Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 02:34 AM JST

PDB ID	:	7EG3
Title	:	Crystal structure of the apoAequorin complex with (S)-HM-daCTZ
Authors	:	Tomabechi, Y.; Shirouzu, M.
Deposited on	:	2021-03-24
Resolution	:	2.09 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:

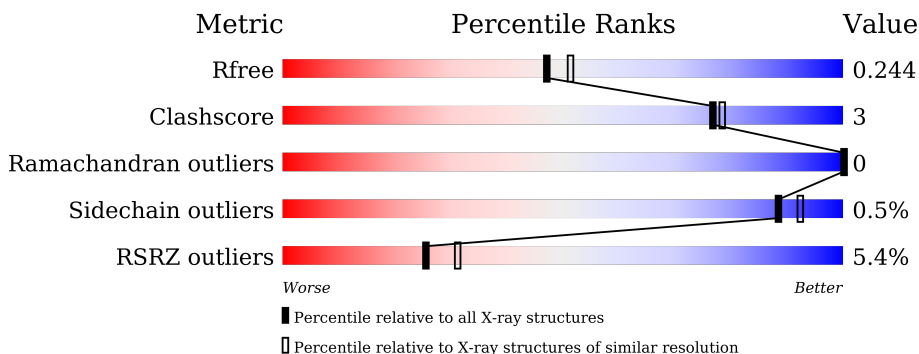|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.09 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	Percentile Ranks	Value
Rfree		0.244
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		0.5%
RSRZ outliers		5.4%

Worse　　　　　　　　　　　　　　　　　　　*Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	198	.% 89% 6% 5%
1	B	198	3% 86% 10% 5%
1	C	198	15% 85% 11% •
1	D	198	8% 88% 7% • •
1	E	198	17% 82% 16% • •
1	F	198	3% 88% 8% •

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Mol	Chain	Length	Quality of chain
1	G	198	5% 85% 11% •
1	H	198	5% 86% 10% •
1	I	198	4% 90% 6% •
1	J	198	5% 94% • •
1	K	198	% 89% 6% 5%
1	L	198	89% 6% • 5%
1	M	198	6% 88% 8% •
1	N	198	5% 90% 6% • •
1	O	198	4% 89% 8% •
1	P	198	4% 91% 6% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 26281 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 Aequorin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	0	0	0
			1509	956	251	294	8			
1	B	189	Total	C	N	O	S	0	0	0
			1509	956	251	294	8			
1	C	190	Total	C	N	O	S	0	0	0
			1519	962	254	295	8			
1	D	190	Total	C	N	O	S	0	0	0
			1519	962	254	295	8			
1	E	194	Total	C	N	O	S	0	0	0
			1559	986	266	299	8			
1	F	191	Total	C	N	O	S	0	0	0
			1529	968	257	296	8			
1	G	190	Total	C	N	O	S	0	0	0
			1519	962	254	295	8			
1	H	190	Total	C	N	O	S	0	0	0
			1519	962	254	295	8			
1	I	190	Total	C	N	O	S	0	0	0
			1519	962	254	295	8			
1	J	193	Total	C	N	O	S	0	0	0
			1549	980	263	298	8			
1	K	188	Total	C	N	O	S	0	0	0
			1505	954	250	293	8			
1	L	188	Total	C	N	O	S	0	0	0
			1505	954	250	293	8			
1	M	190	Total	C	N	O	S	0	0	0
			1519	962	254	295	8			
1	N	190	Total	C	N	O	S	0	0	0
			1519	962	254	295	8			
1	O	192	Total	C	N	O	S	0	0	0
			1539	974	260	297	8			
1	P	192	Total	C	N	O	S	0	0	0
			1539	974	260	297	8			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ALA	-	expression tag	UNP P02592
A	-7	ASN	-	expression tag	UNP P02592
A	-6	SER	-	expression tag	UNP P02592
A	-5	HIS	-	expression tag	UNP P02592
A	-4	HIS	-	expression tag	UNP P02592
A	-3	HIS	-	expression tag	UNP P02592
A	-2	HIS	-	expression tag	UNP P02592
A	-1	HIS	-	expression tag	UNP P02592
A	0	HIS	-	expression tag	UNP P02592
A	1	GLY	-	expression tag	UNP P02592
B	-8	ALA	-	expression tag	UNP P02592
B	-7	ASN	-	expression tag	UNP P02592
B	-6	SER	-	expression tag	UNP P02592
B	-5	HIS	-	expression tag	UNP P02592
B	-4	HIS	-	expression tag	UNP P02592
B	-3	HIS	-	expression tag	UNP P02592
B	-2	HIS	-	expression tag	UNP P02592
B	-1	HIS	-	expression tag	UNP P02592
B	0	HIS	-	expression tag	UNP P02592
B	1	GLY	-	expression tag	UNP P02592
C	-8	ALA	-	expression tag	UNP P02592
C	-7	ASN	-	expression tag	UNP P02592
C	-6	SER	-	expression tag	UNP P02592
C	-5	HIS	-	expression tag	UNP P02592
C	-4	HIS	-	expression tag	UNP P02592
C	-3	HIS	-	expression tag	UNP P02592
C	-2	HIS	-	expression tag	UNP P02592
C	-1	HIS	-	expression tag	UNP P02592
C	0	HIS	-	expression tag	UNP P02592
C	1	GLY	-	expression tag	UNP P02592
D	-8	ALA	-	expression tag	UNP P02592
D	-7	ASN	-	expression tag	UNP P02592
D	-6	SER	-	expression tag	UNP P02592
D	-5	HIS	-	expression tag	UNP P02592
D	-4	HIS	-	expression tag	UNP P02592
D	-3	HIS	-	expression tag	UNP P02592
D	-2	HIS	-	expression tag	UNP P02592
D	-1	HIS	-	expression tag	UNP P02592
D	0	HIS	-	expression tag	UNP P02592
D	1	GLY	-	expression tag	UNP P02592
E	-8	ALA	-	expression tag	UNP P02592
E	-7	ASN	-	expression tag	UNP P02592

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-6	SER	-	expression tag	UNP P02592
E	-5	HIS	-	expression tag	UNP P02592
E	-4	HIS	-	expression tag	UNP P02592
E	-3	HIS	-	expression tag	UNP P02592
E	-2	HIS	-	expression tag	UNP P02592
E	-1	HIS	-	expression tag	UNP P02592
E	0	HIS	-	expression tag	UNP P02592
E	1	GLY	-	expression tag	UNP P02592
F	-8	ALA	-	expression tag	UNP P02592
F	-7	ASN	-	expression tag	UNP P02592
F	-6	SER	-	expression tag	UNP P02592
F	-5	HIS	-	expression tag	UNP P02592
F	-4	HIS	-	expression tag	UNP P02592
F	-3	HIS	-	expression tag	UNP P02592
F	-2	HIS	-	expression tag	UNP P02592
F	-1	HIS	-	expression tag	UNP P02592
F	0	HIS	-	expression tag	UNP P02592
F	1	GLY	-	expression tag	UNP P02592
G	-8	ALA	-	expression tag	UNP P02592
G	-7	ASN	-	expression tag	UNP P02592
G	-6	SER	-	expression tag	UNP P02592
G	-5	HIS	-	expression tag	UNP P02592
G	-4	HIS	-	expression tag	UNP P02592
G	-3	HIS	-	expression tag	UNP P02592
G	-2	HIS	-	expression tag	UNP P02592
G	-1	HIS	-	expression tag	UNP P02592
G	0	HIS	-	expression tag	UNP P02592
G	1	GLY	-	expression tag	UNP P02592
H	-8	ALA	-	expression tag	UNP P02592
H	-7	ASN	-	expression tag	UNP P02592
H	-6	SER	-	expression tag	UNP P02592
H	-5	HIS	-	expression tag	UNP P02592
H	-4	HIS	-	expression tag	UNP P02592
H	-3	HIS	-	expression tag	UNP P02592
H	-2	HIS	-	expression tag	UNP P02592
H	-1	HIS	-	expression tag	UNP P02592
H	0	HIS	-	expression tag	UNP P02592
H	1	GLY	-	expression tag	UNP P02592
I	-8	ALA	-	expression tag	UNP P02592
I	-7	ASN	-	expression tag	UNP P02592
I	-6	SER	-	expression tag	UNP P02592
I	-5	HIS	-	expression tag	UNP P02592

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-4	HIS	-	expression tag	UNP P02592
I	-3	HIS	-	expression tag	UNP P02592
I	-2	HIS	-	expression tag	UNP P02592
I	-1	HIS	-	expression tag	UNP P02592
I	0	HIS	-	expression tag	UNP P02592
I	1	GLY	-	expression tag	UNP P02592
J	-8	ALA	-	expression tag	UNP P02592
J	-7	ASN	-	expression tag	UNP P02592
J	-6	SER	-	expression tag	UNP P02592
J	-5	HIS	-	expression tag	UNP P02592
J	-4	HIS	-	expression tag	UNP P02592
J	-3	HIS	-	expression tag	UNP P02592
J	-2	HIS	-	expression tag	UNP P02592
J	-1	HIS	-	expression tag	UNP P02592
J	0	HIS	-	expression tag	UNP P02592
J	1	GLY	-	expression tag	UNP P02592
K	-8	ALA	-	expression tag	UNP P02592
K	-7	ASN	-	expression tag	UNP P02592
K	-6	SER	-	expression tag	UNP P02592
K	-5	HIS	-	expression tag	UNP P02592
K	-4	HIS	-	expression tag	UNP P02592
K	-3	HIS	-	expression tag	UNP P02592
K	-2	HIS	-	expression tag	UNP P02592
K	-1	HIS	-	expression tag	UNP P02592
K	0	HIS	-	expression tag	UNP P02592
K	1	GLY	-	expression tag	UNP P02592
L	-8	ALA	-	expression tag	UNP P02592
L	-7	ASN	-	expression tag	UNP P02592
L	-6	SER	-	expression tag	UNP P02592
L	-5	HIS	-	expression tag	UNP P02592
L	-4	HIS	-	expression tag	UNP P02592
L	-3	HIS	-	expression tag	UNP P02592
L	-2	HIS	-	expression tag	UNP P02592
L	-1	HIS	-	expression tag	UNP P02592
L	0	HIS	-	expression tag	UNP P02592
L	1	GLY	-	expression tag	UNP P02592
M	-8	ALA	-	expression tag	UNP P02592
M	-7	ASN	-	expression tag	UNP P02592
M	-6	SER	-	expression tag	UNP P02592
M	-5	HIS	-	expression tag	UNP P02592
M	-4	HIS	-	expression tag	UNP P02592
M	-3	HIS	-	expression tag	UNP P02592

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	HIS	-	expression tag	UNP P02592
M	-1	HIS	-	expression tag	UNP P02592
M	0	HIS	-	expression tag	UNP P02592
M	1	GLY	-	expression tag	UNP P02592
N	-8	ALA	-	expression tag	UNP P02592
N	-7	ASN	-	expression tag	UNP P02592
N	-6	SER	-	expression tag	UNP P02592
N	-5	HIS	-	expression tag	UNP P02592
N	-4	HIS	-	expression tag	UNP P02592
N	-3	HIS	-	expression tag	UNP P02592
N	-2	HIS	-	expression tag	UNP P02592
N	-1	HIS	-	expression tag	UNP P02592
N	0	HIS	-	expression tag	UNP P02592
N	1	GLY	-	expression tag	UNP P02592
O	-8	ALA	-	expression tag	UNP P02592
O	-7	ASN	-	expression tag	UNP P02592
O	-6	SER	-	expression tag	UNP P02592
O	-5	HIS	-	expression tag	UNP P02592
O	-4	HIS	-	expression tag	UNP P02592
O	-3	HIS	-	expression tag	UNP P02592
O	-2	HIS	-	expression tag	UNP P02592
O	-1	HIS	-	expression tag	UNP P02592
O	0	HIS	-	expression tag	UNP P02592
O	1	GLY	-	expression tag	UNP P02592
P	-8	ALA	-	expression tag	UNP P02592
P	-7	ASN	-	expression tag	UNP P02592
P	-6	SER	-	expression tag	UNP P02592
P	-5	HIS	-	expression tag	UNP P02592
P	-4	HIS	-	expression tag	UNP P02592
P	-3	HIS	-	expression tag	UNP P02592
P	-2	HIS	-	expression tag	UNP P02592
P	-1	HIS	-	expression tag	UNP P02592
P	0	HIS	-	expression tag	UNP P02592
P	1	GLY	-	expression tag	UNP P02592

