



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 01:27 PM JST

PDB ID : 5ZDP  
Title : Crystal structure of cyanide-insensitive alternative oxidase from *Trypanosoma brucei* with ferulenol  
Authors : Shiba, T.; Inaoka, D.K.; Takahashi, G.; Tsuge, C.; Kido, Y.; Young, L.; Ueda, S.; Balogun, E.O.; Nara, T.; Honma, T.; Tanaka, A.; Inoue, M.; Saimoto, H.; Harada, S.; Moore, A.L.; Kita, K.  
Deposited on : 2018-02-23  
Resolution : 2.71 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (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

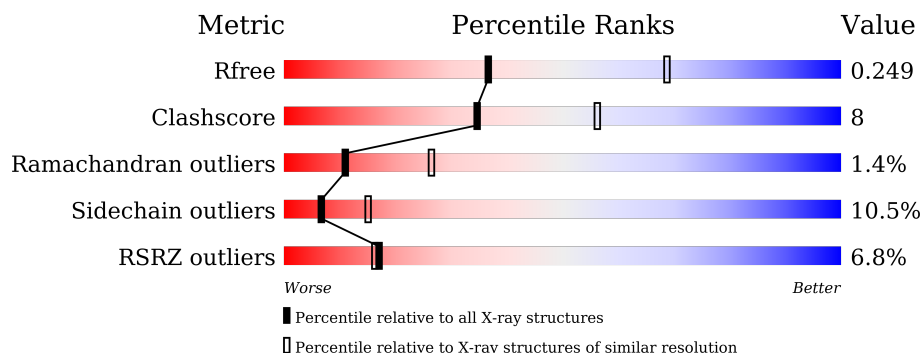
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.71 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	329	 % 60% 18% • 20%
1	B	329	 2% 58% 19% • 20%
1	C	329	 8% 61% 15% 5% 19%
1	D	329	 10% 61% 17% • 19%

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	9AU	D	505	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8796 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.

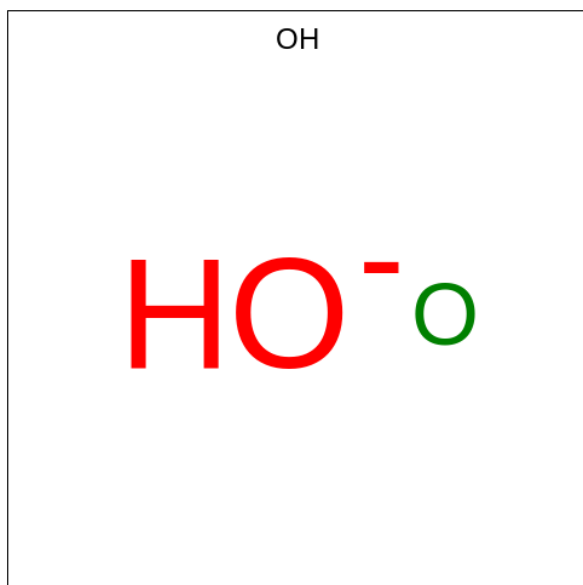
- Molecule 1 is a protein called Alternative oxidase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	264	2146	1375	381	380	10	0	0	0
1	B	263	2137	1369	379	379	10	0	0	0
1	C	266	2162	1386	384	382	10	0	0	0
1	D	265	2153	1380	382	381	10	0	0	0

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

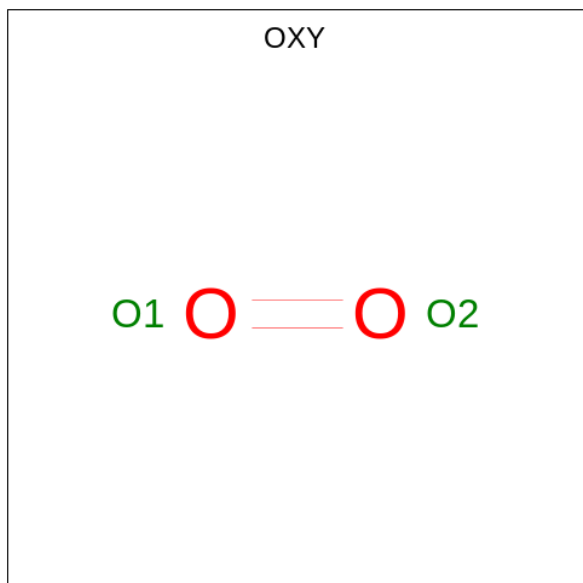
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Fe	0	0
			2	2		
2	B	2	Total	Fe	0	0
			2	2		
2	C	2	Total	Fe	0	0
			2	2		
2	D	2	Total	Fe	0	0
			2	2		

