



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2026 – 10:16 AM UTC

PDB ID : 8BW1 / pdb_00008bw1
Title : Yeast 20S proteasome in complex with an engineered fellutamide derivative (C14QAL)
Authors : Bozhueyuek, K.A.J.; Praeve, L.; Kegler, C.; Kaiser, S.; Shi, Y.; Kuttelochner, W.; Schenk, L.; Groll, M.; Hochberg, G.K.A.; Bode, H.B.
Deposited on : 2022-12-06
Resolution : 3.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

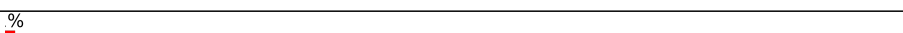
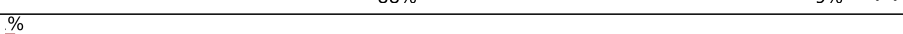
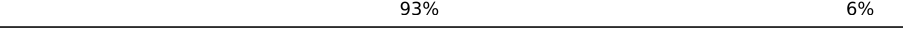
The types of validation reports are described at

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

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

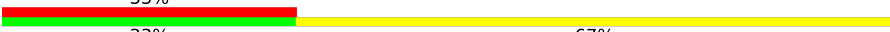
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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Mol	Chain	Length	Quality of chain
3	C	254	
3	Q	254	
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	
15	e	3	

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Mol	Chain	Length	Quality of chain	
15	f	3		
15	g	3		
15	h	3		

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	DCL	e	4	-	-	X	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49555 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			

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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	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	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	230	Total	C	N	O	S	0	0	0
			1797	1137	307	346	7			
13	a	230	Total	C	N	O	S	0	0	0
			1797	1137	307	346	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 a protein called 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-C]PYRAZOLE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	e	3	Total	C	N	O	0	0	0
			22	14	4	4			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	f	3	Total	C	N	O	0	0	0
			22	14	4	4			
15	g	3	Total	C	N	O	0	0	0
			22	14	4	4			
15	h	3	Total	C	N	O	0	0	0
			22	14	4	4			

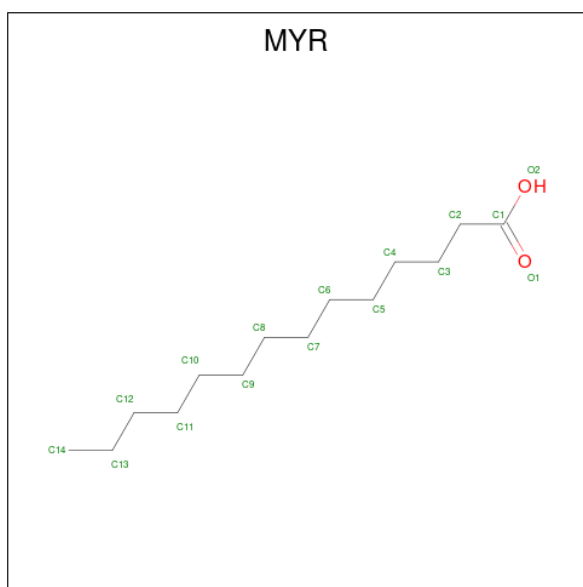
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total	Mg	0	0
			1	1		
16	I	1	Total	Mg	0	0
			1	1		
16	J	1	Total	Mg	0	0
			1	1		
16	K	1	Total	Mg	0	0
			1	1		
16	N	1	Total	Mg	0	0
			1	1		
16	V	1	Total	Mg	0	0
			1	1		
16	Y	1	Total	Mg	0	0
			1	1		
16	Z	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	N	1	Total	Cl	0	0
			1	1		
17	U	1	Total	Cl	0	0
			1	1		

- Molecule 18 is MYRISTIC ACID (CCD ID: MYR) (formula: C₁₄H₂₈O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	e	1	Total	C	O	0	0
			15	14	1		
18	f	1	Total	C	O	0	0
			15	14	1		
18	g	1	Total	C	O	0	0
			15	14	1		
18	h	1	Total	C	O	0	0
			15	14	1		

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	1	Total	O	0	0
			1	1		
19	B	3	Total	O	0	0
			3	3		
19	C	2	Total	O	0	0
			2	2		
19	D	1	Total	O	0	0
			1	1		
19	E	5	Total	O	0	0
			5	5		
19	F	1	Total	O	0	0
			1	1		
19	G	3	Total	O	0	0
			3	3		
19	H	3	Total	O	0	0
			3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	I	2	Total O 2 2	0	0
19	J	4	Total O 4 4	0	0
19	K	7	Total O 7 7	0	0
19	L	6	Total O 6 6	0	0
19	M	6	Total O 6 6	0	0
19	N	4	Total O 4 4	0	0
19	O	1	Total O 1 1	0	0
19	P	6	Total O 6 6	0	0
19	Q	2	Total O 2 2	0	0
19	R	2	Total O 2 2	0	0
19	S	1	Total O 1 1	0	0
19	T	1	Total O 1 1	0	0
19	U	2	Total O 2 2	0	0
19	V	3	Total O 3 3	0	0
19	W	1	Total O 1 1	0	0
19	X	3	Total O 3 3	0	0
19	Y	5	Total O 5 5	0	0
19	Z	3	Total O 3 3	0	0
19	a	3	Total O 3 3	0	0
19	b	1	Total O 1 1	0	0
19	f	1	Total O 1 1	0	0

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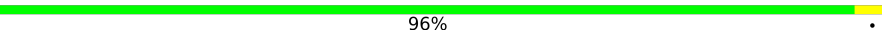
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	h	1	Total	O	0	0
			1	1		

3 Residue-property plots [i](#)

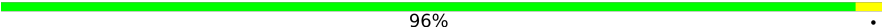
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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:  96%



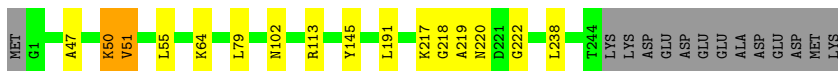
- Molecule 1: Proteasome subunit alpha type-2

Chain O:  96%



- Molecule 2: Proteasome subunit alpha type-3

Chain B:  88% 5% • 5%



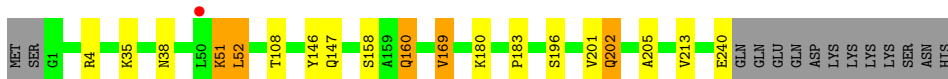
- Molecule 2: Proteasome subunit alpha type-3

Chain P:  88% 6% • 5%



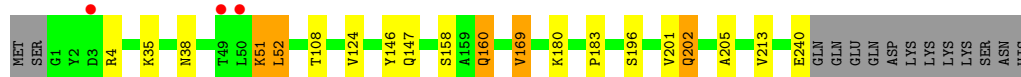
- Molecule 3: Proteasome subunit alpha type-4

Chain C:  87% 6% • 6%

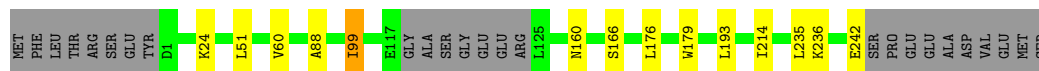


- Molecule 3: Proteasome subunit alpha type-4

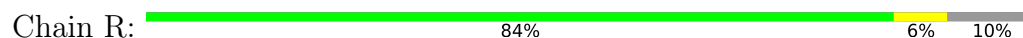
Chain Q:  87% 6% • 6%



• Molecule 4: Proteasome subunit alpha type-5



• Molecule 4: Proteasome subunit alpha type-5



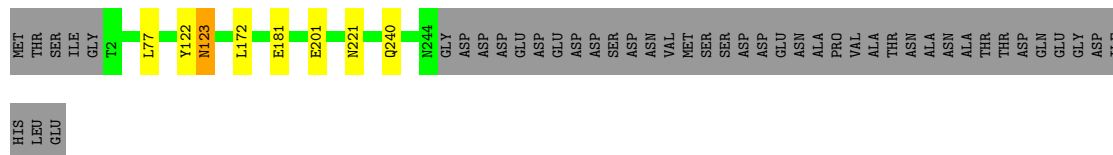
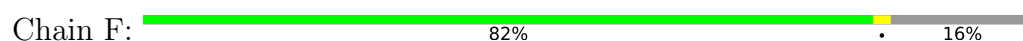
• Molecule 5: Proteasome subunit alpha type-6



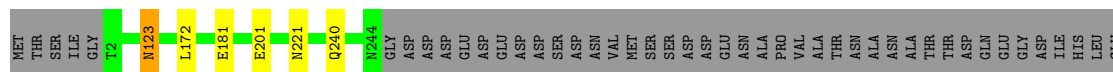
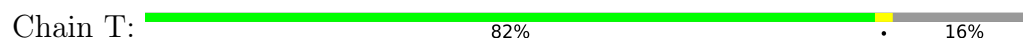
• Molecule 5: Proteasome subunit alpha type-6



