



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 4, 2020 – 12:13 PM EST

PDB ID : 6WV7  
Title : Human VKOR with Chlorophacinone  
Authors : Liu, S.; Sukumar, N.; Li, W.  
Deposited on : 2020-05-05  
Resolution : 2.48 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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 : 2.14.6  
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) : 2.14.6

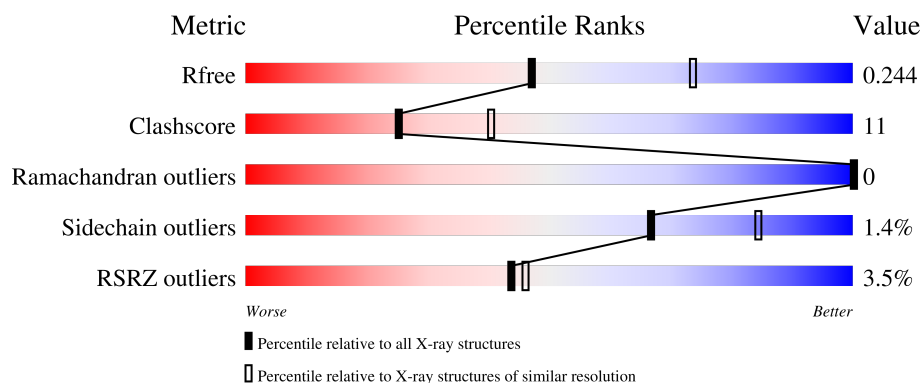
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.48 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	390	
1	B	390	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6401 atoms, of which 30 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 Vitamin K epoxide reductase, termini restrained by green fluorescent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	0	0
			3018	1935	521	548	14			
1	B	389	Total	C	N	O	S	0	0	0
			3096	1981	544	557	14			

There are 34 discrepancies between the modelled and reference sequences:

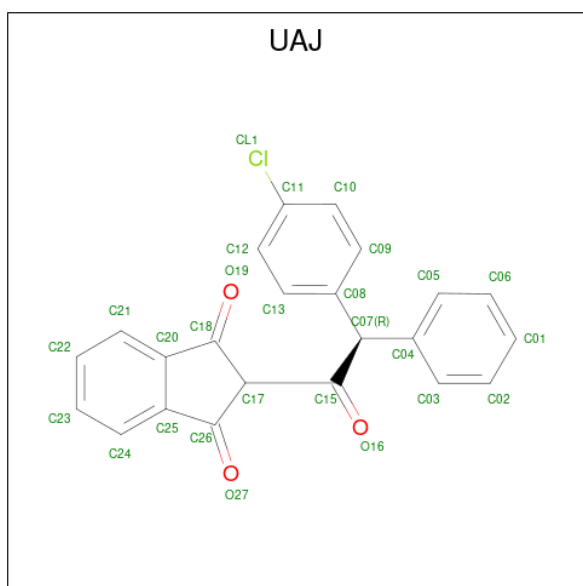
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	ARG	conflict	UNP A0A059PIQ0
A	30	ARG	SER	conflict	UNP A0A059PIQ0
A	66	CRO	THR	chromophore	UNP A0A059PIQ0
A	66	CRO	TYR	chromophore	UNP A0A059PIQ0
A	66	CRO	GLY	chromophore	UNP A0A059PIQ0
A	72	SER	ALA	conflict	UNP A0A059PIQ0
A	80	ARG	GLN	conflict	UNP A0A059PIQ0
A	358	VAL	ALA	conflict	UNP A0A059PIQ0
A	384	HIS	-	expression tag	UNP A0A059PIQ0
A	385	HIS	-	expression tag	UNP A0A059PIQ0
A	386	HIS	-	expression tag	UNP A0A059PIQ0
A	387	HIS	-	expression tag	UNP A0A059PIQ0
A	388	HIS	-	expression tag	UNP A0A059PIQ0
A	389	HIS	-	expression tag	UNP A0A059PIQ0
A	390	HIS	-	expression tag	UNP A0A059PIQ0
A	391	HIS	-	expression tag	UNP A0A059PIQ0
A	392	HIS	-	expression tag	UNP A0A059PIQ0
B	2	SER	ARG	conflict	UNP A0A059PIQ0
B	30	ARG	SER	conflict	UNP A0A059PIQ0
B	66	CRO	THR	chromophore	UNP A0A059PIQ0
B	66	CRO	TYR	chromophore	UNP A0A059PIQ0
B	66	CRO	GLY	chromophore	UNP A0A059PIQ0
B	72	SER	ALA	conflict	UNP A0A059PIQ0
B	80	ARG	GLN	conflict	UNP A0A059PIQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	358	VAL	ALA	conflict	UNP A0A059PIQ0
B	384	HIS	-	expression tag	UNP A0A059PIQ0
B	385	HIS	-	expression tag	UNP A0A059PIQ0
B	386	HIS	-	expression tag	UNP A0A059PIQ0
B	387	HIS	-	expression tag	UNP A0A059PIQ0
B	388	HIS	-	expression tag	UNP A0A059PIQ0
B	389	HIS	-	expression tag	UNP A0A059PIQ0
B	390	HIS	-	expression tag	UNP A0A059PIQ0
B	391	HIS	-	expression tag	UNP A0A059PIQ0
B	392	HIS	-	expression tag	UNP A0A059PIQ0

- Molecule 2 is Chlorophacinone (three-letter code: UAJ) (formula:  $C_{23}H_{15}ClO_3$ ) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	H	O	0	0
			42	23	1	15	3		
2	B	1	Total	C	Cl	H	O	0	0
			42	23	1	15	3		