- Molecule 3 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



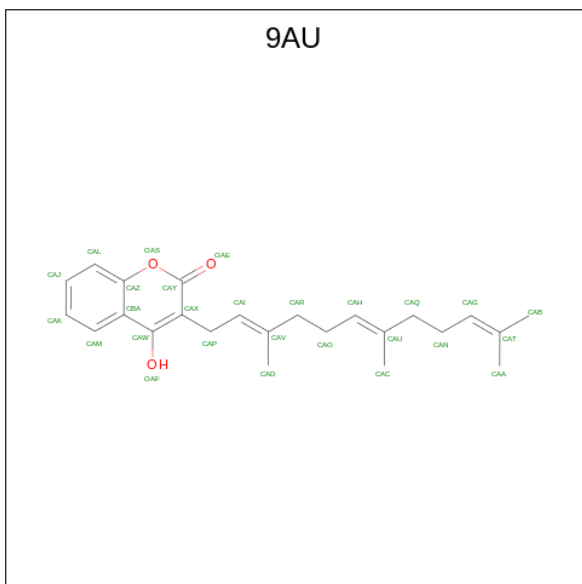
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	B	1	Total O 1 1	0	0
3	C	1	Total O 1 1	0	0
3	D	1	Total O 1 1	0	0

- Molecule 4 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O<sub>2</sub>).



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

- Molecule 5 is 4-oxidanyl-3-[(2 {E},6 {E})-3,7,11-trimethyldodeca-2,6,10-trienyl]chrome n-2-one (three-letter code: 9AU) (formula: C<sub>24</sub>H<sub>30</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 27 24 3	0	0
5	B	1	Total C O 27 24 3	0	0
5	C	1	Total C O 27 24 3	0	0
5	D	1	Total C O 27 24 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	23	Total O 23 23	0	0

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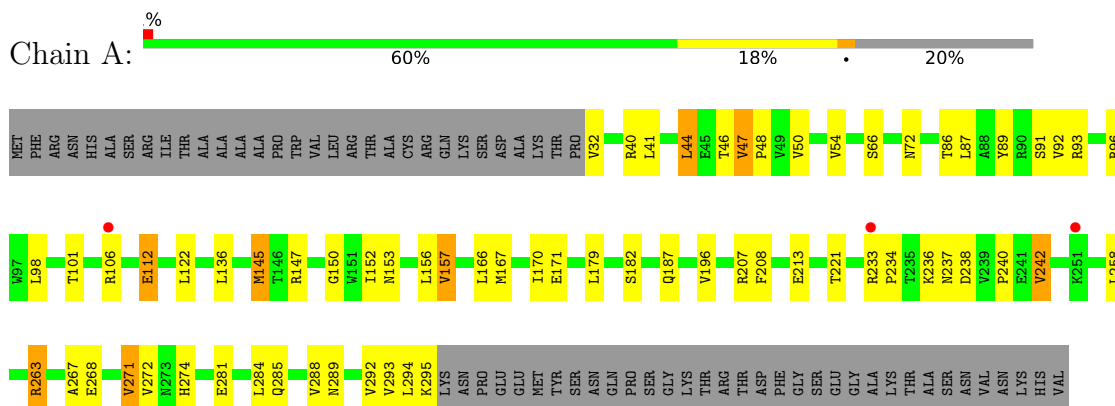
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	B	24	Total 24	O 24	0	0
6	C	14	Total 14	O 14	0	0
6	D	9	Total 9	O 9	0	0