• Molecule 6: Probable proteasome subunit alpha type-7



• Molecule 6: Probable proteasome subunit alpha type-7



• Molecule 7: Proteasome subunit alpha type-1

MTT	SER	GLY	ALA	ALA	ALA	ALA	SER	ALA	ALA	G2	F23	T26	L34	V43	V73	V74	N75	I78	P79	L115	R122	M125	T133	V194	R235	L236	Q242	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	-----

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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|
| Met | Ser | Gly | Ala | Ala | Ala | Ser | Ser | Ala | Ala | G2 | F23 | T26 | L34 | V73 | V74 | N75 | I78 | P79 | L115 | R122 | M125 | T133 | A159 | R235 | L236 | Q242 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|

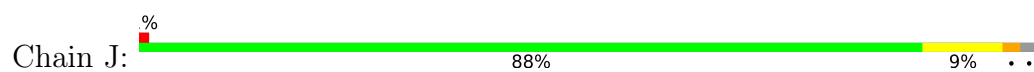
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- [illegible]

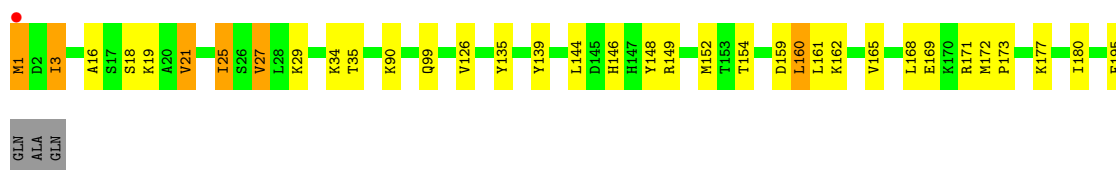
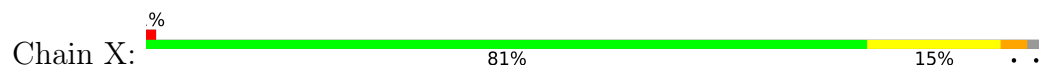
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- | State/DC | Score Range | Color |
|----------|---------------|--------|
| MET | 200 or higher | Green |
| S1 | 200 or higher | Green |
| G9 | 180-199 | Yellow |
| I10 | 180-199 | Yellow |
| V20 | 180-199 | Yellow |
| N37 | 180-199 | Yellow |
| K38 | 180-199 | Yellow |
| K41 | 180-199 | Yellow |
| L62 | 180-199 | Yellow |
| L94 | 180-199 | Yellow |
| V104 | 180-199 | Yellow |
| G105 | 200 or higher | Green |
| P106 | 180-199 | Yellow |
| P118 | 180-199 | Yellow |
| I126 | 160-179 | Orange |
| A141 | 180-199 | Yellow |
| E150 | 180-199 | Yellow |
| S167 | 180-199 | Yellow |
| L171 | 180-199 | Yellow |
| D177 | 180-199 | Yellow |
| W182 | 180-199 | Yellow |
| G183 | 180-199 | Yellow |
| D204 | 180-199 | Yellow |

- | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|
| ME1 | S1 | N7 | G8 | G9 | I10 | V20 | G29 | S36 | S37 | K38 | K41 | L62 | L94 | V104 | G105 | P106 | P118 | I126 | A141 | E150 | S167 | L171 | D177 | G183 | D204 |
|-----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|

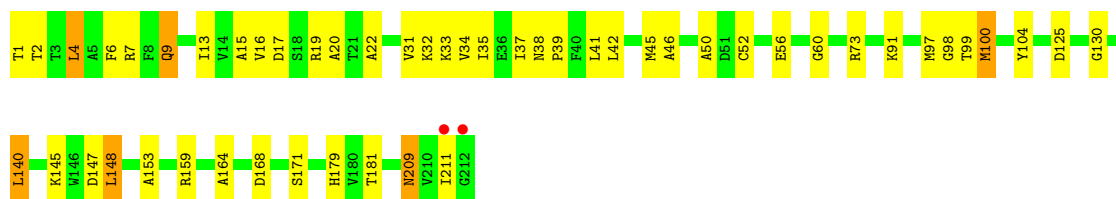
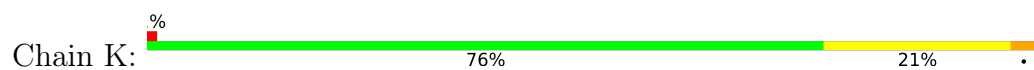
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• Molecule 10: Proteasome subunit beta type-4



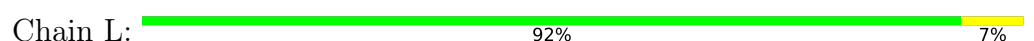
• Molecule 11: Proteasome subunit beta type-5



• Molecule 11: Proteasome subunit beta type-5



• Molecule 12: Proteasome subunit beta type-6



• Molecule 12: Proteasome subunit beta type-6



- Molecule 13: Proteasome subunit beta type-7

Chain M:  89% 7%



- Molecule 13: Proteasome subunit beta type-7

Chain a:  89% 7%



- Molecule 14: Proteasome subunit beta type-1

Chain N:  90% 9%

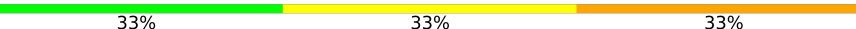


- Molecule 14: Proteasome subunit beta type-1

Chain b:  90% 9%



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

Chain e:  33% 33% 33%



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

Chain f:  33% 67%



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

Chain g:  33% 33% 67%



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

Chain h:

33%

67%


Q2
A3
X4

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	134.97Å 300.87Å 143.98Å 90.00° 112.78° 90.00°	Depositor
Resolution (Å)	30.00 – 3.25 30.00 – 3.25	Depositor EDS
% Data completeness (in resolution range)	95.2 (30.00-3.25) 95.1 (30.00-3.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 3.24Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.174 , 0.212 0.188 , 0.221	Depositor DCC
R_{free} test set	7890 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	81.6	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 73.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	49555	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, DCL, CL, MYR

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	1.00	0/1952	1.40	0/2642
1	O	1.01	0/1952	1.40	0/2642
2	B	1.00	0/1934	1.42	0/2618
2	P	1.00	0/1934	1.41	0/2618
3	C	1.00	0/1910	1.44	0/2586
3	Q	1.00	0/1910	1.44	0/2586
4	D	1.01	0/1837	1.44	0/2475
4	R	1.01	0/1837	1.44	0/2475
5	E	1.01	0/1800	1.41	0/2433
5	S	1.01	0/1800	1.41	0/2433
6	F	0.99	0/1932	1.43	2/2609 (0.1%)
6	T	0.99	0/1932	1.43	0/2609
7	G	0.99	0/1945	1.40	0/2634
7	U	0.99	0/1945	1.40	0/2634
8	H	1.01	0/1750	1.41	0/2373
8	V	1.01	0/1750	1.41	0/2373
9	I	0.98	0/1611	1.39	1/2174 (0.0%)
9	W	0.99	0/1611	1.38	1/2174 (0.0%)
10	J	0.97	0/1589	1.35	0/2142
10	X	0.96	0/1589	1.34	0/2142
11	K	0.98	0/1681	1.43	0/2274
11	Y	0.98	0/1681	1.43	0/2274
12	L	0.97	0/1795	1.34	0/2420
12	Z	0.97	0/1795	1.34	0/2420
13	M	0.99	0/1828	1.36	0/2480
13	a	0.99	0/1828	1.36	0/2480
14	N	0.99	0/1541	1.42	0/2087
14	b	0.99	0/1541	1.42	0/2087
15	e	0.56	0/13	1.26	0/16
15	f	0.63	0/13	0.87	0/16
15	g	0.52	0/13	1.28	0/16
15	h	0.63	0/13	1.14	0/16