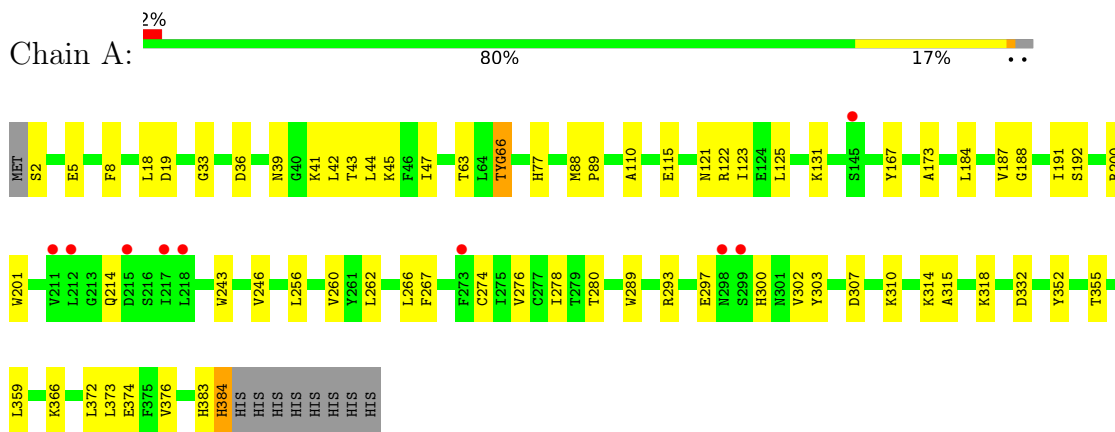
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	99	Total	O	0	0
			99	99		
3	B	104	Total	O	0	0
			104	104		

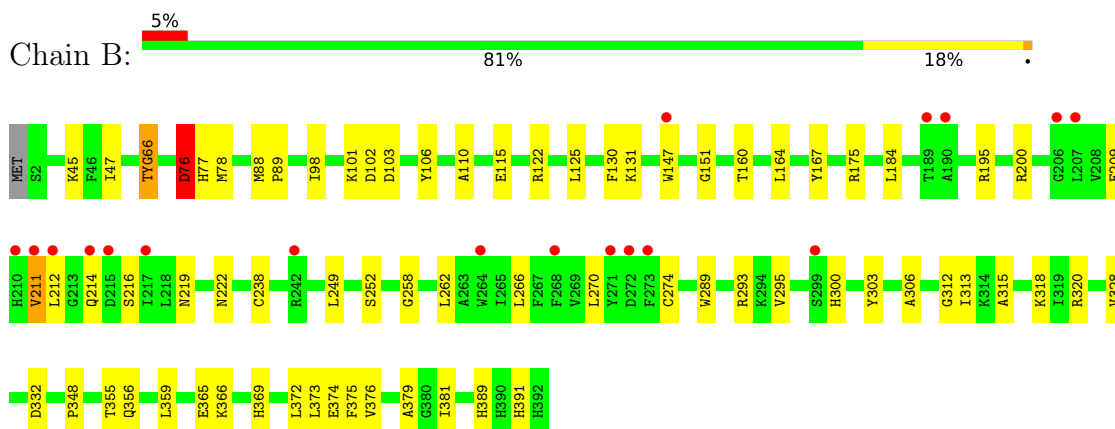
### 3 Residue-property plots

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: Vitamin K epoxide reductase, termini restrained by green fluorescent protein



- Molecule 1: Vitamin K epoxide reductase, termini restrained by green fluorescent protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.56Å 82.57Å 78.78Å 93.39° 97.36° 104.21°	Depositor
Resolution (Å)	34.74 – 2.48 36.90 – 2.48	Depositor EDS
% Data completeness (in resolution range)	86.2 (34.74-2.48) 86.3 (36.90-2.48)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.45 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, $R_{free}$	0.200 , 0.245 0.200 , 0.244	Depositor DCC
$R_{free}$ test set	1582 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.8	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 46.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6401	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UAJ, CRO

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	0.33	0/3064	0.54	0/4151
1	B	0.32	0/3150	0.54	1/4269 (0.0%)
All	All	0.33	0/6214	0.54	1/8420 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	76	ASP	CB-CG-OD1	6.05	123.74	118.30

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	3018	0	2997	64	0
1	B	3096	0	3047	70	0
2	A	27	15	0	5	0
2	B	27	15	0	3	0
3	A	99	0	0	9	0
3	B	104	0	0	20	0
All	All	6371	30	6044	131	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 11.