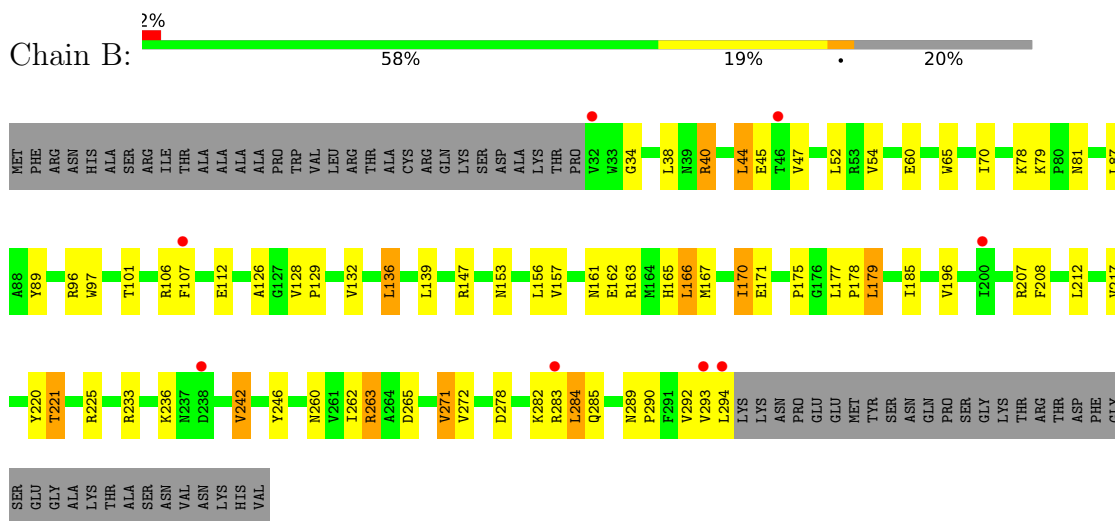
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

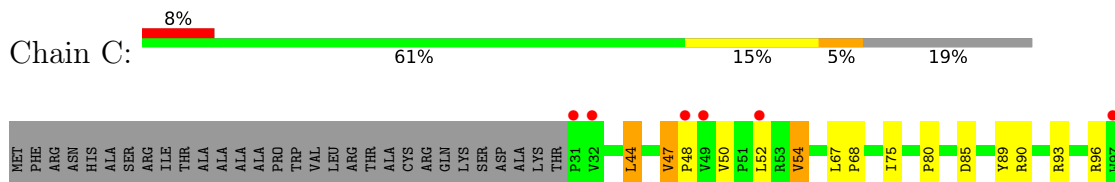
- Molecule 1: Alternative oxidase, mitochondrial