- Molecule 2 is (2 {S})-6-(4-hydroxyphenyl)-2-[(4-hydroxyphenyl)methyl]-4-(phenylmethyl)-2 ,3-dihydroinden-1-one (three-letter code: J2U) (formula: $C_{29}H_{24}O_3$) (labeled as "Ligand of Interest" by depositor).
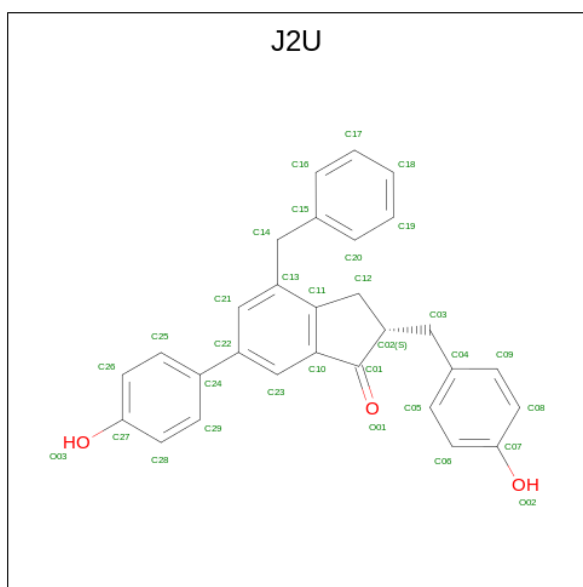
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 32	C 29	O 3	0	0
2	B	1	Total 32	C 29	O 3	0	0
2	C	1	Total 32	C 29	O 3	0	0
2	D	1	Total 32	C 29	O 3	0	0
2	E	1	Total 32	C 29	O 3	0	0
2	F	1	Total 32	C 29	O 3	0	0
2	G	1	Total 32	C 29	O 3	0	0
2	H	1	Total 32	C 29	O 3	0	0
2	I	1	Total 32	C 29	O 3	0	0
2	J	1	Total 32	C 29	O 3	0	0
2	K	1	Total 32	C 29	O 3	0	0
2	L	1	Total 32	C 29	O 3	0	0
2	M	1	Total 32	C 29	O 3	0	0
2	N	1	Total 32	C 29	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	O	1	Total 32	C 29	O 3	0	0
2	P	1	Total 32	C 29	O 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	115	Total 115	O 115	0	0
3	B	60	Total 60	O 60	0	0
3	C	56	Total 56	O 56	0	0
3	D	77	Total 77	O 77	0	0
3	E	50	Total 50	O 50	0	0
3	F	86	Total 86	O 86	0	0
3	G	74	Total 74	O 74	0	0
3	H	75	Total 75	O 75	0	0
3	I	110	Total 110	O 110	0	0
3	J	136	Total 136	O 136	0	0
3	K	80	Total 80	O 80	0	0
3	L	110	Total 110	O 110	0	0
3	M	64	Total 64	O 64	0	0
3	N	73	Total 73	O 73	0	0
3	O	103	Total 103	O 103	0	0
3	P	124	Total 124	O 124	0	0

3 Residue-property plots ⓘ

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.
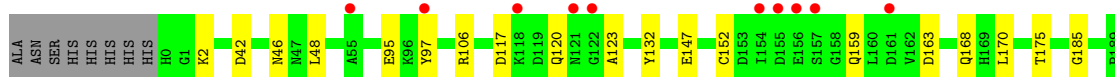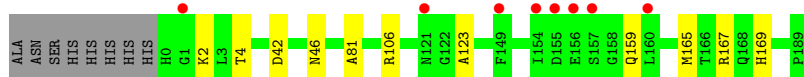
• Molecule 1: Aequorin-2

Chain A:

• Molecule 1: Aequorin-2

Chain B:
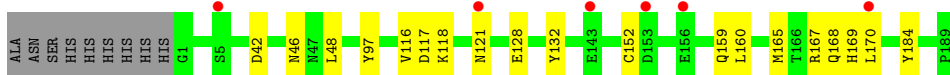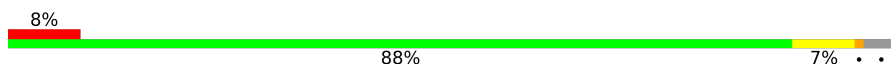
• Molecule 1: Aequorin-2

Chain C:
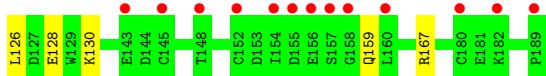
• Molecule 1: Aequorin-2

Chain D:
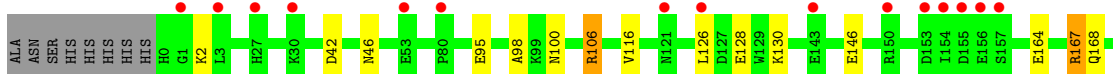
• Molecule 1: Aequorin-2

Chain E:
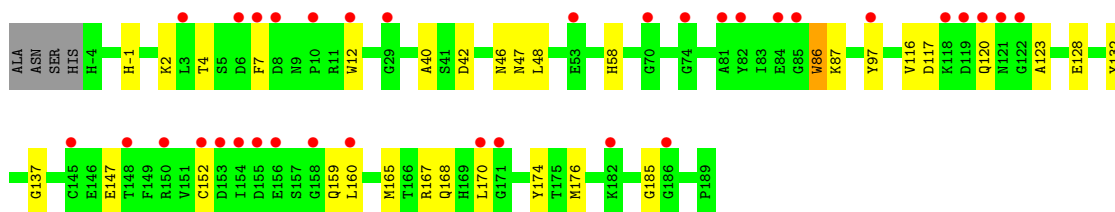
Chain E: 17% / 82% / 16%

- Molecule 1: Aequorin-2

Chain F:
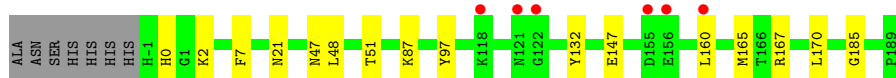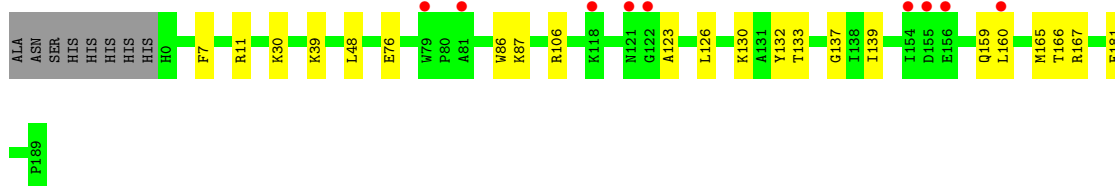
Chain F: 3% / 88% / 8%

- Molecule 1: Aequorin-2

Chain G:

Chain G: 5% / 85% / 11%

- Molecule 1: Aequorin-2

Chain H:

Chain H: 5% / 86% / 10%

- Molecule 1: Aequorin-2

Chain I:

Chain I: 4% / 90% / 6%

- Molecule 1: Aequorin-2

Chain J:

Chain J: 5% / 94%

- Molecule 1: Aequorin-2

Chain K:

• Molecule 1: Aequorin-2

Chain L:
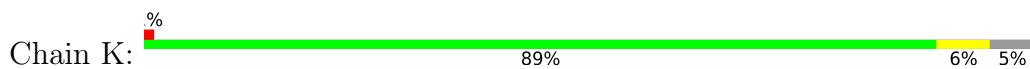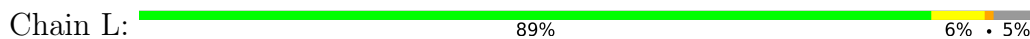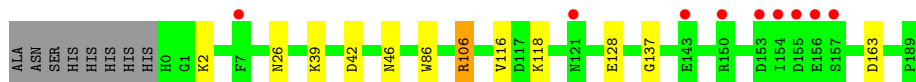

• Molecule 1: Aequorin-2
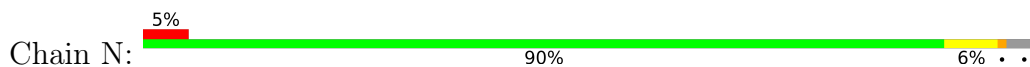
Chain M:

• Molecule 1: Aequorin-2

Chain N:

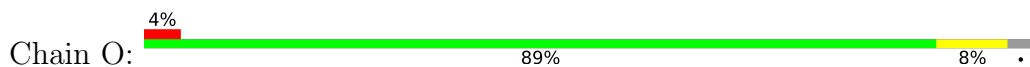• Molecule 1: Aequorin-2

Chain O:

• Molecule 1: Aequorin-2

Chain P:
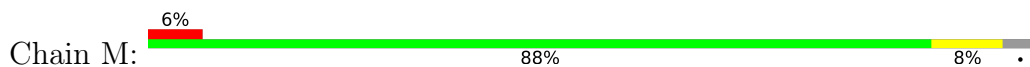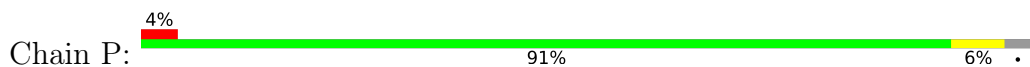
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	90.80Å 98.02Å 121.42Å 77.63° 73.23° 75.22°	Depositor
Resolution (Å)	45.88 – 2.09 46.84 – 2.09	Depositor EDS
% Data completeness (in resolution range)	97.3 (45.88-2.09) 97.4 (46.84-2.09)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.18.2	Depositor
R, R_{free}	0.218 , 0.245 0.218 , 0.244	Depositor DCC
R_{free} test set	2000 reflections (0.91%)	wwPDB-VP
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 42.2	EDS
L-test for twinning[2]	$< |L| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	26281	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.24 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.2713e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

---

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: J2U

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.25	0/1546	0.41	0/2090
1	B	0.24	0/1546	0.38	0/2090
1	C	0.24	0/1557	0.38	0/2105
1	D	0.24	0/1557	0.39	0/2105
1	E	0.24	0/1601	0.38	0/2165
1	F	0.25	0/1568	0.40	0/2120
1	G	0.24	0/1557	0.39	0/2105
1	H	0.24	0/1557	0.38	0/2105
1	I	0.25	0/1557	0.39	0/2105
1	J	0.24	0/1590	0.39	0/2150
1	K	0.24	0/1542	0.38	0/2085
1	L	0.25	0/1542	0.41	0/2085
1	M	0.24	0/1557	0.38	0/2105
1	N	0.24	0/1557	0.38	0/2105
1	O	0.25	0/1579	0.39	0/2135
1	P	0.25	0/1579	0.40	0/2135
All	All	0.24	0/24992	0.39	0/33790

There are no bond length outliers.

There are no bond angle outliers.