All (131) 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:B:214:GLN:NE2	3:B:502:HOH:O	1.90	1.04
1:B:312:GLY:O	3:B:501:HOH:O	1.81	0.98
1:B:101:LYS:NZ	3:B:505:HOH:O	2.01	0.93
1:A:43:THR:HG22	1:A:373:LEU:HD13	1.49	0.91
1:A:2:SER:N	3:A:502:HOH:O	2.10	0.84
1:B:131:LYS:O	3:B:504:HOH:O	1.96	0.83
1:B:306:ALA:HA	3:B:501:HOH:O	1.75	0.83
1:B:209:GLU:OE1	3:B:503:HOH:O	1.95	0.82
1:B:300:HIS:NE2	1:B:355:THR:O	2.12	0.82
1:B:293:ARG:NH1	3:B:508:HOH:O	2.05	0.79
1:B:355:THR:HG22	1:B:376:VAL:HG22	1.65	0.78
1:B:175:ARG:HD2	3:B:521:HOH:O	1.84	0.78
1:B:356:GLN:OE1	3:B:507:HOH:O	2.05	0.75
1:A:66:CRO:HG13	1:A:66:CRO:N2	2.02	0.74
1:B:355:THR:HG22	1:B:376:VAL:HG13	1.68	0.74
1:A:5:GLU:OE2	3:A:501:HOH:O	2.06	0.73
1:B:115:GLU:OE2	1:B:122:ARG:NH1	2.22	0.72
1:A:43:THR:HG22	1:A:373:LEU:CD1	2.21	0.71
1:A:355:THR:HG22	1:A:376:VAL:HG22	1.72	0.71
1:B:76:ASP:OD1	1:B:389:HIS:NE2	2.21	0.71
1:B:214:GLN:HA	1:B:219:ASN:ND2	2.06	0.70
1:A:355:THR:HG22	1:A:376:VAL:HG13	1.74	0.70
1:B:348:PRO:O	3:B:509:HOH:O	2.10	0.70
1:B:212:LEU:HB2	1:B:216:SER:HB2	1.74	0.69
1:A:266:LEU:HD21	1:A:274:CYS:HB3	1.73	0.68
1:B:214:GLN:HA	1:B:219:ASN:HD22	1.57	0.67
1:A:173:ALA:O	3:A:503:HOH:O	2.11	0.67
1:A:121:ASN:ND2	1:A:123:ILE:HD11	2.09	0.67
1:A:280:THR:HG21	2:A:400:UAJ:C01	2.25	0.66
1:A:384:HIS:NE2	3:A:506:HOH:O	2.22	0.63
1:B:212:LEU:CB	1:B:216:SER:HB2	2.29	0.62
1:B:262:LEU:HB3	2:B:400:UAJ:C21	2.32	0.60
1:B:306:ALA:O	3:B:510:HOH:O	2.16	0.59
1:B:313:ILE:HG22	3:B:501:HOH:O	2.02	0.59
1:B:359:LEU:CD2	1:B:372:LEU:HD13	2.33	0.59
1:A:318:LYS:HG2	1:A:332:ASP:OD1	2.03	0.58
1:B:355:THR:HG22	1:B:376:VAL:CG2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:SER:HA	3:B:513:HOH:O	2.05	0.56
1:B:212:LEU:HD13	3:B:549:HOH:O	2.04	0.56
1:A:8:PHE:HZ	1:A:88:MET:HG3	1.70	0.55
1:B:47:ILE:HD13	1:B:369:HIS:HB3	1.87	0.55
1:A:8:PHE:CZ	1:A:88:MET:HG3	2.42	0.55
1:B:355:THR:CG2	1:B:376:VAL:HG22	2.36	0.55
1:B:318:LYS:HG2	1:B:332:ASP:OD1	2.07	0.55
1:B:355:THR:HG22	1:B:376:VAL:CG1	2.37	0.55
1:A:131:LYS:HD3	1:B:184:LEU:HA	1.89	0.55
1:A:66:CRO:N2	1:A:66:CRO:HD1	2.21	0.54
1:A:355:THR:HG22	1:A:376:VAL:CG2	2.38	0.54
1:A:293:ARG:O	1:A:297:GLU:HG3	2.08	0.53
1:B:167:TYR:OH	1:B:184:LEU:HG	2.10	0.52
1:B:76:ASP:OD1	1:B:391:HIS:ND1	2.42	0.52
1:A:122:ARG:NH2	3:A:515:HOH:O	2.43	0.52
1:A:42:LEU:CD1	1:A:374:GLU:HB3	2.40	0.52
1:A:243:TRP:O	1:A:246:VAL:HG22	2.10	0.52
1:B:262:LEU:HD13	2:B:400:UAJ:C18	2.40	0.51
1:A:36:ASP:OD2	1:A:39:ASN:ND2	2.42	0.51
1:B:222:ASN:HB2	2:B:400:UAJ:O16	2.10	0.51
1:B:365:GLU:HB3	1:B:369:HIS:CE1	2.45	0.51
1:A:42:LEU:O	1:A:42:LEU:HD12	2.10	0.51
1:B:88:MET:HB3	1:B:89:PRO:HA	1.93	0.51
1:B:313:ILE:HA	3:B:501:HOH:O	2.11	0.51
1:A:289:TRP:HH2	1:A:293:ARG:HH21	1.58	0.50
1:A:43:THR:CG2	1:A:373:LEU:HD13	2.31	0.50
1:A:267:PHE:HZ	1:A:278:ILE:HD11	1.77	0.50
1:A:355:THR:HG22	1:A:376:VAL:CG1	2.40	0.50
1:A:276:VAL:O	1:A:280:THR:HG23	2.12	0.50
1:A:41:LYS:HE2	3:A:582:HOH:O	2.13	0.49
1:B:151:GLY:HA3	3:B:562:HOH:O	2.12	0.49
1:B:366:LYS:NZ	3:B:522:HOH:O	2.46	0.49
