



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:45 AM UTC

PDB ID : 9QBY / pdb\_00009qby  
Title : Yeast 20S proteasome mutant: beta5\_G128V (b5-propeptide in trans) in complex with ONX0914  
Authors : Huber, E.M.; Heinemeyer, W.; Groll, M.  
Deposited on : 2025-03-04  
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](mailto: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>.

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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

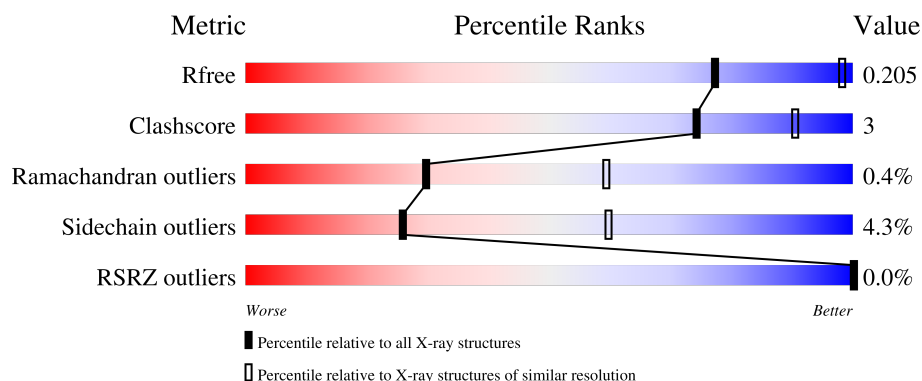
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 2.90 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))
$R_{free}$	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	 97%
1	O	250	 96%
2	B	258	 87% 7% 5%
2	P	258	 87% 7% 5%
3	C	254	 87% 6% 6%





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Mol	Chain	Length	Quality of chain
3	Q	254	 87% 6% • 6%
4	D	260	 85% 5% • 10%
4	R	260	 85% 5% • 10%
5	E	234	 92% 5% • •
5	S	234	 92% 5% • •
6	F	288	 80% • • 16%
6	T	288	 80% • • 16%
7	G	252	 87% 8% • •
7	U	252	 87% 8% • •
8	H	231	 87% 9% • •
8	V	231	 88% 8% • •
9	I	205	 92% 7%
9	W	205	 91% 9%
10	J	198	 89% 6% • •
10	X	198	 87% 8% • •
11	K	211	 78% 19% •
11	Y	211	 80% 17% •
12	L	222	 84% 13% •
12	Z	222	 84% 14% •
13	M	246	 80% 11% • 6%
13	a	246	 82% 12% • 5%
14	N	195	 89% 10% •
14	b	195	 88% 11% •
15	d	4	 50% 50%
15	e	4	 50% 50%

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Mol	Chain	Length	Quality of chain
15	f	4	 50% 50%
15	g	4	 50% 50%
15	h	4	 50% 50%
15	i	4	 50% 50%

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
19	MPD	a	302	-	-	X	-

## 2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 49907 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	225	Total	C	N	O	S	0	0	0
			1712	1078	297	330	7			
8	V	225	Total	C	N	O	S	0	0	0
			1712	1078	297	330	7			

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	211	Total	C	N	O	S	0	0	0
			1640	1044	279	310	7			
11	Y	211	Total	C	N	O	S	0	0	0
			1640	1044	279	310	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	130	VAL	GLY	engineered mutation	UNP P30656
Y	130	VAL	GLY	engineered mutation	UNP P30656

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	232	Total	C	N	O	S	0	0	0
			1815	1148	311	349	7			
13	a	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	195	Total	C	N	O	S	0	0	0
			1505	951	249	298	7			
14	b	195	Total	C	N	O	S	0	0	0
			1505	951	249	298	7			

- Molecule 15 is a protein called 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-C]PYRAZ

OLE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	d	4	Total	C	N	O	0	0	0
			49	35	5	9			
15	e	4	Total	C	N	O	0	0	0
			49	35	5	9			
15	f	4	Total	C	N	O	0	0	0
			49	35	5	9			
15	g	4	Total	C	N	O	0	0	0
			49	35	5	9			
15	h	4	Total	C	N	O	0	0	0
			49	35	5	9			
15	i	4	Total	C	N	O	0	0	0
			49	35	5	9			

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

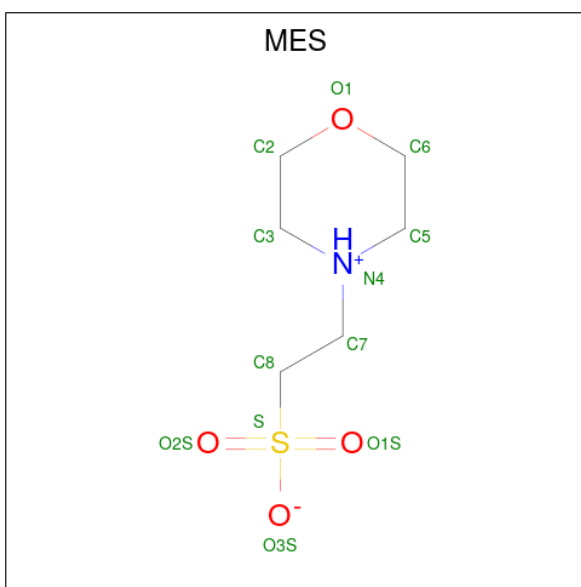
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total	Mg	0	0
			1	1		
16	N	1	Total	Mg	0	0
			1	1		
16	W	1	Total	Mg	0	0
			1	1		

- Molecule 17 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	G	1	Total	Cl	0	0
			1	1		
17	U	1	Total	Cl	0	0
			1	1		

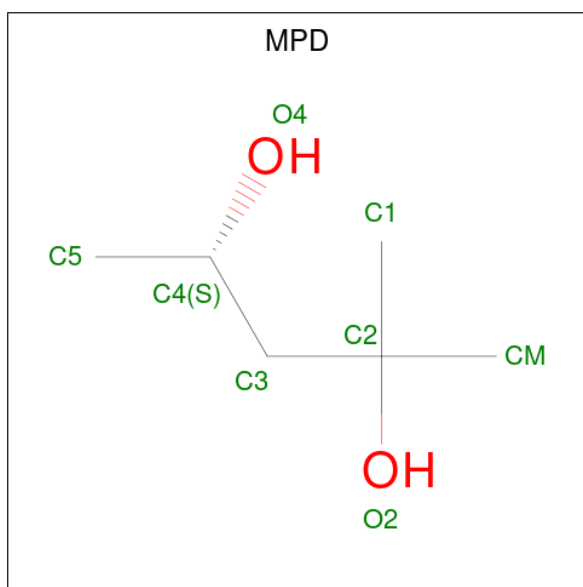
- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	M	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	U	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	V	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
18	a	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 19 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	K	1	Total	C	O	0	0
			8	6	2		
19	a	1	Total	C	O	0	0
			8	6	2		

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	6	Total	O	0	0
			6	6		
20	B	8	Total	O	0	0
			8	8		
20	C	5	Total	O	0	0
			5	5		
20	D	2	Total	O	0	0
			2	2		
20	E	7	Total	O	0	0
			7	7		
20	F	10	Total	O	0	0
			10	10		
20	G	8	Total	O	0	0
			8	8		
20	H	16	Total	O	0	0
			16	16		
20	I	4	Total	O	0	0
			4	4		
20	J	4	Total	O	0	0
			4	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	K	6	Total O 6 6	0	0
20	L	7	Total O 7 7	0	0
20	M	10	Total O 10 10	0	0
20	N	9	Total O 9 9	0	0
20	O	2	Total O 2 2	0	0
20	P	7	Total O 7 7	0	0
20	Q	6	Total O 6 6	0	0
20	R	4	Total O 4 4	0	0
20	S	5	Total O 5 5	0	0
20	T	8	Total O 8 8	0	0
20	U	11	Total O 11 11	0	0
20	V	12	Total O 12 12	0	0
20	W	5	Total O 5 5	0	0
20	X	4	Total O 4 4	0	0
20	Y	8	Total O 8 8	0	0
20	Z	10	Total O 10 10	0	0
20	a	6	Total O 6 6	0	0
20	b	4	Total O 4 4	0	0
20	f	2	Total O 2 2	0	0
20	h	1	Total O 1 1	0	0
20	i	2	Total O 2 2	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

