



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:37 AM UTC

PDB ID : 2OM9 / pdb_00002om9
Title : Ajulemic acid, a synthetic cannabinoid bound to PPAR gamma
Authors : Ambrosio, A.L.B.; Garratt, R.C.
Deposited on : 2007-01-21
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

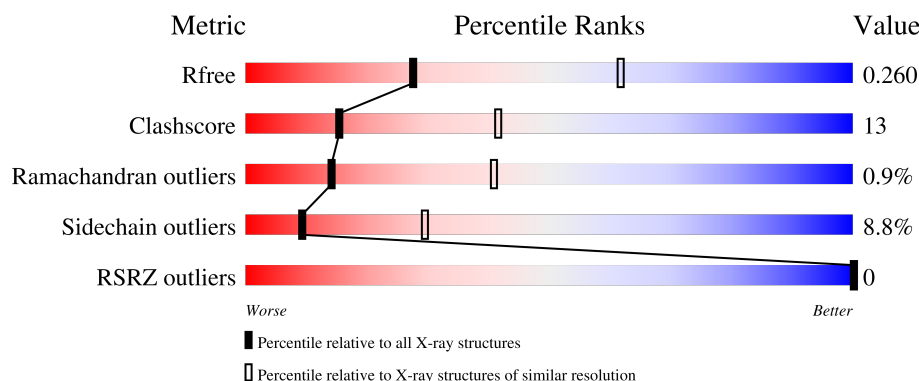
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

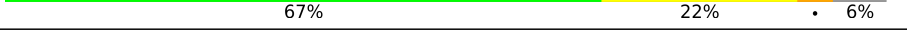
The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 $\leq 5\%$. 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	278	 72% 22% 6%
1	B	278	 68% 23% 6% 3%
1	C	278	 71% 24% 6%
1	D	278	 67% 22% 6% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8965 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.

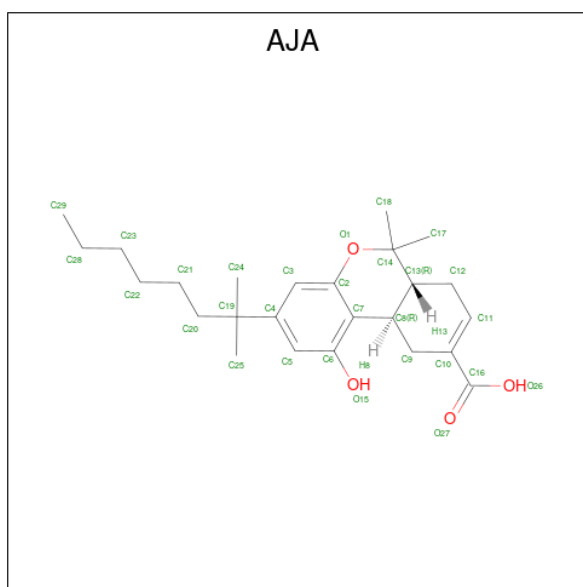
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	1	0
			2171	1401	354	406	10			
1	B	260	Total	C	N	O	S	0	0	0
			2089	1353	341	385	10			
1	C	270	Total	C	N	O	S	0	1	0
			2171	1401	354	406	10			
1	D	260	Total	C	N	O	S	0	0	0
			2089	1353	341	385	10			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	200	GLY	-	expression tag	UNP P37231
A	201	SER	-	expression tag	UNP P37231
A	202	HIS	-	expression tag	UNP P37231
A	203	MET	-	expression tag	UNP P37231
B	200	GLY	-	expression tag	UNP P37231
B	201	SER	-	expression tag	UNP P37231
B	202	HIS	-	expression tag	UNP P37231
B	203	MET	-	expression tag	UNP P37231
C	200	GLY	-	expression tag	UNP P37231
C	201	SER	-	expression tag	UNP P37231
C	202	HIS	-	expression tag	UNP P37231
C	203	MET	-	expression tag	UNP P37231
D	200	GLY	-	expression tag	UNP P37231
D	201	SER	-	expression tag	UNP P37231
D	202	HIS	-	expression tag	UNP P37231
D	203	MET	-	expression tag	UNP P37231

- Molecule 2 is (6AR,10AR)-3-(1,1-DIMETHYLHEPTYL)-1-HYDROXY-6,6-DIMETHYL-6 A,7,10,10A-TETRAHYDRO-6H-BENZO[C]CHROMENE-9-CARBOXYLIC ACID (CCD ID: AJA) (formula: C₂₅H₃₆O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 29 25 4	0	0
2	A	1	Total C O 29 25 4	0	0
2	B	1	Total C O 29 25 4	0	0
2	B	1	Total C O 29 25 4	0	0
2	C	1	Total C O 29 25 4	0	0
2	C	1	Total C O 29 25 4	0	0
2	D	1	Total C O 29 25 4	0	0
2	D	1	Total C O 29 25 4	0	0

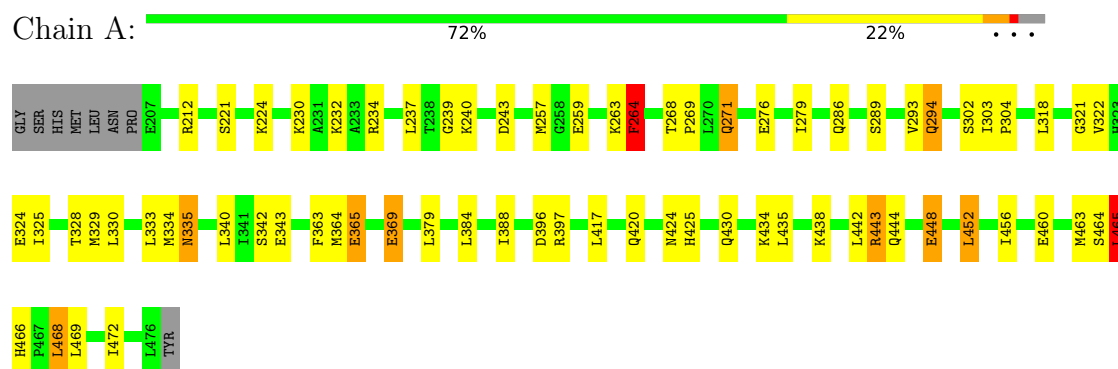
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	65	Total O 65 65	0	0
3	B	46	Total O 46 46	0	0
3	C	61	Total O 61 61	0	0
3	D	41	Total O 41 41	0	0

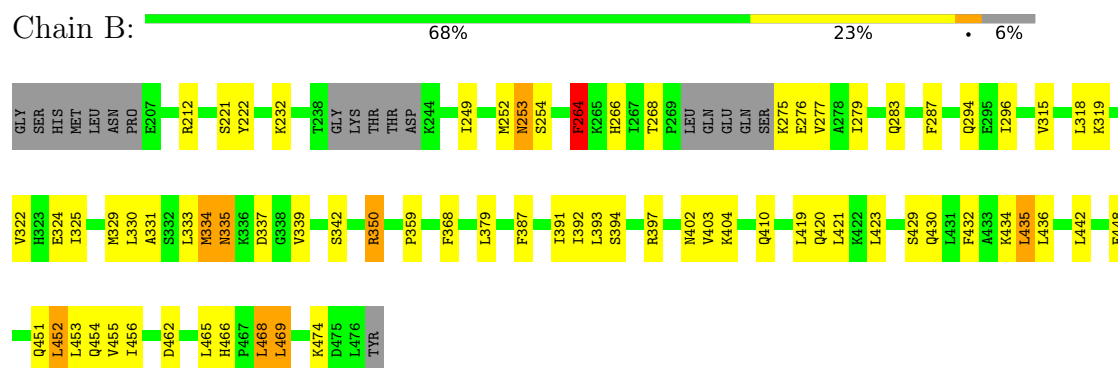
3 Residue-property plots

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.

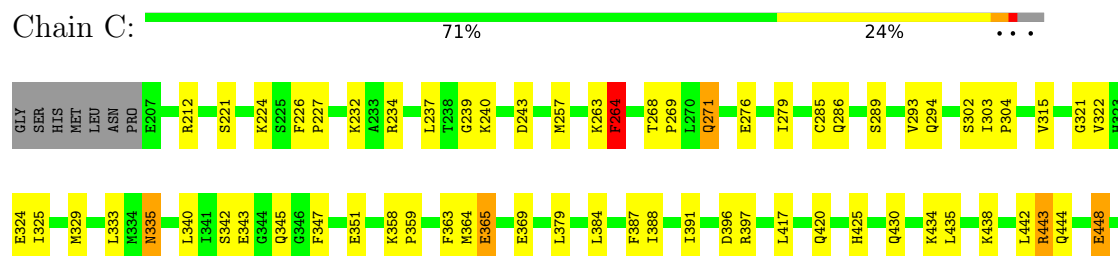
- Molecule 1: Peroxisome proliferator-activated receptor gamma

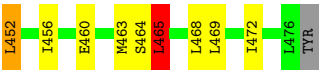


- Molecule 1: Peroxisome proliferator-activated receptor gamma

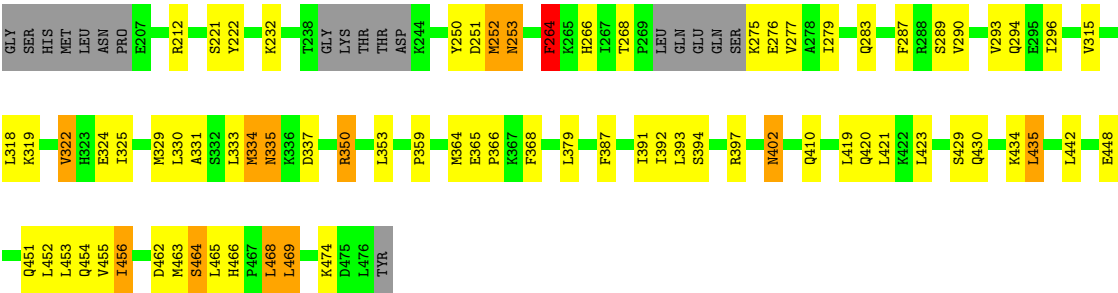


- Molecule 1: Peroxisome proliferator-activated receptor gamma





● Molecule 1: Peroxisome proliferator-activated receptor gamma



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.34Å 78.14Å 104.23Å 100.10° 106.41° 90.01°	Depositor
Resolution (Å)	10.00 – 2.80 10.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.8 (10.00-2.80) 89.2 (10.00-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.217 , 0.267 0.218 , 0.260	Depositor DCC
R_{free} test set	2174 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 16.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.297 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8965	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.66	0/2211	0.96	3/2979 (0.1%)
1	B	0.61	0/2124	0.93	2/2859 (0.1%)
1	C	0.66	0/2211	0.95	3/2979 (0.1%)
1	D	0.61	0/2124	0.93	4/2859 (0.1%)
All	All	0.64	0/8670	0.94	12/11676 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	402	ASN	N-CA-C	6.16	118.81	108.02
1	C	425	HIS	CA-C-N	5.89	125.27	118.85
1	C	425	HIS	C-N-CA	5.89	125.27	118.85
1	B	402	ASN	N-CA-C	5.74	118.23	108.02
1	D	252	MET	N-CA-C	5.69	117.16	111.07
1	D	264	PHE	N-CA-C	5.62	118.71	109.72
1	B	264	PHE	N-CA-C	5.62	118.70	109.72
1	A	425	HIS	CA-C-N	5.56	124.75	118.97
1	A	425	HIS	C-N-CA	5.56	124.75	118.97
1	A	369	GLU	N-CA-C	-5.23	105.66	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	264	PHE	N-CA-C	5.22	118.50	110.42
1	D	322	VAL	N-CA-C	5.03	116.36	110.62