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.99	0/50262	1.40	4/67958 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	183	GLY	CA-C-O	-5.76	118.31	122.45
9	W	183	GLY	CA-C-O	-5.68	118.36	122.45
6	F	77	LEU	CA-C-N	5.05	124.37	120.33
6	F	77	LEU	C-N-CA	5.05	124.37	120.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	4	0
1	O	1915	0	1929	3	0
2	B	1904	0	1904	6	0
2	P	1904	0	1904	7	0
3	C	1881	0	1895	6	0
3	Q	1881	0	1895	7	0
4	D	1813	0	1797	3	0
4	R	1813	0	1797	4	0
5	E	1773	0	1775	6	0
5	S	1773	0	1775	6	0
6	F	1892	0	1883	2	0
6	T	1892	0	1883	1	0
7	G	1907	0	1901	5	0
7	U	1907	0	1901	5	0
8	H	1719	0	1718	36	0
8	V	1719	0	1718	32	0
9	I	1581	0	1574	13	0
9	W	1581	0	1574	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	1561	0	1569	18	0
10	X	1561	0	1569	31	0
11	K	1644	0	1594	40	0
11	Y	1644	0	1594	42	0
12	L	1757	0	1711	13	0
12	Z	1757	0	1711	11	0
13	M	1797	0	1800	7	0
13	a	1797	0	1800	5	0
14	N	1512	0	1481	10	0
14	b	1512	0	1481	11	0
15	e	22	0	23	9	0
15	f	22	0	22	6	0
15	g	22	0	22	2	0
15	h	22	0	22	8	0
16	G	1	0	0	0	0
16	I	1	0	0	0	0
16	J	1	0	0	0	0
16	K	1	0	0	0	0
16	N	1	0	0	0	0
16	V	1	0	0	0	0
16	Y	1	0	0	0	0
16	Z	1	0	0	0	0
17	G	1	0	0	0	0
17	N	1	0	0	0	0
17	U	1	0	0	0	0
18	e	15	0	27	0	0
18	f	15	0	27	2	0
18	g	15	0	27	0	0
18	h	15	0	27	0	0
19	A	1	0	0	0	0
19	B	3	0	0	0	0
19	C	2	0	0	0	0
19	D	1	0	0	0	0
19	E	5	0	0	0	0
19	F	1	0	0	0	0
19	G	3	0	0	0	0
19	H	3	0	0	0	0
19	I	2	0	0	0	0
19	J	4	0	0	0	0
19	K	7	0	0	0	0
19	L	6	0	0	0	0
19	M	6	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	N	4	0	0	0	0
19	O	1	0	0	0	0
19	P	6	0	0	0	0
19	Q	2	0	0	0	0
19	R	2	0	0	0	0
19	S	1	0	0	0	0
19	T	1	0	0	0	0
19	U	2	0	0	0	0
19	V	3	0	0	0	0
19	W	1	0	0	0	0
19	X	3	0	0	0	0
19	Y	5	0	0	0	0
19	Z	3	0	0	0	0
19	a	3	0	0	0	0
19	b	1	0	0	0	0
19	f	1	0	0	0	0
19	h	1	0	0	0	0
All	All	49555	0	49259	316	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 (316) 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)
8:H:2:THR:HG21	8:H:162:GLY:HA3	1.34	1.10
8:H:2:THR:OG1	8:H:169:SER:HB3	1.53	1.08
10:J:139:TYR:OH	10:X:25:ILE:O	1.89	0.91
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.57	0.87
10:X:160:LEU:HD12	10:X:160:LEU:O	1.76	0.86
8:H:2:THR:OG1	8:H:169:SER:CB	2.25	0.84
10:J:155:GLU:OE1	10:J:155:GLU:N	2.13	0.78
10:J:25:ILE:HD11	10:X:135:TYR:HB3	1.65	0.77
15:f:2:GLN:HE21	15:f:2:GLN:CA	1.99	0.75
8:H:18:THR:HG21	8:H:172:ASN:HB2	1.67	0.75
8:V:18:THR:HG21	8:V:172:ASN:HB2	1.67	0.75
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.52	0.75
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.52	0.74
11:K:209:ASN:O	9:W:38:LYS:NZ	2.22	0.72
11:Y:9:GLN:HE21	11:Y:147:ASP:HA	1.55	0.72
10:J:25:ILE:HG12	10:J:25:ILE:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:25:ILE:HD12	10:X:135:TYR:CD1	2.25	0.71
8:V:2:THR:HG21	8:V:162:GLY:HA3	1.72	0.70
11:K:73:ARG:NH2	11:K:104:TYR:O	2.23	0.69
15:h:3:ALA:C	15:h:4:DCL:HD22	2.16	0.68
10:X:160:LEU:HD12	10:X:160:LEU:C	2.18	0.68
15:e:4:DCL:HD13	15:e:4:DCL:N	2.07	0.68
15:h:4:DCL:HD22	15:h:4:DCL:N	2.07	0.67
8:V:20:SER:OG	15:g:2:GLN:NE2	2.27	0.67
10:X:25:ILE:O	10:X:25:ILE:HG12	1.92	0.67
14:b:152:VAL:HA	14:b:175:MET:HE1	1.76	0.67
11:K:9:GLN:HE21	11:K:147:ASP:HA	1.56	0.67
14:N:152:VAL:HA	14:N:175:MET:HE1	1.78	0.66
13:M:228:TYR:HE2	14:b:35:THR:HG21	1.60	0.65
8:V:2:THR:O	8:V:159:ILE:HD12	1.96	0.64
11:Y:4:LEU:C	11:Y:4:LEU:CD1	2.72	0.62
11:K:4:LEU:HD11	11:K:15:ALA:HB3	1.81	0.62
11:Y:73:ARG:NH2	11:Y:104:TYR:O	2.23	0.62
11:Y:27:ALA:CB	15:h:2:GLN:NE2	2.63	0.62
10:X:139:TYR:CE1	10:X:171:ARG:HB3	2.34	0.61
11:Y:27:ALA:HB2	15:h:2:GLN:HE22	1.65	0.61
9:I:38:LYS:NZ	11:Y:209:ASN:O	2.34	0.61
11:Y:9:GLN:NE2	11:Y:147:ASP:HA	2.16	0.60
11:Y:4:LEU:HD22	11:Y:140:LEU:HD21	1.82	0.60
8:V:18:THR:HB	8:V:30:ASN:HD22	1.67	0.60
8:H:2:THR:HG23	8:H:130:GLY:HA3	1.83	0.60
8:V:18:THR:CG2	8:V:172:ASN:HB2	2.32	0.60
11:Y:49:ALA:HB2	15:h:4:DCL:HD21	1.85	0.59
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.67	0.59
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.67	0.59
8:H:18:THR:CG2	8:H:172:ASN:HB2	2.32	0.59
8:H:18:THR:HB	8:H:30:ASN:HD22	1.68	0.58
11:K:45:MET:SD	11:K:52:CYS:HB3	2.42	0.58
10:X:27:VAL:HG12	10:X:27:VAL:O	2.01	0.58
8:V:2:THR:O	8:V:159:ILE:CD1	2.51	0.58
11:K:9:GLN:NE2	11:K:147:ASP:HA	2.18	0.58
11:K:1:THR:O	11:K:130:GLY:HA3	2.04	0.57
15:f:2:GLN:HE21	15:f:2:GLN:N	2.02	0.57
15:f:2:GLN:HE21	15:f:2:GLN:HA	1.69	0.57
10:X:139:TYR:CE1	10:X:171:ARG:CB	2.87	0.56
11:Y:27:ALA:CB	15:h:2:GLN:HE22	2.17	0.56
8:H:2:THR:HG1	8:H:169:SER:HB3	1.65	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.88	0.56
12:L:12:ILE:HD12	12:L:110:ILE:HD12	1.88	0.56
11:K:4:LEU:O	11:K:4:LEU:HD12	2.06	0.55
14:b:7:THR:HG23	14:b:123:PRO:O	2.06	0.55
8:H:3:ILE:HG13	8:H:99:ILE:HD12	1.89	0.55
7:U:23:PHE:O	7:U:26:THR:HB	2.05	0.55
12:Z:12:ILE:HD12	12:Z:110:ILE:HD12	1.88	0.55
7:G:23:PHE:O	7:G:26:THR:HB	2.06	0.55
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.88	0.55
15:e:4:DCL:CD1	15:e:4:DCL:C	2.85	0.54
2:P:217:LYS:C	2:P:219:ALA:H	2.15	0.54
8:H:46:ALA:HA	15:e:4:DCL:HD12	1.90	0.54
11:K:22:ALA:HB2	15:f:2:GLN:NE2	2.23	0.54
8:V:166:ASP:OD2	8:V:169:SER:OG	2.25	0.54
11:K:19:ARG:O	11:K:33:LYS:NZ	2.33	0.53
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.90	0.53
2:B:217:LYS:C	2:B:219:ALA:H	2.15	0.53
12:Z:12:ILE:CD1	12:Z:110:ILE:HD12	2.38	0.53
12:L:194:ARG:CZ	8:V:29:LYS:HE2	2.39	0.53
14:N:35:THR:HG21	13:a:228:TYR:HE2	1.74	0.53
10:X:21:VAL:HG23	10:X:29:LYS:HB3	1.91	0.53
12:L:12:ILE:CD1	12:L:110:ILE:HD12	2.39	0.53
8:V:2:THR:OG1	8:V:169:SER:CB	2.57	0.53
8:H:3:ILE:HD11	8:H:127:LEU:HB3	1.89	0.52
11:K:4:LEU:CD1	11:K:4:LEU:C	2.83	0.52
3:C:35:LYS:HG2	3:C:158:SER:O	2.09	0.52
8:H:29:LYS:HZ1	9:I:150:GLU:CD	2.18	0.52
15:f:4:DCL:N	15:f:4:DCL:HD22	2.24	0.52
10:X:19:LYS:HD2	10:X:180:ILE:HG13	1.91	0.52
13:a:31:GLY:C	13:a:190:ARG:HH21	2.17	0.52
8:H:166:ASP:OD2	8:H:169:SER:OG	2.28	0.52
10:J:155:GLU:H	10:J:155:GLU:CD	2.09	0.52
8:H:19:ARG:O	8:H:33:LYS:NZ	2.43	0.51