Chain A:  97%




- Molecule 1: Proteasome subunit alpha type-2

Chain O:  96%




- Molecule 2: Proteasome subunit alpha type-3

Chain B:  87% 7% 5%




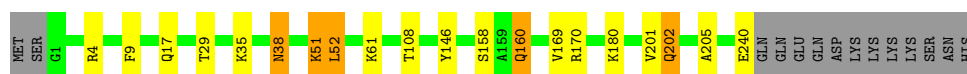
- Molecule 2: Proteasome subunit alpha type-3

Chain P:  87% 7% 5%




- Molecule 3: Proteasome subunit alpha type-4

Chain C:  87% 6% 6%

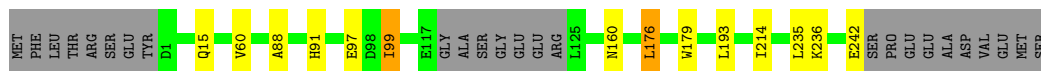
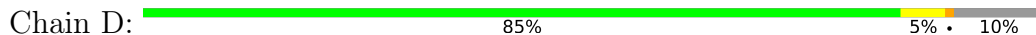


- Molecule 3: Proteasome subunit alpha type-4

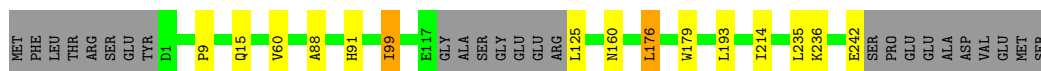
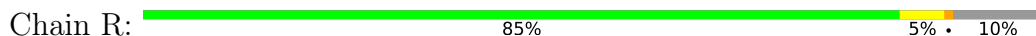
Chain Q:  87% 6% 6%



- Molecule 4: Proteasome subunit alpha type-5



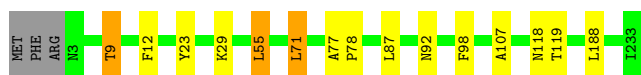
- Molecule 4: Proteasome subunit alpha type-5



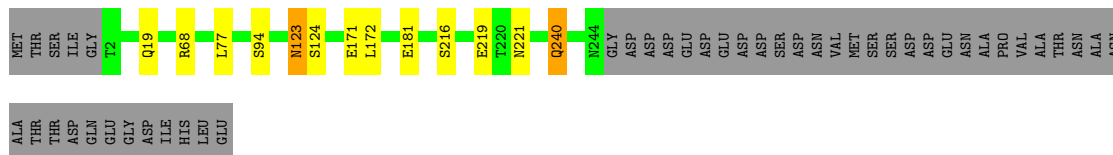
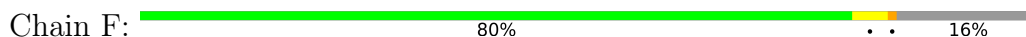
- Molecule 5: Proteasome subunit alpha type-6



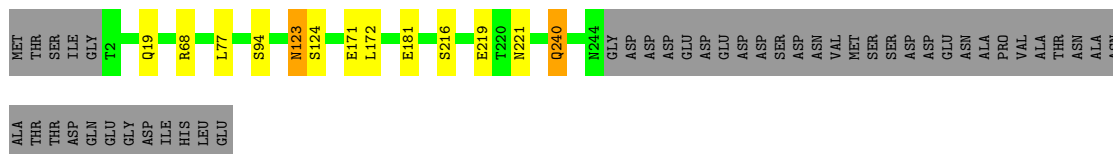
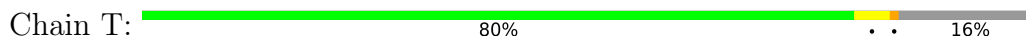
- Molecule 5: Proteasome subunit alpha type-6



- Molecule 6: Probable proteasome subunit alpha type-7



- Molecule 6: Probable proteasome subunit alpha type-7



- Molecule 7: Proteasome subunit alpha type-1

Chain G:  87% 8% . .



- Molecule 7: Proteasome subunit alpha type-1

Chain U:  87% 8% . .



- Molecule 8: Proteasome subunit beta type-2

Chain H:  87% 9% ..



- Molecule 8: Proteasome subunit beta type-2

Chain V:  88% 8% ..



- Molecule 9: Proteasome subunit beta type-3

Chain I:  92% 7%



- Molecule 9: Proteasome subunit beta type-3

Chain W:  91% 9%




- Molecule 10: Proteasome subunit beta type-4

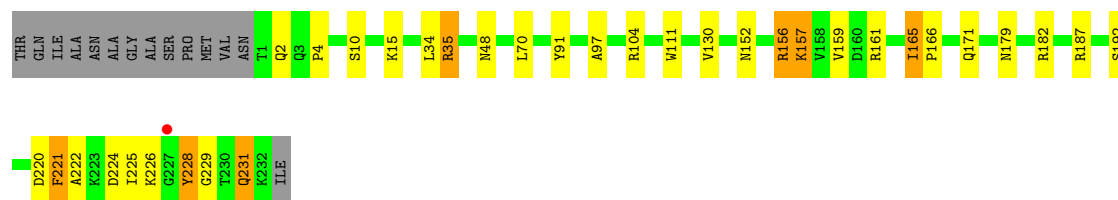
Chain J:  89% 6% ..



- Molecule 10: Proteasome subunit beta type-4

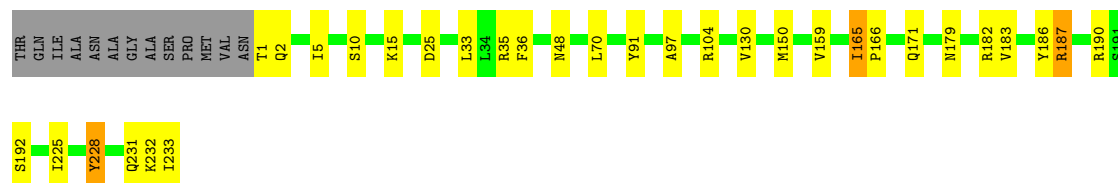
Chain X:  87% 8% . .





• Molecule 13: Proteasome subunit beta type-7

Chain a: 82% 12% 5%



• Molecule 14: Proteasome subunit beta type-1

Chain N: 89% 10%



• Molecule 14: Proteasome subunit beta type-1

Chain b: 88% 11%



• Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE

Chain d: 50% 50%



• Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE

Chain e: 50% 50%



• Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE

Chain f: 50% 50%





- Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE

Chain g:  50% 50%



- Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE

Chain h:  50% 50%



- Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE

Chain i:  50% 50%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.44Å 300.23Å 146.21Å 90.00° 113.30° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.4 (15.00-2.90) 96.4 (15.00-2.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.93 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.177 , 0.211 (Not available) , 0.205	Depositor DCC
$R_{free}$ test set	11466 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.7	Xtriage
Anisotropy	0.983	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 56.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	49907	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MES, 00E, 0A1, MG, A1I44, CL, MPD

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	1.04	0/1952	1.41	0/2642
1	O	1.04	0/1952	1.41	0/2642
2	B	1.02	0/1934	1.42	0/2618
2	P	1.03	0/1934	1.43	0/2618
3	C	1.03	0/1910	1.46	0/2586
3	Q	1.03	0/1910	1.47	0/2586
4	D	1.03	0/1837	1.45	0/2475
4	R	1.03	0/1837	1.45	0/2475
5	E	1.04	0/1800	1.43	2/2433 (0.1%)
5	S	1.04	0/1800	1.44	0/2433
6	F	1.03	0/1932	1.44	2/2609 (0.1%)
6	T	1.02	0/1932	1.44	2/2609 (0.1%)
7	G	1.01	0/1945	1.40	0/2634
7	U	1.02	0/1945	1.41	0/2634
8	H	1.03	0/1743	1.42	0/2363
8	V	1.03	0/1743	1.42	0/2363
9	I	1.02	0/1611	1.42	1/2174 (0.0%)
9	W	1.02	0/1611	1.42	0/2174
10	J	1.00	0/1589	1.42	2/2142 (0.1%)
10	X	1.00	0/1589	1.41	2/2142 (0.1%)
11	K	1.01	0/1677	1.41	0/2269
11	Y	1.00	0/1677	1.39	0/2269
12	L	1.00	0/1795	1.40	0/2420
12	Z	1.01	0/1795	1.40	2/2420 (0.1%)
13	M	1.01	0/1846	1.39	3/2503 (0.1%)
13	a	1.01	0/1855	1.39	2/2514 (0.1%)
14	N	1.00	0/1534	1.39	0/2077
14	b	1.01	0/1534	1.40	0/2077
15	d	0.21	0/4	0.81	0/4
15	e	0.57	0/4	0.47	0/4
15	f	0.95	0/4	0.75	0/4
15	g	0.29	0/4	0.74	0/4