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	239	GLY	Peptide
1	A	264	PHE	Peptide
1	C	239	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2171	0	2238	54	0
1	B	2089	0	2158	57	0
1	C	2171	0	2238	46	0
1	D	2089	0	2158	56	0
2	A	58	0	68	14	0
2	B	58	0	68	12	0
2	C	58	0	68	12	0
2	D	58	0	68	10	0
3	A	65	0	0	3	0
3	B	46	0	0	2	0
3	C	61	0	0	2	0
3	D	41	0	0	3	0
All	All	8965	0	9064	237	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 13.

All (237) 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:D:264:PHE:CD2	2:D:802:AJA:H11	1.90	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:PHE:HB2	2:A:501:AJA:O26	1.76	0.86
1:D:264:PHE:CG	2:D:802:AJA:H11	2.11	0.84
1:C:264:PHE:CD2	2:C:701:AJA:H11	2.12	0.84
1:C:384:LEU:O	1:C:388:ILE:HG12	1.79	0.83
2:C:701:AJA:O15	2:C:701:AJA:H92	1.81	0.80
2:D:802:AJA:H92	2:D:802:AJA:O15	1.81	0.79
1:B:330:LEU:O	1:B:334:MET:HG2	1.84	0.78
1:D:379:LEU:HD11	1:D:435:LEU:HD11	1.66	0.75
1:B:379:LEU:HD11	1:B:435:LEU:HD11	1.69	0.74
1:A:460:GLU:HB3	1:A:463:MET:HE3	1.70	0.74
1:C:460:GLU:HB3	1:C:463:MET:HE3	1.69	0.74
1:C:264:PHE:CG	2:C:701:AJA:H11	2.21	0.74
1:B:468:LEU:HA	2:B:502:AJA:H243	1.69	0.73
1:D:330:LEU:O	1:D:334:MET:HG2	1.88	0.73
1:B:430:GLN:O	1:B:434:LYS:HG3	1.89	0.73
1:A:286:GLN:HE22	1:A:465:LEU:HD23	1.55	0.72
1:A:264:PHE:HB2	2:A:501:AJA:C16	2.18	0.71
1:A:384:LEU:O	1:A:388:ILE:HG12	1.90	0.70
1:A:430:GLN:O	1:A:434:LYS:HG3	1.91	0.70
1:D:430:GLN:O	1:D:434:LYS:HG3	1.92	0.70
1:D:359:PRO:HG2	1:D:456:ILE:HD13	1.74	0.70
1:A:212:ARG:HH12	1:A:420:GLN:HE21	1.39	0.69
1:D:264:PHE:CD2	2:D:802:AJA:C11	2.73	0.69
1:C:286:GLN:HE22	1:C:465:LEU:HD23	1.57	0.69
1:D:212:ARG:HH12	1:D:420:GLN:HE21	1.41	0.69
1:C:302:SER:HB3	3:C:735:HOH:O	1.93	0.68
1:A:466:HIS:CD2	1:A:468:LEU:H	2.11	0.68
1:A:466:HIS:HD2	1:A:468:LEU:H	1.39	0.68
1:B:212:ARG:HH12	1:B:420:GLN:HE21	1.41	0.68
1:A:466:HIS:HE1	3:A:65:HOH:O	1.76	0.68
1:B:264:PHE:HB2	2:B:601:AJA:O26	1.94	0.67
1:D:464:SER:HB2	3:D:839:HOH:O	1.95	0.66
2:C:701:AJA:O15	2:C:701:AJA:C9	2.44	0.66
2:C:702:AJA:H92	2:C:702:AJA:O15	1.96	0.66
2:D:802:AJA:O15	2:D:802:AJA:C9	2.44	0.65
2:B:502:AJA:H92	2:B:502:AJA:O15	1.97	0.65
1:C:430:GLN:O	1:C:434:LYS:HG3	1.96	0.65
1:B:275:LYS:HE2	1:B:462:ASP:HB2	1.78	0.65
2:B:601:AJA:O15	2:B:601:AJA:H92	1.96	0.65
1:A:318:LEU:HB3	2:B:502:AJA:H291	1.78	0.64
2:A:501:AJA:H92	2:A:501:AJA:O15	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:801:AJA:O15	2:D:801:AJA:H92	1.96	0.64
2:C:701:AJA:C3	2:C:701:AJA:H211	2.27	0.64
1:A:468:LEU:HA	2:A:602:AJA:H252	1.79	0.64
2:B:502:AJA:O15	2:B:502:AJA:C9	2.46	0.64
1:C:269:PRO:HB2	1:C:271:GLN:OE1	1.98	0.64
2:A:602:AJA:O15	2:A:602:AJA:H92	1.96	0.64
2:C:702:AJA:O15	2:C:702:AJA:C9	2.46	0.63
1:D:252:MET:SD	1:D:277:VAL:HG11	2.39	0.63
1:A:466:HIS:CE1	2:A:602:AJA:H172	2.33	0.63
2:A:602:AJA:O15	2:A:602:AJA:C9	2.46	0.63
1:B:279:ILE:O	1:B:283:GLN:HG2	1.98	0.63
2:A:501:AJA:O15	2:A:501:AJA:C9	2.46	0.63
2:B:601:AJA:O15	2:B:601:AJA:C9	2.47	0.63
2:D:801:AJA:O15	2:D:801:AJA:C9	2.46	0.62
1:C:276:GLU:HG2	1:C:279:ILE:HD12	1.81	0.62
1:D:275:LYS:HE2	1:D:462:ASP:HB2	1.81	0.62
1:D:325:ILE:HD11	1:D:392:ILE:HG13	1.81	0.62
1:A:468:LEU:HD23	2:A:602:AJA:H252	1.82	0.61
2:A:602:AJA:H222	1:B:315:VAL:HG13	1.82	0.61
1:B:325:ILE:HD11	1:B:392:ILE:HG13	1.81	0.61
1:B:419:LEU:CD1	1:B:423:LEU:HD21	2.30	0.61
1:C:379:LEU:HD11	1:C:435:LEU:HD11	1.83	0.61
1:C:321:GLY:O	1:C:325:ILE:HG12	2.01	0.61
1:B:335:ASN:HD22	1:B:337:ASP:H	1.46	0.60
1:A:269:PRO:HB2	1:A:271:GLN:OE1	2.02	0.60
1:C:263:LYS:HB3	1:C:345:GLN:HE22	1.66	0.60
1:D:279:ILE:O	1:D:283:GLN:HG2	2.01	0.59
1:D:212:ARG:HH12	1:D:420:GLN:NE2	2.00	0.59
1:D:315:VAL:HG13	2:D:801:AJA:H222	1.85	0.59
1:D:387:PHE:CE2	1:D:391:ILE:HD11	2.38	0.58
1:D:335:ASN:HD22	1:D:337:ASP:H	1.49	0.58
1:B:350:ARG:HD3	1:B:368:PHE:CG	2.39	0.58
1:B:212:ARG:HH12	1:B:420:GLN:NE2	2.00	0.58
1:A:276:GLU:HG2	1:A:279:ILE:HD12	1.86	0.57
1:A:363:PHE:HE2	1:A:456:ILE:HD11	1.70	0.57
1:A:230:LYS:NZ	1:A:379:LEU:O	2.25	0.57
1:B:335:ASN:ND2	1:B:337:ASP:H	2.03	0.57
1:D:335:ASN:ND2	1:D:337:ASP:H	2.03	0.57
1:A:468:LEU:HD23	2:A:602:AJA:C25	2.35	0.56
1:B:359:PRO:HG2	1:B:456:ILE:HD13	1.86	0.56
1:C:212:ARG:HH12	1:C:420:GLN:HE21	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:802:AJA:C3	2:D:802:AJA:H211	2.36	0.56
1:B:329:MET:HG3	3:B:104:HOH:O	2.04	0.56
1:D:453:LEU:C	1:D:455:VAL:H	2.12	0.56
1:B:453:LEU:C	1:B:455:VAL:H	2.13	0.56
1:C:464:SER:O	1:C:465:LEU:C	2.48	0.56
1:A:329:MET:HE2	3:A:81:HOH:O	2.05	0.56
1:A:330:LEU:HG	1:A:334:MET:HE3	1.87	0.56
1:D:419:LEU:CD1	1:D:423:LEU:HD21	2.36	0.55
1:B:252:MET:SD	1:B:277:VAL:HG11	2.46	0.55
2:C:702:AJA:H221	2:C:702:AJA:C4	2.36	0.55
1:A:322:VAL:HG21	1:A:472:ILE:HD13	1.88	0.55
1:B:429:SER:O	1:B:430:GLN:HB2	2.06	0.55
1:A:212:ARG:HH22	1:A:420:GLN:HE22	1.55	0.55
1:A:464:SER:O	1:A:465:LEU:C	2.49	0.55
1:D:350:ARG:HD3	1:D:368:PHE:CG	2.42	0.54
1:B:393:LEU:O	1:B:410:GLN:HB2	2.08	0.54
1:C:363:PHE:HE2	1:C:456:ILE:HD11	1.74	0.53
1:D:419:LEU:O	1:D:423:LEU:HD23	2.07	0.53
1:D:325:ILE:HD11	1:D:392:ILE:CG1	2.38	0.53
1:C:315:VAL:HG13	2:C:702:AJA:H222	1.90	0.53
1:D:429:SER:O	1:D:430:GLN:HB2	2.08	0.53
1:C:302:SER:O	1:C:304:PRO:HD3	2.09	0.53
1:C:329:MET:HE2	3:C:726:HOH:O	2.09	0.52
1:A:294:GLN:OE1	1:B:294:GLN:NE2	2.42	0.52
1:B:325:ILE:HD11	1:B:392:ILE:CG1	2.39	0.52
1:C:325:ILE:HD12	1:C:388:ILE:HG23	1.92	0.52
1:B:419:LEU:HD11	1:B:423:LEU:HD21	1.91	0.51
1:B:394:SER:O	1:B:397:ARG:HG2	2.11	0.51
1:A:379:LEU:HD11	1:A:435:LEU:HD11	1.93	0.51
1:D:335:ASN:HD22	1:D:335:ASN:C	2.18	0.51
1:D:359:PRO:HG2	1:D:456:ILE:CD1	2.39	0.51
1:A:259:GLU:HA	1:A:264:PHE:CZ	2.46	0.50
1:B:276:GLU:HG3	1:B:279:ILE:HG12	1.93	0.50