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	1509	0	1434	7	0
1	B	1509	0	1434	12	0
1	C	1519	0	1441	15	0
1	D	1519	0	1441	12	0
1	E	1559	0	1469	19	0
1	F	1529	0	1448	10	0
1	G	1519	0	1441	14	0
1	H	1519	0	1441	12	0
1	I	1519	0	1441	6	0
1	J	1549	0	1462	5	0
1	K	1505	0	1428	6	0
1	L	1505	0	1428	9	0
1	M	1519	0	1441	10	0
1	N	1519	0	1441	8	0
1	O	1539	0	1455	10	0
1	P	1539	0	1455	11	0
2	A	32	0	0	0	0
2	B	32	0	0	0	0
2	C	32	0	0	0	0
2	D	32	0	0	0	0
2	E	32	0	0	0	0
2	F	32	0	0	0	0
2	G	32	0	0	0	0
2	H	32	0	0	0	0
2	I	32	0	0	0	0
2	J	32	0	0	0	0
2	K	32	0	0	0	0
2	L	32	0	0	0	0
2	M	32	0	0	0	0
2	N	32	0	0	0	0
2	O	32	0	0	0	0
2	P	32	0	0	0	0
3	A	115	0	0	0	0
3	B	60	0	0	1	0
3	C	56	0	0	1	0
3	D	77	0	0	2	0
3	E	50	0	0	3	0
3	F	86	0	0	5	0
3	G	74	0	0	1	0
3	H	75	0	0	1	0
3	I	110	0	0	1	0
3	J	136	0	0	1	0
3	K	80	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	110	0	0	2	0
3	M	64	0	0	2	0
3	N	73	0	0	2	0
3	O	103	0	0	1	0
3	P	124	0	0	0	0
All	All	26281	0	23100	145	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 (145) 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)
1:C:2:LYS:HE2	1:C:4:THR:HB	1.64	0.80
1:G:106:ARG:NH2	3:G:301:HOH:O	2.20	0.75
1:F:2:LYS:NZ	3:F:303:HOH:O	2.24	0.70
1:F:51:THR:OG1	3:F:301:HOH:O	2.11	0.69
1:F:21:ASN:ND2	3:F:304:HOH:O	2.25	0.69
1:M:78:ASP:OD2	1:N:118:LYS:NZ	2.26	0.68
1:B:167:ARG:NH2	1:H:95:GLU:OE1	2.31	0.63
1:D:95:GLU:OE2	1:P:167:ARG:NH2	2.32	0.63
1:G:11:ARG:NH2	1:G:181:GLU:OE1	2.34	0.61
1:H:106:ARG:NH2	3:H:307:HOH:O	2.34	0.61
1:D:167:ARG:NH1	1:P:95:GLU:OE1	2.34	0.61
1:E:7:PHE:HB3	1:E:87:LYS:HE2	1.84	0.60
1:I:106:ARG:NH2	3:I:306:HOH:O	2.34	0.60
1:L:157:SER:N	1:L:158:GLY:HA2	2.15	0.60
1:A:157:SER:N	1:A:158:GLY:HA2	2.15	0.60
1:M:106:ARG:NH2	3:M:304:HOH:O	2.34	0.60
1:L:155:ASP:OD1	1:L:157:SER:OG	2.19	0.60
1:D:106:ARG:NH2	3:D:304:HOH:O	2.35	0.59
1:I:81:ALA:HB2	1:P:11:ARG:HD3	1.85	0.59
1:C:42:ASP:OD1	1:C:46:ASN:ND2	2.27	0.59
1:H:106:ARG:NH2	1:H:163:ASP:OD1	2.23	0.59
1:A:42:ASP:OD1	1:A:46:ASN:ND2	2.26	0.58
1:N:42:ASP:OD1	1:N:46:ASN:ND2	2.31	0.57
1:B:42:ASP:OD1	1:B:46:ASN:ND2	2.27	0.56
1:E:-1:HIS:HA	1:K:4:THR:HG22	1.86	0.55
1:B:159:GLN:NE2	3:B:304:HOH:O	2.40	0.54
1:B:48:LEU:HD11	1:B:132:TYR:HD1	1.71	0.54
1:M:116:VAL:HG12	1:M:128:GLU:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:130:LYS:NZ	3:L:302:HOH:O	2.33	0.53
1:D:42:ASP:OD2	1:D:46:ASN:ND2	2.31	0.53
1:E:48:LEU:HD11	1:E:132:TYR:HD1	1.74	0.53
1:C:91:THR:HG23	1:O:0:HIS:HE1	1.73	0.53
1:G:39:LYS:NZ	1:M:42:ASP:OD2	2.42	0.52
1:H:42:ASP:OD2	1:N:39:LYS:NZ	2.41	0.52
1:I:42:ASP:OD2	1:I:46:ASN:ND2	2.28	0.52
1:C:2:LYS:HG2	1:C:4:THR:H	1.75	0.52
1:L:106:ARG:NH2	3:L:313:HOH:O	2.43	0.52
1:A:95:GLU:OE1	1:G:167:ARG:NH2	2.43	0.52
1:F:47:ASN:ND2	3:F:308:HOH:O	2.31	0.52
1:K:97:TYR:CZ	1:K:170:LEU:HB2	2.45	0.51
1:E:2:LYS:NZ	1:E:4:THR:O	2.43	0.51
1:K:7:PHE:HB3	1:K:87:LYS:HE2	1.93	0.50
1:A:97:TYR:CZ	1:A:170:LEU:HB2	2.47	0.49
1:I:123:ALA:HB1	1:I:159:GLN:HB3	1.94	0.49
1:E:116:VAL:HG12	1:E:128:GLU:HB3	1.94	0.49
1:E:42:ASP:OD1	1:E:46:ASN:ND2	2.39	0.49
1:E:47:ASN:ND2	3:E:314:HOH:O	2.44	0.49
1:J:11:ARG:HD3	1:P:81:ALA:HB2	1.95	0.48
1:H:147:GLU:HG2	1:H:185:GLY:HA2	1.95	0.48
1:C:95:GLU:OE1	1:O:167:ARG:NH2	2.47	0.48
1:G:123:ALA:HB1	1:G:159:GLN:HB3	1.96	0.48
1:E:97:TYR:CZ	1:E:170:LEU:HD13	2.49	0.48
1:F:48:LEU:HD11	1:F:132:TYR:HD1	1.77	0.48
1:G:137:GLY:HA3	1:M:46:ASN:HB3	1.96	0.47
1:H:48:LEU:HD11	1:H:132:TYR:HD1	1.78	0.47
1:G:160:LEU:HD11	1:G:165:MET:HG2	1.97	0.47
1:N:2:LYS:HB3	3:N:323:HOH:O	2.14	0.47
1:F:160:LEU:HD21	1:F:165:MET:HE3	1.96	0.47
1:N:26:ASN:ND2	3:N:306:HOH:O	2.45	0.47
1:J:106:ARG:NH2	3:J:313:HOH:O	2.48	0.46
1:C:123:ALA:HB1	1:C:159:GLN:HB3	1.98	0.46
1:B:116:VAL:HG12	1:B:128:GLU:HB3	1.98	0.46
1:K:106:ARG:NH1	3:K:305:HOH:O	2.34	0.46
1:D:100:ASN:O	1:P:106:ARG:NE	2.49	0.46
1:H:152:CYS:SG	1:H:168:GLN:HG3	2.56	0.45
1:B:160:LEU:HD21	1:B:165:MET:SD	2.56	0.45
1:E:12:TRP:HB2	1:E:176:MET:HG3	1.97	0.45
1:E:170:LEU:HD23	1:E:174:TYR:CD2	2.51	0.45
1:B:117:ASP:OD2	1:B:121:ASN:N	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:152:CYS:SG	1:K:168:GLN:HG3	2.57	0.45
1:D:167:ARG:HG3	1:D:168:GLN:N	2.30	0.45
1:C:116:VAL:HG12	1:C:128:GLU:HB3	1.98	0.45
1:E:160:LEU:HD21	1:E:165:MET:SD	2.57	0.45
1:P:123:ALA:HB1	1:P:159:GLN:HB3	1.98	0.45
1:A:100:ASN:HB3	1:G:166:THR:HG21	1.99	0.45
1:L:44:VAL:HB	1:L:115:ILE:HD13	1.98	0.45
1:M:161:ASP:OD1	1:M:162:VAL:N	2.50	0.45
1:C:7:PHE:HB3	1:C:87:LYS:HE2	1.98	0.45
1:P:17:LYS:HD3	1:P:79:TRP:CE2	2.52	0.45
1:A:106:ARG:NH2	1:A:163:ASP:OD1	2.36	0.44
1:F:7:PHE:HB3	1:F:87:LYS:HE2	1.98	0.44
1:G:7:PHE:HB3	1:G:87:LYS:HE2	2.00	0.44
1:D:116:VAL:HG12	1:D:128:GLU:HB3	1.99	0.44
1:E:147:GLU:HG2	1:E:185:GLY:HA2	1.99	0.44
1:L:157:SER:H	1:L:157:SER:HG	1.48	0.44
1:H:123:ALA:HB1	1:H:159:GLN:HB3	1.99	0.44
1:B:118:LYS:HG2	1:B:128:GLU:OE2	2.17	0.44
1:N:116:VAL:HG12	1:N:128:GLU:HB3	2.00	0.44
1:O:2:LYS:NZ	1:O:4:THR:O	2.47	0.44
1:C:126:LEU:HG	1:C:130:LYS:HE3	1.99	0.44
1:C:167:ARG:NH2	1:O:95:GLU:OE1	2.51	0.43
1:E:152:CYS:SG	1:E:168:GLN:HG3	2.58	0.43
1:B:169:HIS:HE2	1:B:184:TYR:HH	1.65	0.43
1:D:98:ALA:HB1	1:P:167:ARG:HG3	2.00	0.43
1:O:116:VAL:HG12	1:O:128:GLU:HB3	2.00	0.43
1:C:69:ALA:HB2	1:C:89:LEU:HD22	2.00	0.43
3:F:335:HOH:O	1:L:91:THR:HG22	2.19	0.43
1:E:123:ALA:HB1	1:E:159:GLN:HB3	1.99	0.43
1:G:30:LYS:HD2	1:G:76:GLU:HB3	2.01	0.43
1:J:62:VAL:HG22	1:J:108:TRP:NE1	2.34	0.43
1:J:58:HIS:O	1:J:62:VAL:HG23	2.19	0.43
1:N:106:ARG:NH1	1:N:163:ASP:OD1	2.39	0.43
1:C:59:LYS:NZ	3:C:311:HOH:O	2.46	0.42
1:F:0:HIS:ND1	1:L:95:GLU:OE2	2.34	0.42
1:L:11:ARG:HH22	1:L:181:GLU:CD	2.22	0.42
1:O:48:LEU:HD11	1:O:132:TYR:HD1	1.84	0.42
1:E:40:ALA:HB1	1:E:58:HIS:HE1	1.84	0.42
1:G:48:LEU:HD11	1:G:132:TYR:HD1	1.84	0.42
1:F:97:TYR:CZ	1:F:170:LEU:HB2	2.55	0.42
1:B:97:TYR:CZ	1:B:170:LEU:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:LYS:HB3	1:C:76:GLU:HB3	2.02	0.42
1:O:121:ASN:ND2	3:O:316:HOH:O	2.49	0.42
1:D:126:LEU:HG	1:D:130:LYS:HE3	2.02	0.42
1:G:11:ARG:HH22	1:G:181:GLU:CD	2.23	0.42
1:H:97:TYR:CZ	1:H:170:LEU:HB2	2.54	0.42
1:B:165:MET:HG3	1:B:169:HIS:CE1	2.55	0.42
1:G:133:THR:HB	1:G:139:ILE:HB	2.02	0.42
1:M:118:LYS:NZ	3:M:317:HOH:O	2.52	0.41
1:F:147:GLU:HG2	1:F:185:GLY:HA2	2.01	0.41
1:E:12:TRP:HZ2	3:E:312:HOH:O	2.03	0.41
1:D:126:LEU:HD21	1:D:146:GLU:HG2	2.02	0.41
1:M:2:LYS:O	1:M:175:THR:HG21	2.20	0.41
1:C:46:ASN:HB3	1:E:137:GLY:HA3	2.02	0.41
1:P:17:LYS:HD3	1:P:79:TRP:CZ2	2.56	0.41
1:H:2:LYS:HG2	1:H:175:THR:HB	2.02	0.41
1:H:46:ASN:HB3	1:N:137:GLY:HA3	2.02	0.41
1:D:164:GLU:OE1	1:D:167:ARG:NH2	2.53	0.41
1:I:2:LYS:NZ	1:I:4:THR:O	2.53	0.41
1:J:188:VAL:HA	1:J:189:PRO:HD3	1.94	0.41
1:K:116:VAL:HG12	1:K:128:GLU:HB3	2.03	0.41
1:O:171:GLY:HA2	1:O:175:THR:OG1	2.21	0.41
1:P:167:ARG:O	1:P:170:LEU:HB3	2.21	0.41
1:H:117:ASP:OD2	1:H:120:GLN:N	2.54	0.41
1:O:7:PHE:HB3	1:O:87:LYS:NZ	2.36	0.41
1:M:165:MET:HG3	1:M:169:HIS:CE1	2.57	0.40
1:C:5:SER:OG	1:O:-2:HIS:N	2.52	0.40
1:G:126:LEU:HG	1:G:130:LYS:HE3	2.03	0.40
1:A:152:CYS:SG	1:A:168:GLN:HG3	2.62	0.40
1:B:152:CYS:SG	1:B:168:GLN:HG3	2.61	0.40
1:D:2:LYS:HD3	3:D:301:HOH:O	2.20	0.40
1:M:48:LEU:HD11	1:M:132:TYR:HD1	1.86	0.40
1:P:97:TYR:CZ	1:P:170:LEU:HB2	2.57	0.40
1:E:86:TRP:HE3	3:E:312:HOH:O	2.05	0.40
1:E:117:ASP:OD2	1:E:120:GLN:N	2.54	0.40
1:I:165:MET:HG3	1:I:169:HIS:CE1	2.56	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	187/198 (94%)	186 (100%)	1 (0%)	0	100	100
1	B	187/198 (94%)	184 (98%)	3 (2%)	0	100	100
1	C	188/198 (95%)	187 (100%)	1 (0%)	0	100	100
1	D	188/198 (95%)	187 (100%)	1 (0%)	0	100	100
1	E	192/198 (97%)	191 (100%)	1 (0%)	0	100	100
1	F	189/198 (96%)	188 (100%)	1 (0%)	0	100	100
1	G	188/198 (95%)	187 (100%)	1 (0%)	0	100	100
1	H	188/198 (95%)	187 (100%)	1 (0%)	0	100	100
1	I	188/198 (95%)	186 (99%)	2 (1%)	0	100	100
1	J	191/198 (96%)	189 (99%)	2 (1%)	0	100	100
1	K	186/198 (94%)	184 (99%)	2 (1%)	0	100	100
1	L	186/198 (94%)	184 (99%)	2 (1%)	0	100	100
1	M	188/198 (95%)	187 (100%)	1 (0%)	0	100	100
1	N	188/198 (95%)	187 (100%)	1 (0%)	0	100	100
1	O	190/198 (96%)	189 (100%)	1 (0%)	0	100	100
1	P	190/198 (96%)	189 (100%)	1 (0%)	0	100	100
All	All	3014/3168 (95%)	2992 (99%)	22 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	157/165 (95%)	157 (100%)	0	100	100
1	B	157/165 (95%)	157 (100%)	0	100	100
1	C	158/165 (96%)	158 (100%)	0	100	100
1	D	158/165 (96%)	156 (99%)	2 (1%)	69	75
1	E	162/165 (98%)	160 (99%)	2 (1%)	71	77
1	F	159/165 (96%)	158 (99%)	1 (1%)	86	90
1	G	158/165 (96%)	157 (99%)	1 (1%)	86	90
1	H	158/165 (96%)	158 (100%)	0	100	100
1	I	158/165 (96%)	157 (99%)	1 (1%)	86	90
1	J	161/165 (98%)	161 (100%)	0	100	100
1	K	157/165 (95%)	156 (99%)	1 (1%)	86	90
1	L	157/165 (95%)	155 (99%)	2 (1%)	69	75
1	M	158/165 (96%)	158 (100%)	0	100	100
1	N	158/165 (96%)	156 (99%)	2 (1%)	69	75
1	O	160/165 (97%)	160 (100%)	0	100	100
1	P	160/165 (97%)	160 (100%)	0	100	100
All	All	2536/2640 (96%)	2524 (100%)	12 (0%)	88	92

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	106	ARG
1	D	167	ARG
1	E	86	TRP
1	E	167	ARG
1	F	167	ARG
1	G	86	TRP
1	I	167	ARG
1	K	86	TRP
1	L	86	TRP
1	L	157	SER
1	N	86	TRP
1	N	106	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	159	GLN
1	F	21	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 ligands 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	#$|Z| > 2$
2	J2U	E	201	-	36,36,36	5.43	11 (30%)	47,51,51	4.52	13 (27%)
2	J2U	J	201	-	36,36,36	5.30	10 (27%)	47,51,51	4.56	14 (29%)
2	J2U	B	201	-	36,36,36	5.39	11 (30%)	47,51,51	4.51	12 (25%)
2	J2U	C	201	-	36,36,36	5.41	11 (30%)	47,51,51	4.50	12 (25%)
2	J2U	L	201	-	36,36,36	5.32	11 (30%)	47,51,51	4.53	14 (29%)
2	J2U	K	201	-	36,36,36	5.35	11 (30%)	47,51,51	4.50	12 (25%)
2	J2U	I	201	-	36,36,36	5.33	11 (30%)	47,51,51	4.49	13 (27%)
2	J2U	N	201	-	36,36,36	5.38	11 (30%)	47,51,51	4.46	13 (27%)
2	J2U	O	201	-	36,36,36	5.32	11 (30%)	47,51,51	4.54	13 (27%)
2	J2U	H	201	-	36,36,36	5.36	11 (30%)	47,51,51	4.57	14 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	J2U	F	201	-	36,36,36	5.34	11 (30%)	47,51,51	4.54	13 (27%)
2	J2U	D	201	-	36,36,36	5.39	11 (30%)	47,51,51	4.52	13 (27%)
2	J2U	G	201	-	36,36,36	5.37	11 (30%)	47,51,51	4.57	14 (29%)
2	J2U	M	201	-	36,36,36	5.38	11 (30%)	47,51,51	4.50	13 (27%)
2	J2U	P	201	-	36,36,36	5.26	10 (27%)	47,51,51	4.57	14 (29%)
2	J2U	A	201	-	36,36,36	5.29	11 (30%)	47,51,51	4.55	15 (31%)