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
15	h	0.63	0/4	0.46	0/4
15	i	0.85	0/4	0.72	0/4
All	All	1.02	0/50243	1.42	18/67925 (0.0%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	77	LEU	CA-C-N	5.46	124.70	120.33
6	T	77	LEU	C-N-CA	5.46	124.70	120.33
13	M	157	LYS	N-CA-C	-5.33	105.52	112.23
9	I	9	GLY	CA-C-O	-5.22	118.11	122.33
10	J	134	GLY	CA-C-N	5.20	127.24	120.28
10	J	134	GLY	C-N-CA	5.20	127.24	120.28
10	X	134	GLY	CA-C-N	5.14	127.17	120.28
10	X	134	GLY	C-N-CA	5.14	127.17	120.28
6	F	77	LEU	CA-C-N	5.13	124.43	120.33
6	F	77	LEU	C-N-CA	5.13	124.43	120.33
12	Z	119	LYS	CA-C-N	5.09	124.80	119.92
12	Z	119	LYS	C-N-CA	5.09	124.80	119.92
5	E	35	VAL	CA-C-N	5.09	125.11	121.65
5	E	35	VAL	C-N-CA	5.09	125.11	121.65
13	M	171	GLN	CA-C-N	5.09	126.97	120.56
13	M	171	GLN	C-N-CA	5.09	126.97	120.56
13	a	171	GLN	CA-C-N	5.06	127.04	120.56
13	a	171	GLN	C-N-CA	5.06	127.04	120.56

There are no chirality outliers.

There are no planarity outliers.

