9	O 9	0	0
16	L	11	Total 11	O 11	0	0
16	M	8	Total 8	O 8	0	0
16	N	6	Total 6	O 6	0	0

Continued on next page...

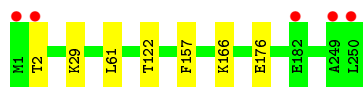
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	O	2	Total 2	O 2	0	0
16	P	9	Total 9	O 9	0	0
16	Q	5	Total 5	O 5	0	0
16	R	3	Total 3	O 3	0	0
16	S	4	Total 4	O 4	0	0
16	T	3	Total 3	O 3	0	0
16	U	10	Total 10	O 10	0	0
16	V	9	Total 9	O 9	0	0
16	W	6	Total 6	O 6	0	0
16	X	5	Total 5	O 5	0	0
16	Y	9	Total 9	O 9	0	0
16	Z	10	Total 10	O 10	0	0
16	a	14	Total 14	O 14	0	0
16	b	5	Total 5	O 5	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 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.

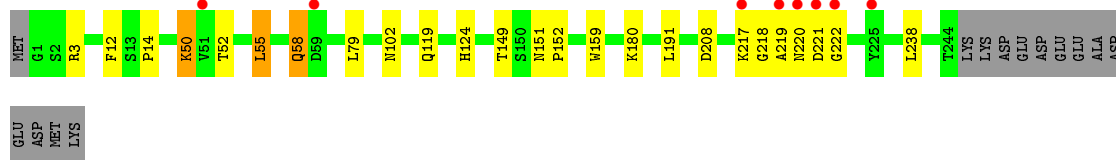
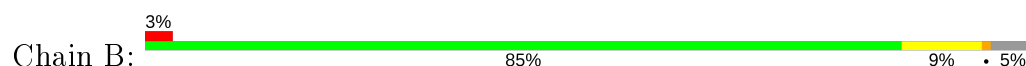
- Molecule 1: Proteasome subunit alpha type-2



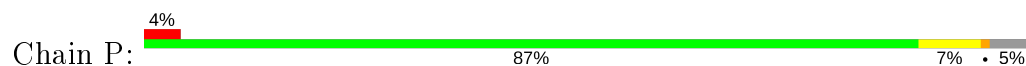
- Molecule 1: Proteasome subunit alpha type-2



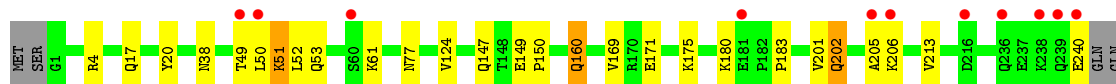
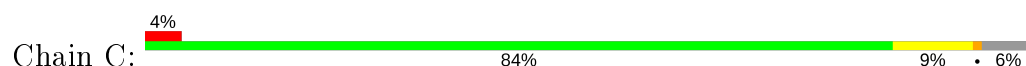
- Molecule 2: Proteasome subunit alpha type-3



- Molecule 2: Proteasome subunit alpha type-3

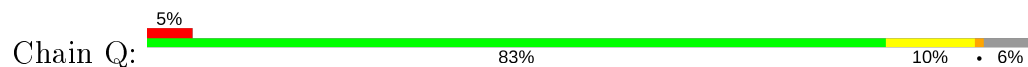


- Molecule 3: Proteasome subunit alpha type-4



GLU
GLN
ASP
LYS
LYS
LYS
LYS
SER
ASN
HIS

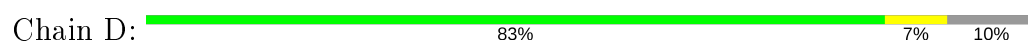
• Molecule 3: Proteasome subunit alpha type-4



MET SER G1 R4 R38 T49 L50 K51 L52 Q53 D84 T55 K61 N77 V124 Q147 T148 E149 P150 Q160 T161 V169 R170 E171 K175 K180 P183 V201 Q202 T203 Q204 A205 K206 V213 E225 T232 Q236 E237 K238 Q239 E240 GLN GLN

GLU
GLN
ASP
LYS
LYS
LYS
SER
ASN
HIS

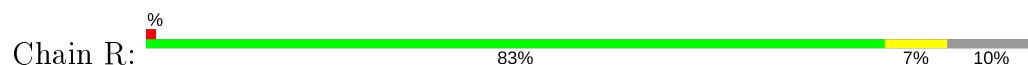
• Molecule 4: Proteasome subunit alpha type-5



MET PHE LEU THR ARG SER GLU TTR D1 L20 L40 L51 C68 A77 I81 H91 I99 L104 E117 GLY ALA SER GLY GLU GLU ARG L125 N160 L176 W179 L190 L193 I214 L235 K236 E242 SER PRQ GLU GLU ALA ASP