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
2	J2U	E	201	-	-	2/12/24/24	0/5/5/5
2	J2U	J	201	-	-	2/12/24/24	0/5/5/5
2	J2U	B	201	-	-	2/12/24/24	0/5/5/5
2	J2U	C	201	-	-	2/12/24/24	0/5/5/5
2	J2U	L	201	-	-	2/12/24/24	0/5/5/5
2	J2U	K	201	-	-	2/12/24/24	0/5/5/5
2	J2U	I	201	-	-	2/12/24/24	0/5/5/5
2	J2U	N	201	-	-	2/12/24/24	0/5/5/5
2	J2U	O	201	-	-	2/12/24/24	0/5/5/5
2	J2U	H	201	-	-	2/12/24/24	0/5/5/5
2	J2U	F	201	-	-	2/12/24/24	0/5/5/5
2	J2U	D	201	-	-	2/12/24/24	0/5/5/5
2	J2U	G	201	-	-	2/12/24/24	0/5/5/5
2	J2U	M	201	-	-	2/12/24/24	0/5/5/5
2	J2U	P	201	-	-	2/12/24/24	0/5/5/5
2	J2U	A	201	-	-	2/12/24/24	0/5/5/5

All (174) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	201	J2U	C10-C01	16.43	1.72	1.47
2	D	201	J2U	C10-C01	16.25	1.71	1.47
2	C	201	J2U	C10-C01	16.24	1.71	1.47
2	N	201	J2U	C10-C01	16.22	1.71	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	201	J2U	C10-C01	16.20	1.71	1.47
2	B	201	J2U	C10-C01	16.16	1.71	1.47
2	G	201	J2U	C10-C01	16.13	1.71	1.47
2	I	201	J2U	C10-C01	16.07	1.71	1.47
2	H	201	J2U	C10-C01	16.06	1.71	1.47
2	K	201	J2U	C10-C01	15.95	1.71	1.47
2	F	201	J2U	C10-C01	15.95	1.71	1.47
2	O	201	J2U	C10-C01	15.90	1.71	1.47
2	L	201	J2U	C10-C01	15.81	1.71	1.47
2	J	201	J2U	C10-C01	15.74	1.71	1.47
2	A	201	J2U	C10-C01	15.68	1.71	1.47
2	P	201	J2U	C10-C01	15.66	1.71	1.47
2	E	201	J2U	C13-C11	14.18	1.60	1.40
2	G	201	J2U	C13-C11	14.16	1.60	1.40
2	H	201	J2U	C13-C11	14.10	1.60	1.40
2	F	201	J2U	C13-C11	14.09	1.60	1.40
2	B	201	J2U	C13-C11	14.01	1.60	1.40
2	M	201	J2U	C13-C11	13.91	1.60	1.40
2	C	201	J2U	C13-C11	13.90	1.60	1.40
2	P	201	J2U	C13-C11	13.86	1.60	1.40
2	J	201	J2U	C13-C11	13.80	1.59	1.40
2	D	201	J2U	C13-C11	13.76	1.59	1.40
2	I	201	J2U	C13-C11	13.73	1.59	1.40
2	L	201	J2U	C13-C11	13.72	1.59	1.40
2	O	201	J2U	C13-C11	13.71	1.59	1.40
2	K	201	J2U	C13-C11	13.71	1.59	1.40
2	N	201	J2U	C13-C11	13.67	1.59	1.40
2	A	201	J2U	C13-C11	13.62	1.59	1.40
2	E	201	J2U	O01-C01	12.53	1.39	1.22
2	B	201	J2U	O01-C01	12.48	1.39	1.22
2	K	201	J2U	O01-C01	12.38	1.39	1.22
2	D	201	J2U	O01-C01	12.34	1.39	1.22
2	M	201	J2U	O01-C01	12.31	1.39	1.22
2	C	201	J2U	O01-C01	12.30	1.39	1.22
2	H	201	J2U	O01-C01	12.29	1.39	1.22
2	G	201	J2U	O01-C01	12.29	1.39	1.22
2	N	201	J2U	O01-C01	12.18	1.39	1.22
2	I	201	J2U	O01-C01	12.17	1.39	1.22
2	O	201	J2U	O01-C01	12.16	1.39	1.22
2	E	201	J2U	C23-C10	12.16	1.58	1.39
2	F	201	J2U	O01-C01	12.11	1.39	1.22
2	C	201	J2U	C23-C10	12.09	1.58	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	201	J2U	O01-C01	12.05	1.39	1.22
2	N	201	J2U	C23-C10	12.04	1.58	1.39
2	D	201	J2U	C23-C10	12.04	1.58	1.39
2	M	201	J2U	C23-C10	12.01	1.58	1.39
2	A	201	J2U	O01-C01	11.99	1.39	1.22
2	J	201	J2U	O01-C01	11.93	1.39	1.22
2	O	201	J2U	C23-C10	11.93	1.58	1.39
2	L	201	J2U	C23-C10	11.92	1.58	1.39
2	I	201	J2U	C23-C10	11.90	1.58	1.39
2	B	201	J2U	C23-C10	11.89	1.58	1.39
2	G	201	J2U	C23-C10	11.89	1.58	1.39
2	K	201	J2U	C23-C10	11.88	1.58	1.39
2	P	201	J2U	C23-C10	11.85	1.58	1.39
2	J	201	J2U	C23-C10	11.84	1.58	1.39
2	A	201	J2U	C23-C10	11.83	1.58	1.39
2	H	201	J2U	C23-C10	11.82	1.58	1.39
2	F	201	J2U	C23-C10	11.79	1.58	1.39
2	P	201	J2U	O01-C01	11.65	1.38	1.22
2	C	201	J2U	C12-C02	-10.36	1.38	1.54
2	N	201	J2U	C12-C02	-10.36	1.38	1.54
2	D	201	J2U	C12-C02	-10.28	1.39	1.54
2	O	201	J2U	C12-C02	-10.27	1.39	1.54
2	K	201	J2U	C12-C02	-10.22	1.39	1.54
2	M	201	J2U	C12-C02	-10.22	1.39	1.54
2	A	201	J2U	C12-C02	-10.21	1.39	1.54
2	J	201	J2U	C12-C02	-10.19	1.39	1.54
2	B	201	J2U	C12-C02	-10.17	1.39	1.54
2	P	201	J2U	C12-C02	-10.15	1.39	1.54
2	L	201	J2U	C12-C02	-10.13	1.39	1.54
2	E	201	J2U	C12-C02	-10.07	1.39	1.54
2	H	201	J2U	C12-C02	-10.06	1.39	1.54
2	I	201	J2U	C12-C02	-10.05	1.39	1.54
2	G	201	J2U	C12-C02	-10.04	1.39	1.54
2	F	201	J2U	C12-C02	-10.02	1.39	1.54
2	N	201	J2U	C12-C11	-7.79	1.41	1.51
2	C	201	J2U	C12-C11	-7.69	1.41	1.51
2	K	201	J2U	C12-C11	-7.68	1.41	1.51
2	D	201	J2U	C12-C11	-7.67	1.41	1.51
2	A	201	J2U	C12-C11	-7.63	1.41	1.51
2	M	201	J2U	C12-C11	-7.56	1.41	1.51
2	G	201	J2U	C12-C11	-7.54	1.41	1.51
2	B	201	J2U	C12-C11	-7.54	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	201	J2U	C12-C11	-7.53	1.41	1.51
2	O	201	J2U	C12-C11	-7.52	1.41	1.51
2	F	201	J2U	C12-C11	-7.51	1.41	1.51
2	H	201	J2U	C12-C11	-7.49	1.41	1.51
2	I	201	J2U	C12-C11	-7.48	1.41	1.51
2	E	201	J2U	C12-C11	-7.46	1.41	1.51
2	J	201	J2U	C12-C11	-7.46	1.41	1.51
2	I	201	J2U	C10-C11	7.32	1.54	1.39
2	J	201	J2U	C10-C11	7.31	1.54	1.39
2	C	201	J2U	C10-C11	7.29	1.54	1.39
2	M	201	J2U	C10-C11	7.28	1.54	1.39
2	E	201	J2U	C10-C11	7.26	1.54	1.39
2	D	201	J2U	C10-C11	7.26	1.54	1.39
2	B	201	J2U	C10-C11	7.25	1.54	1.39
2	N	201	J2U	C10-C11	7.25	1.54	1.39
2	F	201	J2U	C10-C11	7.24	1.54	1.39
2	K	201	J2U	C10-C11	7.23	1.54	1.39
2	P	201	J2U	C12-C11	-7.23	1.42	1.51
2	G	201	J2U	C10-C11	7.19	1.54	1.39
2	O	201	J2U	C10-C11	7.19	1.54	1.39
2	L	201	J2U	C10-C11	7.18	1.54	1.39
2	H	201	J2U	C10-C11	7.16	1.54	1.39
2	A	201	J2U	C10-C11	7.14	1.54	1.39
2	P	201	J2U	C10-C11	7.09	1.53	1.39
2	K	201	J2U	C21-C22	-5.76	1.29	1.39
2	C	201	J2U	C21-C22	-5.76	1.29	1.39
2	N	201	J2U	C21-C22	-5.76	1.29	1.39
2	L	201	J2U	C21-C22	-5.76	1.29	1.39
2	J	201	J2U	C21-C22	-5.75	1.29	1.39
2	D	201	J2U	C21-C22	-5.73	1.29	1.39
2	A	201	J2U	C21-C22	-5.70	1.29	1.39
2	F	201	J2U	C21-C22	-5.69	1.29	1.39
2	P	201	J2U	C21-C22	-5.69	1.29	1.39
2	B	201	J2U	C21-C22	-5.69	1.29	1.39
2	H	201	J2U	C21-C22	-5.67	1.29	1.39
2	E	201	J2U	C21-C22	-5.67	1.30	1.39
2	M	201	J2U	C21-C22	-5.64	1.30	1.39
2	I	201	J2U	C21-C22	-5.63	1.30	1.39
2	G	201	J2U	C21-C22	-5.63	1.30	1.39
2	O	201	J2U	C21-C22	-5.55	1.30	1.39
2	L	201	J2U	C23-C22	-3.78	1.33	1.39
2	P	201	J2U	C23-C22	-3.77	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	201	J2U	C23-C22	-3.70	1.33	1.39
2	I	201	J2U	C23-C22	-3.68	1.33	1.39
2	J	201	J2U	C23-C22	-3.67	1.33	1.39
2	A	201	J2U	C23-C22	-3.67	1.33	1.39
2	O	201	J2U	C23-C22	-3.63	1.33	1.39
2	B	201	J2U	C23-C22	-3.60	1.33	1.39
2	M	201	J2U	C23-C22	-3.56	1.33	1.39
2	F	201	J2U	C23-C22	-3.53	1.33	1.39
2	D	201	J2U	C23-C22	-3.53	1.33	1.39
2	J	201	J2U	C21-C13	-3.51	1.33	1.39
2	H	201	J2U	C23-C22	-3.49	1.33	1.39
2	C	201	J2U	C21-C13	-3.49	1.33	1.39
2	C	201	J2U	C23-C22	-3.47	1.33	1.39
2	G	201	J2U	C23-C22	-3.46	1.33	1.39
2	N	201	J2U	C23-C22	-3.46	1.33	1.39
2	D	201	J2U	C21-C13	-3.46	1.33	1.39
2	N	201	J2U	C21-C13	-3.41	1.33	1.39
2	L	201	J2U	C21-C13	-3.38	1.33	1.39
2	A	201	J2U	C21-C13	-3.37	1.33	1.39
2	I	201	J2U	C21-C13	-3.36	1.33	1.39
2	K	201	J2U	C21-C13	-3.35	1.33	1.39
2	F	201	J2U	C21-C13	-3.35	1.33	1.39
2	P	201	J2U	C21-C13	-3.35	1.33	1.39
2	E	201	J2U	C23-C22	-3.32	1.34	1.39
2	M	201	J2U	C21-C13	-3.31	1.33	1.39
2	H	201	J2U	C21-C13	-3.26	1.33	1.39
2	E	201	J2U	C21-C13	-3.25	1.33	1.39
2	B	201	J2U	C21-C13	-3.24	1.33	1.39
2	O	201	J2U	C21-C13	-3.21	1.34	1.39
2	G	201	J2U	C21-C13	-3.21	1.34	1.39
2	E	201	J2U	C24-C22	2.24	1.54	1.49
2	M	201	J2U	C24-C22	2.18	1.54	1.49
2	B	201	J2U	C24-C22	2.18	1.54	1.49
2	N	201	J2U	C24-C22	2.16	1.54	1.49
2	G	201	J2U	C24-C22	2.15	1.54	1.49
2	D	201	J2U	C24-C22	2.12	1.54	1.49
2	C	201	J2U	C24-C22	2.11	1.54	1.49
2	K	201	J2U	C24-C22	2.10	1.54	1.49
2	H	201	J2U	C24-C22	2.10	1.54	1.49
2	I	201	J2U	C24-C22	2.06	1.54	1.49
2	A	201	J2U	C24-C22	2.06	1.54	1.49
2	O	201	J2U	C24-C22	2.06	1.54	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	201	J2U	C24-C22	2.05	1.54	1.49
2	F	201	J2U	C24-C22	2.03	1.54	1.49