11:K:159:ARG:NH2	10:X:146:HIS:ND1	2.58	0.51
14:N:7:THR:HG23	14:N:123:PRO:O	2.10	0.51
5:S:71:LEU:HD22	5:S:71:LEU:C	2.36	0.51
11:Y:4:LEU:C	11:Y:4:LEU:HD12	2.35	0.51
10:X:165:VAL:HG21	10:X:195:PHE:HE1	1.76	0.51
5:E:71:LEU:C	5:E:71:LEU:HD22	2.36	0.51
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	1.93	0.51
11:K:2:THR:OG1	11:K:171:SER:OG	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:4:LEU:HD12	11:K:4:LEU:C	2.36	0.51
11:Y:19:ARG:O	11:Y:33:LYS:NZ	2.33	0.51
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.93	0.50
11:Y:4:LEU:HD12	11:Y:4:LEU:O	2.11	0.50
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.11	0.50
10:X:19:LYS:CD	10:X:180:ILE:HG13	2.41	0.50
10:J:147:HIS:ND1	10:J:147:HIS:N	2.60	0.50
11:K:1:THR:HG21	11:K:46:ALA:HA	1.93	0.50
13:M:31:GLY:C	13:M:190:ARG:HH21	2.20	0.50
8:H:29:LYS:NZ	9:I:150:GLU:OE1	2.44	0.50
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.47	0.50
11:Y:27:ALA:HB2	15:h:2:GLN:NE2	2.24	0.50
11:Y:50:ALA:HB2	12:Z:128:VAL:HG23	1.93	0.49
15:f:2:GLN:N	15:f:2:GLN:NE2	2.60	0.49
14:N:132:THR:O	14:b:133:PHE:HA	2.12	0.49
8:H:84:LYS:HE2	8:H:119:THR:CG2	2.42	0.49
11:K:37:ILE:HG23	11:K:60:GLY:HA2	1.94	0.49
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.93	0.49
11:Y:2:THR:HG21	11:Y:164:ALA:CB	2.42	0.49
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.47	0.49
8:V:84:LYS:HE2	8:V:119:THR:CG2	2.42	0.49
6:T:123:ASN:C	6:T:123:ASN:HD22	2.21	0.49
8:V:19:ARG:O	8:V:33:LYS:NZ	2.42	0.49
6:F:123:ASN:C	6:F:123:ASN:HD22	2.21	0.49
8:H:3:ILE:HG12	8:H:3:ILE:O	2.12	0.49
8:H:16:ALA:HB3	8:H:34:LEU:HD11	1.95	0.49
8:H:1:THR:OG1	15:e:4:DCL:HD12	2.13	0.49
10:J:146:HIS:HB3	10:J:147:HIS:ND1	2.27	0.49
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.95	0.49
14:b:83:LYS:HG3	14:b:119:VAL:CG2	2.43	0.49
8:H:50:ALA:HB3	9:I:126:ILE:HD11	1.94	0.49
11:K:179:HIS:CE1	11:K:181:THR:HG23	2.48	0.49
11:Y:46:ALA:HB3	11:Y:98:GLY:O	2.13	0.49
9:W:62:LEU:CD1	9:W:104:VAL:HG21	2.42	0.48
9:I:62:LEU:CD1	9:I:104:VAL:HG21	2.43	0.48
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.43	0.48
8:V:1:THR:HG21	8:V:46:ALA:HB2	1.95	0.48
11:Y:50:ALA:CB	12:Z:128:VAL:HG23	2.43	0.48
11:K:159:ARG:CZ	10:X:146:HIS:ND1	2.76	0.48
11:Y:34:VAL:CG1	11:Y:42:LEU:HD22	2.43	0.48
11:K:209:ASN:OD1	11:K:209:ASN:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:22:THR:HG21	10:X:173:PRO:HB3	1.96	0.48
11:K:34:VAL:CG1	11:K:42:LEU:HD22	2.43	0.48
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.95	0.48
11:Y:179:HIS:CE1	11:Y:181:THR:HG23	2.48	0.48
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.13	0.48
7:U:78:ILE:N	7:U:79:PRO:CD	2.77	0.47
1:A:1:MET:HG3	6:F:122:TYR:CZ	2.50	0.47
11:Y:209:ASN:OD1	11:Y:209:ASN:C	2.57	0.47
15:e:4:DCL:HD13	15:e:4:DCL:C	2.43	0.47
13:a:97:ALA:HA	13:a:130:VAL:HG21	1.95	0.47
3:C:51:LYS:O	3:C:52:LEU:HB2	2.13	0.47
7:G:78:ILE:N	7:G:79:PRO:CD	2.77	0.47
8:V:16:ALA:HB3	8:V:34:LEU:HD11	1.96	0.47
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.95	0.47
7:G:34:LEU:C	7:G:34:LEU:HD23	2.40	0.47
8:H:29:LYS:NZ	9:I:150:GLU:OE2	2.48	0.47
10:J:26:SER:HA	10:X:139:TYR:OH	2.15	0.47
1:O:55:LEU:HB3	7:U:159:ALA:O	2.15	0.47
7:U:34:LEU:C	7:U:34:LEU:HD23	2.40	0.47
8:V:84:LYS:HE2	8:V:119:THR:HG23	1.97	0.47
8:V:35:HIS:CB	8:V:56:THR:HG21	2.45	0.47
8:V:20:SER:HB3	8:V:28:ASP:HB3	1.97	0.46
8:H:210:THR:HG21	9:I:167:SER:HB3	1.97	0.46
3:C:108:THR:HG21	3:C:146:TYR:HB3	1.98	0.46
13:M:228:TYR:CE2	14:b:35:THR:HG21	2.46	0.46
10:X:3:ILE:HG23	10:X:18:SER:HB3	1.97	0.46
11:Y:4:LEU:HD11	11:Y:15:ALA:HB3	1.97	0.46
11:K:46:ALA:HB3	11:K:98:GLY:O	2.15	0.46
14:b:8:PHE:CE2	14:b:10:ASP:HB2	2.51	0.46
11:K:56:GLU:OE2	11:K:99:THR:HG21	2.16	0.46
14:N:8:PHE:CE2	14:N:10:ASP:HB2	2.50	0.46
11:Y:25:TRP:CH2	12:Z:144:SER:HA	2.51	0.46
15:e:4:DCL:HD13	15:e:4:DCL:O	2.15	0.46
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.46	0.46
12:L:8:ASN:HA	12:L:30:ILE:O	2.16	0.46
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.64	0.46
8:V:1:THR:HG21	8:V:46:ALA:CB	2.46	0.46
10:X:21:VAL:CG2	10:X:29:LYS:HB3	2.46	0.46
11:Y:13:ILE:HG13	11:Y:153:ALA:HB1	1.97	0.46
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	1.98	0.46
10:J:3:ILE:HG23	10:J:18:SER:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:13:ILE:HG13	11:K:153:ALA:HB1	1.98	0.45
12:L:145:LEU:HD11	8:V:25:ILE:HD11	1.96	0.45
8:H:29:LYS:NZ	9:I:150:GLU:CD	2.73	0.45
8:H:46:ALA:HA	15:e:4:DCL:CD1	2.46	0.45
8:V:3:ILE:HG13	8:V:99:ILE:HD12	1.98	0.45
10:X:149:ARG:HB2	10:X:152:MET:HG3	1.97	0.45
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.15	0.45
2:B:145:TYR:OH	2:B:217:LYS:N	2.49	0.45
12:L:13:LEU:HD11	12:L:150:LEU:HD21	1.98	0.45
14:N:133:PHE:HA	14:b:132:THR:O	2.17	0.45
8:V:2:THR:OG1	8:V:169:SER:HB3	2.16	0.45
11:Y:56:GLU:OE2	11:Y:99:THR:HG21	2.16	0.45
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.47	0.45
3:C:201:VAL:O	3:C:202:GLN:CB	2.63	0.45
2:P:145:TYR:OH	2:P:217:LYS:N	2.49	0.45
8:H:84:LYS:HE2	8:H:119:THR:HG23	1.98	0.45
11:K:20:ALA:CB	11:K:31:VAL:HG21	2.47	0.45
11:K:168:ASP:OD2	11:K:171:SER:OG	2.33	0.45
11:Y:4:LEU:HD22	11:Y:140:LEU:CD2	2.46	0.45
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.82	0.45
8:H:35:HIS:CB	8:H:56:THR:HG21	2.46	0.45
10:X:159:ASP:O	10:X:162:LYS:HB2	2.16	0.45
11:Y:1:THR:O	11:Y:130:GLY:HA3	2.17	0.45
11:Y:20:ALA:CB	11:Y:31:VAL:HG21	2.47	0.45
5:E:77:ALA:N	5:E:78:PRO:CD	2.81	0.44
12:L:106:TYR:CD1	18:f:101:MYR:H81	2.52	0.44
2:P:50:LYS:O	2:P:51:VAL:C	2.60	0.44
3:Q:108:THR:HG21	3:Q:146:TYR:HB3	1.98	0.44
5:S:77:ALA:N	5:S:78:PRO:CD	2.81	0.44
13:M:2:GLN:NE2	19:M:301:HOH:O	2.50	0.44
15:e:3:ALA:C	15:e:4:DCL:HG	2.42	0.44
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.98	0.44
1:O:161:ALA:O	2:P:55:LEU:HD23	2.17	0.44
8:V:210:THR:HG21	9:W:167:SER:HB3	1.99	0.44
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.00	0.44
8:V:2:THR:OG1	8:V:169:SER:OG	2.31	0.44
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.99	0.44
2:B:50:LYS:O	2:B:51:VAL:C	2.60	0.44