VAL
GLU
MET
SER

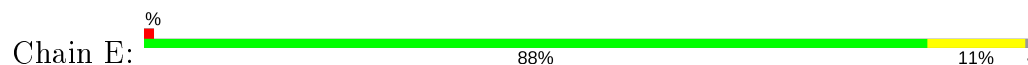
• Molecule 4: Proteasome subunit alpha type-5



MET PHE LEU THR ARG SER GLU TTR D1 L20 L40 L51 C68 A77 I81 I99 L104 E117 GLY ALA SER GLY GLU GLU ARG L125 N160 L176 W179 L190 L193 I214 L235 K236 E242 SER PRQ GLU GLU ALA ASP VAL GLU

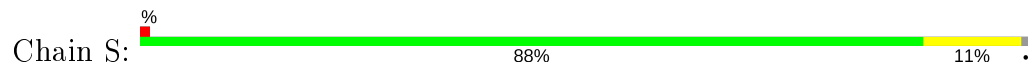
MET
SER

• Molecule 5: Proteasome subunit alpha type-6



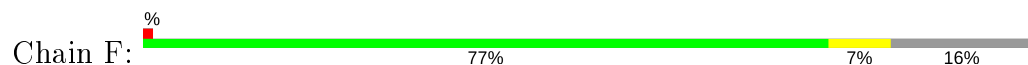
MET PHE ARG N3 D8 T9 V10 F12 L25 K29 E54 L55 L71 L87 N99 A107 Q116 T119 Y122 L155 T158 T174 L175 D176 K180 M184 L188 R201 D202 V207 D208 K217 I233

• Molecule 5: Proteasome subunit alpha type-6



MET PHE ARG N3 D8 T9 V10 F12 L25 K29 E54 L55 L71 L87 N99 A107 Q116 T119 Y122 L155 T158 L175 D176 T177 F178 I179 K180 M184 L188 D202 V207 D208 K217 I233

• Molecule 6: Probable proteasome subunit alpha type-7





- Molecule 9: Proteasome subunit beta type-3

Chain W: 93% 6%



- Molecule 10: Proteasome subunit beta type-4

Chain J: 89% 9% ..



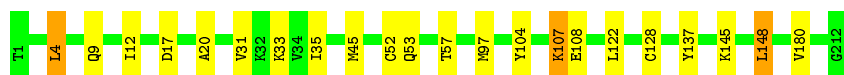
- Molecule 10: Proteasome subunit beta type-4

Chain X: 88% 10% ..



- Molecule 11: Proteasome subunit beta type-5

Chain K: 90% 9% .



- Molecule 11: Proteasome subunit beta type-5

Chain Y: 91% 8% .



- Molecule 12: Proteasome subunit beta type-6

Chain L: 94% 5%




- Molecule 12: Proteasome subunit beta type-6

Chain Z:  94% 5%




- Molecule 13: Proteasome subunit beta type-7

Chain M:  86% 6% 7%

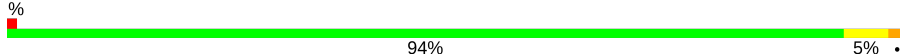


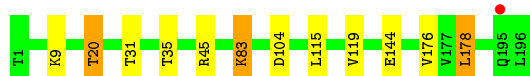
- Molecule 13: Proteasome subunit beta type-7

Chain a:  89% 6% 2%



- Molecule 14: Proteasome subunit beta type-1

Chain N:  94% 5% 1%



- Molecule 14: Proteasome subunit beta type-1

Chain b:  96% 1% 1%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	137.25Å 300.53Å 146.42Å 90.00° 113.73° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.8 (15.00-2.90) 96.8 (15.00-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.180 , 0.201 0.185 , 0.204	Depositor DCC
R_{free} test set	11489 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	64.6	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	49524	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

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

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: 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	0.27	0/1952	0.48	0/2642
1	O	0.27	0/1952	0.48	0/2642
2	B	0.28	0/1934	0.51	0/2618
2	P	0.27	0/1934	0.52	0/2618
3	C	0.28	0/1910	0.53	0/2586
3	Q	0.28	0/1910	0.53	0/2586
4	D	0.27	0/1837	0.50	0/2475
4	R	0.27	0/1837	0.50	0/2475
5	E	0.27	0/1800	0.50	0/2433
5	S	0.27	0/1800	0.50	0/2433
6	F	0.28	0/1932	0.47	0/2609
6	T	0.28	0/1932	0.47	0/2609
7	G	0.28	0/1945	0.49	0/2634
7	U	0.28	0/1945	0.49	0/2634
8	H	0.26	0/1750	0.50	0/2373
8	V	0.25	0/1750	0.49	0/2373
9	I	0.27	0/1611	0.50	0/2174
9	W	0.27	0/1611	0.50	0/2174
10	J	0.27	0/1589	0.50	0/2142
10	X	0.27	0/1589	0.50	0/2142
11	K	0.26	0/1680	0.51	1/2272 (0.0%)
11	Y	0.26	0/1680	0.51	1/2272 (0.0%)
12	L	0.27	0/1795	0.49	0/2420
12	Z	0.27	0/1795	0.49	0/2420
13	M	0.27	0/1817	0.54	0/2465
13	a	0.27	0/1837	0.54	0/2492
14	N	0.26	0/1541	0.48	0/2087
14	b	0.26	0/1541	0.48	0/2087
All	All	0.27	0/50206	0.50	2/67887 (0.0%)