## 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	2	0
1	O	1915	0	1929	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1904	0	1904	9	0
2	P	1904	0	1904	8	0
3	C	1881	0	1895	11	0
3	Q	1881	0	1895	11	0
4	D	1813	0	1797	7	0
4	R	1813	0	1797	6	0
5	E	1773	0	1775	13	0
5	S	1773	0	1775	13	0
6	F	1892	0	1883	5	0
6	T	1892	0	1883	5	0
7	G	1907	0	1901	11	0
7	U	1907	0	1901	13	0
8	H	1712	0	1709	9	0
8	V	1712	0	1709	9	0
9	I	1581	0	1574	9	0
9	W	1581	0	1574	11	0
10	J	1561	0	1569	13	0
10	X	1561	0	1569	15	0
11	K	1640	0	1591	25	0
11	Y	1640	0	1591	23	0
12	L	1757	0	1711	21	0
12	Z	1757	0	1711	20	0
13	M	1815	0	1821	27	0
13	a	1824	0	1832	19	0
14	N	1505	0	1471	17	0
14	b	1505	0	1471	15	0
15	d	49	0	25	2	0
15	e	49	0	25	0	0
15	f	49	0	25	0	0
15	g	49	0	25	2	0
15	h	49	0	25	0	0
15	i	49	0	25	0	0
16	G	1	0	0	0	0
16	N	1	0	0	0	0
16	W	1	0	0	0	0
17	G	1	0	0	0	0
17	U	1	0	0	0	0
18	G	12	0	13	1	0
18	H	12	0	13	0	0
18	M	12	0	13	0	0
18	U	12	0	13	0	0
18	V	12	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	a	12	0	13	0	0
19	K	8	0	14	1	0
19	a	8	0	14	7	0
20	A	6	0	0	0	0
20	B	8	0	0	0	0
20	C	5	0	0	0	0
20	D	2	0	0	0	0
20	E	7	0	0	0	0
20	F	10	0	0	0	0
20	G	8	0	0	0	0
20	H	16	0	0	0	0
20	I	4	0	0	0	0
20	J	4	0	0	0	0
20	K	6	0	0	0	0
20	L	7	0	0	0	0
20	M	10	0	0	0	0
20	N	9	0	0	1	0
20	O	2	0	0	0	0
20	P	7	0	0	0	0
20	Q	6	0	0	0	0
20	R	4	0	0	0	0
20	S	5	0	0	0	0
20	T	8	0	0	0	0
20	U	11	0	0	0	0
20	V	12	0	0	0	0
20	W	5	0	0	0	0
20	X	4	0	0	0	0
20	Y	8	0	0	0	0
20	Z	10	0	0	0	0
20	a	6	0	0	0	0
20	b	4	0	0	0	0
20	f	2	0	0	0	0
20	h	1	0	0	0	0
20	i	2	0	0	0	0
All	All	49907	0	49327	302	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (302) 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)
13:M:152:ASN:O	13:M:156:ARG:HG3	1.43	1.18
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.35	0.91
13:M:152:ASN:O	13:M:156:ARG:CG	2.20	0.88
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.37	0.88
13:M:161:ARG:HG2	13:M:161:ARG:HH11	1.37	0.86
11:K:210:VAL:HG12	11:K:211:ILE:H	1.43	0.84
13:M:4:PRO:HG3	13:M:111:TRP:CD1	2.13	0.83
11:Y:210:VAL:HG12	11:Y:211:ILE:H	1.42	0.82
1:O:12:PHE:H	2:P:20:GLN:HE22	1.38	0.72
19:a:302:MPD:H53	19:a:302:MPD:C1	2.20	0.71
10:J:23:ARG:CZ	11:K:118:ASP:OD2	2.38	0.71
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.40	0.69
3:C:9:PHE:H	4:D:15:GLN:HE22	1.41	0.68
14:b:152:VAL:HA	14:b:175:MET:HE1	1.75	0.67
7:G:23:PHE:O	7:G:26:THR:HB	1.94	0.67
14:N:152:VAL:HA	14:N:175:MET:HE1	1.76	0.67
7:U:23:PHE:O	7:U:26:THR:HB	1.95	0.67
11:Y:65:LEU:O	11:Y:69:ARG:HG3	1.95	0.65
6:T:123:ASN:C	6:T:123:ASN:HD22	2.05	0.64
13:M:161:ARG:HG2	13:M:161:ARG:NH1	2.05	0.64
2:B:12:PHE:H	3:C:17:GLN:HE22	1.45	0.64
5:E:12:PHE:H	6:F:19:GLN:HE22	1.46	0.64
1:A:12:PHE:H	2:B:20:GLN:HE22	1.46	0.63
5:S:12:PHE:H	6:T:19:GLN:HE22	1.47	0.63
10:J:25:ILE:HD12	10:J:25:ILE:O	1.97	0.63
6:F:123:ASN:C	6:F:123:ASN:HD22	2.08	0.61
3:C:160:GLN:HE21	3:C:160:GLN:CA	2.12	0.61
14:N:35:THR:CG2	13:a:228:TYR:HE2	2.13	0.61
19:a:302:MPD:H53	19:a:302:MPD:H11	1.83	0.60
15:d:1:00E:HE1	15:d:3:0A1:HMC3	1.84	0.60
13:M:220:ASP:C	13:M:222:ALA:H	2.10	0.59
15:g:1:00E:HE1	15:g:3:0A1:HMC3	1.84	0.58
11:K:196:LEU:HD22	11:K:200:VAL:HG23	1.86	0.57
13:M:228:TYR:HE1	14:b:35:THR:HG21	1.70	0.57
6:T:123:ASN:HD22	6:T:124:SER:N	2.03	0.57
13:M:228:TYR:HE1	14:b:35:THR:CG2	2.18	0.57
14:N:53:GLN:HG2	13:a:228:TYR:CE1	2.39	0.57
10:X:27:VAL:HG12	10:X:27:VAL:O	2.04	0.57
10:J:140:THR:HG22	10:J:164:CYS:SG	2.44	0.57
13:a:228:TYR:N	13:a:228:TYR:CD2	2.73	0.57
14:N:35:THR:HG21	13:a:228:TYR:HE2	1.70	0.56
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:302:MPD:HM2	19:a:302:MPD:O4	2.05	0.56
6:F:123:ASN:HD22	6:F:124:SER:N	2.04	0.55
11:Y:9:GLN:HG2	11:Y:147:ASP:HA	1.89	0.55
13:M:224:ASP:HB3	8:V:123:TYR:OH	2.08	0.54
10:X:140:THR:HG22	10:X:164:CYS:SG	2.48	0.54
11:K:9:GLN:HG2	11:K:147:ASP:HA	1.88	0.54
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.56	0.53
3:C:38:ASN:C	3:C:38:ASN:HD22	2.16	0.53
13:M:34:LEU:HD12	14:b:164:LYS:O	2.08	0.53
10:J:25:ILE:HD13	10:X:135:TYR:HB3	1.90	0.53
13:a:150:MET:HE1	13:a:187:ARG:HG2	1.91	0.53
11:Y:44:THR:O	11:Y:99:THR:OG1	2.27	0.53
13:M:4:PRO:HG3	13:M:111:TRP:CG	2.44	0.53
13:M:159:VAL:HG23	13:M:159:VAL:O	2.08	0.53
8:H:112:SER:OG	8:H:120:ASP:OD2	2.26	0.52
11:K:44:THR:O	11:K:99:THR:OG1	2.27	0.52
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.09	0.52
3:C:51:LYS:O	3:C:52:LEU:HB2	2.09	0.52
7:G:83:ASN:C	7:G:83:ASN:HD22	2.18	0.52
13:a:165:ILE:HB	13:a:166:PRO:HD3	1.91	0.52
13:M:179:ASN:HD22	13:M:182:ARG:HH11	1.55	0.52
14:N:136:GLY:HA2	14:b:161:GLN:HE21	1.75	0.52
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.75	0.51
13:M:228:TYR:CE2	14:b:53:GLN:HG2	2.46	0.51
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.09	0.51
11:Y:139:VAL:HG13	11:Y:160:SER:HB3	1.92	0.51
3:C:35:LYS:HG2	3:C:158:SER:O	2.09	0.51
8:V:112:SER:OG	8:V:120:ASP:OD2	2.22	0.51
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.93	0.51
19:a:302:MPD:H11	19:a:302:MPD:O4	2.10	0.51
13:M:4:PRO:CG	13:M:111:TRP:CD1	2.92	0.51
11:K:12:ILE:HB	11:K:180:VAL:HB	1.93	0.51
3:Q:38:ASN:C	3:Q:38:ASN:HD22	2.18	0.51
13:a:179:ASN:HD22	13:a:182:ARG:HH11	1.57	0.51
7:G:65:CYS:SG	18:G:303:MES:H31	2.50	0.51
7:U:106:ASP:HB3	7:U:146:TYR:CZ	2.46	0.51
11:K:2:THR:HA	11:K:129:VAL:O	2.11	0.50
8:V:98:LEU:HB2	8:V:113:ILE:HG23	1.93	0.50
11:Y:2:THR:HA	11:Y:129:VAL:O	2.11	0.50
12:Z:100:LYS:HE3	12:Z:103:PHE:O	2.12	0.50
19:a:302:MPD:H53	19:a:302:MPD:H12	1.90	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:135:MET:SD	13:a:187:ARG:NH1	2.84	0.50
12:L:43:VAL:HG12	12:L:205:LEU:HD22	1.94	0.50
14:N:161:GLN:HE21	14:b:136:GLY:HA2	1.77	0.50
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.93	0.50
8:H:98:LEU:HB2	8:H:113:ILE:HG23	1.94	0.50
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.92	0.50
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.77	0.50
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.77	0.50
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.42	0.49
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.93	0.49
7:G:78:ILE:N	7:G:79:PRO:CD	2.75	0.49
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.48	0.49
10:X:26:SER:HB3	11:Y:133:GLN:HB3	1.94	0.49
7:U:78:ILE:N	7:U:79:PRO:CD	2.75	0.49
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	1.93	0.49
13:a:15:LYS:HB2	13:a:165:ILE:HD13	1.94	0.49
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.60	0.49
12:L:145:LEU:O	9:W:147:GLY:HA3	2.13	0.49
13:M:161:ARG:NH1	13:M:161:ARG:CG	2.73	0.48
14:N:35:THR:HG21	13:a:228:TYR:CE2	2.47	0.48
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.48	0.48
7:U:83:ASN:C	7:U:83:ASN:HD22	2.21	0.48
13:M:224:ASP:CB	8:V:123:TYR:OH	2.61	0.48
11:Y:12:ILE:HB	11:Y:180:VAL:HB	1.94	0.48
12:Z:40:GLU:OE1	12:Z:40:GLU:HA	2.13	0.48
14:N:4:MET:HB3	14:N:126:ILE:HG22	1.96	0.48
13:a:159:VAL:HG23	13:a:159:VAL:O	2.13	0.48
2:P:93:HIS:ND1	2:P:113:ARG:HG2	2.29	0.48
12:L:100:LYS:HE3	12:L:103:PHE:O	2.14	0.48
13:M:165:ILE:N	13:M:166:PRO:CD	2.76	0.48
2:B:93:HIS:ND1	2:B:113:ARG:HG2	2.28	0.48
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.49	0.48
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.96	0.48
14:b:4:MET:HB3	14:b:126:ILE:HG22	1.95	0.47
14:b:36:ARG:HG3	14:b:42:TRP:CE2	2.48	0.47
12:L:146:ILE:HG22	12:L:150:LEU:HD22	1.97	0.47
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.61	0.47
3:Q:160:GLN:HE21	3:Q:160:GLN:CA	2.13	0.47
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.78	0.47
12:L:100:LYS:O	12:L:104:PRO:HA	2.14	0.47
12:L:189:THR:HG22	8:V:196:ARG:CZ	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:78:ILE:HG22	7:U:79:PRO:HD3	1.97	0.47
2:P:95:GLN:NE2	9:W:71:ASN:HD22	2.11	0.47
11:K:37:ILE:HG23	11:K:60:GLY:HA2	1.97	0.47
11:K:210:VAL:HG12	11:K:211:ILE:N	2.22	0.47
8:H:196:ARG:CZ	12:Z:189:THR:HG22	2.45	0.47
10:J:23:ARG:NE	11:K:118:ASP:OD2	2.47	0.46
3:Q:160:GLN:HE22	3:Q:170:ARG:HE	1.63	0.46
10:J:4:ILE:HG13	10:J:4:ILE:O	2.14	0.46
10:J:119:ILE:HA	10:J:124:THR:O	2.16	0.46
10:X:23:ARG:HA	10:X:23:ARG:HD2	1.69	0.46
10:X:119:ILE:HA	10:X:124:THR:O	2.15	0.46
12:Z:146:ILE:HG22	12:Z:150:LEU:HD22	1.97	0.46
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.97	0.46
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.45	0.46
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.63	0.46
7:G:106:ASP:HB3	7:G:146:TYR:CZ	2.50	0.46
7:G:167:GLN:HE21	7:G:171:THR:HG23	1.80	0.46
10:J:173:PRO:HG3	10:X:25:ILE:HA	1.97	0.46
12:L:27:THR:HB	12:L:39:TYR:HA	1.97	0.46
14:b:163:ILE:HG23	14:b:170:GLY:HA2	1.98	0.46
5:E:118:ASN:N	5:E:118:ASN:HD22	2.14	0.46
5:S:71:LEU:HD22	5:S:71:LEU:C	2.40	0.46
11:K:197:PHE:HZ	11:K:210:VAL:HG21	1.81	0.46
10:X:4:ILE:HG13	10:X:4:ILE:O	2.15	0.46
3:C:201:VAL:O	3:C:202:GLN:CB	2.64	0.46
12:L:8:ASN:HA	12:L:30:ILE:O	2.15	0.46