1:A:88:MET:HB3	1:A:89:PRO:HA	1.95	0.48
1:A:262:LEU:HD13	2:A:400:UAJ:C17	2.42	0.48
1:B:195:ARG:NH1	3:B:514:HOH:O	2.41	0.48
1:B:209:GLU:N	3:B:516:HOH:O	2.46	0.48
1:A:276:VAL:HG12	2:A:400:UAJ:C06	2.44	0.48
1:A:266:LEU:HD13	2:A:400:UAJ:C23	2.45	0.47
1:A:184:LEU:HA	1:B:131:LYS:HD3	1.95	0.47
1:B:47:ILE:HD13	1:B:369:HIS:CB	2.44	0.47
1:A:110:ALA:HA	1:A:122:ARG:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:THR:CG2	1:A:123:ILE:HG21	2.45	0.47
1:B:249:LEU:HD22	1:B:295:VAL:HG21	1.98	0.46
1:B:373:LEU:HD23	1:B:374:GLU:N	2.30	0.46
1:B:110:ALA:HA	1:B:122:ARG:O	2.16	0.46
1:A:121:ASN:HD21	1:A:123:ILE:HD11	1.78	0.46
1:A:303:TYR:O	1:A:315:ALA:HA	2.16	0.46
1:A:359:LEU:CD2	1:A:372:LEU:HD13	2.47	0.45
1:B:115:GLU:CD	1:B:122:ARG:HH12	2.20	0.45
1:A:188:GLY:HA3	3:A:535:HOH:O	2.17	0.45
1:B:303:TYR:O	1:B:315:ALA:HA	2.17	0.45
1:A:187:VAL:HB	1:A:191:ILE:CG2	2.47	0.45
1:A:66:CRO:HG11	1:A:374:GLU:OE1	2.17	0.45
1:A:45:LYS:HE2	1:A:47:ILE:HD11	1.97	0.45
1:B:102:ASP:O	1:B:131:LYS:HE3	2.16	0.45
1:A:167:TYR:OH	1:A:184:LEU:HG	2.17	0.45
1:A:262:LEU:HD13	2:A:400:UAJ:C26	2.48	0.44
1:A:18:LEU:HD23	1:A:18:LEU:C	2.37	0.44
1:A:125:LEU:HD23	1:A:125:LEU:C	2.38	0.44
1:A:77:HIS:CE1	1:A:383:HIS:HB2	2.53	0.44
1:B:211:VAL:O	1:B:212:LEU:HB2	2.17	0.44
1:A:359:LEU:HD22	1:A:372:LEU:HD13	2.00	0.43
1:A:131:LYS:NZ	1:B:184:LEU:O	2.48	0.43
1:B:77:HIS:NE2	1:B:381:ILE:O	2.48	0.43
1:A:77:HIS:CD2	1:A:383:HIS:HB2	2.54	0.43
1:B:45:LYS:HE2	1:B:47:ILE:HD11	2.00	0.43
1:B:373:LEU:HD22	1:B:375:PHE:CE2	2.54	0.43
1:B:147:TRP:HA	1:B:238:CYS:O	2.18	0.43
1:B:125:LEU:C	1:B:125:LEU:HD23	2.39	0.43
1:A:18:LEU:HD23	1:A:19:ASP:N	2.34	0.42
1:A:192:SER:HB2	3:A:565:HOH:O	2.18	0.42
1:A:310:LYS:NZ	3:A:513:HOH:O	2.39	0.42
1:A:33:GLY:HA3	1:A:44:LEU:HD23	2.00	0.42
1:B:214:GLN:CA	1:B:219:ASN:HD22	2.30	0.42
1:B:379:ALA:HB1	3:B:538:HOH:O	2.19	0.42
1:A:267:PHE:CZ	1:A:278:ILE:HD11	2.53	0.42
1:A:302:VAL:O	1:A:352:TYR:HA	2.18	0.42
1:B:266:LEU:O	1:B:270:LEU:O	2.38	0.42
1:A:66:CRO:N2	1:A:66:CRO:CG1	2.78	0.42
1:B:98:ILE:HB	1:B:106:TYR:HB2	2.02	0.42
1:A:256:LEU:O	1:A:260:VAL:HG23	2.20	0.42
1:B:289:TRP:HH2	1:B:293:ARG:HH21	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:ARG:HB3	1:B:328:VAL:CG1	2.51	0.41
1:B:266:LEU:HD21	1:B:274:CYS:HB3	2.02	0.41
1:B:103:ASP:OD1	1:B:130:PHE:HA	2.19	0.41
1:A:115:GLU:OE2	1:A:122:ARG:NH1	2.54	0.41
1:B:66:CRO:HD1	1:B:66:CRO:N2	2.35	0.41
1:B:160:THR:O	1:B:164:LEU:HG	2.20	0.41
1:A:384:HIS:N	1:A:384:HIS:CD2	2.89	0.41
1:B:258:GLY:O	1:B:262:LEU:HG	2.21	0.41
1:B:77:HIS:CD2	1:B:78:MET:HG3	2.56	0.40
1:B:359:LEU:HD22	1:B:372:LEU:HD13	2.03	0.40
1:A:187:VAL:HB	1:A:191:ILE:HB	2.03	0.40
1:A:307:ASP:OD2	1:A:314:LYS:HD2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	376/390 (96%)	368 (98%)	8 (2%)	0	100	100
1	B	384/390 (98%)	374 (97%)	10 (3%)	0	100	100
All	All	760/780 (97%)	742 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	328/339 (97%)	322 (98%)	6 (2%)	59	80
1	B	336/339 (99%)	333 (99%)	3 (1%)	78	91
All	All	664/678 (98%)	655 (99%)	9 (1%)	67	84