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	B	0	1
2	P	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	4	LEU	CA-CB-CG	5.20	127.27	115.30
11	K	4	LEU	CA-CB-CG	5.15	127.16	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	50	LYS	Peptide
2	P	50	LYS	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	1915	0	1929	1	0
1	O	1915	0	1929	2	0
2	B	1904	0	1904	10	0
2	P	1904	0	1904	5	0
3	C	1881	0	1895	7	0
3	Q	1881	0	1895	7	0
4	D	1813	0	1797	4	0
4	R	1813	0	1797	3	0
5	E	1773	0	1775	6	0
5	S	1773	0	1775	6	0
6	F	1892	0	1883	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	T	1892	0	1883	4	0
7	G	1907	0	1901	3	0
7	U	1907	0	1901	5	0
8	H	1719	0	1719	2	0
8	V	1719	0	1719	3	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	6	0
10	J	1561	0	1569	7	0
10	X	1561	0	1569	8	0
11	K	1643	0	1591	9	0
11	Y	1643	0	1591	8	0
12	L	1757	0	1711	2	0
12	Z	1757	0	1711	2	0
13	M	1786	0	1790	5	0
13	a	1806	0	1808	0	0
14	N	1512	0	1481	6	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	I	3	0	0	0	0
15	J	1	0	0	0	0
15	K	2	0	0	0	0
15	L	1	0	0	0	0
15	N	2	0	0	0	0
15	Z	1	0	0	0	0
16	A	8	0	0	0	0
16	B	7	0	0	0	0
16	C	7	0	0	0	0
16	D	7	0	0	0	0
16	E	6	0	0	0	0
16	F	6	0	0	0	0
16	G	7	0	0	0	0
16	H	14	0	0	0	0
16	I	5	0	0	0	0
16	J	10	0	0	0	0
16	K	9	0	0	0	0
16	L	11	0	0	0	0
16	M	8	0	0	0	0
16	N	6	0	0	0	0
16	O	2	0	0	0	0
16	P	9	0	0	0	0
16	Q	5	0	0	0	0
16	R	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	S	4	0	0	0	0
16	T	3	0	0	0	0
16	U	10	0	0	0	0
16	V	9	0	0	0	0
16	W	6	0	0	0	0
16	X	5	0	0	0	0
16	Y	9	0	0	0	0
16	Z	10	0	0	0	0
16	a	14	0	0	0	0
16	b	5	0	0	0	0
All	All	49524	0	49056	119	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (119) 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)
3:C:51:LYS:O	3:C:52:LEU:HB2	1.99	0.61
10:X:126:VAL:HG12	10:X:128:LEU:HG	1.82	0.61
10:J:126:VAL:HG12	10:J:128:LEU:HG	1.82	0.61
3:Q:51:LYS:O	3:Q:52:LEU:HB2	1.99	0.61
2:B:12:PHE:H	3:C:17:GLN:HE22	1.49	0.61
11:K:53:GLN:O	11:K:57:THR:HG23	2.02	0.59
11:Y:53:GLN:O	11:Y:57:THR:HG23	2.02	0.59
2:B:217:LYS:O	2:B:219:ALA:N	2.39	0.56
2:P:217:LYS:O	2:P:219:ALA:N	2.40	0.55
4:R:99:ILE:HD11	4:R:104:LEU:HB2	1.90	0.54
3:C:201:VAL:O	3:C:202:GLN:CB	2.56	0.53
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.90	0.53
14:N:20:THR:HG22	14:N:31:THR:OG1	2.09	0.53
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.91	0.53
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.56	0.52
4:D:99:ILE:HD11	4:D:104:LEU:HB2	1.90	0.52
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.92	0.52
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.90	0.52
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.92	0.52
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.92	0.52
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.91	0.52
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.40	0.51
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.92	0.51
5:S:12:PHE:H	6:T:19:GLN:HE22	1.58	0.51
7:G:187:GLU:HG2	7:G:192:LYS:HB3	1.93	0.50
7:U:187:GLU:HG2	7:U:192:LYS:HB3	1.94	0.50
5:E:12:PHE:H	6:F:19:GLN:HE22	1.59	0.50
11:K:128:CYS:HB2	11:K:137:TYR:CE2	2.47	0.50
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.93	0.49
10:J:3:ILE:HG23	10:J:18:SER:HB3	1.95	0.48
10:X:3:ILE:HG23	10:X:18:SER:HB3	1.95	0.48
11:Y:128:CYS:HB2	11:Y:137:TYR:CE2	2.48	0.48
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.48	0.48
13:M:159:VAL:O	13:M:159:VAL:HG23	2.13	0.48
12:Z:164:THR:O	12:Z:167:LYS:HE3	2.14	0.47
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.95	0.47
12:L:164:THR:O	12:L:167:LYS:HE3	2.15	0.47
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.97	0.47
14:N:35:THR:CG2	14:N:45:ARG:HE	2.28	0.47
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.98	0.46
12:L:23:LEU:HD13	12:L:43:VAL:HG13	1.97	0.46
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.97	0.46
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.98	0.46
14:N:20:THR:CG2	14:N:31:THR:OG1	2.64	0.45
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.97	0.45
8:V:3:ILE:HG22	8:V:99:ILE:HD12	1.98	0.45
2:B:149:THR:HG1	2:B:159:TRP:HE1	1.63	0.45
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.98	0.45
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.52	0.45
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.99	0.45
10:J:162:LYS:HG3	10:J:195:PHE:CZ	2.52	0.45
8:H:3:ILE:HG22	8:H:99:ILE:HD12	1.98	0.44
9:I:98:ARG:HD2	9:I:126:ILE:HG12	1.99	0.44
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.47	0.44
1:A:176:GLU:HG2	2:B:55:LEU:HD22	1.98	0.44
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.53	0.44
5:E:9:THR:HG21	5:E:119:THR:HA	1.99	0.44