1:C:322:VAL:HG21	1:C:472:ILE:HD13	1.92	0.50
1:A:328:THR:HG21	1:A:388:ILE:HD11	1.93	0.50
1:C:212:ARG:HH22	1:C:420:GLN:HE22	1.60	0.50
1:B:419:LEU:O	1:B:423:LEU:HD23	2.11	0.50
1:B:452:LEU:HD12	3:B:26:HOH:O	2.11	0.50
1:D:392:ILE:HG22	1:D:393:LEU:HD22	1.92	0.50
1:A:365:GLU:OE1	1:A:365:GLU:HA	2.12	0.49
1:B:212:ARG:HH22	1:B:420:GLN:HE22	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:ASN:HD22	1:B:335:ASN:C	2.20	0.49
1:A:452:LEU:O	1:A:456:ILE:HG12	2.13	0.49
1:C:335:ASN:C	1:C:335:ASN:HD22	2.19	0.49
1:C:279:ILE:HG12	1:C:463:MET:HE1	1.94	0.48
1:A:302:SER:O	1:A:304:PRO:HD3	2.13	0.48
1:D:393:LEU:O	1:D:410:GLN:HB2	2.14	0.48
1:D:324:GLU:HG2	1:D:442:LEU:HB3	1.95	0.48
1:A:289:SER:O	1:A:293:VAL:HG23	2.14	0.48
1:B:466:HIS:HB3	1:B:469:LEU:HD22	1.95	0.48
1:A:263:LYS:O	1:A:263:LYS:HG2	2.13	0.47
1:D:252:MET:HE1	1:D:277:VAL:HG21	1.95	0.47
1:B:387:PHE:CE2	1:B:391:ILE:HD11	2.50	0.47
1:C:396:ASP:CG	1:C:443:ARG:HH12	2.23	0.47
1:C:434:LYS:O	1:C:438:LYS:HG2	2.15	0.47
1:C:324:GLU:OE2	1:C:397:ARG:NH1	2.36	0.47
1:C:324:GLU:OE2	1:C:443:ARG:HG3	2.14	0.47
1:C:417:LEU:HD21	1:C:435:LEU:HD23	1.96	0.47
1:B:331:ALA:HA	1:B:334:MET:HG3	1.96	0.47
1:B:419:LEU:O	1:B:423:LEU:CD2	2.63	0.46
1:A:335:ASN:C	1:A:335:ASN:HD22	2.22	0.46
1:D:253:ASN:ND2	1:D:253:ASN:H	2.12	0.46
1:D:419:LEU:O	1:D:423:LEU:CD2	2.64	0.46
1:D:276:GLU:HG3	1:D:279:ILE:HG12	1.97	0.46
1:B:324:GLU:HG2	1:B:442:LEU:HB3	1.97	0.46
1:D:279:ILE:CD1	1:D:463:MET:HE1	2.46	0.46
1:C:387:PHE:CE2	1:C:391:ILE:HD11	2.51	0.46
1:C:452:LEU:O	1:C:456:ILE:HG12	2.15	0.46
1:D:419:LEU:HD11	1:D:423:LEU:HD21	1.96	0.46
1:D:331:ALA:HA	1:D:334:MET:HG3	1.98	0.46
1:A:212:ARG:HH12	1:A:420:GLN:NE2	2.10	0.46
1:A:364:MET:O	1:A:365:GLU:C	2.58	0.46
2:B:502:AJA:H253	2:B:502:AJA:H212	1.55	0.46
1:D:466:HIS:HB3	1:D:469:LEU:HD22	1.97	0.45
1:A:444:GLN:NE2	1:A:448:GLU:OE2	2.50	0.45
1:A:321:GLY:O	1:A:325:ILE:HG12	2.17	0.45
1:D:394:SER:O	1:D:397:ARG:HG2	2.17	0.45
1:A:460:GLU:CB	1:A:463:MET:HE3	2.45	0.45
1:D:325:ILE:O	1:D:329:MET:HG2	2.17	0.45
1:A:434:LYS:O	1:A:438:LYS:HG2	2.17	0.45
1:B:419:LEU:HD12	1:B:423:LEU:CD2	2.47	0.45
2:D:802:AJA:H211	2:D:802:AJA:H3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:ASN:HD22	1:C:335:ASN:H	1.65	0.44
1:B:350:ARG:HB2	1:B:368:PHE:CZ	2.52	0.44
1:C:335:ASN:C	1:C:335:ASN:ND2	2.75	0.44
1:A:466:HIS:HD2	1:A:468:LEU:N	2.13	0.44
2:A:602:AJA:H121	3:A:65:HOH:O	2.17	0.44
1:B:392:ILE:HG22	1:B:393:LEU:HD22	1.98	0.44
1:D:253:ASN:ND2	1:D:253:ASN:N	2.65	0.44
2:A:602:AJA:H242	2:A:602:AJA:H211	1.69	0.44
1:B:466:HIS:CE1	2:B:502:AJA:H172	2.53	0.44
1:C:358:LYS:HA	1:C:359:PRO:HA	1.70	0.44
1:D:252:MET:CE	1:D:277:VAL:HG21	2.47	0.44
1:A:417:LEU:HD21	1:A:435:LEU:HD23	1.99	0.44
1:B:324:GLU:CD	1:B:397:ARG:HH22	2.26	0.44
1:C:264:PHE:CD2	2:C:701:AJA:C11	2.95	0.44
1:B:432:PHE:O	1:B:436:LEU:HG	2.17	0.43
1:D:250:TYR:CE2	1:D:251:ASP:OD1	2.71	0.43
1:C:444:GLN:NE2	1:C:448:GLU:OE2	2.51	0.43
1:A:237:LEU:HD21	1:A:340:LEU:HG	2.00	0.43
1:B:296:ILE:HG21	1:B:322:VAL:HG12	2.00	0.43
1:D:353:LEU:HD13	1:D:364:MET:HG3	2.01	0.43
2:B:601:AJA:H212	2:B:601:AJA:H253	1.82	0.43
1:D:365:GLU:N	1:D:366:PRO:HD2	2.34	0.43
1:D:296:ILE:HG21	1:D:322:VAL:HG12	2.00	0.43
1:B:419:LEU:CD1	1:B:423:LEU:CD2	2.96	0.43
2:C:701:AJA:C3	2:C:701:AJA:C21	2.97	0.43
1:A:324:GLU:OE2	1:A:443:ARG:HG3	2.19	0.43
1:C:364:MET:O	1:C:365:GLU:C	2.61	0.43
1:B:264:PHE:HB2	2:B:601:AJA:C16	2.48	0.42
1:B:325:ILE:O	1:B:329:MET:HG2	2.19	0.42
1:C:289:SER:O	1:C:293:VAL:HG23	2.18	0.42
1:D:402:ASN:HB2	3:D:819:HOH:O	2.18	0.42
1:B:252:MET:CE	1:B:277:VAL:HG21	2.49	0.42
1:B:212:ARG:HD2	1:B:212:ARG:HA	1.73	0.42
1:D:266:HIS:CE1	1:D:287:PHE:CE1	3.08	0.42
1:A:328:THR:HG21	1:A:388:ILE:CD1	2.50	0.42
1:B:403:VAL:O	1:B:404:LYS:C	2.61	0.42
1:B:266:HIS:CE1	1:B:287:PHE:CE1	3.08	0.42
1:C:303:ILE:O	1:C:304:PRO:C	2.62	0.42
1:B:342:SER:OG	2:B:601:AJA:O27	2.28	0.42
1:B:253:ASN:H	1:B:253:ASN:ND2	2.17	0.42
2:A:602:AJA:C4	2:A:602:AJA:H221	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:LEU:O	1:B:455:VAL:HB	2.20	0.42
1:D:402:ASN:HA	3:D:834:HOH:O	2.19	0.42
1:A:396:ASP:CG	1:A:443:ARG:HH12	2.28	0.41
1:A:303:ILE:O	1:A:304:PRO:C	2.63	0.41
1:A:324:GLU:OE2	1:A:397:ARG:NH1	2.39	0.41
1:D:212:ARG:HD2	1:D:212:ARG:HA	1.73	0.41
1:A:424:ASN:O	1:C:351:GLU:HG2	2.19	0.41
1:D:421:LEU:HD11	1:D:435:LEU:HD22	2.02	0.41
1:B:421:LEU:HD11	1:B:435:LEU:HD22	2.01	0.41
1:D:290:VAL:HG13	1:D:468:LEU:HD12	2.03	0.41
1:C:237:LEU:HD21	1:C:340:LEU:HG	2.03	0.41
1:A:325:ILE:O	1:A:329:MET:HG3	2.21	0.41
1:C:442:LEU:HD23	1:C:442:LEU:HA	1.89	0.41
1:C:285:CYS:SG	2:C:701:AJA:H222	2.61	0.41
1:D:350:ARG:HD2	1:D:365:GLU:OE1	2.21	0.41
1:A:212:ARG:HH22	1:A:420:GLN:NE2	2.17	0.41
1:C:226:PHE:HA	1:C:227:PRO:HD2	1.91	0.41
1:D:279:ILE:HD13	1:D:463:MET:HE1	2.02	0.41
1:D:289:SER:O	1:D:293:VAL:HG23	2.20	0.41
1:D:453:LEU:C	1:D:455:VAL:N	2.79	0.41
1:A:335:ASN:C	1:A:335:ASN:ND2	2.78	0.41
1:A:442:LEU:HD23	1:A:442:LEU:HA	1.89	0.41
1:D:324:GLU:CD	1:D:397:ARG:HH22	2.29	0.41
1:C:325:ILE:O	1:C:329:MET:HG3	2.21	0.40
1:C:365:GLU:OE1	1:C:365:GLU:HA	2.20	0.40
1:A:318:LEU:O	1:A:322:VAL:HG13	2.21	0.40
1:B:253:ASN:ND2	1:B:253:ASN:N	2.69	0.40
1:C:335:ASN:HD21	1:C:347:PHE:HZ	1.68	0.40
1:B:252:MET:HE1	1:B:277:VAL:HG21	2.03	0.40
1:B:334:MET:HE3	1:B:339:VAL:HG21	2.02	0.40
1:B:249:ILE:HA	1:B:254:SER:HB3	2.04	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	269/278 (97%)	254 (94%)	13 (5%)	2 (1%)	18	47
1	B	254/278 (91%)	234 (92%)	18 (7%)	2 (1%)	16	44
1	C	269/278 (97%)	254 (94%)	13 (5%)	2 (1%)	18	47
1	D	254/278 (91%)	236 (93%)	15 (6%)	3 (1%)	10	34
All	All	1046/1112 (94%)	978 (94%)	59 (6%)	9 (1%)	14	41