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	ARG
1	A	201	TRP
1	A	214	GLN
1	A	300	HIS
1	A	366	LYS
1	A	384	HIS
1	B	76	ASP
1	B	200	ARG
1	B	211	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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
1	CRO	A	66	1	23,23,24	2.73	8 (34%)	30,32,34	2.70	11 (36%)
1	CRO	B	66	1	23,23,24	2.51	8 (34%)	30,32,34	2.93	10 (33%)

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
1	CRO	A	66	1	-	6/12/31/32	0/2/2/2
1	CRO	B	66	1	-	3/12/31/32	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	CRO	C1-N2	7.19	1.42	1.32
1	B	66	CRO	C1-N2	6.78	1.42	1.32
1	A	66	CRO	CA2-C2	6.26	1.54	1.48
1	A	66	CRO	C1-N3	5.09	1.45	1.37
1	B	66	CRO	CA2-C2	4.71	1.53	1.48
1	B	66	CRO	C1-N3	4.36	1.44	1.37
1	B	66	CRO	CB2-CA2	-4.28	1.31	1.35
1	A	66	CRO	C2-N3	3.66	1.48	1.39
1	A	66	CRO	CG2-CB2	3.65	1.53	1.46
1	B	66	CRO	C2-N3	3.57	1.48	1.39
1	A	66	CRO	CB2-CA2	-3.29	1.32	1.35
1	B	66	CRO	CG2-CB2	3.07	1.52	1.46
1	A	66	CRO	O2-C2	-2.21	1.18	1.23
1	B	66	CRO	O2-C2	-2.16	1.18	1.23
1	A	66	CRO	CA2-N2	2.08	1.43	1.38
1	B	66	CRO	CA2-N2	2.01	1.42	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	CRO	O2-C2-CA2	-9.56	125.59	130.96
1	B	66	CRO	CA2-C2-N3	7.57	106.95	103.37
1	A	66	CRO	CA2-C2-N3	7.54	106.94	103.37
1	A	66	CRO	O2-C2-CA2	-5.83	127.68	130.96
1	B	66	CRO	C2-N3-C1	-5.64	105.11	107.97
1	A	66	CRO	CG2-CB2-CA2	-5.03	123.78	129.94
1	A	66	CRO	C2-N3-C1	-4.77	105.55	107.97
1	A	66	CRO	CA2-N2-C1	4.49	109.08	105.77
1	A	66	CRO	CB2-CA2-C2	3.40	126.33	122.28
1	B	66	CRO	CG2-CB2-CA2	-3.38	125.81	129.94
1	A	66	CRO	C2-CA2-N2	-3.32	106.61	108.93
1	B	66	CRO	CA2-N2-C1	3.14	108.09	105.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	CRO	CA1-C1-N3	-3.13	120.99	124.75
1	B	66	CRO	CA1-C1-N3	-3.10	121.03	124.75
1	B	66	CRO	O3-C3-CA3	-3.07	117.11	126.39
1	A	66	CRO	C1-CA1-N1	-2.59	105.76	109.96
1	B	66	CRO	C2-CA2-N2	-2.56	107.14	108.93
1	A	66	CRO	CA1-C1-N2	2.34	127.16	123.89
1	B	66	CRO	CA3-N3-C2	2.21	128.86	123.80
1	A	66	CRO	O3-C3-CA3	-2.17	119.84	126.39
1	B	66	CRO	CD2-CG2-CD1	2.02	120.63	117.64

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66	CRO	N2-C1-CA1-CB1
1	A	66	CRO	N3-C1-CA1-CB1
1	A	66	CRO	C2-CA2-CB2-CG2
1	B	66	CRO	C2-CA2-CB2-CG2
1	A	66	CRO	N2-CA2-CB2-CG2
1	B	66	CRO	N2-CA2-CB2-CG2
1	A	66	CRO	C1-CA1-CB1-OG1
1	A	66	CRO	C3-CA3-N3-C2
1	B	66	CRO	C3-CA3-N3-C2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	66	CRO	4	0
1	B	66	CRO	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 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	UAJ	A	400	-	28,30,30	1.58	6 (21%)	37,43,43	1.48	9 (24%)
2	UAJ	B	400	-	28,30,30	1.63	4 (14%)	37,43,43	2.00	11 (29%)

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	UAJ	A	400	-	-	3/16/32/32	0/4/4/4
2	UAJ	B	400	-	-	1/16/32/32	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	UAJ	C20-C18	5.54	1.55	1.47
2	A	400	UAJ	C25-C26	4.48	1.54	1.47
2	A	400	UAJ	C20-C18	4.41	1.54	1.47
2	B	400	UAJ	C25-C26	3.91	1.53	1.47
2	A	400	UAJ	O27-C26	-2.81	1.18	1.22
2	B	400	UAJ	O19-C18	-2.65	1.18	1.22
2	A	400	UAJ	O16-C15	-2.46	1.17	1.21
2	B	400	UAJ	O27-C26	-2.45	1.18	1.22
2	A	400	UAJ	O19-C18	-2.21	1.19	1.22
2	A	400	UAJ	C11-CL1	2.04	1.78	1.74

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	UAJ	O16-C15-C07	-5.55	112.29	120.39
2	B	400	UAJ	C09-C08-C07	-4.14	112.34	120.85
2	B	400	UAJ	C12-C11-CL1	3.32	124.54	119.35
2	B	400	UAJ	C13-C08-C07	3.04	127.10	120.85
2	B	400	UAJ	C20-C25-C26	-3.00	107.72	110.03
2	B	400	UAJ	C10-C11-CL1	-2.98	114.69	119.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	UAJ	C12-C13-C08	-2.95	118.23	121.20
2	B	400	UAJ	O27-C26-C25	-2.80	123.69	127.11
2	B	400	UAJ	O16-C15-C17	-2.79	116.31	120.39
2	B	400	UAJ	C12-C13-C08	-2.71	118.47	121.20
2	A	400	UAJ	O16-C15-C07	-2.69	116.47	120.39
2	A	400	UAJ	C25-C20-C18	-2.54	108.08	110.03
2	A	400	UAJ	C09-C08-C07	-2.54	115.64	120.85
2	A	400	UAJ	C24-C25-C26	2.47	132.17	128.65
2	A	400	UAJ	O16-C15-C17	-2.42	116.86	120.39
2	A	400	UAJ	C20-C25-C26	-2.39	108.19	110.03
2	B	400	UAJ	C21-C20-C18	2.34	131.98	128.65
2	A	400	UAJ	C13-C08-C09	2.27	121.12	118.29
2	A	400	UAJ	O19-C18-C20	-2.25	124.36	127.11
2	B	400	UAJ	C05-C04-C07	-2.17	116.39	120.85