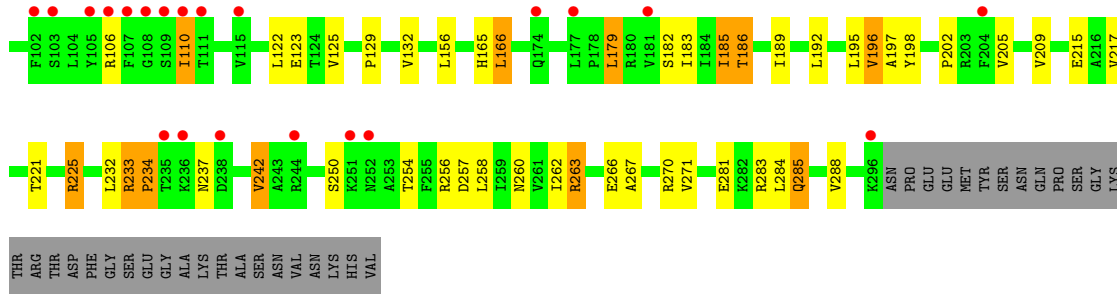


- Molecule 1: Alternative oxidase, mitochondrial

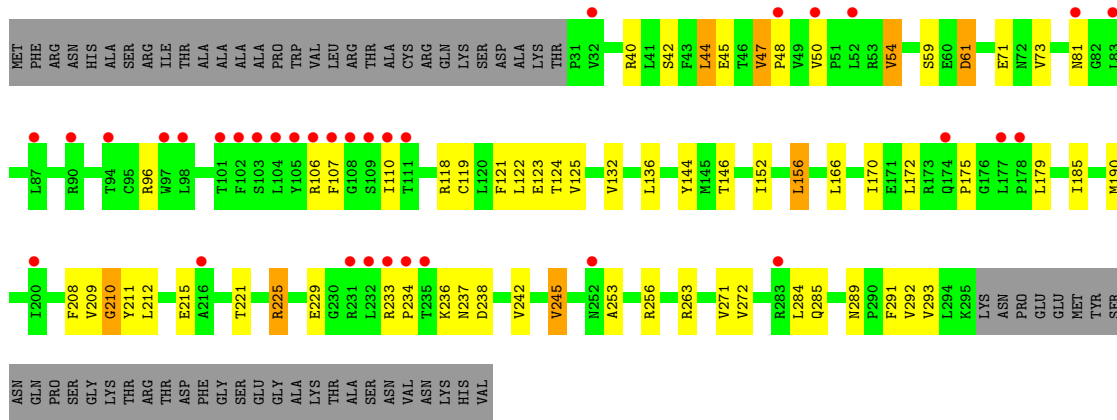


- Molecule 1: Alternative oxidase, mitochondrial





• Molecule 1: Alternative oxidase, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	259.50Å 63.11Å 138.27Å 90.00° 122.21° 90.00°	Depositor
Resolution (Å)	39.32 – 2.71 39.32 – 2.71	Depositor EDS
% Data completeness (in resolution range)	92.6 (39.32-2.71) 94.8 (39.32-2.71)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.57 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.192 , 0.249 0.203 , 0.249	Depositor DCC
$R_{free}$ test set	2582 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.9	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 58.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.216 for -h-2*1,-k,l	Xtriage
Reported twinning fraction	0.539 for H, K, L 0.461 for H+4/2L, -K, -L	Depositor
Outliers	0 of 49577 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8796	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: OXY, 9AU, OH, FE

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	0.50	0/2195	0.76	0/2982
1	B	0.51	0/2186	0.76	1/2971 (0.0%)
1	C	0.51	0/2212	0.71	2/3004 (0.1%)
1	D	0.42	0/2203	0.65	0/2993
All	All	0.49	0/8796	0.72	3/11950 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	96	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	C	225	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	C	225	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts i

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2146	0	2175	43	0
1	B	2137	0	2162	46	0
1	C	2162	0	2196	42	0
1	D	2153	0	2183	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	1	0
3	C	1	0	0	1	0
3	D	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	27	0	0	4	0
5	B	27	0	0	2	0
5	C	27	0	0	6	0
5	D	27	0	0	2	0
6	A	23	0	0	1	0
6	B	24	0	0	1	0
6	C	14	0	0	1	0
6	D	9	0	0	1	0
All	All	8796	0	8716	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 8.