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	ASP
1	A	465	LEU
1	C	243	ASP
1	C	465	LEU
1	B	454	GLN
1	D	454	GLN
1	D	474	LYS
1	B	474	LYS
1	D	456	ILE

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	244/250 (98%)	221 (91%)	23 (9%)	8	27
1	B	234/250 (94%)	215 (92%)	19 (8%)	11	33
1	C	244/250 (98%)	221 (91%)	23 (9%)	8	27
1	D	234/250 (94%)	213 (91%)	21 (9%)	9	28
All	All	956/1000 (96%)	870 (91%)	86 (9%)	9	28

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	SER
1	A	224	LYS
1	A	232	LYS
1	A	234	ARG
1	A	240	LYS
1	A	257	MET
1	A	264	PHE
1	A	268	THR
1	A	271	GLN
1	A	294	GLN
1	A	333	LEU
1	A	335	ASN
1	A	342	SER
1	A	343[A]	GLU
1	A	343[B]	GLU
1	A	365	GLU
1	A	369	GLU
1	A	443	ARG
1	A	448	GLU
1	A	452	LEU
1	A	465	LEU
1	A	468	LEU
1	A	469	LEU
1	B	221	SER
1	B	222	TYR
1	B	232	LYS
1	B	253	ASN
1	B	264	PHE
1	B	268	THR
1	B	318	LEU
1	B	319	LYS
1	B	333	LEU
1	B	334	MET
1	B	335	ASN
1	B	350	ARG
1	B	435	LEU
1	B	448	GLU
1	B	451	GLN
1	B	452	LEU
1	B	465	LEU
1	B	468	LEU
1	B	469	LEU
1	C	221	SER

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Mol	Chain	Res	Type
1	C	224	LYS
1	C	232	LYS
1	C	234	ARG
1	C	240	LYS
1	C	257	MET
1	C	264	PHE
1	C	268	THR
1	C	271	GLN
1	C	294	GLN
1	C	333	LEU
1	C	335	ASN
1	C	342	SER
1	C	343[A]	GLU
1	C	343[B]	GLU
1	C	365	GLU
1	C	369	GLU
1	C	443	ARG
1	C	448	GLU
1	C	452	LEU
1	C	465	LEU
1	C	468	LEU
1	C	469	LEU
1	D	221	SER
1	D	222	TYR
1	D	232	LYS
1	D	253	ASN
1	D	264	PHE
1	D	268	THR
1	D	294	GLN
1	D	318	LEU
1	D	319	LYS
1	D	333	LEU
1	D	334	MET
1	D	335	ASN
1	D	350	ARG
1	D	435	LEU
1	D	448	GLU
1	D	451	GLN
1	D	452	LEU
1	D	464	SER
1	D	465	LEU
1	D	468	LEU

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Mol	Chain	Res	Type
1	D	469	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	GLN
1	A	335	ASN
1	A	345	GLN
1	A	410	GLN
1	A	420	GLN
1	A	466	HIS
1	B	253	ASN
1	B	266	HIS
1	B	283	GLN
1	B	308	ASN
1	B	335	ASN
1	B	410	GLN
1	B	412	ASN
1	B	420	GLN
1	B	437	GLN
1	B	470	GLN
1	C	273	GLN
1	C	286	GLN
1	C	335	ASN
1	C	345	GLN
1	C	402	ASN
1	C	410	GLN
1	C	420	GLN
1	D	253	ASN
1	D	266	HIS
1	D	283	GLN
1	D	308	ASN
1	D	335	ASN
1	D	410	GLN
1	D	412	ASN
1	D	420	GLN
1	D	437	GLN
1	D	470	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	AJA	D	802	-	31,31,31	0.95	3 (9%)	47,47,47	1.27	5 (10%)
2	AJA	C	702	-	31,31,31	0.94	3 (9%)	47,47,47	1.27	4 (8%)
2	AJA	D	801	-	31,31,31	0.94	3 (9%)	47,47,47	1.27	4 (8%)
2	AJA	C	701	-	31,31,31	0.95	3 (9%)	47,47,47	1.27	5 (10%)
2	AJA	A	602	-	31,31,31	0.95	3 (9%)	47,47,47	1.27	4 (8%)
2	AJA	A	501	-	31,31,31	0.95	3 (9%)	47,47,47	1.27	4 (8%)
2	AJA	B	502	-	31,31,31	0.95	3 (9%)	47,47,47	1.27	4 (8%)
2	AJA	B	601	-	31,31,31	0.94	3 (9%)	47,47,47	1.27	4 (8%)

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	AJA	D	802	-	-	9/17/45/45	0/3/3/3
2	AJA	C	702	-	-	6/17/45/45	0/3/3/3
2	AJA	D	801	-	-	6/17/45/45	0/3/3/3
2	AJA	C	701	-	-	6/17/45/45	0/3/3/3
2	AJA	A	602	-	-	11/17/45/45	0/3/3/3
2	AJA	A	501	-	-	8/17/45/45	0/3/3/3
2	AJA	B	502	-	-	7/17/45/45	0/3/3/3
2	AJA	B	601	-	-	8/17/45/45	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	AJA	C7-C8	-2.49	1.48	1.51
2	D	802	AJA	C7-C8	-2.49	1.48	1.51
2	A	602	AJA	C7-C8	-2.40	1.48	1.51
2	D	801	AJA	C7-C8	-2.40	1.48	1.51
2	A	501	AJA	C7-C8	-2.40	1.48	1.51
2	A	602	AJA	O1-C14	-2.36	1.42	1.47
2	B	502	AJA	C7-C8	-2.34	1.48	1.51
2	C	702	AJA	C7-C8	-2.34	1.48	1.51
2	B	601	AJA	C7-C8	-2.33	1.48	1.51
2	C	702	AJA	O1-C14	-2.31	1.42	1.47
2	B	502	AJA	O1-C14	-2.30	1.42	1.47
2	D	801	AJA	O1-C14	-2.29	1.42	1.47
2	B	601	AJA	O1-C14	-2.28	1.43	1.47
2	A	501	AJA	O1-C14	-2.28	1.43	1.47
2	D	802	AJA	O1-C14	-2.23	1.43	1.47
2	C	701	AJA	O1-C14	-2.21	1.43	1.47
2	B	502	AJA	C19-C4	-2.13	1.50	1.53
2	A	501	AJA	C19-C4	-2.11	1.50	1.53
2	C	701	AJA	C19-C4	-2.10	1.50	1.53
2	B	601	AJA	C19-C4	-2.10	1.50	1.53
2	A	602	AJA	C19-C4	-2.09	1.50	1.53
2	C	702	AJA	C19-C4	-2.07	1.50	1.53
2	D	802	AJA	C19-C4	-2.06	1.50	1.53
2	D	801	AJA	C19-C4	-2.06	1.50	1.53

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	AJA	C6-C7-C2	3.68	120.10	116.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	802	AJA	C6-C7-C2	3.68	120.09	116.63
2	A	501	AJA	C6-C7-C2	3.56	119.99	116.63
2	C	702	AJA	C6-C7-C2	3.56	119.98	116.63
2	B	502	AJA	C6-C7-C2	3.56	119.98	116.63
2	A	602	AJA	C6-C7-C2	3.53	119.95	116.63
2	B	601	AJA	C6-C7-C2	3.53	119.95	116.63
2	D	801	AJA	C6-C7-C2	3.52	119.95	116.63
2	C	702	AJA	C21-C20-C19	-3.10	110.96	117.01
2	A	602	AJA	C21-C20-C19	-3.10	110.97	117.01
2	A	501	AJA	C21-C20-C19	-3.09	110.99	117.01
2	D	801	AJA	C21-C20-C19	-3.08	111.00	117.01
2	B	601	AJA	C21-C20-C19	-3.08	111.00	117.01
2	D	802	AJA	C21-C20-C19	-3.07	111.01	117.01
2	C	701	AJA	C21-C20-C19	-3.07	111.02	117.01
2	B	502	AJA	C21-C20-C19	-3.06	111.04	117.01
2	C	701	AJA	C8-C9-C10	-2.92	109.25	113.74
2	D	802	AJA	C8-C9-C10	-2.89	109.29	113.74
2	A	501	AJA	C8-C9-C10	-2.80	109.42	113.74
2	D	801	AJA	C8-C9-C10	-2.78	109.45	113.74
2	B	601	AJA	C8-C9-C10	-2.78	109.46	113.74
2	C	702	AJA	C8-C9-C10	-2.76	109.48	113.74
2	B	502	AJA	C8-C9-C10	-2.76	109.49	113.74
2	A	602	AJA	C8-C9-C10	-2.75	109.50	113.74
2	B	502	AJA	C6-C7-C8	-2.67	118.99	122.28
2	C	702	AJA	C6-C7-C8	-2.67	119.00	122.28
2	D	801	AJA	C6-C7-C8	-2.64	119.03	122.28
2	A	602	AJA	C6-C7-C8	-2.62	119.06	122.28
2	B	601	AJA	C6-C7-C8	-2.62	119.06	122.28
2	A	501	AJA	C6-C7-C8	-2.61	119.07	122.28
2	D	802	AJA	C6-C7-C8	-2.42	119.30	122.28
2	C	701	AJA	C6-C7-C8	-2.41	119.32	122.28
2	C	701	AJA	C14-O1-C2	2.03	121.42	117.57
2	D	802	AJA	C14-O1-C2	2.03	121.42	117.57