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.82	0.44
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.00	0.43
10:J:177:LYS:NZ	10:X:169:GLU:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:50:ALA:HB2	12:L:128:VAL:HG23	2.01	0.43
11:K:100:MET:HE2	11:K:100:MET:HB2	1.76	0.43
9:W:36:SER:HB2	10:X:126:VAL:HG11	2.00	0.43
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.18	0.43
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	2.01	0.43
11:K:6:PHE:HA	11:K:125:ASP:O	2.18	0.43
11:K:20:ALA:HB2	11:K:31:VAL:HG21	2.01	0.43
11:Y:41:LEU:HD23	11:Y:41:LEU:HA	1.81	0.43
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.54	0.43
2:B:47:ALA:HB1	2:B:64:LYS:HD2	2.01	0.43
2:B:50:LYS:HD3	2:B:50:LYS:HA	1.78	0.43
11:Y:100:MET:HE2	11:Y:100:MET:HB2	1.76	0.43
14:b:14:LEU:N	14:b:14:LEU:HD12	2.34	0.43
1:A:64:VAL:HG11	1:A:212:ALA:HB3	2.01	0.42
10:J:50:ALA:O	11:K:91:LYS:NZ	2.52	0.42
13:M:187:ARG:NH1	8:V:139:GLU:OE1	2.42	0.42
12:Z:146:ILE:HG22	12:Z:150:LEU:HD22	2.02	0.42
2:P:47:ALA:HB1	2:P:64:LYS:HD2	2.01	0.42
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	2.01	0.42
10:J:169:GLU:O	10:X:177:LYS:NZ	2.51	0.42
10:X:139:TYR:CE1	10:X:171:ARG:HB2	2.55	0.42
10:X:168:LEU:O	10:X:172:MET:HB2	2.20	0.42
11:Y:104:TYR:CD1	11:Y:104:TYR:C	2.97	0.42
8:H:24:PRO:O	12:Z:196:ILE:HG12	2.20	0.42
14:b:45:ARG:HB3	14:b:52:THR:HB	2.00	0.42
1:A:104:TYR:HH	8:H:64:GLU:CD	2.26	0.42
11:K:179:HIS:CE1	11:K:181:THR:CG2	3.03	0.42
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	2.01	0.42
8:H:47:GLY:O	15:e:4:DCL:CD1	2.68	0.42
11:K:104:TYR:CD1	11:K:104:TYR:C	2.98	0.42
4:R:24:LYS:O	4:R:166:SER:HA	2.20	0.42
8:V:112:SER:HB3	8:V:125:LEU:HD13	2.00	0.42
11:Y:179:HIS:CE1	11:Y:181:THR:CG2	3.03	0.42
11:K:145:LYS:HB2	11:K:148:LEU:HD13	2.02	0.42
14:N:14:LEU:HD12	14:N:14:LEU:N	2.34	0.42
4:D:24:LYS:O	4:D:166:SER:HA	2.20	0.42
8:H:112:SER:HB3	8:H:125:LEU:HD13	2.00	0.42
5:S:71:LEU:C	5:S:71:LEU:CD2	2.93	0.42
2:B:217:LYS:C	2:B:219:ALA:N	2.78	0.42
5:E:71:LEU:C	5:E:71:LEU:CD2	2.93	0.42
12:L:146:ILE:HG22	12:L:150:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:64:VAL:HG11	1:O:212:ALA:HB3	2.02	0.42
10:J:168:LEU:O	10:J:172:MET:HB2	2.19	0.41
14:N:45:ARG:HB3	14:N:52:THR:HB	2.01	0.41
8:V:3:ILE:HG22	8:V:16:ALA:HB1	2.01	0.41
8:H:1:THR:O	8:H:128:GLY:HA3	2.20	0.41
8:H:34:LEU:N	8:H:34:LEU:HD12	2.35	0.41
11:K:140:LEU:HD12	11:K:140:LEU:HA	1.88	0.41
7:U:73:VAL:HG12	7:U:133:THR:HB	2.01	0.41
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.02	0.41
10:J:25:ILE:CD1	10:X:135:TYR:HB3	2.45	0.41
11:K:2:THR:HG21	11:K:164:ALA:CB	2.50	0.41
11:K:32:LYS:HE2	11:K:32:LYS:HB3	1.75	0.41
12:L:194:ARG:NH2	8:V:29:LYS:HE2	2.35	0.41
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.03	0.41
8:V:34:LEU:HD12	8:V:34:LEU:N	2.36	0.41
5:E:9:THR:HG21	5:E:119:THR:HA	2.01	0.41
5:E:68:HIS:HE1	5:E:102:LEU:O	2.04	0.41
9:I:141:ALA:HB2	9:I:177:ASP:HB2	2.03	0.41
5:S:9:THR:HG21	5:S:119:THR:HA	2.01	0.41
8:V:2:THR:N	8:V:17:ASP:OD1	2.45	0.41
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.02	0.41
12:L:5:TYR:CE2	18:f:101:MYR:H112	2.56	0.41
14:N:159:LEU:HD12	14:N:173:ILE:HG23	2.03	0.41
10:X:144:LEU:O	10:X:148:TYR:HB2	2.21	0.41
11:Y:3:THR:HG22	11:Y:16:VAL:HB	2.03	0.41
13:a:48:ASN:H	13:a:48:ASN:HD22	1.68	0.41
15:g:4:DCL:HD22	15:g:4:DCL:HA	1.75	0.41
1:A:226:GLY:HA3	8:H:186:TYR:O	2.21	0.41
7:G:73:VAL:HG12	7:G:133:THR:HB	2.01	0.41
8:H:137:VAL:HG21	8:H:161:ALA:HB2	2.03	0.41
9:I:94:LEU:HD11	9:I:106:PRO:HG2	2.02	0.41
9:W:94:LEU:HD11	9:W:106:PRO:HG2	2.02	0.41
10:X:1:MET:HB3	10:X:34:LYS:HE3	2.03	0.41
11:Y:12:ILE:HB	11:Y:180:VAL:HB	2.03	0.41
11:Y:16:VAL:HG23	11:Y:17:ASP:O	2.20	0.41
11:Y:45:MET:SD	11:Y:52:CYS:HB3	2.60	0.41
13:a:165:ILE:HB	13:a:166:PRO:HD3	2.03	0.41
14:b:159:LEU:HD12	14:b:173:ILE:HG23	2.03	0.41
11:K:16:VAL:HG23	11:K:17:ASP:O	2.20	0.41
11:K:42:LEU:HD23	11:K:42:LEU:HA	1.95	0.41
8:H:4:VAL:HG13	8:H:159:ILE:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:114:LEU:HD23	2:P:114:LEU:HA	1.94	0.40
9:W:7:ASN:HA	9:W:29:GLY:O	2.21	0.40
9:W:141:ALA:HB2	9:W:177:ASP:HB2	2.03	0.40
11:Y:86:LEU:HD13	11:Y:86:LEU:C	2.47	0.40
5:S:68:HIS:HE1	5:S:102:LEU:O	2.05	0.40
8:V:29:LYS:NZ	9:W:150:GLU:OE2	2.55	0.40
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.03	0.40
3:C:169:VAL:HG23	3:C:196:SER:HB2	2.02	0.40
5:E:80:ALA:HB2	5:E:129:VAL:HG21	2.02	0.40
7:G:43:VAL:HG11	7:G:194:VAL:HA	2.04	0.40
11:K:41:LEU:HD23	11:K:41:LEU:HA	1.82	0.40
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.04	0.40
15:h:2:GLN:HE21	15:h:2:GLN:HB3	1.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	30	59
1	O	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	30	59
2	B	242/258 (94%)	232 (96%)	6 (2%)	4 (2%)	7	29
2	P	242/258 (94%)	232 (96%)	6 (2%)	4 (2%)	7	29
3	C	238/254 (94%)	231 (97%)	4 (2%)	3 (1%)	9	34
3	Q	238/254 (94%)	231 (97%)	4 (2%)	3 (1%)	9	34
4	D	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
4	R	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
5	E	229/234 (98%)	219 (96%)	10 (4%)	0	100	100
5	S	229/234 (98%)	219 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	236 (99%)	3 (1%)	0	100	100
8	H	224/232 (97%)	219 (98%)	5 (2%)	0	100	100
8	V	224/232 (97%)	218 (97%)	6 (3%)	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%)	5 (3%)	0	100	100
10	X	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
11	K	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
11	Y	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
12	Z	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
13	M	228/246 (93%)	220 (96%)	8 (4%)	0	100	100
13	a	228/246 (93%)	220 (96%)	8 (4%)	0	100	100
14	N	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
14	b	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
15	e	1/3 (33%)	0	1 (100%)	0	100	100
15	f	1/3 (33%)	1 (100%)	0	0	100	100
15	g	1/3 (33%)	1 (100%)	0	0	100	100
15	h	1/3 (33%)	1 (100%)	0	0	100	100
All	All	6282/6626 (95%)	6103 (97%)	163 (3%)	16 (0%)	36	66