All (212) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	201	J2U	C11-C12-C02	20.00	124.22	103.46
2	G	201	J2U	C11-C12-C02	20.00	124.21	103.46
2	E	201	J2U	C11-C12-C02	19.97	124.18	103.46
2	F	201	J2U	C11-C12-C02	19.89	124.10	103.46
2	C	201	J2U	C11-C12-C02	19.89	124.10	103.46
2	M	201	J2U	C11-C12-C02	19.89	124.10	103.46
2	B	201	J2U	C11-C12-C02	19.86	124.06	103.46
2	P	201	J2U	C11-C12-C02	19.77	123.97	103.46
2	O	201	J2U	C11-C12-C02	19.76	123.96	103.46
2	D	201	J2U	C11-C12-C02	19.70	123.90	103.46
2	A	201	J2U	C11-C12-C02	19.65	123.85	103.46
2	J	201	J2U	C11-C12-C02	19.64	123.84	103.46
2	N	201	J2U	C11-C12-C02	19.62	123.82	103.46
2	I	201	J2U	C11-C12-C02	19.60	123.80	103.46
2	L	201	J2U	C11-C12-C02	19.57	123.77	103.46
2	K	201	J2U	C11-C12-C02	19.49	123.68	103.46
2	N	201	J2U	C23-C10-C01	11.55	142.54	128.40
2	C	201	J2U	C23-C10-C01	11.44	142.41	128.40
2	D	201	J2U	C23-C10-C01	11.44	142.40	128.40
2	E	201	J2U	C23-C10-C01	11.32	142.26	128.40
2	M	201	J2U	C23-C10-C01	11.25	142.17	128.40
2	P	201	J2U	O01-C01-C02	11.15	130.82	124.76
2	G	201	J2U	C23-C10-C01	11.14	142.03	128.40
2	B	201	J2U	C23-C10-C01	11.13	142.02	128.40
2	I	201	J2U	C23-C10-C01	11.01	141.88	128.40
2	O	201	J2U	C23-C10-C01	11.00	141.86	128.40
2	J	201	J2U	C23-C10-C01	10.99	141.85	128.40
2	K	201	J2U	C23-C10-C01	10.98	141.85	128.40
2	H	201	J2U	C23-C10-C01	10.95	141.80	128.40
2	A	201	J2U	C23-C10-C01	10.91	141.76	128.40
2	L	201	J2U	C23-C10-C01	10.84	141.66	128.40
2	F	201	J2U	C23-C10-C01	10.74	141.55	128.40
2	E	201	J2U	C23-C10-C11	-10.73	113.69	123.12
2	J	201	J2U	O01-C01-C02	10.70	130.58	124.76
2	G	201	J2U	C23-C10-C11	-10.63	113.78	123.12
2	B	201	J2U	C23-C10-C11	-10.62	113.79	123.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	201	J2U	C23-C10-C11	-10.61	113.80	123.12
2	N	201	J2U	C23-C10-C11	-10.59	113.81	123.12
2	M	201	J2U	C23-C10-C11	-10.51	113.89	123.12
2	P	201	J2U	C23-C10-C01	10.51	141.26	128.40
2	C	201	J2U	C23-C10-C11	-10.44	113.94	123.12
2	A	201	J2U	O01-C01-C02	10.40	130.41	124.76
2	H	201	J2U	C23-C10-C11	-10.35	114.03	123.12
2	L	201	J2U	O01-C01-C02	10.33	130.38	124.76
2	O	201	J2U	O01-C01-C02	10.20	130.30	124.76
2	F	201	J2U	O01-C01-C02	10.18	130.29	124.76
2	K	201	J2U	C23-C10-C11	-10.18	114.18	123.12
2	O	201	J2U	C23-C10-C11	-10.17	114.19	123.12
2	H	201	J2U	O01-C01-C02	10.09	130.25	124.76
2	I	201	J2U	C23-C10-C11	-10.08	114.27	123.12
2	F	201	J2U	C23-C10-C11	-10.06	114.28	123.12
2	J	201	J2U	C23-C10-C11	-10.02	114.32	123.12
2	A	201	J2U	C23-C10-C11	-9.96	114.37	123.12
2	L	201	J2U	C23-C10-C11	-9.90	114.42	123.12
2	K	201	J2U	O01-C01-C02	9.81	130.09	124.76
2	G	201	J2U	O01-C01-C02	9.68	130.02	124.76
2	D	201	J2U	O01-C01-C02	9.31	129.82	124.76
2	I	201	J2U	O01-C01-C02	9.30	129.82	124.76
2	P	201	J2U	C23-C10-C11	-9.27	114.98	123.12
2	B	201	J2U	O01-C01-C02	9.14	129.73	124.76
2	C	201	J2U	O01-C01-C02	8.91	129.60	124.76
2	M	201	J2U	O01-C01-C02	8.87	129.58	124.76
2	P	201	J2U	C10-C11-C13	-8.85	110.97	120.78
2	L	201	J2U	C10-C11-C13	-8.69	111.14	120.78
2	E	201	J2U	O01-C01-C02	8.63	129.45	124.76
2	A	201	J2U	C10-C11-C13	-8.58	111.26	120.78
2	F	201	J2U	C10-C11-C13	-8.42	111.44	120.78
2	I	201	J2U	C10-C11-C13	-8.41	111.45	120.78
2	K	201	J2U	C10-C11-C13	-8.41	111.45	120.78
2	J	201	J2U	C10-C11-C13	-8.40	111.46	120.78
2	G	201	J2U	C10-C11-C13	-8.24	111.64	120.78
2	D	201	J2U	C10-C11-C13	-8.23	111.65	120.78
2	O	201	J2U	C10-C11-C13	-8.22	111.66	120.78
2	H	201	J2U	C10-C11-C13	-8.21	111.67	120.78
2	C	201	J2U	C10-C11-C13	-8.21	111.67	120.78
2	E	201	J2U	C10-C11-C13	-8.21	111.68	120.78
2	B	201	J2U	C10-C11-C13	-8.19	111.69	120.78
2	N	201	J2U	O01-C01-C02	8.19	129.21	124.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	201	J2U	C10-C11-C13	-8.17	111.72	120.78
2	N	201	J2U	C10-C11-C13	-8.01	111.90	120.78
2	P	201	J2U	C12-C11-C13	6.35	145.05	128.53
2	F	201	J2U	C12-C11-C13	6.28	144.87	128.53
2	L	201	J2U	C12-C11-C13	6.28	144.87	128.53
2	H	201	J2U	C12-C11-C13	6.22	144.69	128.53
2	A	201	J2U	C12-C11-C13	6.21	144.67	128.53
2	G	201	J2U	C12-C11-C13	6.21	144.67	128.53
2	B	201	J2U	C12-C11-C13	6.19	144.63	128.53
2	J	201	J2U	C12-C11-C13	6.16	144.56	128.53
2	I	201	J2U	C12-C11-C13	6.16	144.55	128.53
2	E	201	J2U	C12-C11-C13	6.15	144.53	128.53
2	K	201	J2U	C12-C11-C13	6.14	144.49	128.53
2	M	201	J2U	C12-C11-C13	6.13	144.46	128.53
2	O	201	J2U	C12-C11-C13	6.11	144.42	128.53
2	C	201	J2U	C12-C11-C13	6.08	144.33	128.53
2	D	201	J2U	C12-C11-C13	6.05	144.27	128.53
2	N	201	J2U	C12-C11-C13	5.91	143.91	128.53
2	J	201	J2U	C23-C22-C21	5.83	126.93	118.31
2	H	201	J2U	C23-C22-C21	5.70	126.74	118.31
2	F	201	J2U	C23-C22-C21	5.70	126.74	118.31
2	N	201	J2U	C23-C22-C21	5.67	126.69	118.31
2	C	201	J2U	C23-C22-C21	5.61	126.61	118.31
2	O	201	J2U	C23-C22-C21	5.61	126.60	118.31
2	P	201	J2U	C23-C22-C21	5.61	126.60	118.31
2	D	201	J2U	C23-C22-C21	5.59	126.57	118.31
2	I	201	J2U	C23-C22-C21	5.58	126.56	118.31
2	M	201	J2U	C23-C22-C21	5.57	126.54	118.31
2	G	201	J2U	C23-C22-C21	5.54	126.50	118.31
2	A	201	J2U	C23-C22-C21	5.53	126.49	118.31
2	K	201	J2U	C23-C22-C21	5.53	126.48	118.31
2	B	201	J2U	C23-C22-C21	5.51	126.45	118.31
2	A	201	J2U	C21-C13-C11	5.51	125.56	119.28
2	L	201	J2U	C23-C22-C21	5.47	126.40	118.31
2	E	201	J2U	C21-C13-C11	5.47	125.52	119.28
2	E	201	J2U	C23-C22-C21	5.47	126.39	118.31
2	D	201	J2U	C21-C13-C11	5.47	125.51	119.28
2	G	201	J2U	C21-C13-C11	5.46	125.50	119.28
2	L	201	J2U	C21-C13-C11	5.45	125.49	119.28
2	K	201	J2U	C21-C13-C11	5.27	125.29	119.28
2	P	201	J2U	C21-C13-C11	5.26	125.27	119.28
2	B	201	J2U	C21-C13-C11	5.25	125.27	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	201	J2U	C21-C13-C11	5.24	125.25	119.28
2	C	201	J2U	C21-C13-C11	5.23	125.24	119.28
2	F	201	J2U	C21-C13-C11	5.23	125.24	119.28
2	I	201	J2U	C21-C13-C11	5.22	125.23	119.28
2	M	201	J2U	C21-C13-C11	5.22	125.23	119.28
2	J	201	J2U	C21-C13-C11	5.19	125.20	119.28
2	N	201	J2U	C21-C13-C11	5.19	125.20	119.28
2	O	201	J2U	C21-C13-C11	5.17	125.17	119.28
2	H	201	J2U	C12-C11-C10	-4.54	103.64	110.64
2	B	201	J2U	C12-C11-C10	-4.52	103.68	110.64
2	F	201	J2U	C12-C11-C10	-4.51	103.69	110.64
2	G	201	J2U	C12-C11-C10	-4.51	103.69	110.64
2	E	201	J2U	C12-C11-C10	-4.44	103.79	110.64
2	G	201	J2U	C23-C22-C24	-4.44	113.52	120.86
2	M	201	J2U	C12-C11-C10	-4.43	103.82	110.64
2	O	201	J2U	C12-C11-C10	-4.36	103.92	110.64
2	P	201	J2U	C12-C11-C10	-4.32	103.98	110.64
2	J	201	J2U	C12-C11-C10	-4.32	103.98	110.64
2	C	201	J2U	C12-C11-C10	-4.31	104.00	110.64
2	L	201	J2U	C12-C11-C10	-4.31	104.00	110.64
2	I	201	J2U	C12-C11-C10	-4.30	104.01	110.64
2	H	201	J2U	C23-C22-C24	-4.29	113.77	120.86
2	K	201	J2U	C12-C11-C10	-4.27	104.06	110.64
2	A	201	J2U	C12-C11-C10	-4.26	104.07	110.64
2	D	201	J2U	C12-C11-C10	-4.26	104.08	110.64
2	N	201	J2U	C12-C11-C10	-4.18	104.20	110.64
2	B	201	J2U	C23-C22-C24	-4.15	114.00	120.86
2	F	201	J2U	C23-C22-C24	-4.13	114.03	120.86
2	L	201	J2U	C23-C22-C24	-4.12	114.06	120.86
2	A	201	J2U	C23-C22-C24	-4.11	114.07	120.86
2	K	201	J2U	C23-C22-C24	-3.99	114.27	120.86
2	O	201	J2U	C23-C22-C24	-3.90	114.41	120.86
2	E	201	J2U	C23-C22-C24	-3.87	114.47	120.86
2	M	201	J2U	C23-C22-C24	-3.84	114.51	120.86
2	P	201	J2U	C23-C22-C24	-3.66	114.81	120.86
2	N	201	J2U	C23-C22-C24	-3.53	115.02	120.86
2	I	201	J2U	C23-C22-C24	-3.53	115.03	120.86
2	D	201	J2U	C23-C22-C24	-3.52	115.04	120.86
2	I	201	J2U	C03-C02-C01	-3.49	109.17	115.58
2	J	201	J2U	C23-C22-C24	-3.41	115.23	120.86
2	P	201	J2U	C12-C02-C01	-3.37	103.02	104.68
2	O	201	J2U	C04-C03-C02	-3.35	107.58	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	201	J2U	C03-C02-C01	-3.34	109.45	115.58
2	B	201	J2U	C03-C02-C01	-3.31	109.50	115.58
2	L	201	J2U	C03-C02-C01	-3.29	109.53	115.58
2	K	201	J2U	C04-C03-C02	-3.29	107.68	113.72
2	N	201	J2U	C03-C02-C01	-3.27	109.58	115.58
2	K	201	J2U	C03-C02-C01	-3.24	109.63	115.58
2	N	201	J2U	C04-C03-C02	-3.20	107.84	113.72
2	A	201	J2U	C03-C02-C01	-3.12	109.85	115.58
2	C	201	J2U	C23-C22-C24	-3.09	115.75	120.86
2	M	201	J2U	C03-C02-C01	-3.07	109.95	115.58
2	J	201	J2U	C03-C02-C01	-3.05	109.99	115.58
2	I	201	J2U	C04-C03-C02	-3.01	108.19	113.72
2	D	201	J2U	C03-C02-C01	-2.97	110.12	115.58
2	E	201	J2U	C03-C02-C01	-2.90	110.25	115.58
2	O	201	J2U	C03-C02-C01	-2.88	110.30	115.58
2	F	201	J2U	C03-C02-C01	-2.87	110.32	115.58
2	C	201	J2U	C03-C02-C01	-2.81	110.41	115.58
2	B	201	J2U	C04-C03-C02	-2.81	108.56	113.72
2	G	201	J2U	C03-C02-C01	-2.76	110.52	115.58
2	H	201	J2U	C12-C02-C01	-2.74	103.33	104.68
2	H	201	J2U	C03-C02-C01	-2.68	110.66	115.58
2	E	201	J2U	C04-C03-C02	-2.63	108.89	113.72
2	A	201	J2U	C12-C02-C01	-2.61	103.39	104.68
2	L	201	J2U	C04-C03-C02	-2.61	108.93	113.72
2	J	201	J2U	C12-C02-C01	-2.60	103.40	104.68
2	J	201	J2U	C04-C03-C02	-2.59	108.96	113.72
2	D	201	J2U	C04-C03-C02	-2.58	108.98	113.72
2	C	201	J2U	C12-C02-C01	-2.57	103.41	104.68
2	F	201	J2U	C12-C02-C01	-2.54	103.43	104.68
2	G	201	J2U	C12-C02-C01	-2.54	103.43	104.68
2	P	201	J2U	O01-C01-C10	-2.53	124.02	127.11
2	P	201	J2U	C04-C03-C02	-2.46	109.21	113.72
2	M	201	J2U	C04-C03-C02	-2.39	109.33	113.72
2	L	201	J2U	C25-C24-C22	-2.38	117.22	121.36
2	L	201	J2U	C12-C02-C01	-2.37	103.51	104.68
2	H	201	J2U	C25-C24-C22	-2.37	117.26	121.36
2	A	201	J2U	C13-C14-C15	-2.34	108.92	114.22
2	O	201	J2U	C12-C02-C01	-2.34	103.53	104.68
2	E	201	J2U	C12-C02-C01	-2.30	103.55	104.68
2	G	201	J2U	C04-C03-C02	-2.28	109.54	113.72
2	A	201	J2U	C04-C03-C02	-2.27	109.54	113.72
2	F	201	J2U	C25-C24-C22	-2.25	117.46	121.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	201	J2U	C04-C03-C02	-2.20	109.68	113.72
2	M	201	J2U	C12-C02-C01	-2.16	103.61	104.68
2	A	201	J2U	C25-C24-C22	-2.11	117.70	121.36
2	I	201	J2U	C12-C02-C01	-2.09	103.65	104.68
2	N	201	J2U	C25-C24-C22	-2.06	117.79	121.36
2	G	201	J2U	C25-C24-C22	-2.05	117.81	121.36
2	D	201	J2U	C12-C02-C01	-2.04	103.67	104.68
2	J	201	J2U	O01-C01-C10	-2.04	124.62	127.11