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	UAJ	C08-C07-C15-C17
2	B	400	UAJ	C07-C15-C17-C18
2	A	400	UAJ	C04-C07-C15-O16
2	A	400	UAJ	C07-C15-C17-C18

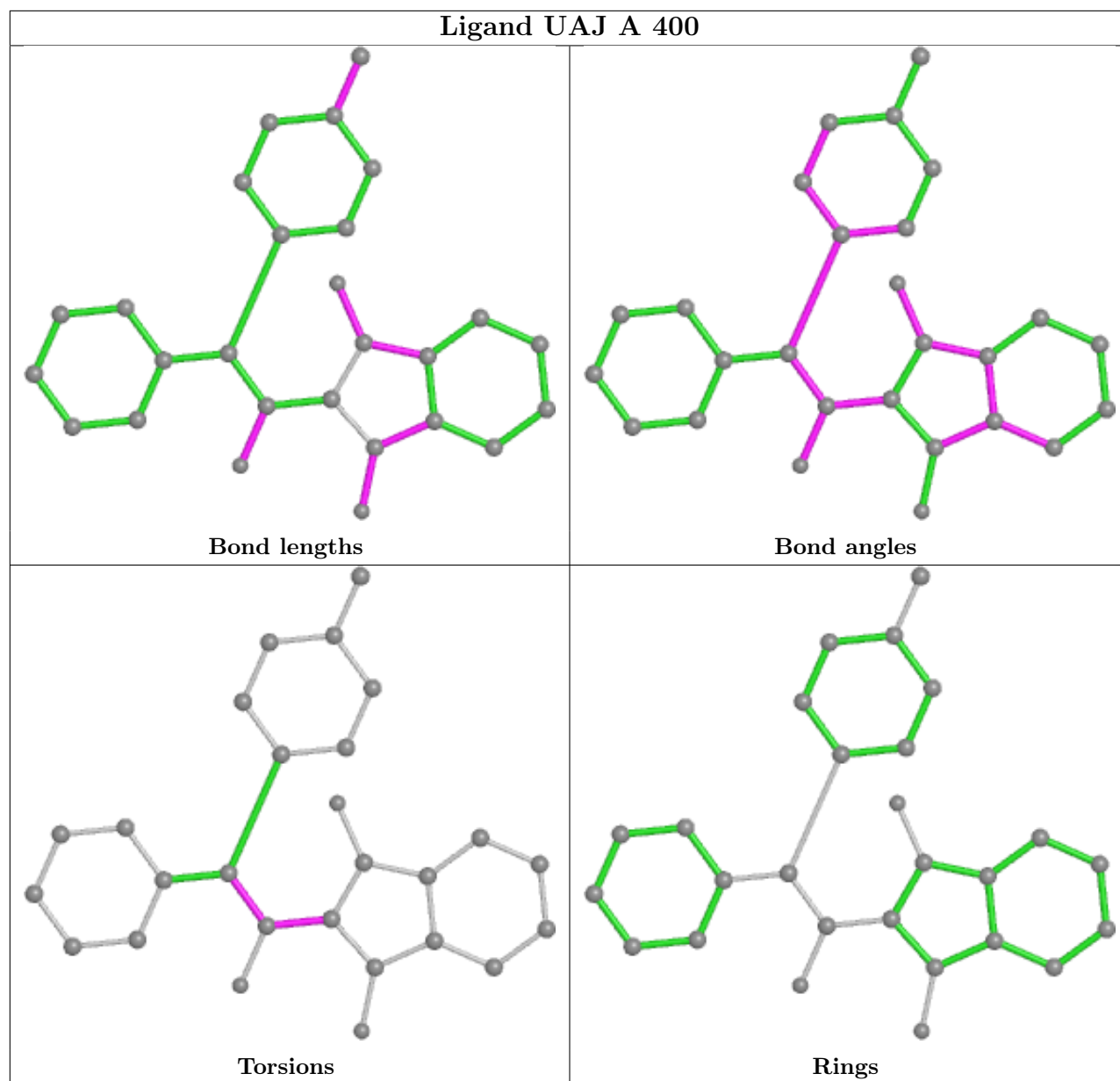
There are no ring outliers.