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.45	0.46
12:Z:100:LYS:O	12:Z:104:PRO:HA	2.16	0.46
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.98	0.46
9:I:125:LEU:HD21	15:d:1:00E:HD2	1.98	0.46
14:N:13:ILE:HG21	14:N:175:MET:HE2	1.98	0.46
12:L:35:ILE:HG22	12:L:35:ILE:O	2.16	0.45
13:M:228:TYR:CD1	13:M:228:TYR:N	2.84	0.45
11:Y:16:VAL:HG21	11:Y:34:VAL:HG23	1.97	0.45
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.98	0.45
11:Y:197:PHE:HZ	11:Y:210:VAL:HG21	1.81	0.45
10:J:26:SER:HB3	11:K:133:GLN:HB3	1.97	0.45
11:K:143:ASN:HB2	11:K:156:LEU:HD13	1.99	0.45
12:L:29:ASN:O	12:L:36:ASN:HB2	2.16	0.45
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.99	0.45
12:Z:165:ASN:C	12:Z:165:ASN:HD22	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.63	0.45
12:L:23:LEU:HD13	12:L:43:VAL:HG13	1.98	0.45
5:E:71:LEU:C	5:E:71:LEU:HD22	2.42	0.45
6:F:240:GLN:HE21	6:F:240:GLN:HA	1.81	0.45
13:M:15:LYS:HB2	13:M:165:ILE:HD13	1.98	0.45
9:W:125:LEU:HD21	15:g:1:00E:HD2	1.99	0.45
14:b:83:LYS:HG3	14:b:119:VAL:CG2	2.46	0.45
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.46	0.45
12:Z:42:LYS:HB2	12:Z:42:LYS:HE2	1.87	0.45
10:J:23:ARG:O	10:J:23:ARG:HG3	2.14	0.44
1:O:55:LEU:HB3	7:U:159:ALA:O	2.17	0.44
5:S:77:ALA:N	5:S:78:PRO:CD	2.80	0.44
11:Y:143:ASN:HB2	11:Y:156:LEU:HD13	1.99	0.44
19:a:302:MPD:C1	19:a:302:MPD:C5	2.88	0.44
4:D:176:LEU:HA	5:E:55:LEU:HD21	1.99	0.44
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.99	0.44
13:M:221:PHE:O	13:M:221:PHE:CD2	2.70	0.44
11:K:35:ILE:HB	11:K:45:MET:HE2	1.99	0.44
14:N:192:GLU:HB3	20:N:302:HOH:O	2.16	0.44
10:X:1:MET:HE1	10:X:134:GLY:HA3	1.98	0.44
11:Y:210:VAL:CG1	11:Y:211:ILE:H	2.23	0.44
3:C:29:THR:OG1	3:C:61:LYS:NZ	2.48	0.44
11:K:16:VAL:HG21	11:K:34:VAL:HG23	1.98	0.44
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.53	0.44
4:R:91:HIS:CD2	4:R:99:ILE:HG22	2.53	0.44
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.00	0.44
10:X:1:MET:HE2	10:X:1:MET:HB3	1.78	0.44
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	1.99	0.44
12:Z:29:ASN:O	12:Z:36:ASN:HB2	2.18	0.44
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.99	0.44
11:K:210:VAL:CG1	11:K:211:ILE:H	2.24	0.44
2:P:50:LYS:HD3	2:P:50:LYS:HA	1.85	0.44
10:J:1:MET:HE1	10:J:134:GLY:HA3	1.99	0.44
7:U:165:LYS:HD2	7:U:205:LEU:HD22	2.00	0.44
14:N:133:PHE:CE1	13:a:33:LEU:HD13	2.53	0.44
5:S:71:LEU:C	5:S:71:LEU:CD2	2.91	0.44
7:G:78:ILE:HG22	7:G:79:PRO:HD3	1.99	0.44
11:K:176:ASN:ND2	11:K:190:ASN:HB2	2.33	0.44
11:Y:35:ILE:HB	11:Y:45:MET:HE2	2.00	0.44
11:Y:158:LYS:HB2	11:Y:177:LEU:HD11	2.00	0.44
13:a:25:ASP:HB2	13:a:192:SER:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:83:ASN:C	7:G:83:ASN:ND2	2.76	0.43
6:T:240:GLN:HE21	6:T:240:GLN:HA	1.82	0.43
2:B:47:ALA:HB1	2:B:64:LYS:HD2	2.01	0.43
5:E:77:ALA:N	5:E:78:PRO:CD	2.82	0.43
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	2.15	0.43
13:a:5:ILE:HD12	19:a:302:MPD:CM	2.49	0.43
2:B:145:TYR:OH	2:B:217:LYS:HB2	2.18	0.43
8:H:112:SER:HB3	8:H:125:LEU:HD13	2.00	0.43
8:V:210:THR:HG21	9:W:167:SER:HB3	2.00	0.43
14:b:176:VAL:HG12	14:b:178:LEU:HD13	2.00	0.43
11:K:148:LEU:HD23	11:K:153:ALA:HA	2.01	0.43
9:W:58:ASP:OD2	10:X:93:ARG:NH2	2.52	0.43
13:a:97:ALA:HA	13:a:130:VAL:HG21	2.00	0.43
7:G:165:LYS:HD2	7:G:205:LEU:HD22	2.01	0.43
13:a:183:VAL:O	13:a:186:TYR:HB2	2.19	0.43
4:R:9:PRO:HA	5:S:23:TYR:CD1	2.54	0.43
7:U:167:GLN:HE21	7:U:171:THR:HG23	1.82	0.43
8:V:137:VAL:HG21	8:V:161:ALA:HB2	2.01	0.43
1:A:149:GLN:O	1:A:156:TYR:HA	2.19	0.42
2:P:145:TYR:OH	2:P:217:LYS:HB2	2.19	0.42
14:b:13:ILE:HG21	14:b:175:MET:HE2	2.00	0.42
2:P:47:ALA:HB1	2:P:64:LYS:HD2	2.00	0.42
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.19	0.42
7:G:34:LEU:C	7:G:34:LEU:HD23	2.45	0.42
11:K:19:ARG:O	11:K:33:LYS:NZ	2.51	0.42
11:K:176:ASN:HD21	11:K:190:ASN:HB2	1.84	0.42
14:N:35:THR:HG22	13:a:228:TYR:HE2	1.84	0.42
5:S:118:ASN:N	5:S:118:ASN:HD22	2.16	0.42
10:X:28:LEU:O	11:Y:136:ALA:HB2	2.18	0.42
1:O:149:GLN:O	1:O:156:TYR:HA	2.19	0.42
7:U:73:VAL:HG12	7:U:133:THR:HB	2.01	0.42
2:B:50:LYS:O	2:B:51:VAL:C	2.62	0.42
5:E:71:LEU:C	5:E:71:LEU:CD2	2.93	0.42
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.00	0.42
11:K:90:TYR:HH	19:K:301:MPD:HO2	1.66	0.42
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	2.16	0.42
8:V:113:ILE:HB	8:V:119:THR:HG22	2.01	0.42
11:K:158:LYS:HB2	11:K:177:LEU:HD11	2.01	0.42
12:L:165:ASN:C	12:L:165:ASN:HD22	2.27	0.42
7:U:106:ASP:HB3	7:U:146:TYR:CE1	2.55	0.42
4:D:91:HIS:CD2	4:D:99:ILE:HG22	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:35:ARG:NH2	14:N:114:PRO:HB3	2.34	0.42
3:Q:77:ASN:HD22	3:Q:77:ASN:N	2.18	0.42
3:C:160:GLN:HE22	3:C:170:ARG:HE	1.67	0.42
7:U:34:LEU:C	7:U:34:LEU:HD23	2.44	0.42
7:U:83:ASN:C	7:U:83:ASN:ND2	2.77	0.42
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	2.02	0.42
5:E:9:THR:HG21	5:E:119:THR:HA	2.02	0.42
11:Y:176:ASN:HD21	11:Y:190:ASN:HB2	1.84	0.42
12:Z:111:ILE:HG12	12:Z:123:TYR:HB2	2.02	0.42
5:E:65:CYS:SG	5:E:71:LEU:CD1	3.08	0.41
12:L:42:LYS:O	12:L:53:SER:OG	2.26	0.41
5:E:98:PHE:O	13:M:91:TYR:HA	2.20	0.41
9:W:7:ASN:HA	9:W:29:GLY:O	2.20	0.41
9:W:94:LEU:HD11	9:W:106:PRO:HG2	2.01	0.41
7:G:73:VAL:HG12	7:G:133:THR:HB	2.02	0.41
8:H:19:ARG:O	8:H:33:LYS:NZ	2.53	0.41
9:I:94:LEU:HD11	9:I:106:PRO:HG2	2.01	0.41
13:M:179:ASN:HD22	13:M:182:ARG:NH1	2.17	0.41
4:R:176:LEU:HA	5:S:55:LEU:HD21	2.01	0.41
9:I:147:GLY:HA3	12:Z:145:LEU:O	2.21	0.41
13:M:228:TYR:CE1	14:b:35:THR:HG21	2.53	0.41
5:S:9:THR:HG21	5:S:119:THR:HA	2.02	0.41
11:Y:176:ASN:ND2	11:Y:190:ASN:HB2	2.35	0.41
11:K:66:HIS:O	11:K:70:GLU:HG2	2.20	0.41
2:B:95:GLN:NE2	9:I:71:ASN:HD22	2.17	0.41
12:L:111:ILE:HG12	12:L:123:TYR:HB2	2.01	0.41
8:V:35:HIS:HD2	8:V:56:THR:OG1	2.04	0.41
11:Y:148:LEU:HD23	11:Y:153:ALA:HA	2.02	0.41
4:D:97:GLU:OE1	12:L:75:TYR:OH	2.23	0.41
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.03	0.41
3:Q:108:THR:HG21	3:Q:146:TYR:HB3	2.03	0.41
11:K:20:ALA:HB2	11:K:31:VAL:HG21	2.03	0.41
10:X:35:THR:HG21	10:X:182:LYS:HD2	2.03	0.41
6:F:216:SER:HB3	6:F:219:GLU:HB2	2.03	0.41
8:H:137:VAL:HG21	8:H:161:ALA:HB2	2.02	0.41
11:K:39:PRO:O	11:K:184:GLY:HA2	2.20	0.41
13:M:231:GLN:HE21	13:M:231:GLN:HB2	1.46	0.41
11:Y:37:ILE:HB	11:Y:41:LEU:HB3	2.03	0.41
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.55	0.41
13:a:35:ARG:HD3	13:a:36:PHE:CE2	2.56	0.41
12:L:16:ALA:O	12:L:135:GLN:NE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:98:PHE:O	13:a:91:TYR:HA	2.21	0.41
11:Y:86:LEU:HD13	11:Y:86:LEU:C	2.46	0.41
10:X:92:ILE:HG21	10:X:122:LEU:HA	2.01	0.40
8:H:113:ILE:HB	8:H:119:THR:HG22	2.02	0.40
9:I:58:ASP:OD2	10:J:93:ARG:NH2	2.55	0.40
10:J:35:THR:HG21	10:J:182:LYS:HD2	2.03	0.40
10:X:1:MET:HE3	10:X:2:ASP:O	2.22	0.40
3:C:108:THR:HG21	3:C:146:TYR:HB3	2.04	0.40
6:T:216:SER:HB3	6:T:219:GLU:HB2	2.03	0.40
11:Y:41:LEU:HD23	11:Y:41:LEU:HA	1.91	0.40
12:Z:124:SER:HB2	12:Z:137:ARG:HG2	2.04	0.40
2:B:145:TYR:OH	2:B:217:LYS:N	2.55	0.40
5:E:92:ASN:ND2	12:L:70:ASN:HD21	2.20	0.40
14:b:134:ILE:HG21	14:b:158:SER:O	2.22	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%)	238 (96%)	9 (4%)	1 (0%)	30	59
1	O	248/250 (99%)	240 (97%)	7 (3%)	1 (0%)	30	59
2	B	242/258 (94%)	232 (96%)	6 (2%)	4 (2%)	7	26
2	P	242/258 (94%)	232 (96%)	6 (2%)	4 (2%)	7	26
3	C	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	16	44
3	Q	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	16	44
4	D	231/260 (89%)	224 (97%)	7 (3%)	0	100	100
4	R	231/260 (89%)	224 (97%)	7 (3%)	0	100	100
5	E	229/234 (98%)	222 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	S	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
6	F	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
6	T	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
7	G	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
7	U	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
8	H	223/231 (96%)	221 (99%)	2 (1%)	0	100	100
8	V	223/231 (96%)	221 (99%)	2 (1%)	0	100	100
9	I	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
9	W	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
10	J	193/198 (98%)	188 (97%)	4 (2%)	1 (0%)	24	54
10	X	193/198 (98%)	186 (96%)	6 (3%)	1 (0%)	24	54
11	K	209/211 (99%)	199 (95%)	8 (4%)	2 (1%)	12	39
11	Y	209/211 (99%)	198 (95%)	9 (4%)	2 (1%)	12	39
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	230/246 (94%)	220 (96%)	8 (4%)	2 (1%)	14	41
13	a	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
14	N	193/195 (99%)	189 (98%)	4 (2%)	0	100	100
14	b	193/195 (99%)	189 (98%)	4 (2%)	0	100	100
15	d	1/4 (25%)	1 (100%)	0	0	100	100
15	e	1/4 (25%)	1 (100%)	0	0	100	100
15	f	1/4 (25%)	1 (100%)	0	0	100	100
15	g	1/4 (25%)	1 (100%)	0	0	100	100
15	h	1/4 (25%)	1 (100%)	0	0	100	100
15	i	1/4 (25%)	1 (100%)	0	0	100	100
All	All	6283/6632 (95%)	6100 (97%)	161 (3%)	22 (0%)	30	59