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.99	0.44
5:S:9:THR:HG21	5:S:119:THR:HA	1.99	0.44
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	2.00	0.44
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	1.97	0.44
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.53	0.44
14:N:35:THR:HG21	14:N:45:ARG:HE	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:55:LEU:HB3	7:U:159:ALA:O	2.17	0.44
10:X:162:LYS:HG3	10:X:195:PHE:CZ	2.53	0.43
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.47	0.43
2:P:58:GLN:NE2	2:P:208:ASP:HA	2.34	0.43
6:T:172:LEU:HD13	6:T:195:ILE:HD13	2.01	0.43
6:F:172:LEU:HD13	6:F:195:ILE:HD13	2.01	0.43
9:I:101:PRO:HB3	9:I:126:ILE:HD12	2.00	0.43
9:W:98:ARG:HD2	9:W:126:ILE:HG12	2.00	0.43
11:K:17:ASP:OD1	11:K:33:LYS:NZ	2.52	0.43
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.01	0.42
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.02	0.42
9:W:101:PRO:HB3	9:W:126:ILE:HD12	2.00	0.42
10:J:132:ALA:HB1	10:J:136:SER:HB2	2.01	0.42
11:Y:17:ASP:OD1	11:Y:33:LYS:NZ	2.52	0.42
10:X:132:ALA:HB1	10:X:136:SER:HB2	2.02	0.42
10:J:168:LEU:O	10:J:172:MET:HB2	2.20	0.42
5:S:155:LEU:HD13	5:S:158:THR:HB	2.02	0.42
5:E:155:LEU:HD13	5:E:158:THR:HB	2.02	0.42
10:X:168:LEU:O	10:X:172:MET:HB2	2.20	0.42
2:B:3:ARG:HB3	5:E:122:TYR:OH	2.19	0.42
13:M:96:LEU:O	13:M:100:MET:HG2	2.20	0.42
13:M:187:ARG:NH1	8:V:139:GLU:OE1	2.47	0.42
2:B:58:GLN:NE2	2:B:208:ASP:HA	2.34	0.41
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.03	0.41
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.41
6:T:146:MET:CE	6:T:161:THR:HB	2.50	0.41
4:D:77:ALA:O	4:D:81:ILE:HG12	2.20	0.41
6:F:34:ILE:HG12	6:F:196:ILE:HD11	2.03	0.41
9:I:141:ALA:HB2	9:I:177:ASP:HB2	2.03	0.41
6:T:34:ILE:HG12	6:T:196:ILE:HD11	2.02	0.41
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.03	0.41
7:U:78:ILE:N	7:U:79:PRO:CD	2.83	0.41
9:I:9:GLY:HA3	9:I:41:LYS:HE2	2.03	0.41
5:S:176:ASP:O	5:S:180:LYS:HD3	2.20	0.41
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.86	0.41
4:R:77:ALA:O	4:R:81:ILE:HG12	2.21	0.41
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.86	0.41
11:K:107:LYS:HG3	11:K:108:GLU:HG3	2.03	0.41
11:K:45:MET:HG3	11:K:52:CYS:HB2	2.03	0.41
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.02	0.41
10:X:149:ARG:O	10:X:152:MET:HG3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	2.03	0.41
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.02	0.41
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.51	0.41
3:Q:232:THR:O	3:Q:236:GLN:HG3	2.21	0.41
5:E:176:ASP:O	5:E:180:LYS:HD3	2.20	0.41
3:Q:160:GLN:HG3	3:Q:161:THR:N	2.36	0.41
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.51	0.41
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.03	0.41
11:K:12:ILE:HB	11:K:180:VAL:HB	2.03	0.40
6:F:146:MET:CE	6:F:161:THR:HB	2.51	0.40
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.03	0.40
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.52	0.40
11:Y:12:ILE:HB	11:Y:180:VAL:HB	2.04	0.40
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	240 (97%)	6 (2%)	2 (1%)	19	51
1	O	248/250 (99%)	240 (97%)	6 (2%)	2 (1%)	19	51
2	B	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	9	31
2	P	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	9	31
3	C	238/254 (94%)	231 (97%)	4 (2%)	3 (1%)	12	37
3	Q	238/254 (94%)	231 (97%)	4 (2%)	3 (1%)	12	37
4	D	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
4	R	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
5	E	229/234 (98%)	224 (98%)	5 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	S	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
6	F	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
6	T	241/288 (84%)	237 (98%)	4 (2%)	0	100	100
7	G	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
7	U	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
8	H	224/232 (97%)	217 (97%)	6 (3%)	1 (0%)	34	66
8	V	224/232 (97%)	217 (97%)	6 (3%)	1 (0%)	34	66
9	I	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
9	W	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
10	J	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
10	X	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
11	K	210/212 (99%)	203 (97%)	7 (3%)	0	100	100
11	Y	210/212 (99%)	203 (97%)	7 (3%)	0	100	100
12	L	220/222 (99%)	216 (98%)	3 (1%)	1 (0%)	29	61
12	Z	220/222 (99%)	216 (98%)	3 (1%)	1 (0%)	29	61
13	M	226/246 (92%)	219 (97%)	7 (3%)	0	100	100
13	a	229/246 (93%)	222 (97%)	5 (2%)	2 (1%)	17	48
14	N	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
14	b	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
All	All	6277/6614 (95%)	6118 (98%)	135 (2%)	24 (0%)	34	66