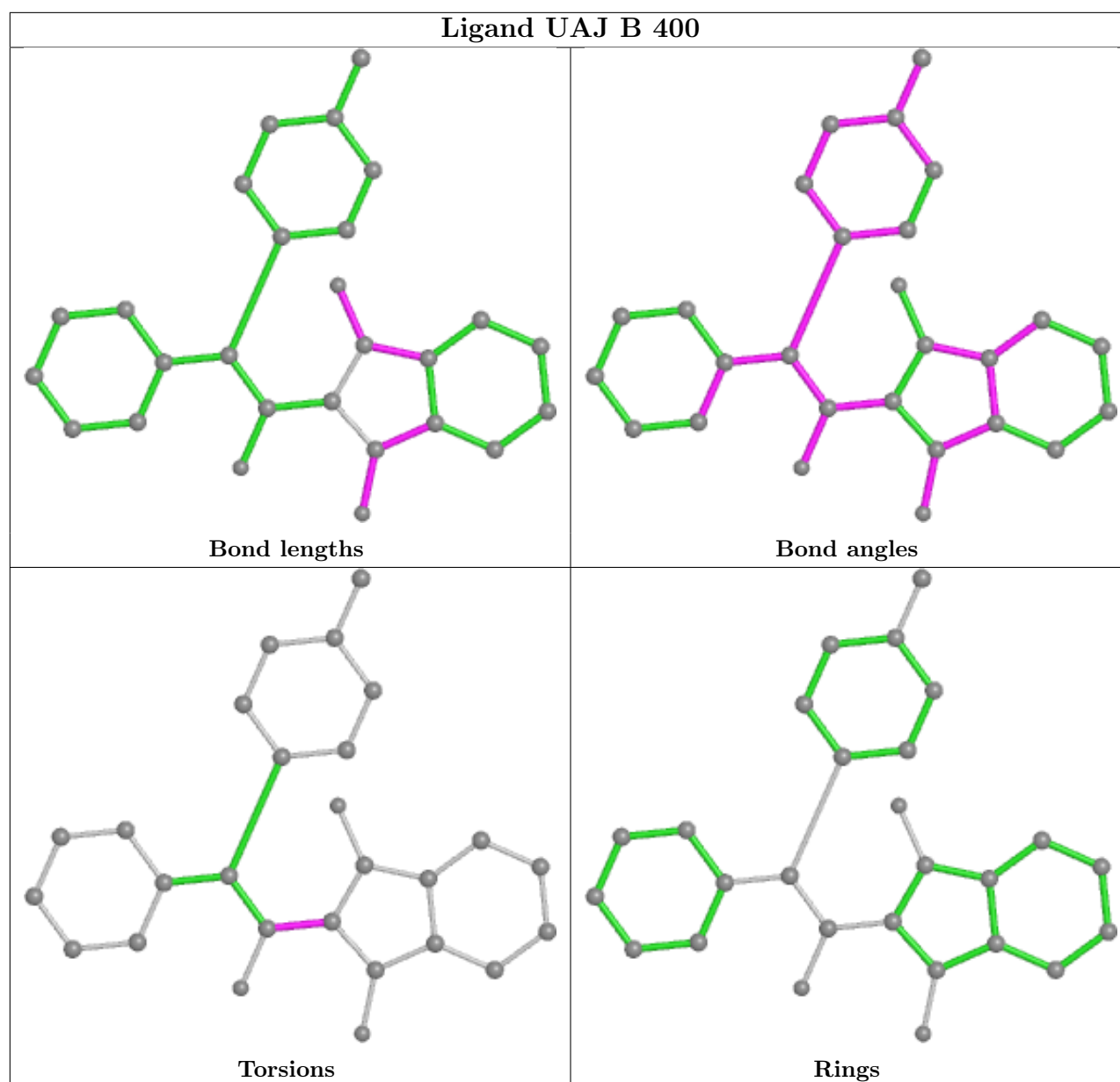
2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	UAJ	5	0
2	B	400	UAJ	3	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

### 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	380/390 (97%)	-0.15	9 (2%) 59 61	21, 34, 64, 84	0
1	B	388/390 (99%)	-0.06	18 (4%) 32 34	21, 39, 72, 94	0
All	All	768/780 (98%)	-0.11	27 (3%) 44 46	21, 37, 67, 94	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	189	THR	6.8
1	B	212	LEU	5.3
1	A	211	VAL	5.0
1	A	217	ILE	4.3
1	A	215	ASP	3.4
1	B	217	ILE	3.3
1	B	190	ALA	3.1
1	A	299	SER	3.0
1	B	214	GLN	2.9
1	A	298	ASN	2.8
1	B	215	ASP	2.8
1	A	212	LEU	2.8
1	B	299	SER	2.8
1	B	206	GLY	2.7
1	B	264	TRP	2.7
1	B	268	PHE	2.7
1	A	145	SER	2.6
1	B	271	TYR	2.6
1	A	218	LEU	2.5
1	B	211	VAL	2.5
1	B	273	PHE	2.4
1	B	147	TRP	2.3
1	A	273	PHE	2.2
1	B	207	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	242	ARG	2.2
1	B	210	HIS	2.2
1	B	272	ASP	2.1

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	CRO	A	66	22/23	0.96	0.15	22,28,35,39	0
1	CRO	B	66	22/23	0.98	0.16	19,26,29,35	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