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	218	GLY
3	C	202	GLN

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Mol	Chain	Res	Type
2	P	51	VAL
2	P	218	GLY
3	Q	202	GLN
1	A	2	THR
2	B	220	ASN
2	B	221	ASP
3	C	205	ALA
11	K	210	VAL
11	K	211	ILE
1	O	2	THR
2	P	220	ASN
2	P	221	ASP
3	Q	205	ALA
11	Y	210	VAL
11	Y	211	ILE
13	M	221	PHE
10	J	9	VAL
13	M	229	GLY
10	X	9	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	209/209 (100%)	205 (98%)	4 (2%)	50	79
1	O	209/209 (100%)	205 (98%)	4 (2%)	50	79
2	B	203/216 (94%)	198 (98%)	5 (2%)	42	74
2	P	203/216 (94%)	198 (98%)	5 (2%)	42	74
3	C	212/226 (94%)	204 (96%)	8 (4%)	29	64
3	Q	212/226 (94%)	204 (96%)	8 (4%)	29	64
4	D	194/215 (90%)	186 (96%)	8 (4%)	27	61
4	R	194/215 (90%)	185 (95%)	9 (5%)	24	57
5	E	190/193 (98%)	184 (97%)	6 (3%)	34	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	S	190/193 (98%)	185 (97%)	5 (3%)	40	73
6	F	201/239 (84%)	193 (96%)	8 (4%)	28	62
6	T	201/239 (84%)	193 (96%)	8 (4%)	28	62
7	G	206/210 (98%)	197 (96%)	9 (4%)	25	59
7	U	206/210 (98%)	197 (96%)	9 (4%)	25	59
8	H	184/189 (97%)	173 (94%)	11 (6%)	17	47
8	V	184/189 (97%)	172 (94%)	12 (6%)	15	44
9	I	172/173 (99%)	169 (98%)	3 (2%)	53	82
9	W	172/173 (99%)	169 (98%)	3 (2%)	53	82
10	J	173/175 (99%)	165 (95%)	8 (5%)	24	57
10	X	173/175 (99%)	164 (95%)	9 (5%)	21	52
11	K	169/169 (100%)	157 (93%)	12 (7%)	13	40
11	Y	169/169 (100%)	157 (93%)	12 (7%)	13	40
12	L	185/185 (100%)	173 (94%)	12 (6%)	15	44
12	Z	185/185 (100%)	172 (93%)	13 (7%)	14	40
13	M	198/208 (95%)	183 (92%)	15 (8%)	12	36
13	a	199/208 (96%)	185 (93%)	14 (7%)	14	40
14	N	161/161 (100%)	157 (98%)	4 (2%)	42	74
14	b	161/161 (100%)	156 (97%)	5 (3%)	35	69
All	All	5315/5536 (96%)	5086 (96%)	229 (4%)	26	60

All (229) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	55	LEU
2	B	79	LEU
2	B	102	ASN
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN

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Mol	Chain	Res	Type
3	C	51	LYS
3	C	52	LEU
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	240	GLU
4	D	60	VAL
4	D	99	ILE
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	55	LEU
5	E	71	LEU
5	E	118	ASN
5	E	188	LEU
6	F	68	ARG
6	F	94	SER
6	F	123	ASN
6	F	171	GLU
6	F	172	LEU
6	F	181	GLU
6	F	221	ASN
6	F	240	GLN
7	G	13	GLU
7	G	26	THR
7	G	83	ASN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	208	GLU
7	G	235	ARG
7	G	236	LEU
8	H	20	SER
8	H	22	GLN
8	H	31	CYS
8	H	34	LEU
8	H	35	HIS