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
2	B	218	GLY
2	B	222	GLY
3	C	202	GLN
1	O	2	THR
2	P	218	GLY
2	P	222	GLY
3	Q	202	GLN
1	A	166	LYS
3	C	205	ALA
1	O	166	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	Q	205	ALA
2	B	220	ASN
2	P	220	ASN
8	H	9	ASN
8	V	9	ASN
12	L	165	ASN
12	Z	165	ASN
2	B	221	ASP
3	C	183	PRO
2	P	221	ASP
3	Q	183	PRO
13	a	83	ALA
13	a	229	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	205 (98%)	4 (2%)	57	84
1	O	209/209 (100%)	205 (98%)	4 (2%)	57	84
2	B	203/216 (94%)	193 (95%)	10 (5%)	25	57
2	P	203/216 (94%)	193 (95%)	10 (5%)	25	57
3	C	212/226 (94%)	195 (92%)	17 (8%)	12	33
3	Q	212/226 (94%)	195 (92%)	17 (8%)	12	33
4	D	194/215 (90%)	180 (93%)	14 (7%)	14	39
4	R	194/215 (90%)	180 (93%)	14 (7%)	14	39
5	E	190/193 (98%)	173 (91%)	17 (9%)	9	29
5	S	190/193 (98%)	174 (92%)	16 (8%)	11	31
6	F	201/239 (84%)	187 (93%)	14 (7%)	15	41
6	T	201/239 (84%)	187 (93%)	14 (7%)	15	41
7	G	206/210 (98%)	195 (95%)	11 (5%)	22	54
7	U	206/210 (98%)	195 (95%)	11 (5%)	22	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	185/190 (97%)	177 (96%)	8 (4%)	29	62
8	V	185/190 (97%)	177 (96%)	8 (4%)	29	62
9	I	172/173 (99%)	168 (98%)	4 (2%)	50	80
9	W	172/173 (99%)	168 (98%)	4 (2%)	50	80
10	J	173/175 (99%)	166 (96%)	7 (4%)	31	65
10	X	173/175 (99%)	166 (96%)	7 (4%)	31	65
11	K	168/169 (99%)	161 (96%)	7 (4%)	30	63
11	Y	168/169 (99%)	161 (96%)	7 (4%)	30	63
12	L	185/185 (100%)	176 (95%)	9 (5%)	25	57
12	Z	185/185 (100%)	176 (95%)	9 (5%)	25	57
13	M	195/208 (94%)	186 (95%)	9 (5%)	27	60
13	a	197/208 (95%)	188 (95%)	9 (5%)	27	60
14	N	162/162 (100%)	155 (96%)	7 (4%)	29	62
14	b	162/162 (100%)	155 (96%)	7 (4%)	29	62
All	All	5312/5540 (96%)	5037 (95%)	275 (5%)	23	55