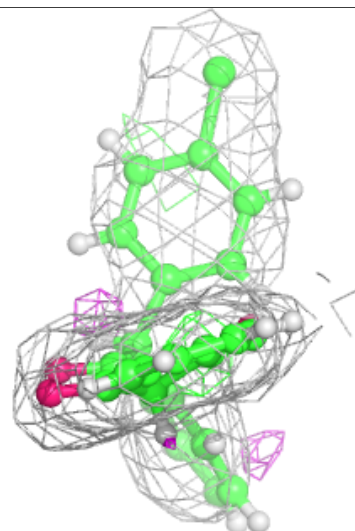
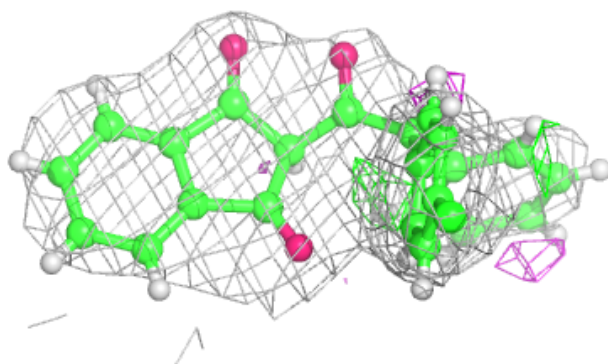
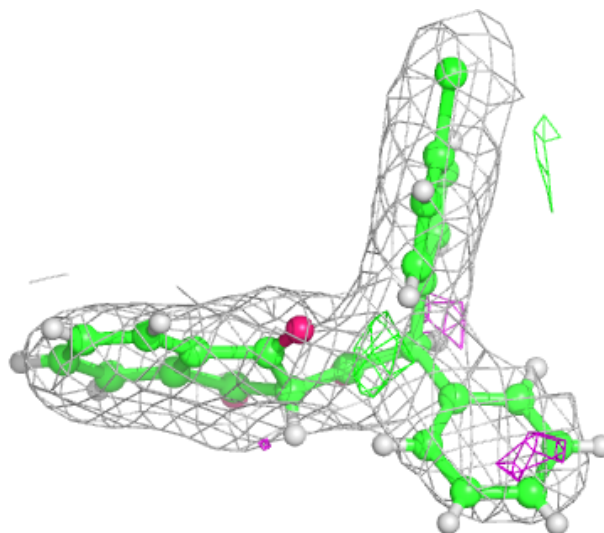
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

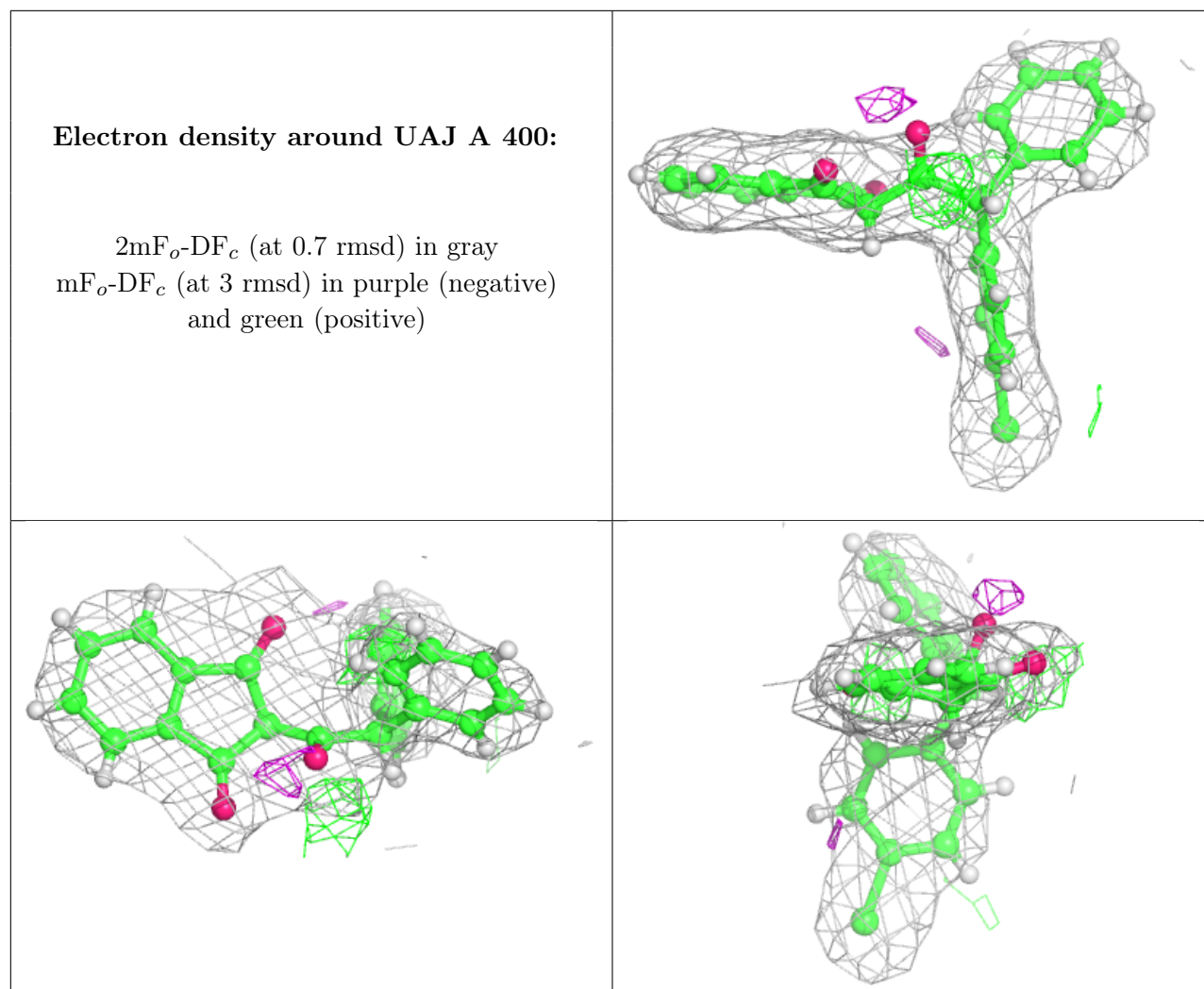
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	UAJ	B	400	27/27	0.92	0.17	33,44,56,60	0
2	UAJ	A	400	27/27	0.94	0.16	16,37,48,55	0

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 UAJ B 400:**

$2mF_o-DF_c$  (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.