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	J2U	C12-C02-C03-C04
2	B	201	J2U	C12-C02-C03-C04
2	C	201	J2U	C12-C02-C03-C04
2	D	201	J2U	C12-C02-C03-C04
2	E	201	J2U	C12-C02-C03-C04
2	F	201	J2U	C12-C02-C03-C04
2	G	201	J2U	C12-C02-C03-C04
2	H	201	J2U	C12-C02-C03-C04
2	I	201	J2U	C12-C02-C03-C04
2	J	201	J2U	C12-C02-C03-C04
2	K	201	J2U	C12-C02-C03-C04
2	L	201	J2U	C12-C02-C03-C04
2	M	201	J2U	C12-C02-C03-C04
2	N	201	J2U	C12-C02-C03-C04
2	O	201	J2U	C12-C02-C03-C04
2	P	201	J2U	C12-C02-C03-C04
2	B	201	J2U	C01-C02-C03-C04
2	C	201	J2U	C01-C02-C03-C04
2	F	201	J2U	C01-C02-C03-C04
2	H	201	J2U	C01-C02-C03-C04
2	J	201	J2U	C01-C02-C03-C04
2	P	201	J2U	C01-C02-C03-C04
2	A	201	J2U	C01-C02-C03-C04
2	D	201	J2U	C01-C02-C03-C04
2	E	201	J2U	C01-C02-C03-C04
2	G	201	J2U	C01-C02-C03-C04
2	I	201	J2U	C01-C02-C03-C04
2	K	201	J2U	C01-C02-C03-C04
2	L	201	J2U	C01-C02-C03-C04

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Mol	Chain	Res	Type	Atoms
2	M	201	J2U	C01-C02-C03-C04
2	N	201	J2U	C01-C02-C03-C04
2	O	201	J2U	C01-C02-C03-C04

There are no ring outliers.

No monomer is involved in short contacts.

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 then 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.

Ligand J2U E 201

Bond lengths

Bond angles

Torsions

Rings

Ligand J2U J 201

Bond lengths

Bond angles

Torsions

Rings

Ligand J2U B 201

Bond lengths

Bond angles

Torsions

Rings

Ligand J2U C 201

Bond lengths

Bond angles

Torsions

Rings

Ligand J2U L 201

Bond lengths

Bond angles

Torsions

Rings

Ligand J2U K 201

Bond lengths

Bond angles

Torsions

Rings

Ligand J2U I 201

Bond lengths

Bond angles

Torsions

Rings

Ligand J2U N 201

Bond lengths

Bond angles

Torsions

Rings

Ligand J2U O 201

Bond lengths

Bond angles

Torsions

Rings

Ligand J2U H 201

Bond lengths

Bond angles

Torsions

Rings

Ligand J2U F 201

Bond lengths

Bond angles

Torsions

Rings

Ligand J2U D 201

Bond lengths

Bond angles

Torsions

Rings

Ligand J2U G 201

Bond lengths

Bond angles

Torsions

Rings

Ligand J2U M 201

Bond lengths

Bond angles

Torsions

Rings

Ligand J2U P 201

Bond lengths

Bond angles

Torsions

Rings

Ligand J2U A 201

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	189/198 (95%)	0.24	2 (1%)	80	84	18, 28, 40, 57	0
1	B	189/198 (95%)	0.48	6 (3%)	47	54	20, 36, 55, 69	0
1	C	190/198 (95%)	1.03	30 (15%)	2	2	28, 44, 59, 79	0
1	D	190/198 (95%)	0.57	16 (8%)	11	14	21, 35, 53, 66	0
1	E	194/198 (97%)	1.05	34 (17%)	1	1	30, 46, 67, 78	0
1	F	191/198 (96%)	0.46	6 (3%)	49	55	22, 30, 52, 69	0
1	G	190/198 (95%)	0.49	9 (4%)	31	37	26, 35, 52, 62	0
1	H	190/198 (95%)	0.53	10 (5%)	26	32	20, 35, 55, 79	0
1	I	190/198 (95%)	0.46	8 (4%)	36	42	20, 29, 52, 67	0
1	J	193/198 (97%)	0.44	9 (4%)	31	37	17, 27, 51, 66	0
1	K	188/198 (94%)	0.32	2 (1%)	80	84	21, 33, 47, 57	0
1	L	188/198 (94%)	0.26	0	100	100	19, 29, 41, 53	0
1	M	190/198 (95%)	0.59	11 (5%)	23	28	25, 38, 55, 73	0
1	N	190/198 (95%)	0.53	9 (4%)	31	37	19, 35, 57, 77	0
1	O	192/198 (96%)	0.47	7 (3%)	42	49	20, 30, 53, 66	0
1	P	192/198 (96%)	0.45	7 (3%)	42	49	17, 26, 50, 64	0
All	All	3046/3168 (96%)	0.53	166 (5%)	25	31	17, 34, 55, 79	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	158	GLY	7.0
1	H	156	GLU	5.8
1	C	154	ILE	5.5
1	J	-3	HIS	5.5
1	I	157	SER	5.0