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
2	P	51	VAL
3	Q	202	GLN
1	A	2	THR
2	B	218	GLY
2	B	222	GLY

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Mol	Chain	Res	Type
1	O	2	THR
2	P	218	GLY
2	P	222	GLY
2	B	220	ASN
2	P	220	ASN
3	C	205	ALA
3	Q	205	ALA
3	C	183	PRO
3	Q	183	PRO

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%)	204 (98%)	5 (2%)	43	64
1	O	209/209 (100%)	204 (98%)	5 (2%)	43	64
2	B	203/216 (94%)	196 (97%)	7 (3%)	32	57
2	P	203/216 (94%)	196 (97%)	7 (3%)	32	57
3	C	212/226 (94%)	202 (95%)	10 (5%)	23	51
3	Q	212/226 (94%)	202 (95%)	10 (5%)	23	51
4	D	194/215 (90%)	185 (95%)	9 (5%)	24	51
4	R	194/215 (90%)	184 (95%)	10 (5%)	21	48
5	E	190/193 (98%)	184 (97%)	6 (3%)	34	58
5	S	190/193 (98%)	184 (97%)	6 (3%)	34	58
6	F	201/239 (84%)	195 (97%)	6 (3%)	36	59
6	T	201/239 (84%)	195 (97%)	6 (3%)	36	59
7	G	206/210 (98%)	199 (97%)	7 (3%)	32	57
7	U	206/210 (98%)	199 (97%)	7 (3%)	32	57
8	H	185/190 (97%)	175 (95%)	10 (5%)	20	47
8	V	185/190 (97%)	177 (96%)	8 (4%)	26	52
9	I	172/173 (99%)	168 (98%)	4 (2%)	44	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	W	172/173 (99%)	169 (98%)	3 (2%)	53	69
10	J	173/175 (99%)	167 (96%)	6 (4%)	32	56
10	X	173/175 (99%)	163 (94%)	10 (6%)	18	45
11	K	169/169 (100%)	159 (94%)	10 (6%)	18	45
11	Y	169/169 (100%)	158 (94%)	11 (6%)	15	42
12	L	185/185 (100%)	183 (99%)	2 (1%)	65	75
12	Z	185/185 (100%)	183 (99%)	2 (1%)	65	75
13	M	196/208 (94%)	191 (97%)	5 (3%)	40	62
13	a	196/208 (94%)	191 (97%)	5 (3%)	40	62
14	N	162/162 (100%)	157 (97%)	5 (3%)	35	59
14	b	162/162 (100%)	157 (97%)	5 (3%)	35	59
15	e	1/1 (100%)	1 (100%)	0	100	100
15	f	1/1 (100%)	0	1 (100%)	0	0
15	g	1/1 (100%)	1 (100%)	0	100	100
15	h	1/1 (100%)	0	1 (100%)	0	0
All	All	5318/5544 (96%)	5129 (96%)	189 (4%)	31	56

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	29	LYS
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	50	LYS
2	B	55	LEU
2	B	79	LEU
2	B	102	ASN
2	B	113	ARG
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	51	LYS
3	C	52	LEU
3	C	147	GLN

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Mol	Chain	Res	Type
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	213	VAL
3	C	240	GLU
4	D	51	LEU
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	188	LEU
5	E	231	LYS
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
6	F	221	ASN
6	F	240	GLN
7	G	26	THR
7	G	75	ASN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	235	ARG
7	G	236	LEU
8	H	2	THR
8	H	3	ILE
8	H	4	VAL
8	H	12	VAL
8	H	25	ILE
8	H	68	LEU
8	H	113	ILE
8	H	127	LEU
8	H	169	SER

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Mol	Chain	Res	Type
8	H	196	ARG
9	I	37	ASN
9	I	126	ILE
9	I	171	LEU
9	I	182	TRP
10	J	3	ILE
10	J	25	ILE
10	J	35	THR
10	J	90	LYS
10	J	99	GLN
10	J	147	HIS
11	K	4	LEU
11	K	7	ARG
11	K	9	GLN
11	K	35	ILE
11	K	97	MET
11	K	100	MET
11	K	140	LEU
11	K	148	LEU
11	K	209	ASN
11	K	211	ILE
12	L	23	LEU
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	187	ARG
14	N	9	LYS
14	N	104	ASP
14	N	107	LYS
14	N	119	VAL
14	N	159	LEU
1	O	1	MET
1	O	29	LYS
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	55	LEU
2	P	79	LEU
2	P	102	ASN

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Mol	Chain	Res	Type
2	P	113	ARG
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	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	213	VAL
3	Q	240	GLU
4	R	51	LEU
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
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
5	S	231	LYS
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	221	ASN
6	T	240	GLN
7	U	26	THR
7	U	75	ASN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	235	ARG
7	U	236	LEU

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Mol	Chain	Res	Type
8	V	4	VAL
8	V	12	VAL
8	V	25	ILE
8	V	68	LEU
8	V	113	ILE
8	V	127	LEU
8	V	169	SER
8	V	196	ARG
9	W	37	ASN
9	W	126	ILE
9	W	171	LEU
10	X	1	MET
10	X	3	ILE
10	X	21	VAL
10	X	25	ILE
10	X	27	VAL
10	X	35	THR
10	X	90	LYS
10	X	99	GLN
10	X	154	THR
10	X	160	LEU
11	Y	1	THR
11	Y	4	LEU
11	Y	7	ARG
11	Y	9	GLN
11	Y	35	ILE
11	Y	97	MET
11	Y	100	MET
11	Y	140	LEU
11	Y	148	LEU
11	Y	209	ASN
11	Y	211	ILE
12	Z	23	LEU
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	187	ARG
14	b	9	LYS
14	b	104	ASP
14	b	107	LYS

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Mol	Chain	Res	Type
14	b	119	VAL
14	b	159	LEU
15	f	2	GLN
15	h	2	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (159) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	124	HIS
2	B	176	GLN
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	123	ASN
6	F	191	GLN
6	F	203	ASN
6	F	240	GLN
7	G	30	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN

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Mol	Chain	Res	Type
7	G	167	GLN
7	G	175	ASN
8	H	9	ASN
8	H	30	ASN
8	H	189	ASN
8	H	200	GLN
9	I	63	ASN
9	I	88	GLN
9	I	168	GLN
9	I	203	GLN
10	J	37	GLN
10	J	55	GLN
10	J	63	ASN
10	J	78	GLN
11	K	9	GLN
11	K	85	ASN
11	K	133	GLN
11	K	143	ASN
11	K	176	ASN
11	K	179	HIS
12	L	3	ASN
12	L	29	ASN
12	L	36	ASN
12	L	49	ASN
12	L	70	ASN
12	L	80	ASN
12	L	135	GLN
12	L	152	ASN
12	L	153	GLN
12	L	158	ASN
12	L	159	GLN
12	L	197	GLN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	149	HIS
13	M	194	ASN
13	M	213	GLN
14	N	28	ASN
14	N	141	ASN
14	N	161	GLN

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Mol	Chain	Res	Type
1	O	119	GLN
1	O	123	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	124	HIS
2	P	176	GLN
2	P	220	ASN
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	225	ASN
5	S	68	HIS
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	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	175	ASN
8	V	9	ASN
8	V	30	ASN
8	V	57	GLN
8	V	165	ASN

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Mol	Chain	Res	Type
8	V	189	ASN
8	V	194	ASN
9	W	44	HIS
9	W	63	ASN
9	W	88	GLN
9	W	168	GLN
9	W	203	GLN
10	X	37	GLN
10	X	55	GLN
10	X	63	ASN
11	Y	9	GLN
11	Y	85	ASN
11	Y	133	GLN
11	Y	143	ASN
11	Y	176	ASN
11	Y	179	HIS
12	Z	3	ASN
12	Z	29	ASN
12	Z	36	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	79	HIS
12	Z	80	ASN
12	Z	135	GLN
12	Z	152	ASN
12	Z	153	GLN
12	Z	155	ASN
12	Z	158	ASN
12	Z	197	GLN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	194	ASN
13	a	213	GLN
14	b	28	ASN
14	b	141	ASN
14	b	161	GLN
15	f	2	GLN
15	g	2	GLN
15	h	2	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	DCL	h	4	15,11	7,7,7	0.40	0	6,8,8	1.11	1 (16%)
15	DCL	f	4	15	7,7,7	0.79	0	6,8,8	1.35	1 (16%)
15	DCL	g	4	8,15	7,7,7	0.24	0	6,8,8	0.84	0
15	DCL	e	4	8,15	7,7,7	0.85	1 (14%)	6,8,8	0.93	1 (16%)