All (275) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	61	LEU
1	A	122	THR
1	A	157	PHE
2	B	50	LYS
2	B	52	THR
2	B	55	LEU
2	B	58	GLN
2	B	79	LEU
2	B	102	ASN
2	B	119	GLN
2	B	180	LYS
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	49	THR
3	C	50	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	51	LYS
3	C	53	GLN
3	C	61	LYS
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	171	GLU
3	C	175	LYS
3	C	180	LYS
3	C	206	LYS
3	C	213	VAL
3	C	240	GLU
4	D	20	LEU
4	D	40	LEU
4	D	51	LEU
4	D	68	CYS
4	D	99	ILE
4	D	117	GLU
4	D	125	LEU
4	D	176	LEU
4	D	190	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	3	ASN
5	E	8	ASP
5	E	9	THR
5	E	10	VAL
5	E	25	LEU
5	E	29	LYS
5	E	54	GLU
5	E	55	LEU
5	E	71	LEU
5	E	99	ASN
5	E	116	GLN
5	E	174	THR
5	E	184	ASN
5	E	188	LEU
5	E	207	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	208	ASP
5	E	217	LYS
6	F	14	ASP
6	F	96	LYS
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	171	GLU
6	F	172	LEU
6	F	181	GLU
6	F	187	GLU
6	F	198	LEU
6	F	201	GLU
6	F	202	ASP
6	F	214	TRP
6	F	221	ASN
7	G	13	GLU
7	G	26	THR
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	122	ARG
7	G	125	MET
7	G	166	GLN
7	G	235	ARG
7	G	236	LEU
7	G	242	GLN
8	H	13	VAL
8	H	30	ASN
8	H	55	VAL
8	H	68	LEU
8	H	106	THR
8	H	153	LYS
8	H	195	VAL
8	H	196	ARG
9	I	37	ASN
9	I	126	ILE
9	I	171	LEU
9	I	192	ASP
10	J	3	ILE
10	J	23	ARG
10	J	35	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	J	78	GLN
10	J	90	LYS
10	J	99	GLN
10	J	110	LYS
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	97	MET
11	K	104	TYR
11	K	107	LYS
11	K	148	LEU
12	L	3	ASN
12	L	18	GLU
12	L	23	LEU
12	L	31	THR
12	L	108	HIS
12	L	136	CYS
12	L	150	LEU
12	L	172	LEU
12	L	173	LYS
13	M	2	GLN
13	M	43	ILE
13	M	48	ASN
13	M	104	ARG
13	M	146	PHE
13	M	161	ARG
13	M	187	ARG
13	M	206	LEU
13	M	212	LEU
14	N	9	LYS
14	N	20	THR
14	N	83	LYS
14	N	104	ASP
14	N	115	LEU
14	N	144	GLU
14	N	178	LEU
1	O	29	LYS
1	O	61	LEU
1	O	122	THR
1	O	157	PHE
2	P	50	LYS
2	P	52	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	55	LEU
2	P	58	GLN
2	P	79	LEU
2	P	102	ASN
2	P	119	GLN
2	P	180	LYS
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	49	THR
3	Q	50	LEU
3	Q	51	LYS
3	Q	53	GLN
3	Q	61	LYS
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	171	GLU
3	Q	175	LYS
3	Q	180	LYS
3	Q	206	LYS
3	Q	213	VAL
3	Q	240	GLU
4	R	20	LEU
4	R	40	LEU
4	R	51	LEU
4	R	68	CYS
4	R	99	ILE
4	R	117	GLU
4	R	125	LEU
4	R	176	LEU
4	R	190	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	3	ASN
5	S	8	ASP
5	S	9	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	S	10	VAL
5	S	25	LEU
5	S	29	LYS
5	S	54	GLU
5	S	55	LEU
5	S	71	LEU
5	S	99	ASN
5	S	116	GLN
5	S	184	ASN
5	S	188	LEU
5	S	207	VAL
5	S	208	ASP
5	S	217	LYS
6	T	14	ASP
6	T	96	LYS
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	171	GLU
6	T	172	LEU
6	T	181	GLU
6	T	187	GLU