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	AJA	C9-C10-C16-O27
2	A	501	AJA	C11-C10-C16-O27
2	A	501	AJA	C9-C10-C16-O26
2	A	501	AJA	C11-C10-C16-O26

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Mol	Chain	Res	Type	Atoms
2	A	602	AJA	C9-C10-C16-O27
2	A	602	AJA	C11-C10-C16-O27
2	A	602	AJA	C9-C10-C16-O26
2	A	602	AJA	C11-C10-C16-O26
2	B	502	AJA	C4-C19-C20-C21
2	B	502	AJA	C25-C19-C20-C21
2	B	601	AJA	C9-C10-C16-O27
2	B	601	AJA	C11-C10-C16-O27
2	B	601	AJA	C9-C10-C16-O26
2	B	601	AJA	C11-C10-C16-O26
2	C	701	AJA	C9-C10-C16-O27
2	C	701	AJA	C11-C10-C16-O27
2	C	701	AJA	C9-C10-C16-O26
2	C	701	AJA	C11-C10-C16-O26
2	C	702	AJA	C24-C19-C20-C21
2	D	801	AJA	C4-C19-C20-C21
2	D	801	AJA	C24-C19-C20-C21
2	D	802	AJA	C9-C10-C16-O27
2	D	802	AJA	C11-C10-C16-O27
2	D	802	AJA	C9-C10-C16-O26
2	D	802	AJA	C11-C10-C16-O26
2	B	502	AJA	C20-C21-C22-C23
2	D	801	AJA	C20-C21-C22-C23
2	B	502	AJA	C21-C22-C23-C28
2	D	801	AJA	C21-C22-C23-C28
2	D	802	AJA	C20-C21-C22-C23
2	B	601	AJA	C20-C21-C22-C23
2	A	602	AJA	C20-C21-C22-C23
2	B	502	AJA	C19-C20-C21-C22
2	C	701	AJA	C20-C21-C22-C23
2	C	702	AJA	C20-C21-C22-C23
2	A	602	AJA	C24-C19-C20-C21
2	B	502	AJA	C24-C19-C20-C21
2	D	801	AJA	C25-C19-C20-C21
2	A	602	AJA	C19-C20-C21-C22
2	A	501	AJA	C20-C21-C22-C23
2	A	602	AJA	C21-C22-C23-C28
2	D	802	AJA	C21-C22-C23-C28
2	D	801	AJA	C19-C20-C21-C22
2	C	702	AJA	C19-C20-C21-C22
2	B	601	AJA	C19-C20-C21-C22
2	A	501	AJA	C21-C22-C23-C28

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Mol	Chain	Res	Type	Atoms
2	C	701	AJA	C21-C22-C23-C28
2	C	702	AJA	C25-C19-C20-C21
2	C	702	AJA	C4-C19-C20-C21
2	D	802	AJA	C22-C23-C28-C29
2	B	502	AJA	C22-C23-C28-C29
2	A	602	AJA	C22-C23-C28-C29
2	B	601	AJA	C22-C23-C28-C29
2	C	702	AJA	C21-C22-C23-C28
2	A	602	AJA	C25-C19-C20-C21
2	D	802	AJA	C24-C19-C4-C3
2	A	501	AJA	C25-C19-C4-C5
2	B	601	AJA	C25-C19-C20-C21
2	A	602	AJA	C4-C19-C20-C21
2	D	802	AJA	C24-C19-C4-C5
2	A	501	AJA	C25-C19-C4-C3

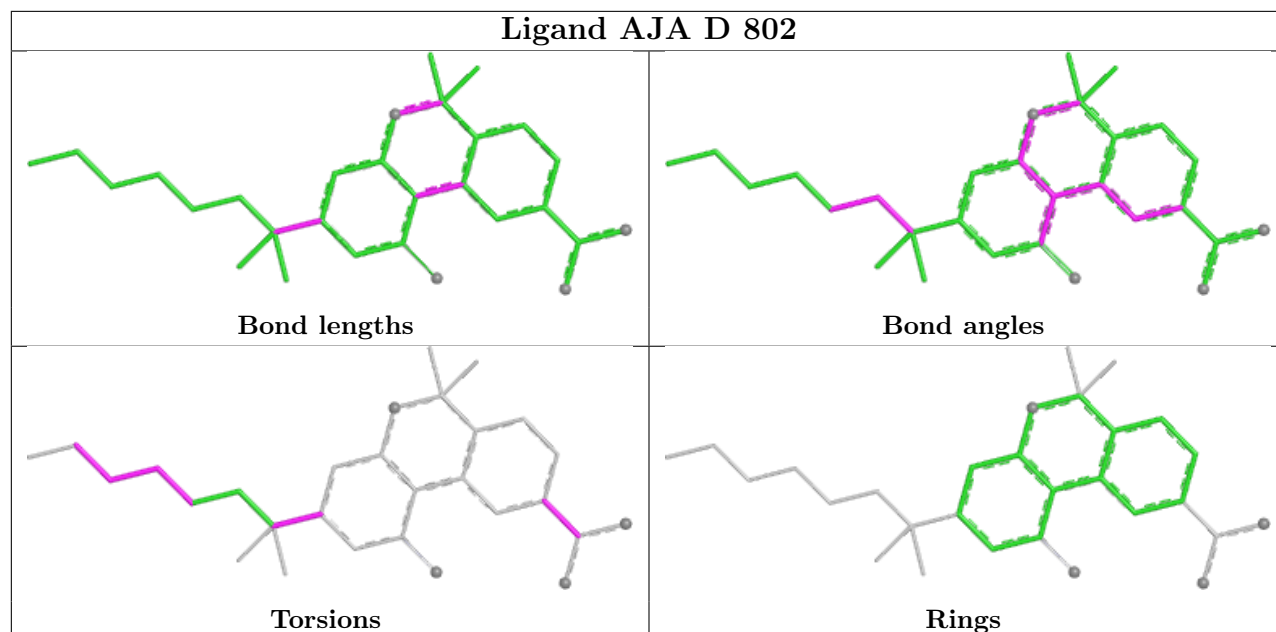
There are no ring outliers.

8 monomers are involved in 48 short contacts:

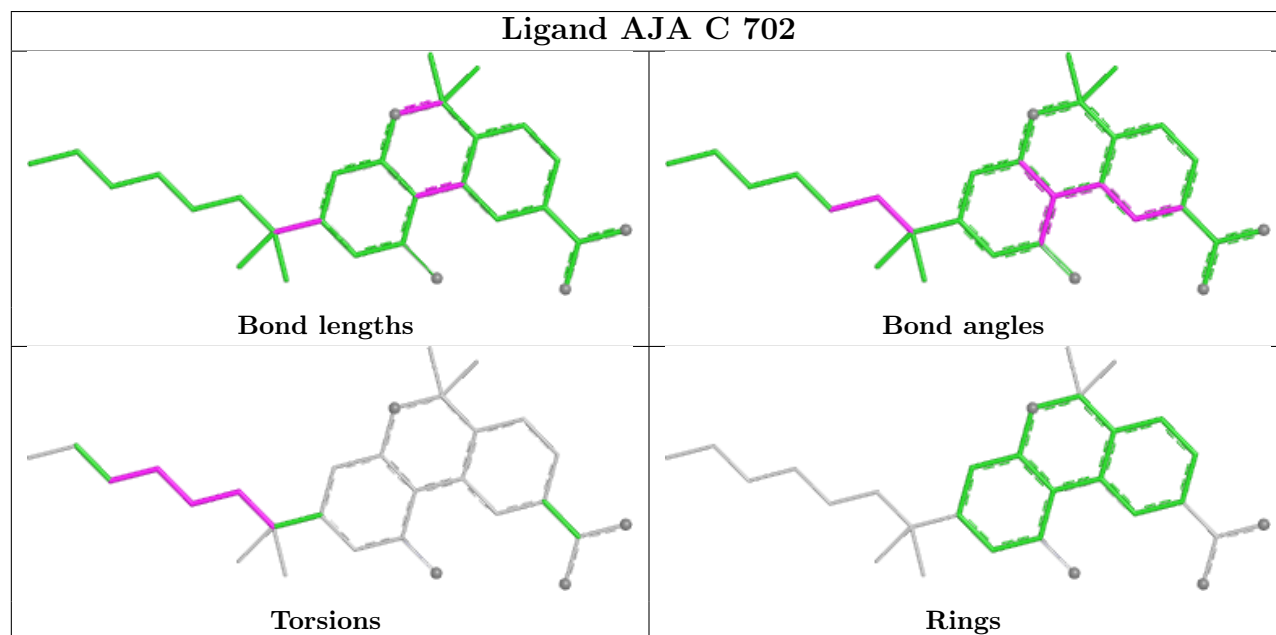
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	802	AJA	7	0
2	C	702	AJA	4	0
2	D	801	AJA	3	0
2	C	701	AJA	8	0
2	A	602	AJA	10	0
2	A	501	AJA	4	0
2	B	502	AJA	6	0
2	B	601	AJA	6	0

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.