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:185:ILE:C	1:C:185:ILE:HD12	1.58	1.18
1:C:185:ILE:HD12	1:C:185:ILE:O	1.64	0.97
1:C:185:ILE:C	1:C:185:ILE:CD1	2.34	0.95
1:A:44:LEU:O	1:A:47:VAL:HG13	1.70	0.91
1:C:217:VAL:O	1:C:221:THR:HG22	1.74	0.87
1:C:75:ILE:HD11	1:C:221:THR:HG21	1.58	0.84
1:C:185:ILE:O	1:C:185:ILE:CD1	2.30	0.79
1:C:262:ILE:O	1:C:266:GLU:HG2	1.84	0.78
1:B:208:PHE:CE2	1:B:212:LEU:HD11	2.22	0.75
1:A:96:ARG:HA	5:A:505:9AU:CAD	2.18	0.72
1:B:289:ASN:O	1:B:292:VAL:HG22	1.91	0.71
1:A:221:THR:HG22	1:A:263:ARG:HH21	1.56	0.71
1:A:147:ARG:HA	1:B:167:MET:HE2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:LEU:H	1:B:294:LEU:HD22	1.56	0.69
1:C:263:ARG:HD3	6:C:604:HOH:O	1.93	0.69
1:B:153:ASN:O	1:B:157:VAL:HG22	1.93	0.67
1:D:208:PHE:CE2	1:D:212:LEU:HD11	2.31	0.65
1:D:185:ILE:HD11	6:D:609:HOH:O	1.96	0.65
1:A:167:MET:HE2	1:B:147:ARG:HA	1.78	0.65
3:C:503:OH:O	5:C:505:9AU:CAK	2.46	0.64
1:A:236:LYS:O	1:A:238:ASP:N	2.31	0.63
1:C:185:ILE:HD12	1:C:186:THR:N	2.12	0.63
1:D:40:ARG:NH2	1:D:42:SER:O	2.31	0.63
1:B:112:GLU:OE2	1:B:236:LYS:HG2	1.99	0.62
1:C:123:GLU:OE2	1:C:123:GLU:HA	2.00	0.60
1:D:289:ASN:O	1:D:292:VAL:HG22	2.01	0.60
1:D:292:VAL:HG23	1:D:293:VAL:HG23	1.82	0.60
1:A:207:ARG:HD3	1:A:274:HIS:CD2	2.37	0.59
1:B:161:ASN:ND2	1:B:246:TYR:OH	2.30	0.58
1:B:217:VAL:O	1:B:221:THR:HG23	2.03	0.58
1:A:293:VAL:O	1:A:295:LYS:N	2.37	0.58
1:B:294:LEU:HD22	1:B:294:LEU:N	2.19	0.58
1:C:185:ILE:HD11	1:C:189:ILE:HD12	1.85	0.58
1:C:185:ILE:HD11	1:C:189:ILE:CD1	2.34	0.57
1:A:44:LEU:HG	1:B:278:ASP:HB3	1.87	0.57
5:A:505:9AU:CAI	5:A:505:9AU:OAF	2.52	0.57
1:A:145:MET:HB3	1:B:170:ILE:HG13	1.87	0.57
1:B:44:LEU:O	1:B:47:VAL:HG13	2.04	0.57
1:D:122:LEU:HD13	5:D:505:9AU:CAW	2.35	0.56
3:B:503:OH:O	5:B:505:9AU:CAK	2.54	0.56
1:A:207:ARG:NH1	6:A:602:HOH:O	2.40	0.55
1:C:234:PRO:O	1:C:237:ASN:ND2	2.41	0.54
1:A:147:ARG:HA	1:B:167:MET:CE	2.37	0.54
1:C:75:ILE:HD11	1:C:221:THR:CG2	2.33	0.54
1:A:89:TYR:OH	1:D:225:ARG:HG3	2.08	0.53
1:C:96:ARG:HA	5:C:505:9AU:CAD	2.38	0.53
1:C:166:LEU:HD22	1:C:166:LEU:O	2.10	0.53
1:C:44:LEU:O	1:C:44:LEU:HD22	2.10	0.52
1:A:47:VAL:HG12	1:B:290:PRO:HG3	1.92	0.52
1:B:65:TRP:HB3	1:B:70:ILE:HD13	1.93	0.51
1:A:46:THR:O	1:A:50:VAL:HG13	2.12	0.50
1:A:271:VAL:CG1	1:B:40:ARG:O	2.60	0.50
1:C:182:SER:O	1:C:186:THR:OG1	2.28	0.50
5:C:505:9AU:CAI	5:C:505:9AU:OAF	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:ARG:NH1	1:C:215:GLU:OE1	2.39	0.49
1:A:213:GLU:OE1	1:A:213:GLU:HA	2.12	0.49
5:D:505:9AU:CAI	5:D:505:9AU:OAF	2.61	0.49
1:C:254:THR:OG1	1:C:257:ASP:OD1	2.27	0.48
1:D:47:VAL:O	1:D:50:VAL:HG12	2.13	0.48
1:A:293:VAL:C	1:A:295:LYS:H	2.17	0.48
1:C:179:LEU:O	1:C:183:ILE:HD12	2.13	0.48
1:C:258:LEU:C	1:C:258:LEU:HD23	2.35	0.47
1:B:97:TRP:O	1:B:101:THR:HG23	2.15	0.47
1:D:125:VAL:HG13	1:D:190:MET:HG3	1.97	0.47
1:A:112:GLU:OE1	1:A:234:PRO:HA	2.15	0.47
1:B:207:ARG:O	1:B:208:PHE:C	2.51	0.46