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Mol	Chain	Res	Type
8	H	38	SER
8	H	68	LEU
8	H	113	ILE
8	H	127	LEU
8	H	196	ARG
8	H	213	LEU
9	I	37	ASN
9	I	151	SER
9	I	171	LEU
10	J	1	MET
10	J	23	ARG
10	J	25	ILE
10	J	35	THR
10	J	92	ILE
10	J	140	THR
10	J	149	ARG
10	J	174	MET
11	K	31	VAL
11	K	35	ILE
11	K	71	LYS
11	K	73	ARG
11	K	130	VAL
11	K	142	SER
11	K	148	LEU
11	K	149	SER
11	K	152	ASP
11	K	186	ILE
11	K	196	LEU
11	K	209	ASN
12	L	1	GLN
12	L	23	LEU
12	L	34	SER
12	L	35	ILE
12	L	42	LYS
12	L	49	ASN
12	L	71	SER
12	L	128	VAL
12	L	130	SER
12	L	150	LEU
12	L	165	ASN
12	L	189	THR
13	M	2	GLN

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Mol	Chain	Res	Type
13	M	10	SER
13	M	35	ARG
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	156	ARG
13	M	157	LYS
13	M	165	ILE
13	M	187	ARG
13	M	192	SER
13	M	225	ILE
13	M	226	LYS
13	M	228	TYR
13	M	231	GLN
14	N	9	LYS
14	N	107	LYS
14	N	119	VAL
14	N	178	LEU
1	O	1	MET
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	55	LEU
2	P	79	LEU
2	P	102	ASN
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	51	LYS
3	Q	52	LEU
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	240	GLU
4	R	60	VAL
4	R	99	ILE
4	R	125	LEU
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU

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Mol	Chain	Res	Type
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	55	LEU
5	S	71	LEU
5	S	188	LEU
6	T	68	ARG
6	T	94	SER
6	T	123	ASN
6	T	171	GLU
6	T	172	LEU
6	T	181	GLU
6	T	221	ASN
6	T	240	GLN
7	U	13	GLU
7	U	26	THR
7	U	83	ASN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	208	GLU
7	U	235	ARG
7	U	236	LEU
8	V	20	SER
8	V	22	GLN
8	V	31	CYS
8	V	34	LEU
8	V	35	HIS
8	V	38	SER
8	V	68	LEU
8	V	80	LEU
8	V	113	ILE
8	V	125	LEU
8	V	127	LEU
8	V	196	ARG
9	W	37	ASN
9	W	151	SER
9	W	171	LEU
10	X	1	MET
10	X	7	ILE
10	X	25	ILE

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Mol	Chain	Res	Type
10	X	27	VAL
10	X	35	THR
10	X	92	ILE
10	X	140	THR
10	X	149	ARG
10	X	174	MET
11	Y	31	VAL
11	Y	35	ILE
11	Y	69	ARG
11	Y	72	GLU
11	Y	130	VAL
11	Y	139	VAL
11	Y	142	SER
11	Y	148	LEU
11	Y	149	SER
11	Y	152	ASP
11	Y	186	ILE
11	Y	209	ASN
12	Z	1	GLN
12	Z	23	LEU
12	Z	34	SER
12	Z	35	ILE
12	Z	38	ARG
12	Z	42	LYS
12	Z	49	ASN
12	Z	71	SER
12	Z	128	VAL
12	Z	130	SER
12	Z	150	LEU
12	Z	165	ASN
12	Z	189	THR
13	a	1	THR
13	a	2	GLN
13	a	10	SER
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	165	ILE
13	a	187	ARG
13	a	190	ARG
13	a	225	ILE
13	a	228	TYR

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Mol	Chain	Res	Type
13	a	231	GLN
13	a	232	LYS
13	a	233	ILE
14	b	9	LYS
14	b	107	LYS
14	b	119	VAL
14	b	172	VAL
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (179) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	124	HIS
2	B	155	ASN
2	B	176	GLN
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN
3	C	92	GLN
3	C	147	GLN
3	C	160	GLN
3	C	165	ASN
3	C	176	ASN
3	C	233	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	106	GLN
4	D	146	GLN
4	D	160	ASN
4	D	198	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN

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Mol	Chain	Res	Type
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	140	ASN
6	F	191	GLN
6	F	203	ASN
6	F	240	GLN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
7	G	231	ASN
8	H	22	GLN
8	H	30	ASN
8	H	35	HIS
8	H	66	HIS
8	H	165	ASN
8	H	189	ASN
8	H	200	GLN
9	I	63	ASN
9	I	88	GLN
10	J	10	GLN
10	J	55	GLN
10	J	63	ASN
10	J	65	GLN
10	J	118	GLN
10	J	147	HIS
10	J	191	GLN
11	K	85	ASN
11	K	176	ASN
11	K	190	ASN
11	K	191	HIS
11	K	209	ASN
12	L	1	GLN

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Mol	Chain	Res	Type
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	80	ASN
12	L	159	GLN
12	L	165	ASN
13	M	18	ASN
13	M	26	ASN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	179	ASN
14	N	69	GLN
14	N	141	ASN
14	N	161	GLN
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	124	HIS
2	P	155	ASN
2	P	167	ASN
2	P	176	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	92	GLN
3	Q	115	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	165	ASN
3	Q	176	ASN
3	Q	233	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	146	GLN
4	R	160	ASN
4	R	198	GLN
4	R	225	ASN
5	S	68	HIS

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Mol	Chain	Res	Type
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	140	ASN
6	T	191	GLN
6	T	203	ASN
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
7	U	231	ASN
8	V	22	GLN
8	V	30	ASN
8	V	35	HIS
8	V	66	HIS
8	V	165	ASN
8	V	189	ASN
8	V	200	GLN
9	W	44	HIS
9	W	63	ASN
9	W	88	GLN
10	X	10	GLN
10	X	55	GLN
10	X	63	ASN
10	X	65	GLN
10	X	118	GLN
10	X	147	HIS
10	X	191	GLN
11	Y	85	ASN

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Mol	Chain	Res	Type
11	Y	176	ASN
11	Y	190	ASN
11	Y	191	HIS
11	Y	209	ASN
12	Z	1	GLN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	76	HIS
12	Z	80	ASN
12	Z	159	GLN
12	Z	165	ASN
13	a	18	ASN
13	a	26	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	69	GLN
14	b	141	ASN
14	b	161	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	00E	g	1	15	9,9,10	0.73	0	10,10,12	1.35	1 (10%)
15	0A1	h	3	15	12,13,14	1.46	1 (8%)	11,16,18	0.92	0
15	0A1	f	3	15	12,13,14	1.55	1 (8%)	11,16,18	0.78	0
15	00E	f	1	15	9,9,10	0.86	1 (11%)	10,10,12	1.27	2 (20%)
15	00E	e	1	15	9,9,10	0.88	0	10,10,12	1.26	2 (20%)
15	00E	h	1	15	9,9,10	0.84	0	10,10,12	1.34	1 (10%)
15	0A1	g	3	15	12,13,14	1.44	1 (8%)	11,16,18	0.79	0
15	0A1	i	3	15	12,13,14	1.56	1 (8%)	11,16,18	0.76	0
15	00E	i	1	15	9,9,10	0.85	0	10,10,12	1.28	2 (20%)
15	00E	d	1	15	9,9,10	0.79	0	10,10,12	1.34	2 (20%)
15	0A1	d	3	15	12,13,14	1.54	1 (8%)	11,16,18	0.88	0
15	0A1	e	3	15	12,13,14	1.55	1 (8%)	11,16,18	0.98	1 (9%)

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	00E	g	1	15	-	0/2/11/12	0/1/1/1
15	0A1	h	3	15	-	0/7/8/10	0/1/1/1
15	0A1	f	3	15	-	2/7/8/10	0/1/1/1
15	00E	f	1	15	-	0/2/11/12	0/1/1/1
15	00E	e	1	15	-	0/2/11/12	0/1/1/1
15	00E	h	1	15	-	0/2/11/12	0/1/1/1
15	0A1	g	3	15	-	0/7/8/10	0/1/1/1
15	0A1	i	3	15	-	2/7/8/10	0/1/1/1
15	00E	i	1	15	-	0/2/11/12	0/1/1/1
15	00E	d	1	15	-	0/2/11/12	0/1/1/1
15	0A1	d	3	15	-	0/7/8/10	0/1/1/1
15	0A1	e	3	15	-	0/7/8/10	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	i	3	0A1	CB-CG	-5.01	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	e	3	0A1	CB-CG	-4.96	1.39	1.51
15	f	3	0A1	CB-CG	-4.93	1.39	1.51
15	d	3	0A1	CB-CG	-4.87	1.39	1.51
15	h	3	0A1	CB-CG	-4.65	1.40	1.51
15	g	3	0A1	CB-CG	-4.51	1.40	1.51
15	f	1	00E	CA-C	2.01	1.56	1.49