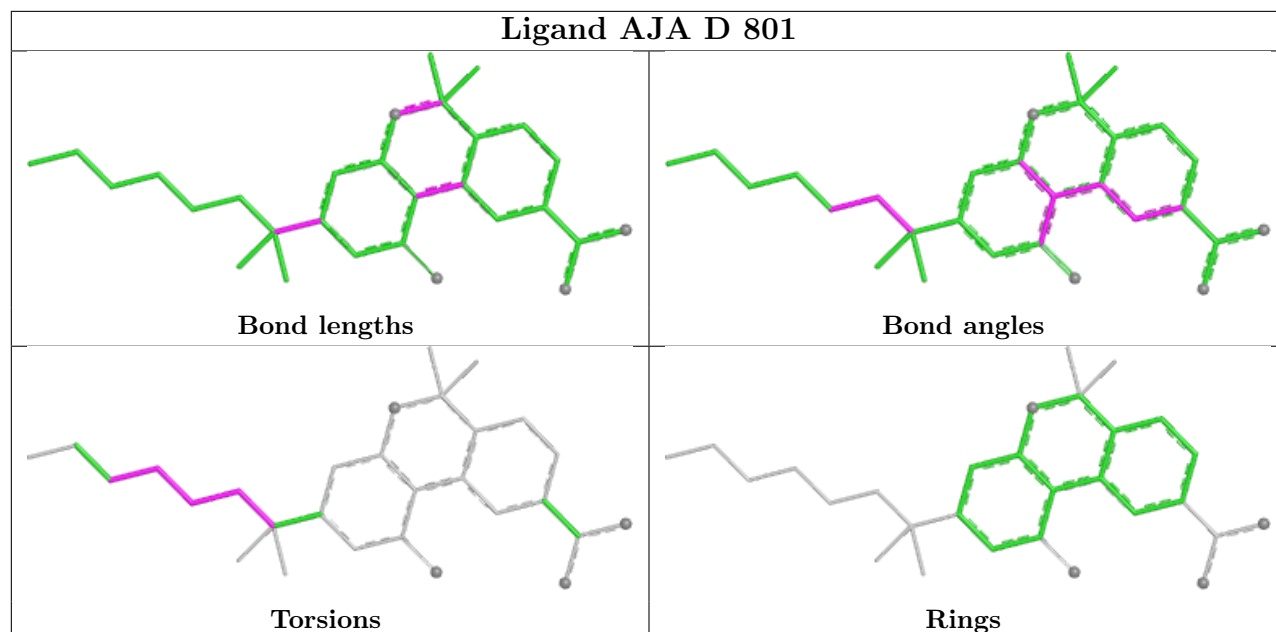
Ligand AJA D 802



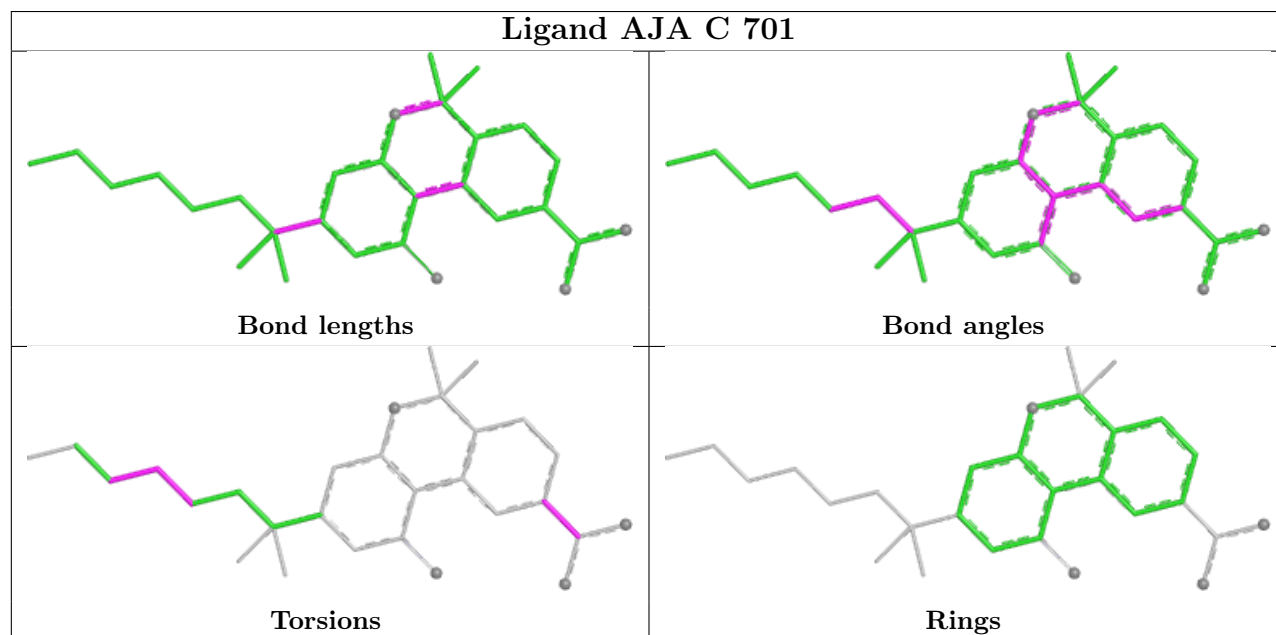
Ligand AJA C 702



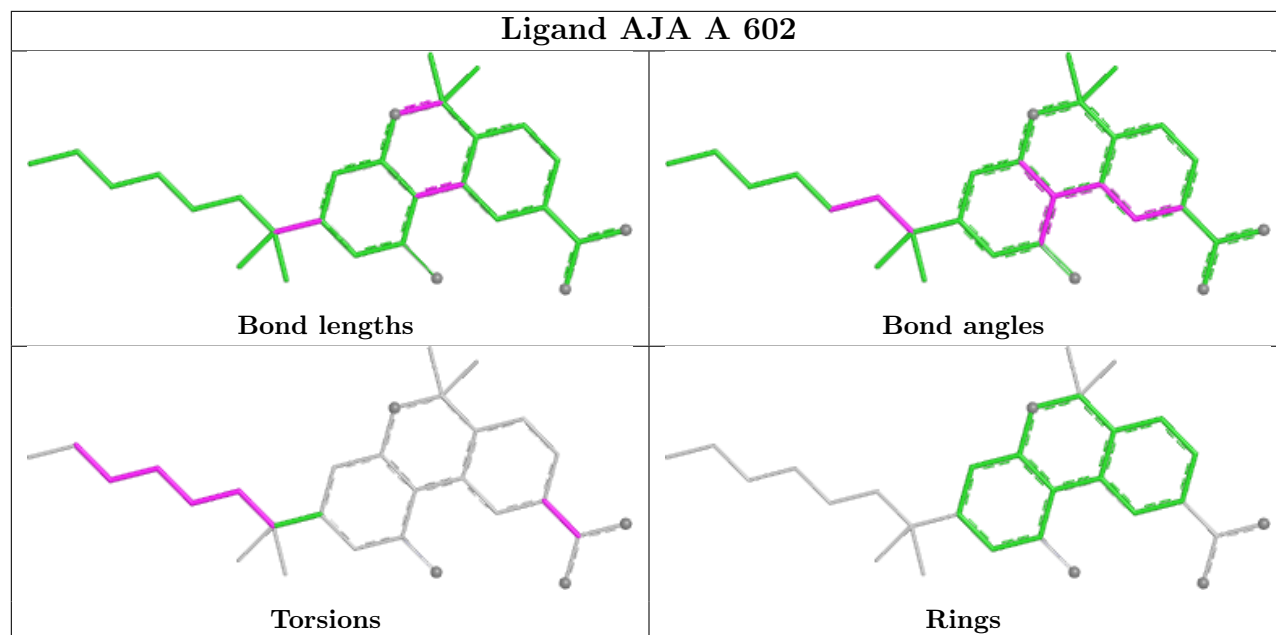
Ligand AJA D 801



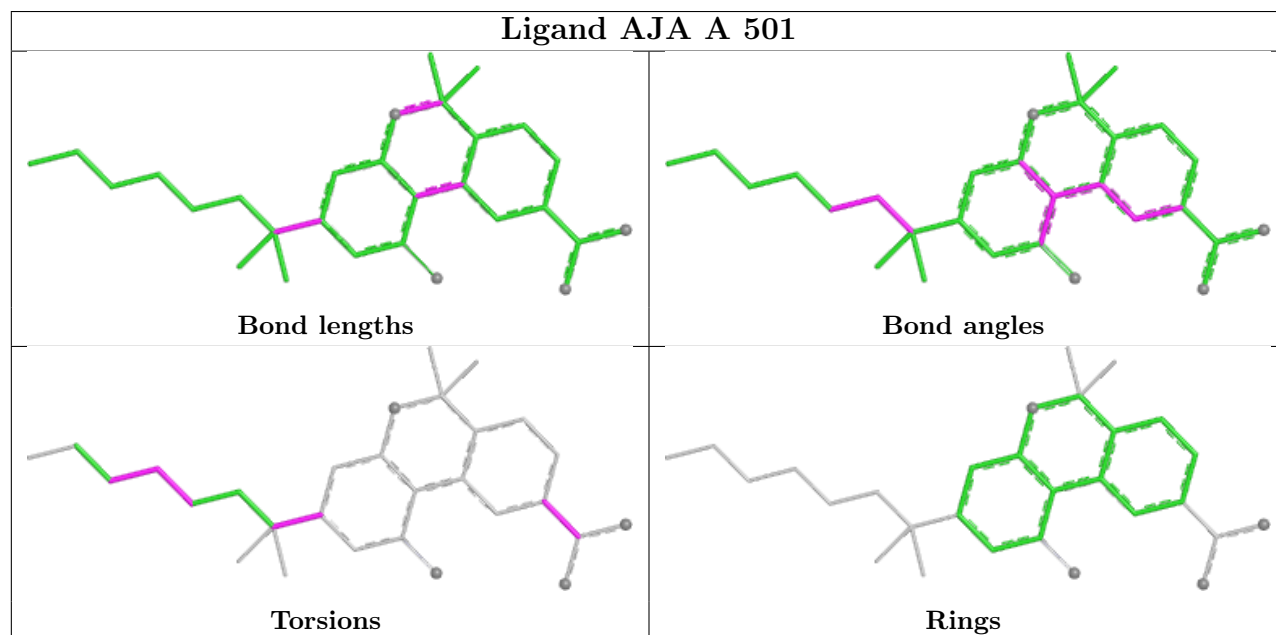
Ligand AJA C 701

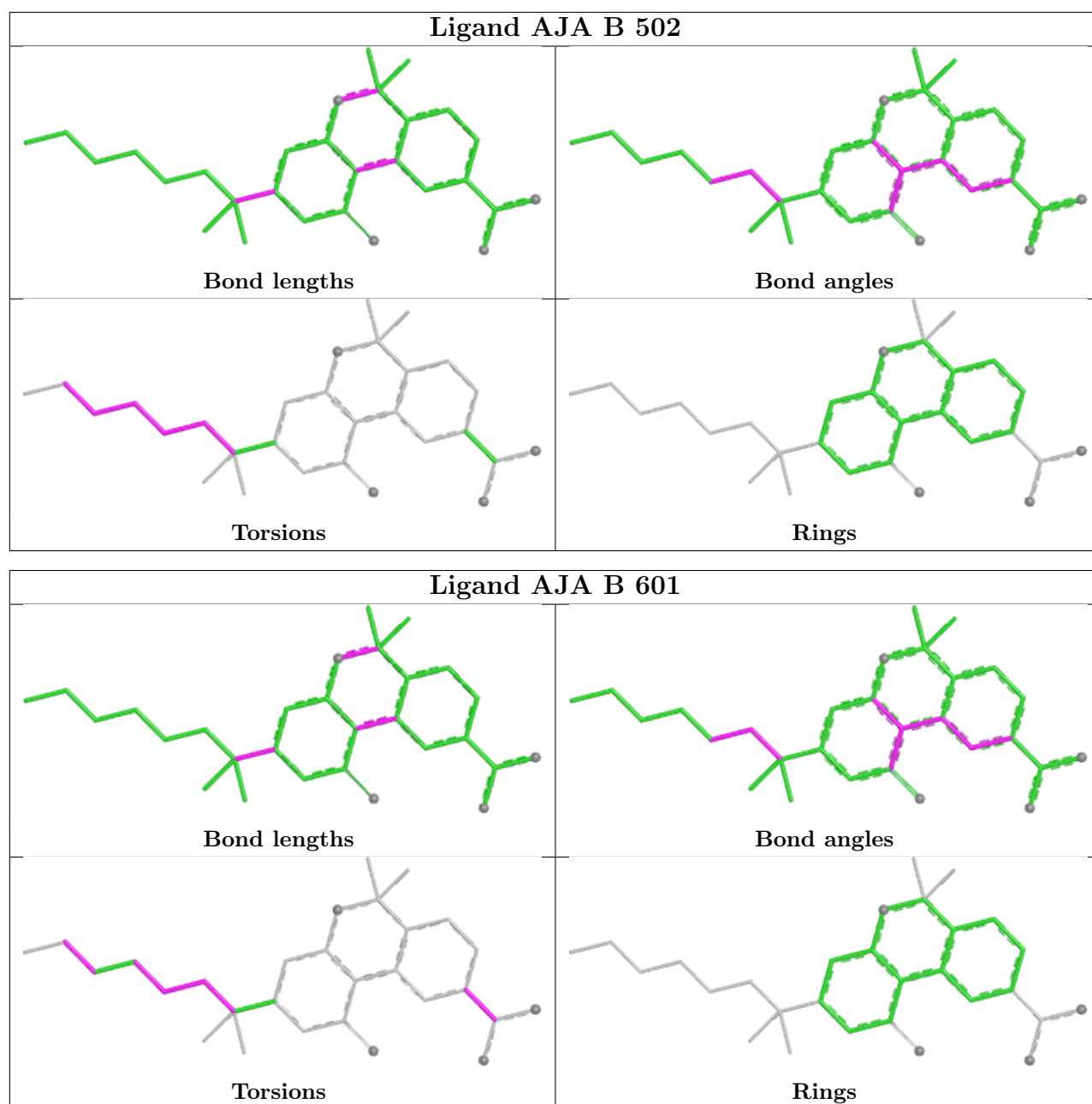


Ligand AJA A 602



Ligand AJA A 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	270/278 (97%)	-1.71	0 100 100	16, 32, 55, 70	7 (2%)
1	B	260/278 (93%)	-1.60	0 100 100	17, 41, 75, 80	7 (2%)
1	C	270/278 (97%)	-1.71	0 100 100	16, 32, 55, 70	7 (2%)
1	D	260/278 (93%)	-1.63	0 100 100	16, 39, 74, 81	7 (2%)
All	All	1060/1112 (95%)	-1.66	0 100 100	16, 36, 69, 81	28 (2%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