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Mol	Chain	Res	Type	RSRZ
1	G	121	ASN	4.9
1	E	121	ASN	4.8
1	H	118	LYS	4.8
1	F	121	ASN	4.7
1	C	180	CYS	4.6
1	O	121	ASN	4.6
1	G	155	ASP	4.6
1	E	160	LEU	4.5
1	J	122	GLY	4.5
1	E	158	GLY	4.5
1	H	121	ASN	4.5
1	C	156	GLU	4.4
1	N	121	ASN	4.4
1	E	155	ASP	4.3
1	D	155	ASP	4.2
1	C	10	PRO	4.1
1	C	157	SER	3.9
1	D	1	GLY	3.9
1	E	122	GLY	3.9
1	E	85	GLY	3.9
1	B	121	ASN	3.8
1	E	150	ARG	3.8
1	N	156	GLU	3.6
1	E	154	ILE	3.6
1	M	158	GLY	3.6
1	J	160	LEU	3.5
1	E	10	PRO	3.5
1	C	118	LYS	3.5
1	P	157	SER	3.5
1	N	155	ASP	3.5
1	M	69	ALA	3.5
1	G	156	GLU	3.5
1	I	121	ASN	3.4
1	H	155	ASP	3.4
1	E	152	CYS	3.4
1	P	122	GLY	3.4
1	M	156	GLU	3.4
1	E	74	GLY	3.4
1	N	157	SER	3.3
1	M	155	ASP	3.3
1	P	121	ASN	3.3
1	O	158	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	124	ILE	3.2
1	D	153	ASP	3.2
1	N	153	ASP	3.2
1	E	70	GLY	3.1
1	F	155	ASP	3.1
1	J	121	ASN	3.0
1	C	80	PRO	3.0
1	G	118	LYS	3.0
1	C	155	ASP	3.0
1	E	53	GLU	2.9
1	H	122	GLY	2.9
1	C	2	LYS	2.9
1	P	53	GLU	2.9
1	M	154	ILE	2.9
1	D	157	SER	2.9
1	C	152	CYS	2.9
1	A	1	GLY	2.9
1	I	154	ILE	2.9
1	M	153	ASP	2.9
1	J	155	ASP	2.9
1	O	155	ASP	2.8
1	C	27	HIS	2.8
1	E	8	ASP	2.8
1	M	118	LYS	2.8
1	N	150	ARG	2.8
1	C	189	PRO	2.8
1	H	161	ASP	2.8
1	O	126	LEU	2.8
1	D	154	ILE	2.8
1	C	182	LYS	2.8
1	H	97	TYR	2.7
1	B	153	ASP	2.7
1	F	156	GLU	2.7
1	E	182	LYS	2.7
1	E	118	LYS	2.7
1	A	157	SER	2.7
1	O	154	ILE	2.7
1	G	122	GLY	2.6
1	G	154	ILE	2.6
1	J	53	GLU	2.6
1	H	157	SER	2.6
1	C	1	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	P	155	ASP	2.6
1	M	48	LEU	2.6
1	E	120	GLN	2.6
1	B	156	GLU	2.6
1	B	170	LEU	2.6
1	E	170	LEU	2.6
1	N	154	ILE	2.6
1	E	156	GLU	2.5
1	D	143	GLU	2.5
1	C	143	GLU	2.5
1	H	154	ILE	2.5
1	E	29	GLY	2.5
1	I	155	ASP	2.5
1	C	145	CYS	2.5
1	C	53	GLU	2.5
1	P	156	GLU	2.5
1	E	7	PHE	2.5
1	O	123	ALA	2.5
1	C	79	TRP	2.5
1	J	-2	HIS	2.5
1	D	182	LYS	2.5
1	D	126	LEU	2.4
1	G	160	LEU	2.4
1	E	84	GLU	2.4
1	B	5	SER	2.4
1	F	122	GLY	2.4
1	D	53	GLU	2.4
1	D	3	LEU	2.4
1	I	1	GLY	2.4
1	N	7	PHE	2.3
1	D	156	GLU	2.3
1	E	145	CYS	2.3
1	D	27	HIS	2.3
1	E	97	TYR	2.3
1	C	160	LEU	2.3
1	E	81	ALA	2.3
1	E	148	THR	2.3
1	C	0	HIS	2.3
1	D	150	ARG	2.3
1	P	154	ILE	2.3
1	I	160	LEU	2.2
1	N	143	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	83	ILE	2.2
1	H	55	ALA	2.2
1	D	80	PRO	2.2
1	E	153	ASP	2.2
1	M	150	ARG	2.2
1	M	80	PRO	2.2
1	I	149	PHE	2.1
1	C	116	VAL	2.1
1	B	143	GLU	2.1
1	E	82	TYR	2.1
1	C	148	THR	2.1
1	D	121	ASN	2.1
1	E	119	ASP	2.1
1	M	27	HIS	2.1
1	C	14	GLY	2.1
1	E	186	GLY	2.1
1	F	160	LEU	2.1
1	O	122	GLY	2.1
1	K	152	CYS	2.1
1	D	30	LYS	2.1
1	F	118	LYS	2.1
1	E	3	LEU	2.1
1	C	84	GLU	2.1
1	J	-1	HIS	2.1
1	J	118	LYS	2.1
1	C	115	ILE	2.0
1	G	81	ALA	2.0
1	E	171	GLY	2.0
1	E	6	ASP	2.0
1	G	79	TRP	2.0
1	K	139	ILE	2.0
1	E	12	TRP	2.0
1	I	156	GLU	2.0
1	C	90	ALA	2.0
1	C	70	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	J2U	C	201	32/32	0.89	0.16	26,32,39,43	0
2	J2U	K	201	32/32	0.90	0.17	18,26,30,32	0
2	J2U	M	201	32/32	0.90	0.16	23,29,36,39	0
2	J2U	A	201	32/32	0.91	0.17	16,21,27,27	0
2	J2U	E	201	32/32	0.92	0.16	27,33,41,42	0
2	J2U	H	201	32/32	0.93	0.16	19,26,35,37	0
2	J2U	I	201	32/32	0.93	0.15	17,23,28,34	0
2	J2U	J	201	32/32	0.93	0.15	16,19,28,31	0
2	J2U	B	201	32/32	0.93	0.15	24,29,33,39	0
2	J2U	G	201	32/32	0.93	0.13	18,24,29,31	0
2	J2U	N	201	32/32	0.93	0.15	20,25,31,31	0
2	J2U	O	201	32/32	0.93	0.15	17,22,28,30	0
2	J2U	L	201	32/32	0.94	0.15	16,22,27,27	0
2	J2U	D	201	32/32	0.94	0.14	23,26,32,33	0
2	J2U	P	201	32/32	0.94	0.15	13,20,25,28	0
2	J2U	F	201	32/32	0.95	0.15	16,22,27,35	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 J2U C 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
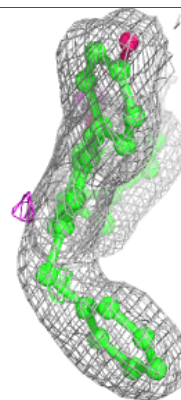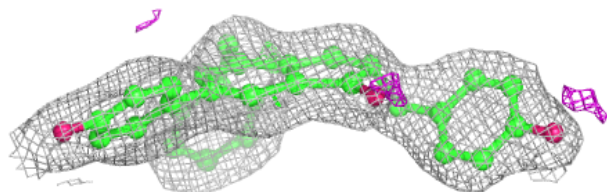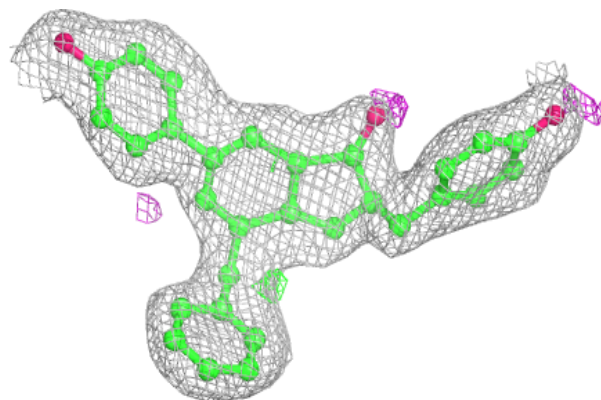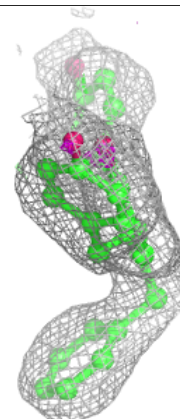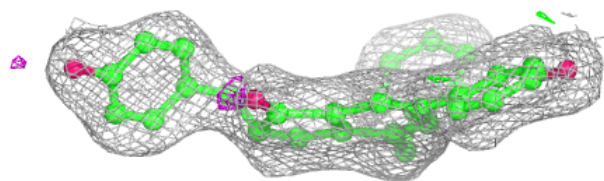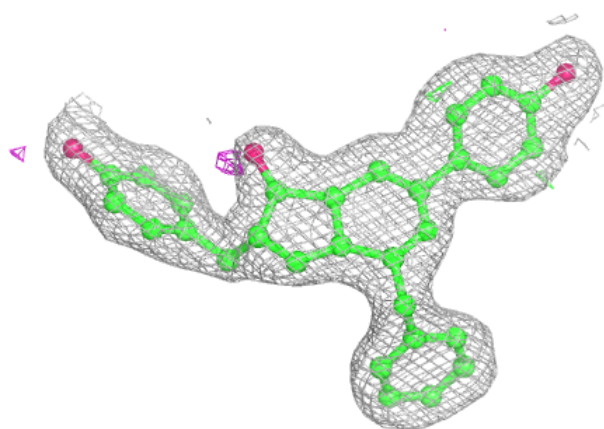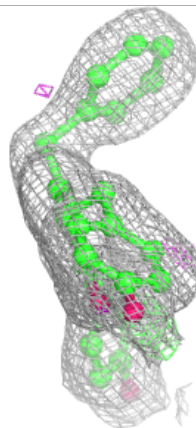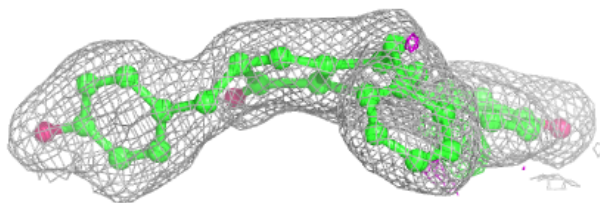mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
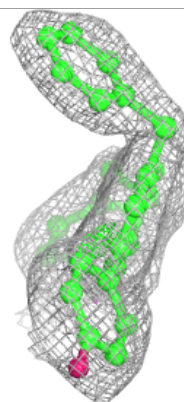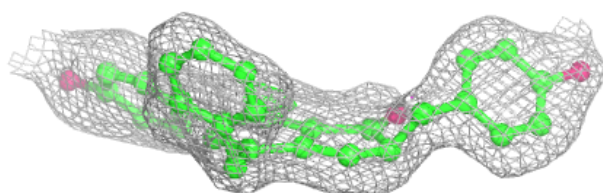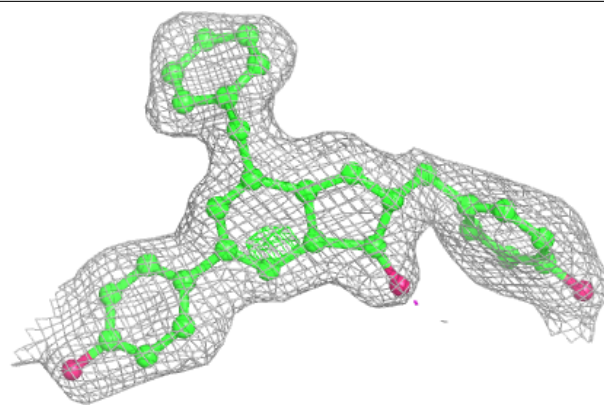
Electron density around J2U K 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
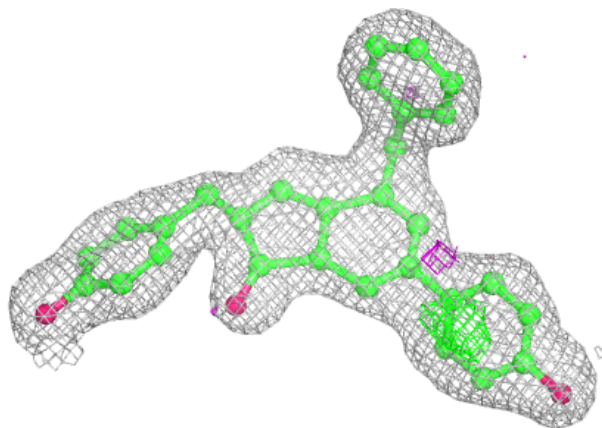and green (positive)
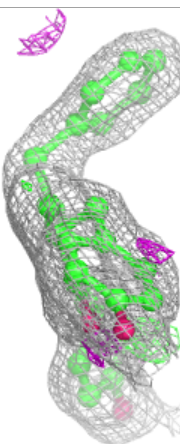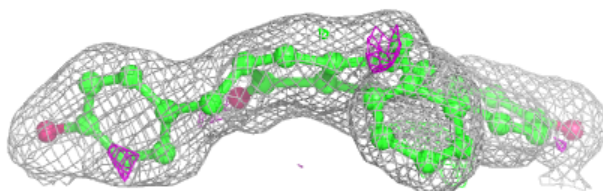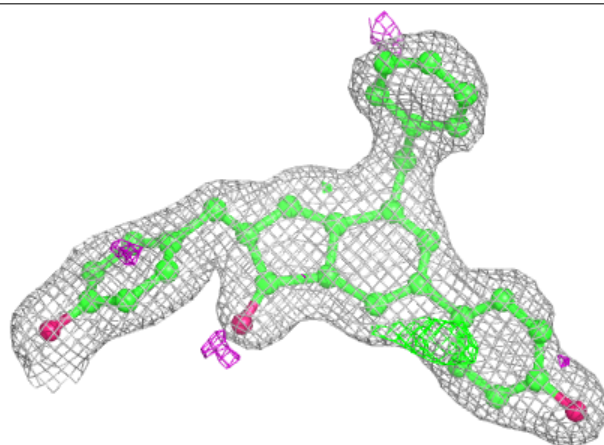
Electron density around J2U M 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
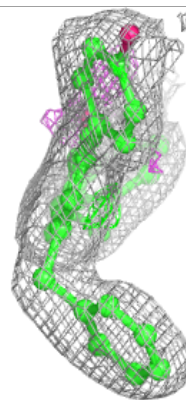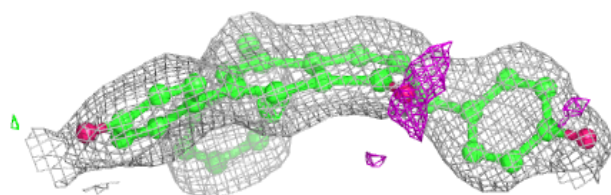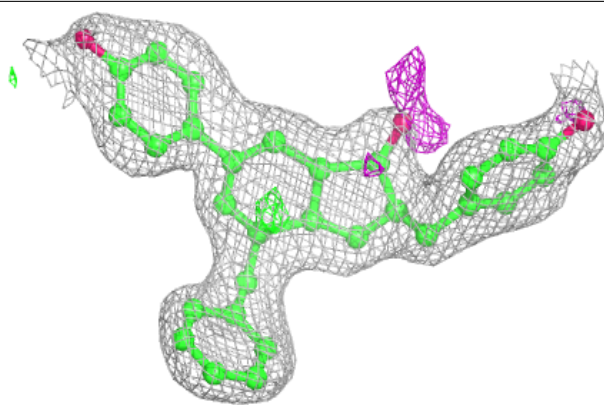
Electron density around J2U A 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
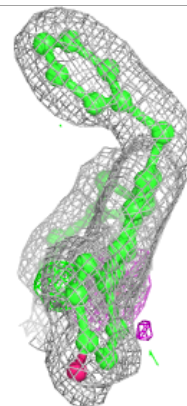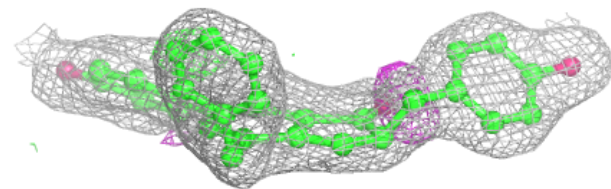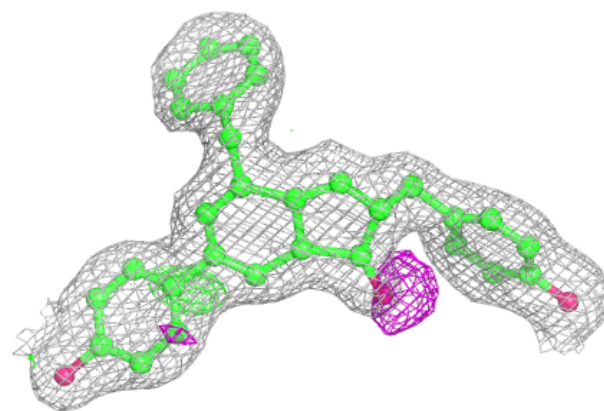
Electron density around J2U E 201:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
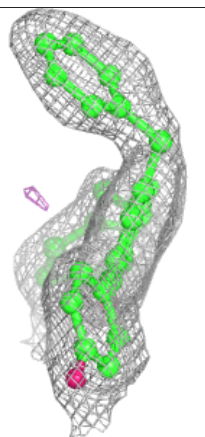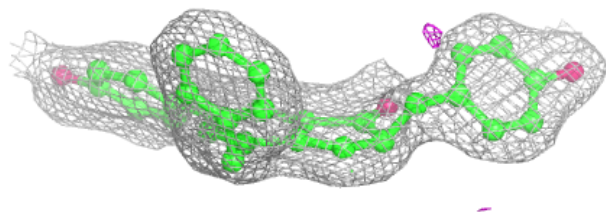and green (positive)
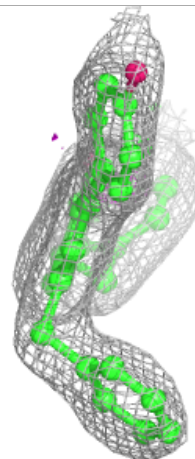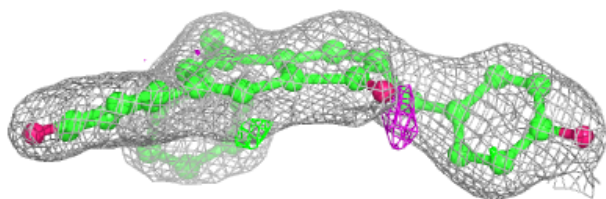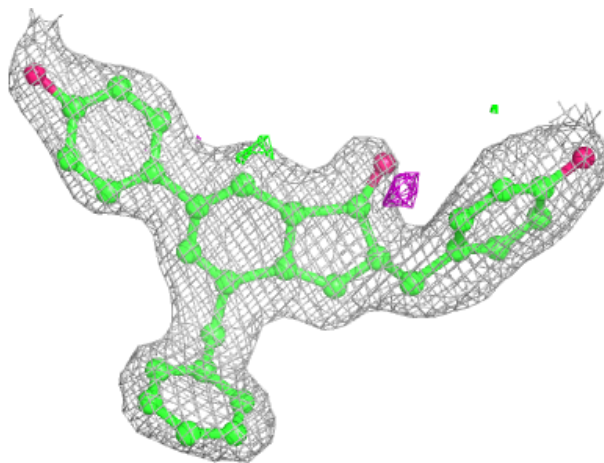
Electron density around J2U H 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
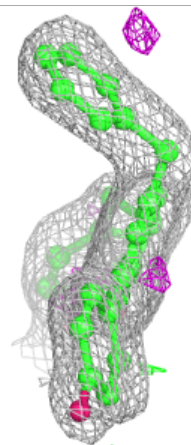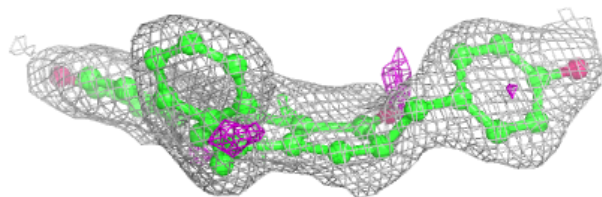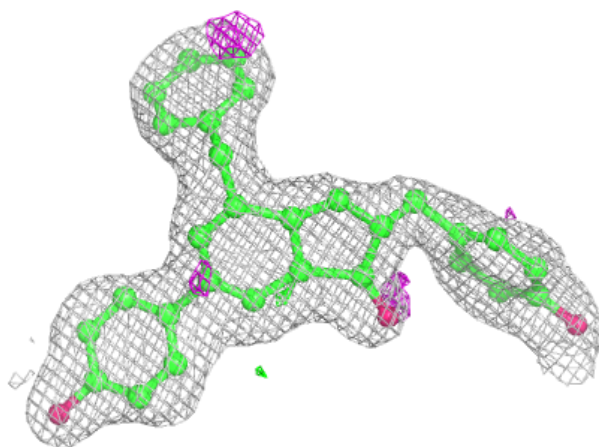
Electron density around J2U I 201:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
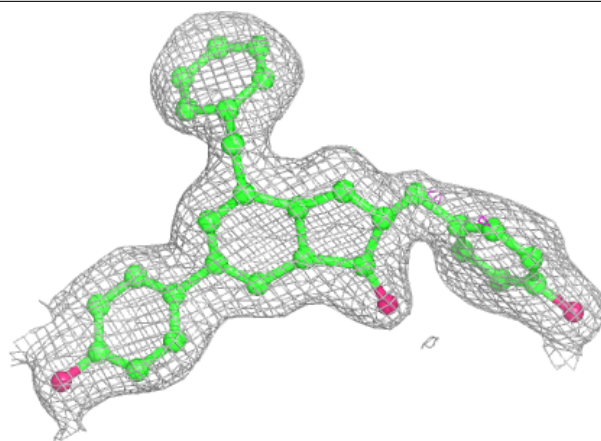and green (positive)
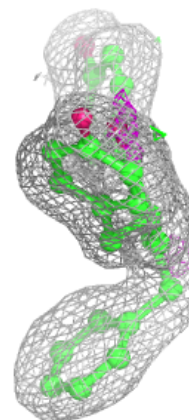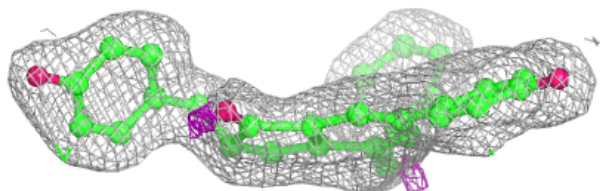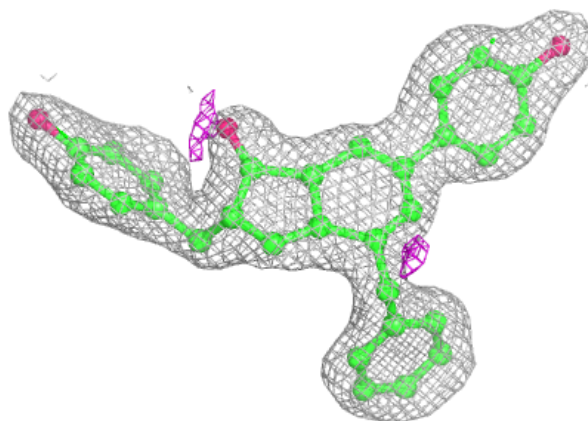
Electron density around J2U J 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
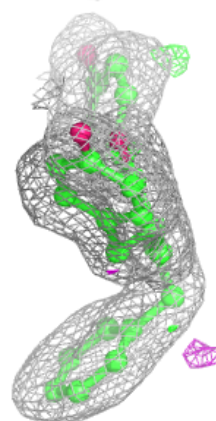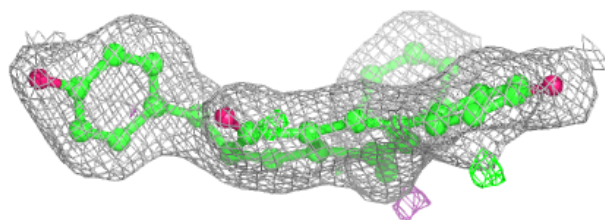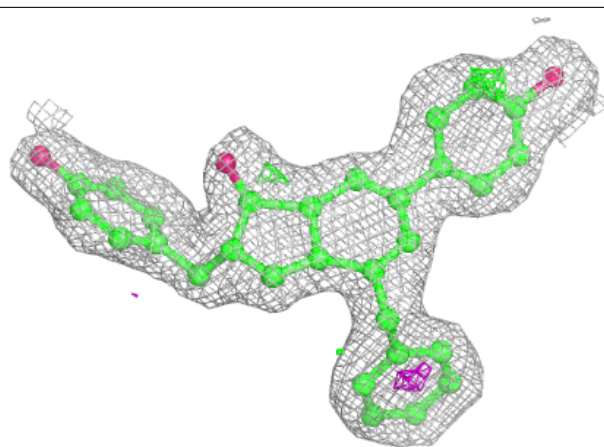
Electron density around J2U B 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
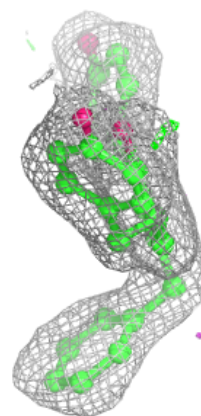mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
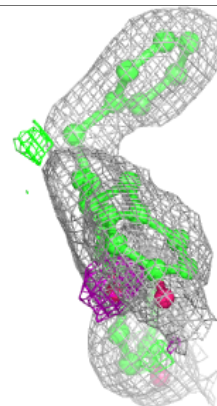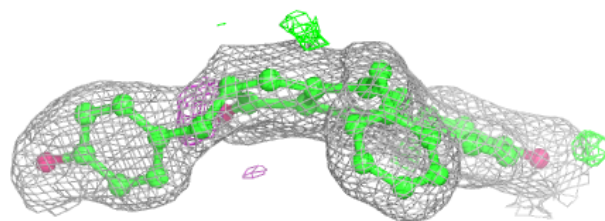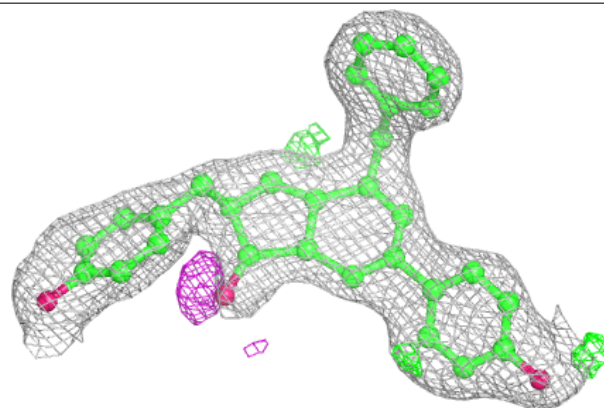
Electron density around J2U G 201:

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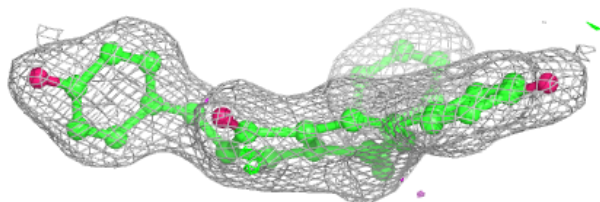and green (positive)
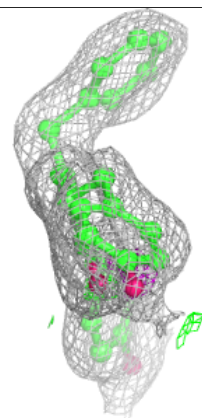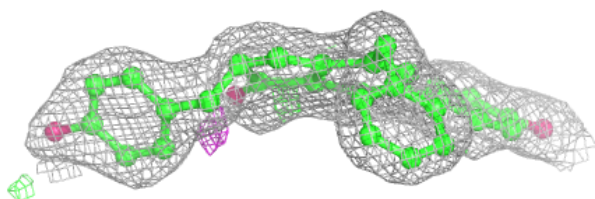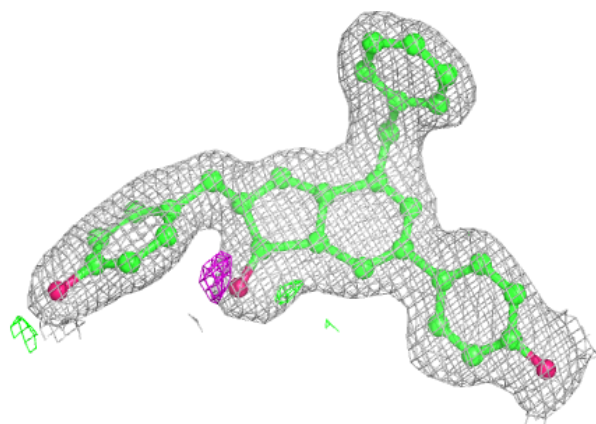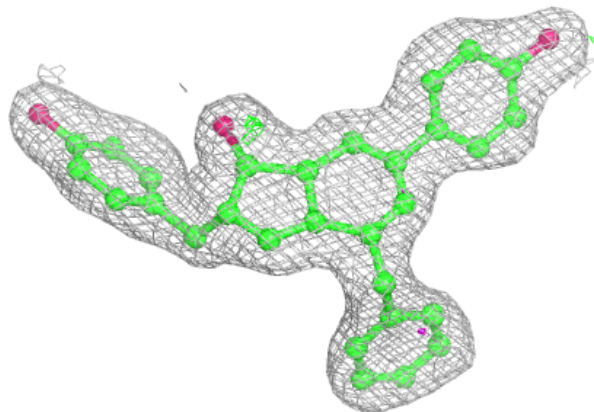

Electron density around J2U N 201:

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

Electron density around J2U O 201:

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

Electron density around J2U L 201:

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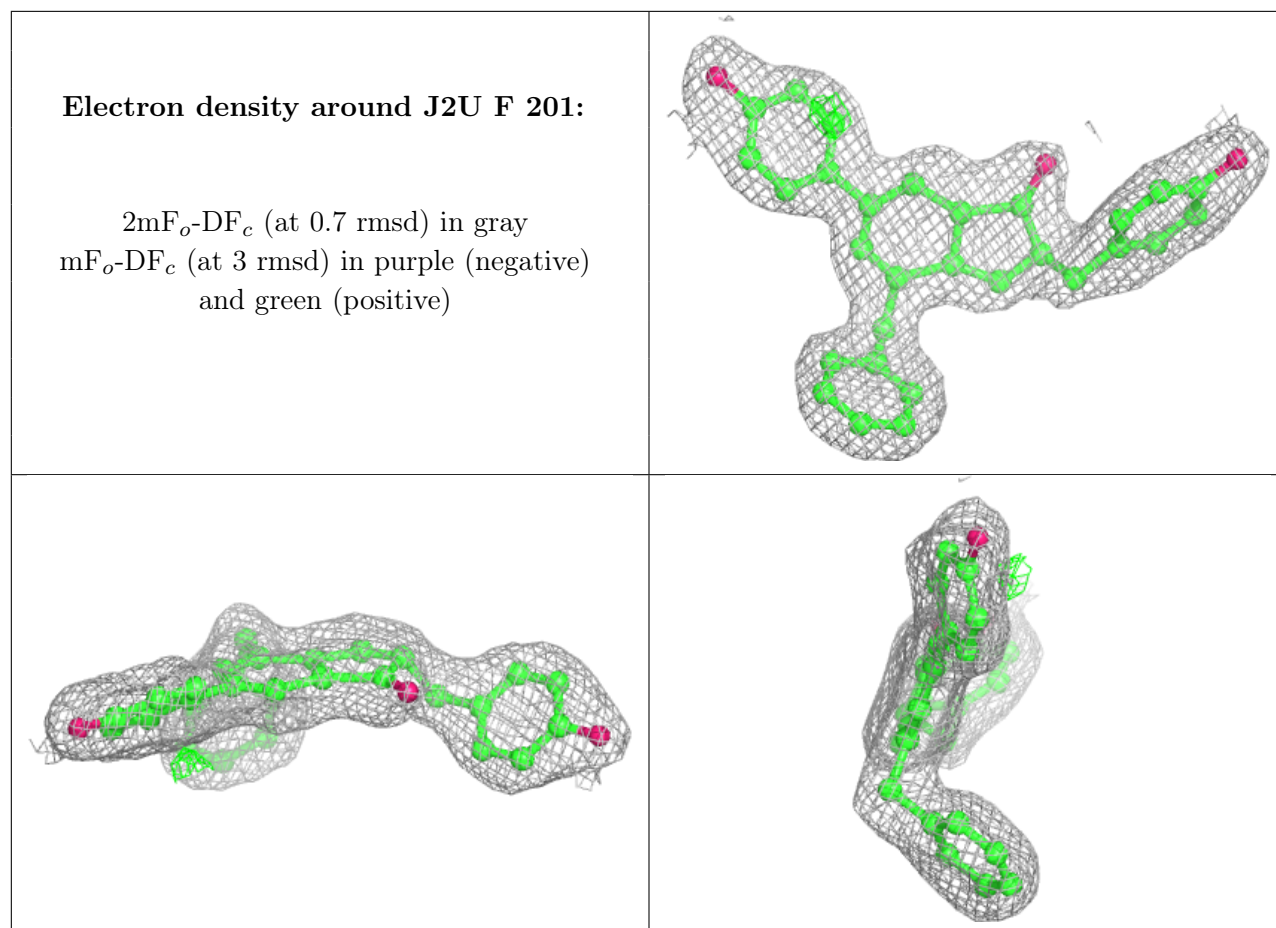and green (positive)

Electron density around J2U D 201:

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

Electron density around J2U P 201:

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

Electron density around J2U F 201:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.