6	T	198	LEU
6	T	201	GLU
6	T	202	ASP
6	T	214	TRP
6	T	221	ASN
7	U	13	GLU
7	U	26	THR
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	122	ARG
7	U	125	MET
7	U	166	GLN
7	U	235	ARG
7	U	236	LEU
7	U	242	GLN
8	V	13	VAL
8	V	30	ASN
8	V	55	VAL
8	V	68	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	V	106	THR
8	V	153	LYS
8	V	195	VAL
8	V	196	ARG
9	W	37	ASN
9	W	126	ILE
9	W	171	LEU
9	W	192	ASP
10	X	3	ILE
10	X	23	ARG
10	X	35	THR
10	X	78	GLN
10	X	90	LYS
10	X	99	GLN
10	X	110	LYS
11	Y	4	LEU
11	Y	9	GLN
11	Y	35	ILE
11	Y	97	MET
11	Y	104	TYR
11	Y	107	LYS
11	Y	148	LEU
12	Z	3	ASN
12	Z	18	GLU
12	Z	23	LEU
12	Z	31	THR
12	Z	108	HIS
12	Z	136	CYS
12	Z	150	LEU
12	Z	172	LEU
12	Z	173	LYS
13	a	2	GLN
13	a	43	ILE
13	a	48	ASN
13	a	104	ARG
13	a	146	PHE
13	a	161	ARG
13	a	187	ARG
13	a	206	LEU
13	a	212	LEU
14	b	9	LYS
14	b	20	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	b	83	LYS
14	b	104	ASP
14	b	115	LEU
14	b	144	GLU
14	b	178	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	146	GLN
4	D	225	ASN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
8	H	66	HIS
9	I	37	ASN
10	J	55	GLN
11	K	85	ASN
11	K	176	ASN
11	K	208	ASN
12	L	3	ASN
12	L	158	ASN
13	M	48	ASN
13	M	102	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	176	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	146	GLN
4	R	225	ASN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
7	U	175	ASN
8	V	66	HIS
9	W	37	ASN
10	X	55	GLN
11	Y	85	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	79	HIS
12	Z	158	ASN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	-0.39	5 (2%) 65 63	38, 54, 92, 131	0
1	O	250/250 (100%)	-0.36	7 (2%) 53 49	46, 64, 109, 144	0
2	B	244/258 (94%)	-0.35	8 (3%) 46 41	40, 61, 109, 177	0
2	P	244/258 (94%)	-0.22	10 (4%) 37 32	47, 65, 115, 178	0
3	C	240/254 (94%)	-0.18	11 (4%) 32 29	41, 66, 134, 164	0
3	Q	240/254 (94%)	-0.04	13 (5%) 25 22	46, 76, 156, 178	0
4	D	235/260 (90%)	-0.37	1 (0%) 92 93	48, 68, 104, 145	0
4	R	235/260 (90%)	-0.27	2 (0%) 84 84	51, 72, 112, 144	0
5	E	231/234 (98%)	-0.29	3 (1%) 77 77	52, 72, 109, 149	0
5	S	231/234 (98%)	-0.21	3 (1%) 77 77	53, 78, 122, 168	0
6	F	243/288 (84%)	-0.45	4 (1%) 72 71	42, 60, 107, 146	0
6	T	243/288 (84%)	-0.34	4 (1%) 72 71	44, 69, 128, 164	0
7	G	241/252 (95%)	-0.50	1 (0%) 92 93	41, 56, 93, 134	0
7	U	241/252 (95%)	-0.44	3 (1%) 79 79	43, 59, 97, 130	0
8	H	226/232 (97%)	-0.34	6 (2%) 54 50	43, 55, 94, 170	0
8	V	226/232 (97%)	-0.22	8 (3%) 44 38	45, 60, 99, 185	0
9	I	204/205 (99%)	-0.65	1 (0%) 91 91	38, 52, 82, 111	0
9	W	204/205 (99%)	-0.60	1 (0%) 91 91	40, 56, 91, 114	0
10	J	195/198 (98%)	-0.48	2 (1%) 82 82	39, 58, 86, 144	0
10	X	195/198 (98%)	-0.42	3 (1%) 73 73	39, 61, 90, 150	0
11	K	212/212 (100%)	-0.47	0 100 100	42, 58, 83, 100	0
11	Y	212/212 (100%)	-0.51	0 100 100	41, 56, 81, 104	0
12	L	222/222 (100%)	-0.53	1 (0%) 91 91	42, 58, 92, 141	0