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	g	1	00E	C-CA-NB	-2.77	107.50	112.80
15	d	1	00E	C-CA-NB	-2.73	107.58	112.80
15	h	1	00E	OZ-CE1-CD1	-2.61	106.16	111.77
15	e	1	00E	OZ-CE1-CD1	-2.39	106.63	111.77
15	e	3	0A1	CM-OH-CZ	2.24	122.31	117.50
15	f	1	00E	OZ-CE1-CD1	-2.22	106.98	111.77
15	i	1	00E	OZ-CE1-CD1	-2.16	107.13	111.77
15	d	1	00E	OZ-CE1-CD1	-2.10	107.24	111.77
15	i	1	00E	C-CA-NB	-2.01	108.95	112.80
15	e	1	00E	C-CA-NB	-2.01	108.95	112.80
15	f	1	00E	C-CA-NB	-2.01	108.97	112.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	f	3	0A1	C-CA-CB-CG
15	i	3	0A1	C-CA-CB-CG
15	f	3	0A1	N-CA-CB-CG
15	i	3	0A1	N-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	g	1	00E	2	0
15	g	3	0A1	1	0
15	d	1	00E	2	0
15	d	3	0A1	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
19	MPD	a	302	-	7,7,7	0.38	0	9,10,10	0.35	0
18	MES	H	301	-	12,12,12	0.73	0	15,16,16	0.29	0
18	MES	M	301	-	12,12,12	0.67	0	15,16,16	0.35	0
19	MPD	K	301	-	7,7,7	0.14	0	9,10,10	0.45	0
18	MES	U	302	-	12,12,12	0.76	0	15,16,16	0.38	0
18	MES	G	303	-	12,12,12	0.77	0	15,16,16	0.32	0
18	MES	V	301	-	12,12,12	0.73	0	15,16,16	0.34	0
18	MES	a	301	-	12,12,12	0.71	0	15,16,16	0.31	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	MPD	a	302	-	-	3/5/5/5	-
18	MES	H	301	-	-	1/6/14/14	0/1/1/1
18	MES	M	301	-	-	0/6/14/14	0/1/1/1
19	MPD	K	301	-	-	2/5/5/5	-
18	MES	U	302	-	-	3/6/14/14	0/1/1/1
18	MES	G	303	-	-	1/6/14/14	0/1/1/1
18	MES	V	301	-	-	0/6/14/14	0/1/1/1
18	MES	a	301	-	-	0/6/14/14	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	U	302	MES	C7-C8-S-O2S
19	a	302	MPD	C2-C3-C4-C5
18	U	302	MES	C7-C8-S-O3S
18	G	303	MES	N4-C7-C8-S
18	U	302	MES	C7-C8-S-O1S
19	K	301	MPD	C2-C3-C4-C5
18	H	301	MES	N4-C7-C8-S
19	a	302	MPD	O2-C2-C3-C4
19	K	301	MPD	C2-C3-C4-O4
19	a	302	MPD	CM-C2-C3-C4

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	a	302	MPD	7	0
19	K	301	MPD	1	0
18	G	303	MES	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	250/250 (100%)	-0.83	0 100 100	43, 60, 91, 131	0
1	O	250/250 (100%)	-0.84	0 100 100	46, 66, 100, 156	0
2	B	244/258 (94%)	-0.74	0 100 100	45, 66, 112, 154	0
2	P	244/258 (94%)	-0.74	0 100 100	48, 69, 110, 149	0
3	C	240/254 (94%)	-0.77	0 100 100	46, 70, 126, 143	0
3	Q	240/254 (94%)	-0.69	1 (0%) 88 85	53, 80, 142, 168	0
4	D	235/260 (90%)	-0.84	0 100 100	49, 71, 99, 123	0
4	R	235/260 (90%)	-0.79	0 100 100	49, 72, 102, 126	0
5	E	231/234 (98%)	-0.78	0 100 100	51, 74, 106, 137	0
5	S	231/234 (98%)	-0.73	0 100 100	51, 80, 116, 141	0
6	F	243/288 (84%)	-0.84	0 100 100	44, 67, 101, 141	0
6	T	243/288 (84%)	-0.80	0 100 100	46, 70, 117, 134	0
7	G	241/252 (95%)	-0.90	0 100 100	43, 60, 92, 145	0
7	U	241/252 (95%)	-0.86	0 100 100	44, 62, 95, 125	0
8	H	225/231 (97%)	-0.89	0 100 100	41, 56, 87, 123	0
8	V	225/231 (97%)	-0.86	0 100 100	46, 59, 92, 149	0
9	I	204/205 (99%)	-0.91	0 100 100	42, 60, 86, 108	0
9	W	204/205 (99%)	-0.93	0 100 100	43, 60, 88, 114	0
10	J	195/198 (98%)	-0.86	0 100 100	43, 64, 94, 123	0
10	X	195/198 (98%)	-0.89	0 100 100	46, 67, 94, 134	0
11	K	211/211 (100%)	-0.75	0 100 100	46, 68, 110, 129	0
11	Y	211/211 (100%)	-0.78	0 100 100	47, 67, 113, 133	0
12	L	222/222 (100%)	-0.88	0 100 100	47, 61, 92, 115	0
12	Z	222/222 (100%)	-0.88	0 100 100	44, 60, 88, 110	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	232/246 (94%)	-0.79	1 (0%) 88 85	41, 59, 87, 109	0
13	a	233/246 (94%)	-0.83	0 100 100	40, 58, 84, 120	0
14	N	195/195 (100%)	-0.96	0 100 100	41, 55, 85, 106	0
14	b	195/195 (100%)	-0.93	0 100 100	40, 55, 84, 110	0
15	d	1/4 (25%)	-0.26	0 100 100	59, 59, 59, 59	0
15	e	1/4 (25%)	-0.12	0 100 100	71, 71, 71, 71	0
15	f	1/4 (25%)	0.69	0 100 100	92, 92, 92, 92	0
15	g	1/4 (25%)	-0.35	0 100 100	61, 61, 61, 61	0
15	h	1/4 (25%)	-0.57	0 100 100	75, 75, 75, 75	0
15	i	1/4 (25%)	-0.40	0 100 100	84, 84, 84, 84	0
All	All	6343/6632 (95%)	-0.83	2 (0%) 100 100	40, 64, 106, 168	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	50	LEU	3.6
13	M	227	GLY	2.6

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
15	00E	f	1	9/10	0.90	0.11	98,115,123,125	0
15	00E	i	1	9/10	0.90	0.11	88,113,120,122	0
15	00E	h	1	9/10	0.92	0.09	80,85,89,90	0
15	0A1	h	3	13/14	0.93	0.08	66,71,93,101	0
15	0A1	e	3	13/14	0.96	0.07	64,69,86,89	0
15	0A1	f	3	13/14	0.96	0.08	81,91,97,97	0
15	00E	d	1	9/10	0.96	0.07	73,81,83,85	0
15	0A1	i	3	13/14	0.96	0.07	80,86,98,99	0
15	00E	e	1	9/10	0.97	0.06	72,80,94,97	0
15	00E	g	1	9/10	0.97	0.06	65,77,84,85	0
15	0A1	d	3	13/14	0.98	0.04	53,58,65,66	0
15	0A1	g	3	13/14	0.98	0.05	61,63,67,68	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
19	MPD	K	301	8/8	0.88	0.15	90,97,98,111	0
18	MES	G	303	12/12	0.91	0.13	92,153,170,176	0
18	MES	a	301	12/12	0.92	0.10	125,129,133,133	0
16	MG	W	301	1/1	0.93	0.18	143,143,143,143	0
18	MES	M	301	12/12	0.93	0.12	126,137,147,151	0
19	MPD	a	302	8/8	0.93	0.10	80,102,107,111	0
18	MES	U	302	12/12	0.95	0.10	108,131,136,141	0
18	MES	V	301	12/12	0.96	0.10	92,106,111,115	0
18	MES	H	301	12/12	0.96	0.09	79,94,99,100	0
17	CL	U	301	1/1	0.99	0.05	60,60,60,60	0
16	MG	N	201	1/1	0.99	0.06	72,72,72,72	0
17	CL	G	302	1/1	0.99	0.06	59,59,59,59	0
16	MG	G	301	1/1	1.00	0.02	75,75,75,75	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.