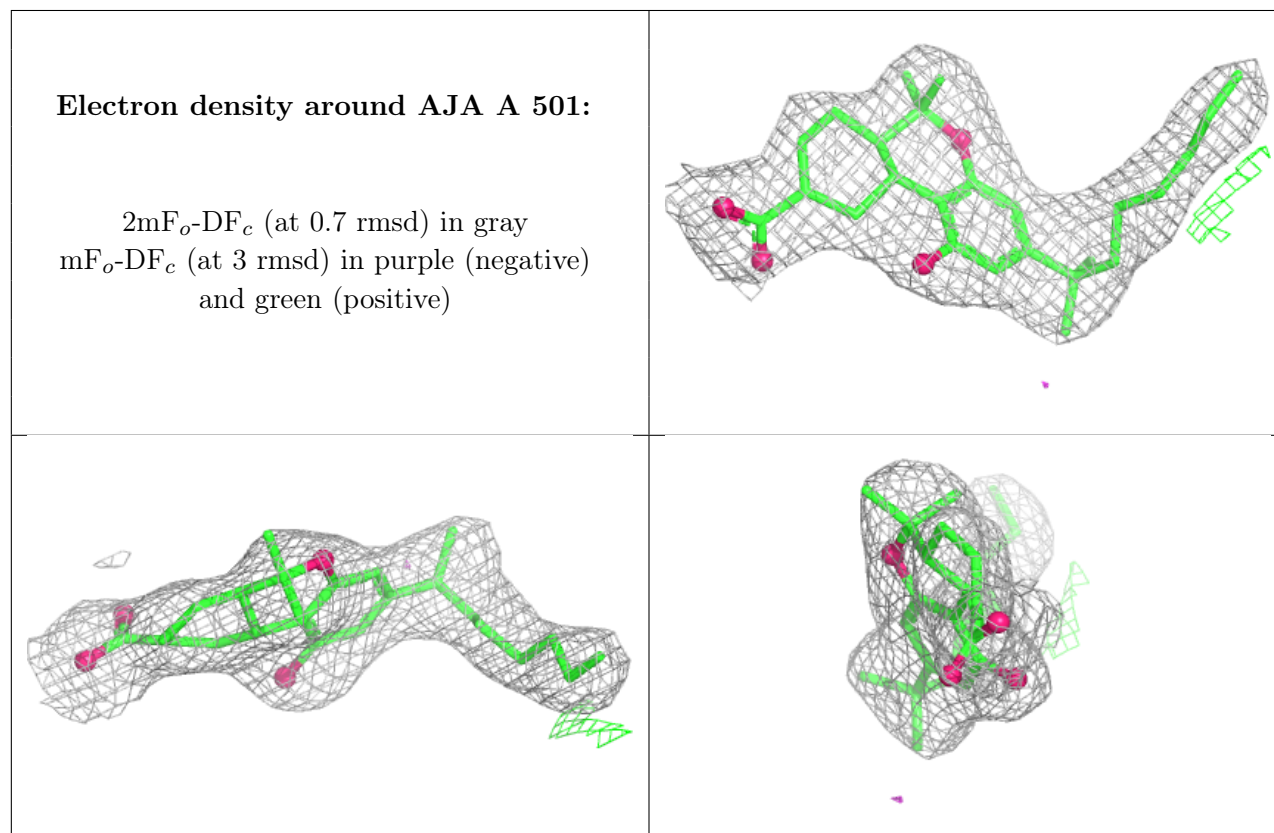
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	AJA	A	501	29/29	0.99	0.03	21,27,30,32	0
2	AJA	A	602	29/29	0.99	0.03	22,29,33,36	0
2	AJA	B	601	29/29	0.99	0.04	43,45,46,47	0
2	AJA	C	701	29/29	0.99	0.03	30,33,37,39	0

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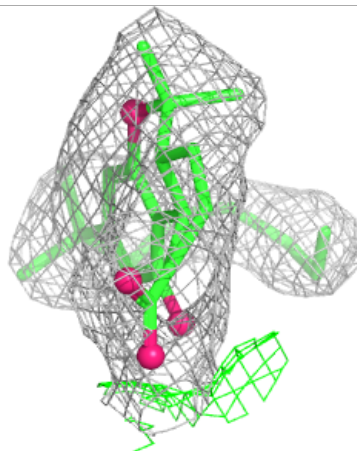
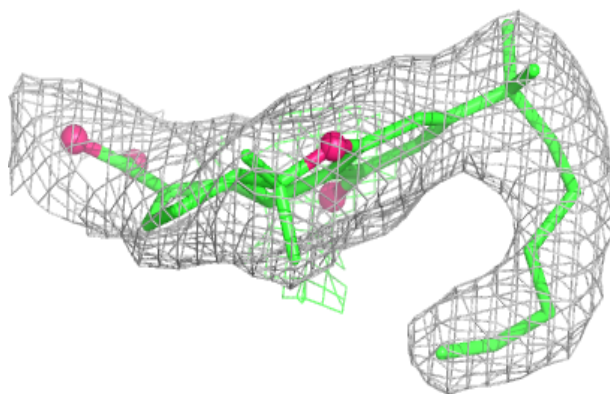
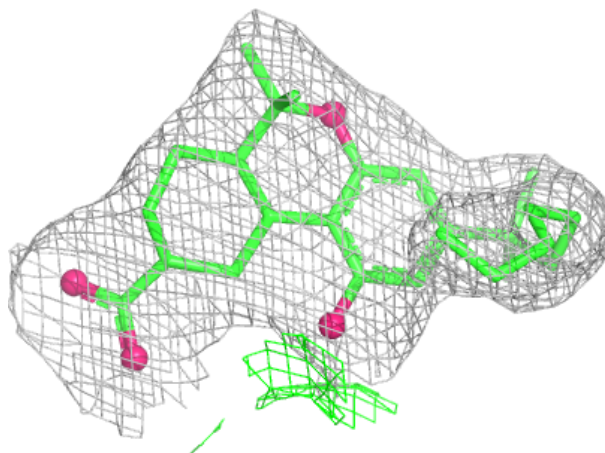
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AJA	D	801	29/29	0.99	0.04	25,27,32,33	0
2	AJA	C	702	29/29	1.00	0.03	28,29,34,35	0
2	AJA	B	502	29/29	1.00	0.03	28,29,33,37	0
2	AJA	D	802	29/29	1.00	0.03	37,42,46,47	0

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.