12	Z	222/222 (100%)	-0.47	1 (0%) 91 91	34, 57, 90, 129	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	228/246 (92%)	-0.52	2 (0%) 84 84	37, 56, 85, 102	0
13	a	231/246 (93%)	-0.50	4 (1%) 70 69	38, 57, 86, 109	0
14	N	196/196 (100%)	-0.55	1 (0%) 91 91	38, 52, 85, 121	0
14	b	196/196 (100%)	-0.49	1 (0%) 91 91	40, 53, 85, 119	0
All	All	6337/6614 (95%)	-0.39	106 (1%) 70 69	34, 61, 106, 185	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	V	224	GLN	9.0
10	X	1	MET	8.7
3	Q	206	LYS	7.6
8	V	226	GLU	7.5
3	Q	49	THR	7.5
8	H	224	GLN	7.4
2	B	221	ASP	7.2
2	P	219	ALA	7.1
8	H	223	ILE	6.5
8	V	223	ILE	6.4
8	V	222	ASP	6.3
3	C	206	LYS	5.8
8	H	225	GLU	5.5
3	Q	50	LEU	5.4
8	V	225	GLU	5.4
8	V	221	CYS	5.4
2	P	220	ASN	5.1
10	J	1	MET	5.0
2	B	219	ALA	4.6
2	P	221	ASP	4.5
2	B	220	ASN	4.4
8	H	222	ASP	4.4
9	W	1	SER	4.3
2	P	51	VAL	4.3
8	H	226	GLU	4.2
3	Q	238	LYS	4.2
8	H	221	CYS	4.1
2	P	59	ASP	4.1
12	L	174	TYR	4.0
3	C	49	THR	4.0
3	Q	236	GLN	3.9
5	S	202	ASP	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	X	193	ASP	3.8
1	O	249	ALA	3.8
5	E	202	ASP	3.5
6	T	244	ASN	3.5
3	Q	239	GLN	3.5
2	P	222	GLY	3.4
6	F	244	ASN	3.4
2	P	60	THR	3.4
2	P	52	THR	3.3
1	A	1	MET	3.2
3	C	50	LEU	3.2
7	U	222	ASP	3.1
1	A	249	ALA	3.1
10	J	194	ASP	3.1
6	F	205	GLU	3.1
10	X	194	ASP	3.0
3	C	240	GLU	3.0
3	C	205	ALA	3.0
3	C	216	ASP	3.0
2	B	59	ASP	2.9
13	a	230	THR	2.9
9	I	1	SER	2.9
12	Z	174	TYR	2.9
2	B	51	VAL	2.9
3	C	239	GLN	2.8
3	Q	237	GLU	2.8
7	U	242	GLN	2.7
1	O	1	MET	2.7
1	A	250	LEU	2.7
3	Q	240	GLU	2.6
13	a	231	GLN	2.6
4	R	1	ASP	2.6
4	R	242	GLU	2.5
1	O	2	THR	2.5
3	C	60	SER	2.5
1	A	182	GLU	2.5
3	C	236	GLN	2.5
3	C	238	LYS	2.5
13	a	1	THR	2.5
1	O	231	LYS	2.5
2	P	225	TYR	2.5
1	O	201	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	201	ARG	2.4
6	T	230	ASP	2.4
1	O	250	LEU	2.4
2	P	203	SER	2.4
6	T	243	ILE	2.4
4	D	242	GLU	2.4
3	C	181	GLU	2.3
1	A	2	THR	2.3
3	Q	202	GLN	2.3
13	a	216	ASN	2.3
3	Q	203	THR	2.3
14	N	195	GLN	2.3
7	G	222	ASP	2.3
6	F	241	LYS	2.2
2	B	217	LYS	2.2
14	b	195	GLN	2.2
1	O	52	SER	2.2
6	T	215	CYS	2.2
3	Q	204	GLY	2.2
13	M	47	ASP	2.2
5	S	54	GLU	2.2
13	M	216	ASN	2.2
6	F	181	GLU	2.1
2	B	222	GLY	2.1
3	Q	55	THR	2.1
5	S	122	TYR	2.1
2	B	225	TYR	2.1
7	U	2	GLY	2.1
8	V	198	GLU	2.0
5	E	122	TYR	2.0
8	V	145	ASP	2.0
3	Q	225	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
15	MG	I	302	1/1	0.71	0.22	110,110,110,110	0
15	MG	N	202	1/1	0.81	0.38	69,69,69,69	0
15	MG	K	302	1/1	0.86	0.48	70,70,70,70	0
15	MG	N	201	1/1	0.94	0.12	50,50,50,50	0
15	MG	Z	301	1/1	0.96	0.28	64,64,64,64	0
15	MG	G	301	1/1	0.97	0.07	55,55,55,55	0
15	MG	J	201	1/1	0.97	0.21	50,50,50,50	0
15	MG	L	301	1/1	0.97	0.07	67,67,67,67	0
15	MG	I	301	1/1	0.99	0.46	71,71,71,71	0
15	MG	K	301	1/1	0.99	0.10	57,57,57,57	0
15	MG	I	303	1/1	0.99	0.06	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.