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	DCL	h	4	15,11	-	2/6/6/6	-
15	DCL	f	4	15	-	1/6/6/6	-
15	DCL	g	4	8,15	-	3/6/6/6	-
15	DCL	e	4	8,15	-	5/6/6/6	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	e	4	DCL	C-CA	2.19	1.56	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	f	4	DCL	CG-CB-CA	-2.34	107.92	116.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	h	4	DCL	CG-CB-CA	-2.26	108.19	116.37
15	e	4	DCL	CG-CB-CA	-2.01	109.08	116.37

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	e	4	DCL	O-C-CA-N
15	e	4	DCL	O-C-CA-CB
15	e	4	DCL	N-CA-CB-CG
15	h	4	DCL	N-CA-CB-CG
15	g	4	DCL	O-C-CA-CB
15	g	4	DCL	O-C-CA-N
15	h	4	DCL	CA-CB-CG-CD2
15	g	4	DCL	CA-CB-CG-CD2
15	f	4	DCL	CA-CB-CG-CD2
15	e	4	DCL	C-CA-CB-CG
15	e	4	DCL	CA-CB-CG-CD1

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	h	4	DCL	3	0
15	f	4	DCL	1	0
15	g	4	DCL	1	0
15	e	4	DCL	9	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 11 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
18	MYR	h	101	15	13,14,15	0.35	0	12,13,15	0.82	0
18	MYR	f	101	15	13,14,15	0.40	0	12,13,15	0.75	0
18	MYR	g	101	15	13,14,15	0.35	0	12,13,15	0.84	0
18	MYR	e	101	15	13,14,15	0.32	0	12,13,15	0.84	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	MYR	h	101	15	-	5/12/12/13	-
18	MYR	f	101	15	-	3/12/12/13	-
18	MYR	g	101	15	-	6/12/12/13	-
18	MYR	e	101	15	-	3/12/12/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	g	101	MYR	C10-C11-C12-C13
18	g	101	MYR	C2-C3-C4-C5
18	e	101	MYR	C9-C10-C11-C12
18	g	101	MYR	C9-C10-C11-C12
18	g	101	MYR	C11-C10-C9-C8
18	g	101	MYR	C4-C5-C6-C7
18	e	101	MYR	C5-C6-C7-C8
18	h	101	MYR	C4-C5-C6-C7
18	f	101	MYR	C9-C10-C11-C12
18	h	101	MYR	C11-C10-C9-C8
18	g	101	MYR	C6-C7-C8-C9
18	h	101	MYR	C11-C12-C13-C14
18	e	101	MYR	C6-C7-C8-C9
18	f	101	MYR	C7-C8-C9-C10

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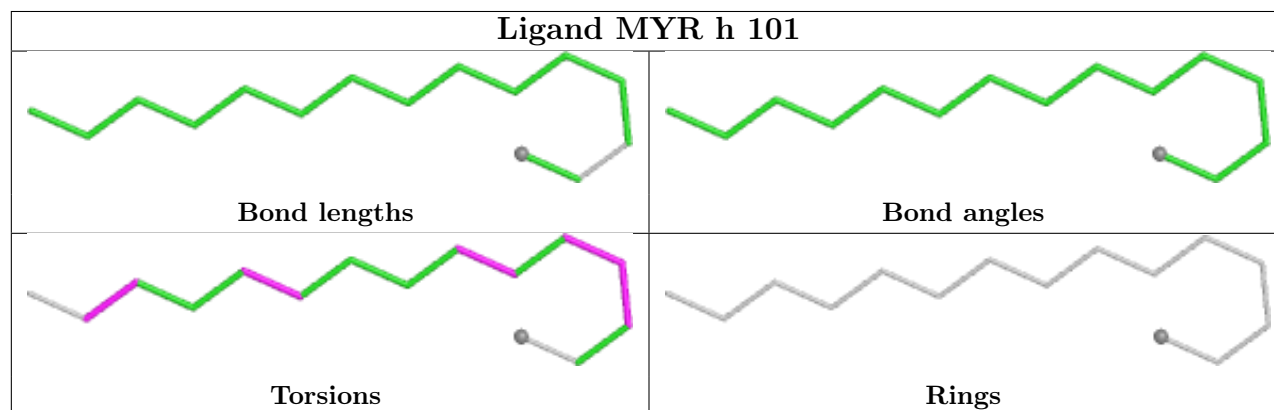
Mol	Chain	Res	Type	Atoms
18	f	101	MYR	C11-C10-C9-C8
18	h	101	MYR	C2-C3-C4-C5
18	h	101	MYR	C1-C2-C3-C4

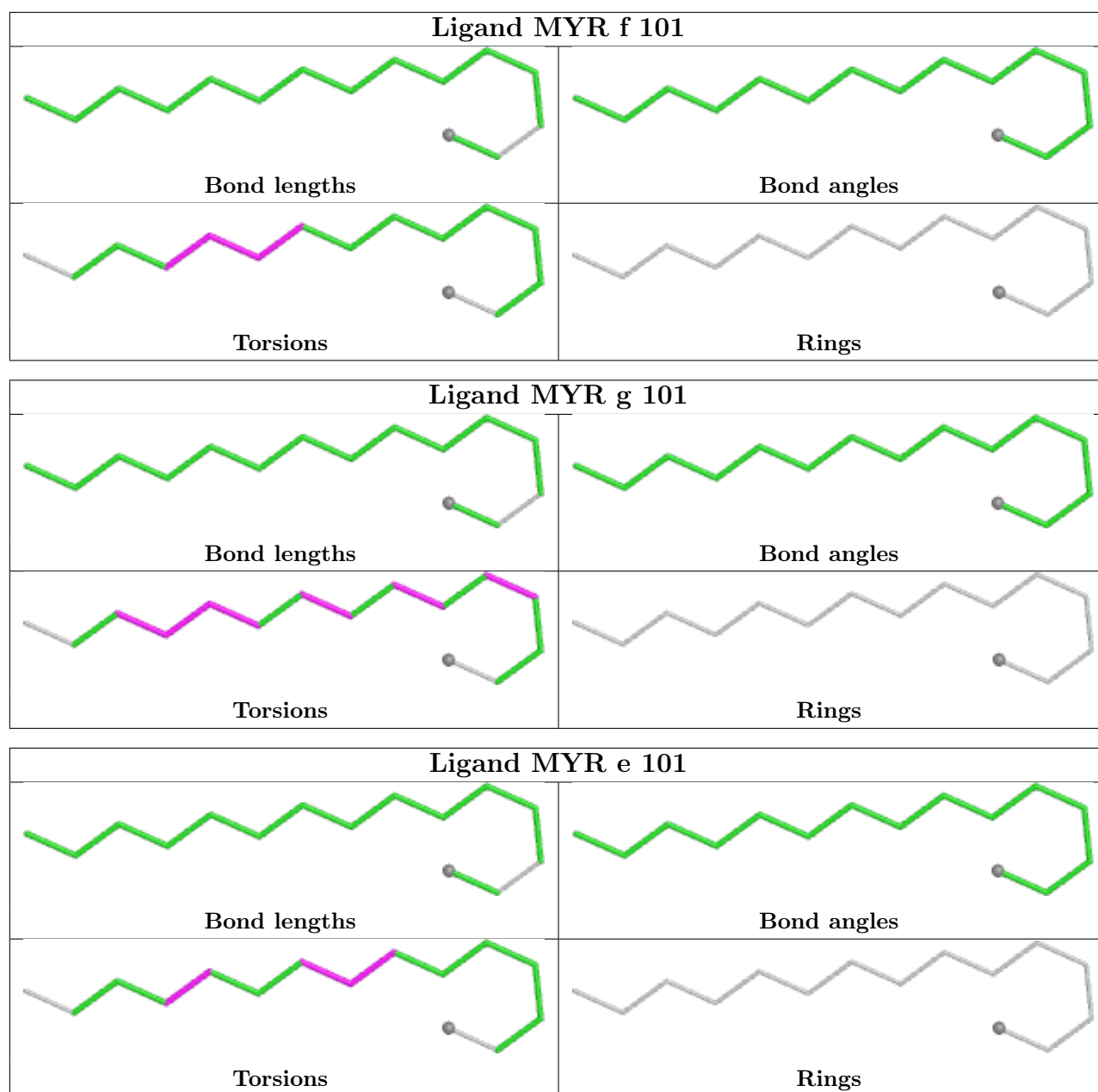
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	f	101	MYR	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	-0.52	0 100 100	71, 90, 129, 157	0
1	O	250/250 (100%)	-0.51	0 100 100	76, 99, 137, 168	0
2	B	244/258 (94%)	-0.39	0 100 100	73, 98, 153, 206	0
2	P	244/258 (94%)	-0.34	0 100 100	83, 103, 159, 188	0
3	C	240/254 (94%)	-0.45	1 (0%) 88 78	73, 103, 156, 174	0
3	Q	240/254 (94%)	-0.34	3 (1%) 75 56	85, 118, 184, 200	0
4	D	235/260 (90%)	-0.49	0 100 100	75, 101, 130, 161	0
4	R	235/260 (90%)	-0.41	0 100 100	80, 110, 145, 176	0
5	E	231/234 (98%)	-0.49	0 100 100	76, 104, 141, 163	0
5	S	231/234 (98%)	-0.43	0 100 100	76, 111, 151, 176	0
6	F	243/288 (84%)	-0.51	0 100 100	68, 95, 132, 166	0
6	T	243/288 (84%)	-0.54	0 100 100	73, 102, 145, 167	0
7	G	241/252 (95%)	-0.55	0 100 100	66, 92, 124, 159	0
7	U	241/252 (95%)	-0.48	0 100 100	72, 94, 125, 169	0
8	H	226/232 (97%)	-0.36	1 (0%) 88 78	70, 87, 121, 186	0
8	V	226/232 (97%)	-0.40	1 (0%) 88 78	73, 91, 125, 206	0
9	I	204/205 (99%)	-0.54	0 100 100	65, 85, 113, 141	0
9	W	204/205 (99%)	-0.57	0 100 100	69, 87, 116, 143	0
10	J	195/198 (98%)	-0.55	1 (0%) 87 76	67, 87, 113, 136	0
10	X	195/198 (98%)	-0.54	1 (0%) 87 76	69, 91, 116, 149	0
11	K	212/212 (100%)	-0.43	2 (0%) 81 65	70, 89, 123, 143	0
11	Y	212/212 (100%)	-0.51	1 (0%) 87 76	72, 92, 128, 146	0
12	L	222/222 (100%)	-0.50	0 100 100	68, 88, 130, 153	0
12	Z	222/222 (100%)	-0.49	0 100 100	68, 90, 126, 157	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	230/246 (93%)	-0.54	0 100 100	63, 86, 113, 119	0
13	a	230/246 (93%)	-0.57	1 (0%) 88 78	64, 84, 111, 119	0
14	N	196/196 (100%)	-0.64	0 100 100	66, 78, 112, 131	0
14	b	196/196 (100%)	-0.63	0 100 100	68, 80, 109, 127	0
15	e	2/3 (66%)	0.80	0 100 100	115, 115, 115, 116	0
15	f	2/3 (66%)	0.34	0 100 100	92, 92, 92, 92	0
15	g	2/3 (66%)	1.60	1 (50%) 0 0	119, 119, 119, 122	0
15	h	2/3 (66%)	0.11	0 100 100	97, 97, 97, 101	0
All	All	6346/6626 (95%)	-0.49	13 (0%) 91 85	63, 94, 141, 206	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	K	211	ILE	4.2
8	V	223	ILE	3.6
3	Q	50	LEU	3.1
15	g	3	ALA	3.0
11	Y	211	ILE	2.6
3	Q	49	THR	2.6
10	X	1	MET	2.5
3	C	50	LEU	2.4
3	Q	3	ASP	2.3
11	K	212	GLY	2.2
13	a	1	THR	2.1
10	J	1	MET	2.1
8	H	223	ILE	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	DCL	e	4	8/8	0.77	0.23	114,117,119,119	0
15	DCL	g	4	8/8	0.90	0.29	112,119,122,123	0
15	DCL	f	4	8/8	0.94	0.14	85,92,99,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	DCL	h	4	8/8	0.94	0.14	94,101,107,112	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