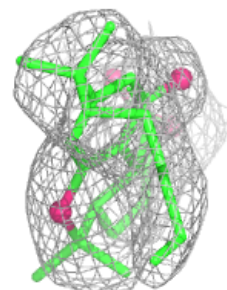
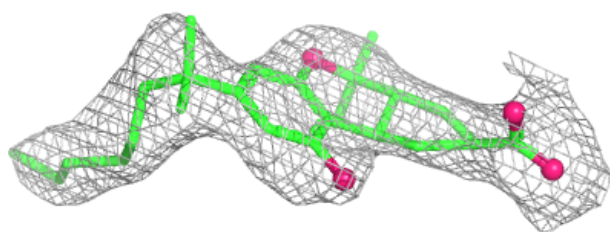
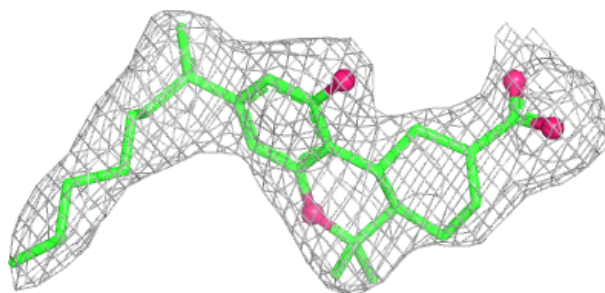
Electron density around AJA A 602:

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

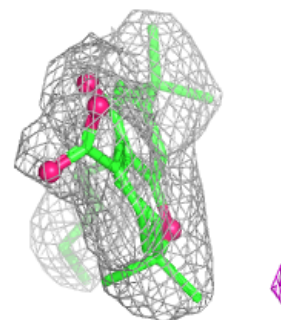
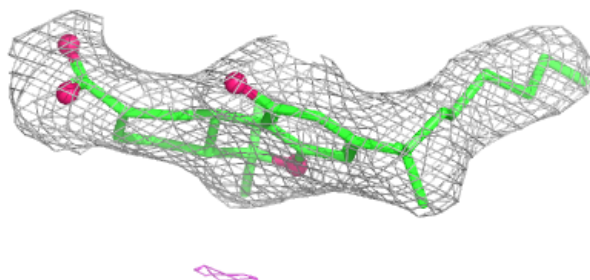
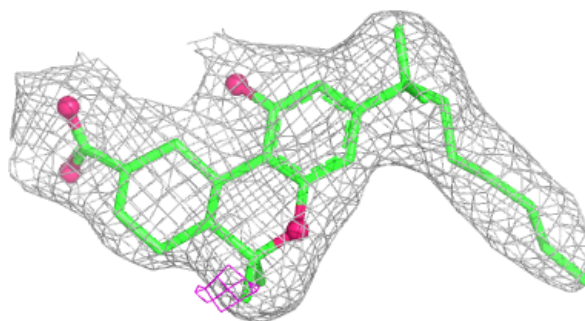


Electron density around AJA B 601:

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

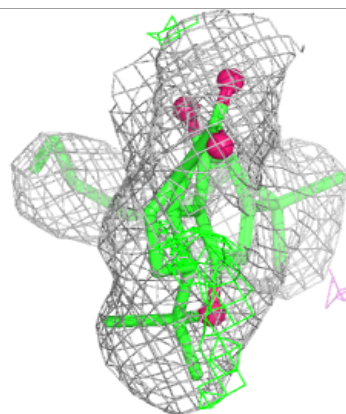
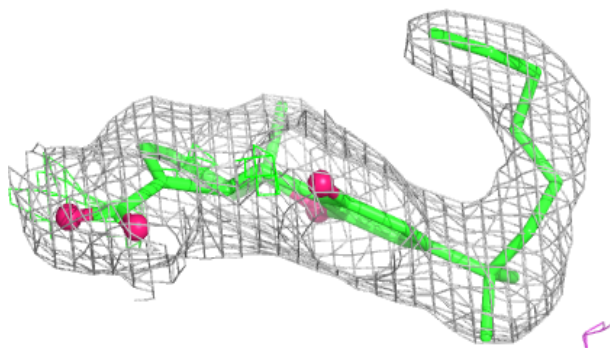
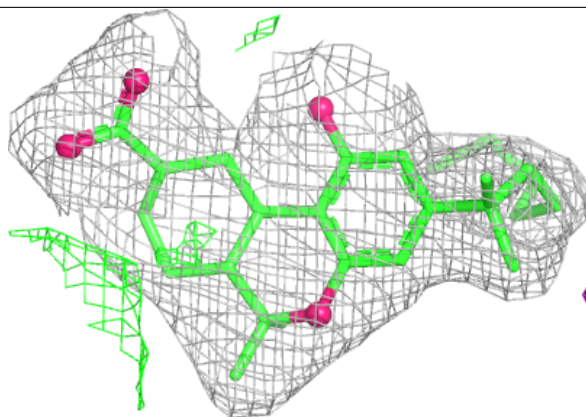
**Electron density around AJA C 701:**

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

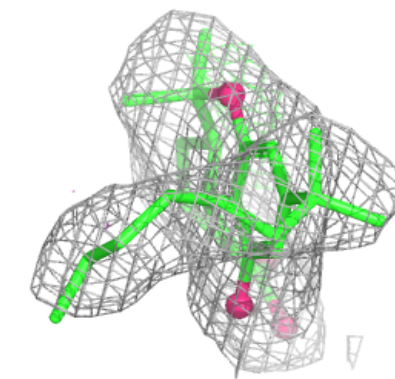
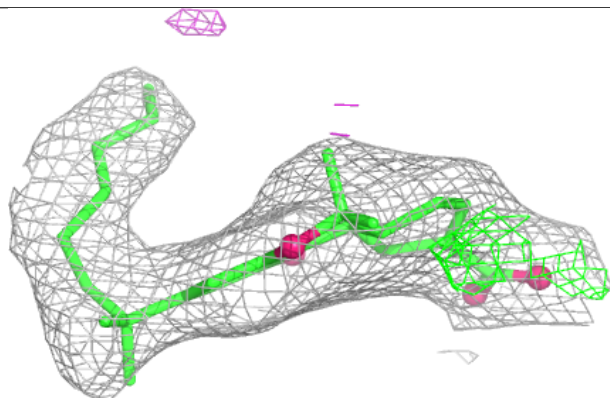
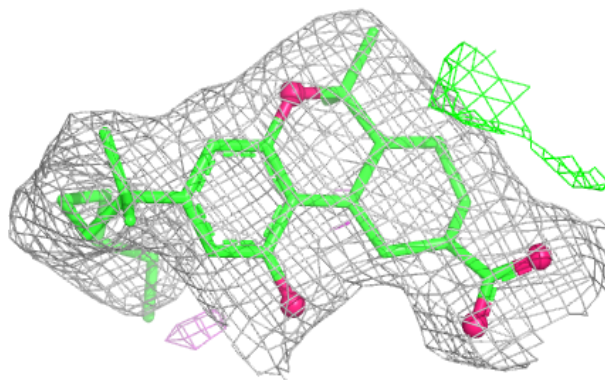


Electron density around AJA D 801:

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

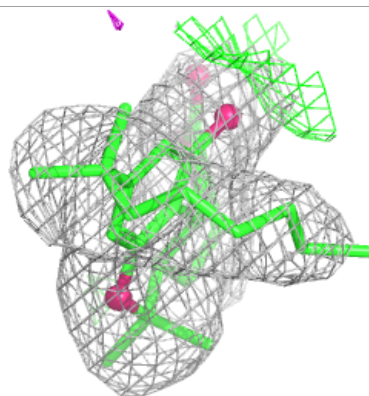
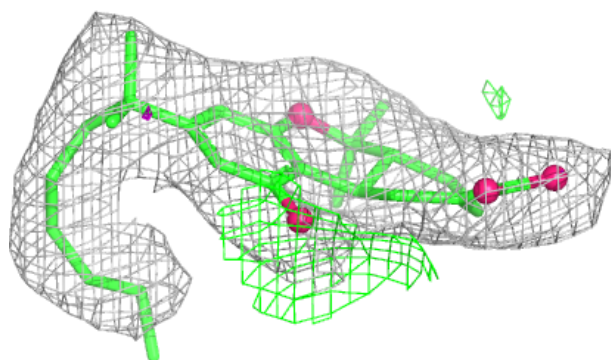
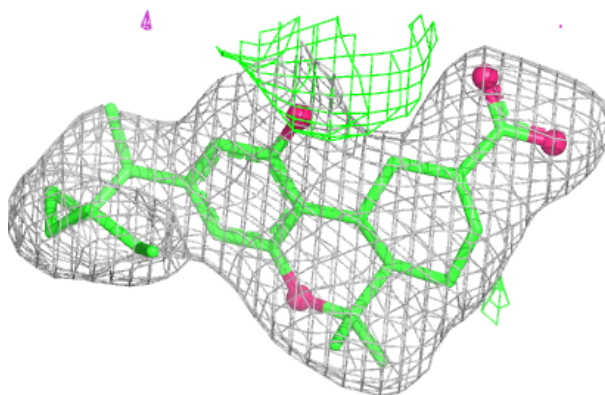
**Electron density around AJA C 702:**

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

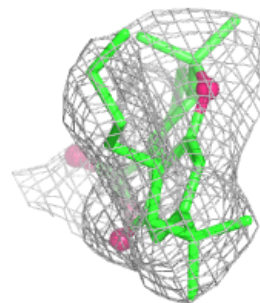
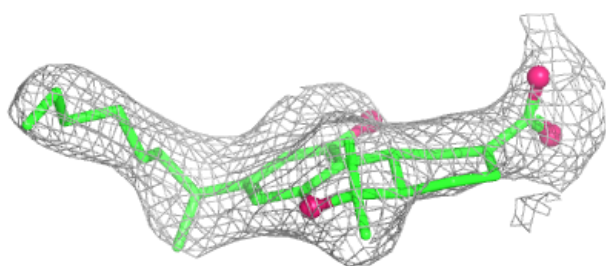
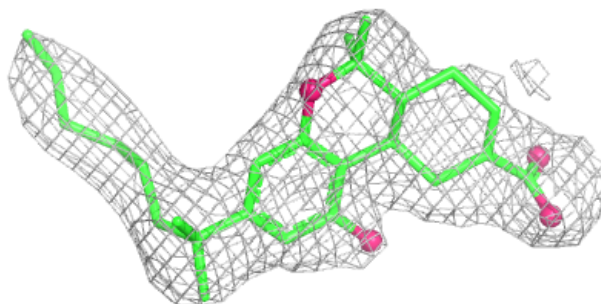


Electron density around AJA B 502:

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

**Electron density around AJA D 802:**

$2mF_o-DF_c$ (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.