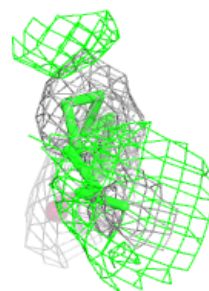
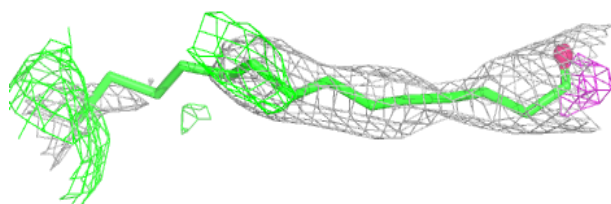
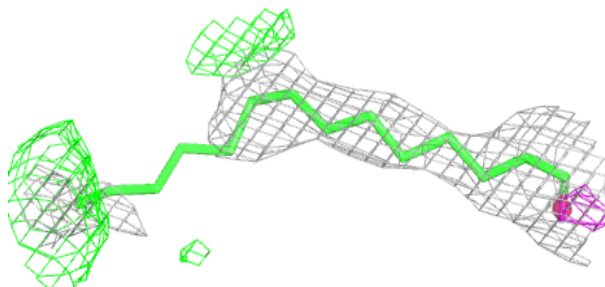
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
18	MYR	h	101	15/16	0.73	0.23	89,93,101,101	0
18	MYR	g	101	15/16	0.79	0.23	112,117,136,137	0
18	MYR	f	101	15/16	0.79	0.21	81,85,103,103	0
18	MYR	e	101	15/16	0.81	0.21	108,114,128,128	0
16	MG	G	301	1/1	0.93	0.07	77,77,77,77	0
16	MG	Z	301	1/1	0.96	0.09	83,83,83,83	0
17	CL	N	202	1/1	0.97	0.07	100,100,100,100	0
16	MG	J	201	1/1	0.98	0.03	44,44,44,44	0
17	CL	U	301	1/1	0.98	0.10	70,70,70,70	0
16	MG	K	301	1/1	0.98	0.08	95,95,95,95	0
16	MG	N	201	1/1	0.98	0.05	78,78,78,78	0
16	MG	I	301	1/1	0.98	0.04	89,89,89,89	0
17	CL	G	302	1/1	0.98	0.06	61,61,61,61	0
16	MG	V	301	1/1	0.99	0.11	111,111,111,111	0
16	MG	Y	301	1/1	0.99	0.05	82,82,82,82	0

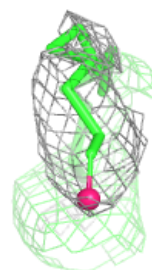
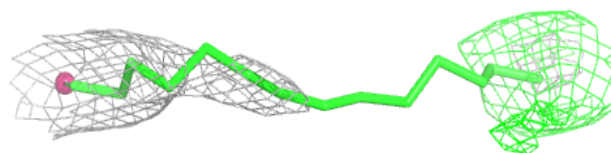
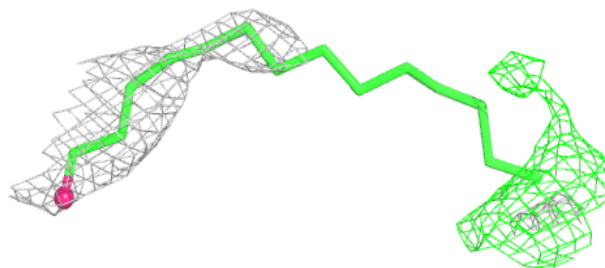
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around MYR h 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

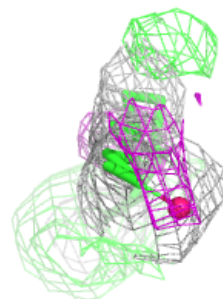
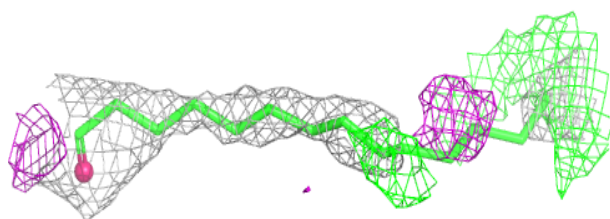
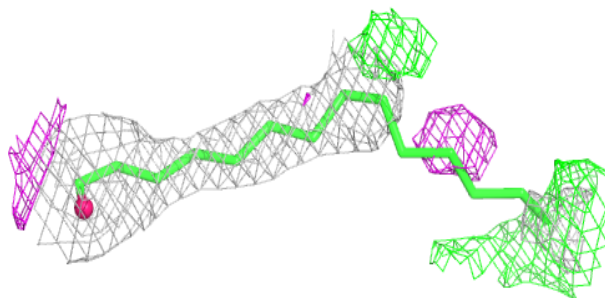
**Electron density around MYR g 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

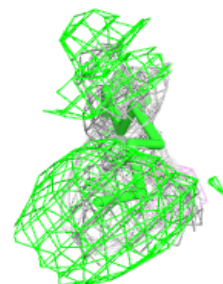
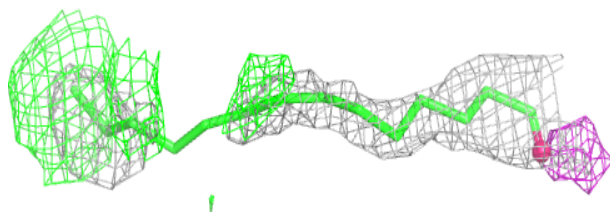
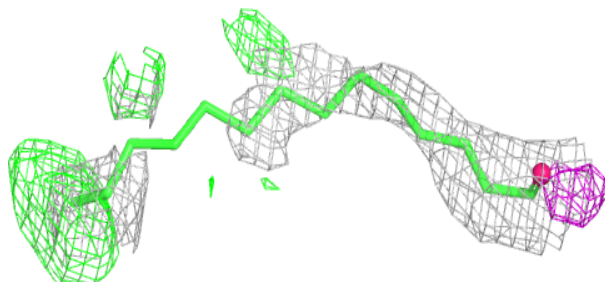


Electron density around MYR f 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around MYR e 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.