1:B:293:VAL:O	1:B:294:LEU:C	2.54	0.46
1:D:209:VAL:O	1:D:210:GLY:C	2.54	0.46
1:A:147:ARG:NH1	1:B:171:GLU:OE2	2.48	0.46
1:B:262:ILE:O	1:B:265:ASP:HB2	2.16	0.46
1:C:47:VAL:HG13	1:C:48:PRO:HD3	1.98	0.46
1:A:32:VAL:O	1:A:32:VAL:HG13	2.17	0.45
1:C:196:VAL:O	1:C:197:ALA:C	2.54	0.45
1:A:47:VAL:HG22	1:A:48:PRO:HD3	1.99	0.45
1:C:165:HIS:CE1	1:C:266:GLU:OE1	2.70	0.45
1:A:150:GLY:HA3	1:A:292:VAL:HG11	1.98	0.45
1:A:47:VAL:HG21	1:B:284:LEU:HD23	1.98	0.45
1:A:147:ARG:HD3	1:B:167:MET:CE	2.46	0.45
1:D:44:LEU:O	1:D:47:VAL:HG13	2.17	0.45
1:A:171:GLU:OE1	1:A:240:PRO:HB3	2.16	0.45
1:A:167:MET:CE	1:B:147:ARG:HA	2.47	0.45
1:D:73:VAL:HB	1:D:263:ARG:HH11	1.80	0.45
1:B:54:VAL:CG2	1:B:242:VAL:HG13	2.47	0.45
1:D:175:PRO:CB	1:D:179:LEU:HD12	2.47	0.45
1:B:220:TYR:HB3	1:B:263:ARG:HB2	1.99	0.44
1:B:221:THR:HG22	1:B:263:ARG:HE	1.81	0.44
1:A:87:LEU:O	1:A:91:SER:OG	2.32	0.44
1:A:293:VAL:C	1:A:295:LYS:N	2.71	0.44
1:C:122:LEU:HD13	5:C:505:9AU:CAX	2.47	0.44
1:B:175:PRO:CB	1:B:179:LEU:HD12	2.48	0.44
1:A:207:ARG:HD3	1:A:274:HIS:HD2	1.83	0.43
1:A:289:ASN:O	1:A:292:VAL:HG22	2.18	0.43
1:B:163:ARG:O	1:B:167:MET:HG2	2.17	0.43
1:C:233:ARG:O	1:C:234:PRO:C	2.57	0.43
1:A:41:LEU:HD22	1:B:78:LYS:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:VAL:HG22	1:B:242:VAL:HG13	2.01	0.43
1:C:267:ALA:O	1:C:270:ARG:HB3	2.17	0.43
1:D:152:ILE:HG22	1:D:156:LEU:HD22	2.01	0.43
1:A:268:GLU:O	1:A:272:VAL:HG23	2.19	0.43
1:B:79:LYS:HE3	1:C:256:ARG:HD3	1.99	0.43
1:D:272:VAL:HA	1:D:291:PHE:CZ	2.54	0.43
1:B:282:LYS:O	1:B:283:ARG:HB2	2.18	0.42
1:C:283:ARG:HA	1:C:285:GLN:HE21	1.84	0.42
1:A:187:GLN:NE2	1:B:139:LEU:HB3	2.34	0.42
1:C:67:LEU:HB2	1:C:68:PRO:HD3	2.01	0.42
1:C:185:ILE:CD1	1:C:189:ILE:CD1	2.97	0.42
1:D:121:PHE:O	1:D:124:THR:OG1	2.27	0.42
1:B:89:TYR:OH	1:C:225:ARG:NE	2.43	0.42
1:C:89:TYR:CE1	1:C:93:ARG:HD3	2.54	0.42
1:D:71:GLU:OE2	1:D:256:ARG:NH2	2.47	0.42
1:D:211:TYR:O	1:D:215:GLU:HG2	2.20	0.42
1:C:186:THR:HG23	5:C:505:9AU:CAA	2.50	0.42
1:C:205:VAL:O	1:C:209:VAL:HG23	2.20	0.42
1:A:92:VAL:HG23	1:A:208:PHE:CD1	2.54	0.42
1:B:65:TRP:CB	1:B:70:ILE:HD13	2.49	0.42
1:D:96:ARG:NH1	1:D:215:GLU:OE1	2.49	0.42
1:D:144:TYR:O	1:D:146:THR:HG23	2.20	0.42
1:A:96:ARG:CA	5:A:505:9AU:CAD	2.95	0.42
1:A:153:ASN:O	1:A:157:VAL:HG13	2.19	0.42
1:B:177:LEU:N	1:B:178:PRO:CD	2.83	0.42
1:B:34:GLY:O	1:B:38:LEU:HG	2.20	0.42
1:D:54:VAL:HG13	1:D:242:VAL:HA	2.02	0.42
1:A:93:ARG:NE	1:D:229:GLU:OE2	2.47	0.41
5:B:505:9AU:OAF	5:B:505:9AU:CAI	2.68	0.41
1:C:122:LEU:HD13	5:C:505:9AU:CAW	2.50	0.41
1:C:125:VAL:O	1:C:129:PRO:HD3	2.20	0.41
1:D:47:VAL:N	1:D:48:PRO:CD	2.82	0.41
1:A:122:LEU:HD13	5:A:505:9AU:CAW	2.50	0.41
1:A:145:MET:HG3	1:B:166:LEU:HD21	2.02	0.41
1:D:119:CYS:O	1:D:123:GLU:HG2	2.20	0.41
1:B:271:VAL:O	1:B:272:VAL:C	2.59	0.41
1:A:267:ALA:O	1:A:271:VAL:HG22	2.20	0.41
1:C:198:TYR:CE1	1:C:202:PRO:HB3	2.55	0.41
1:B:132:VAL:O	1:B:136:LEU:HD22	2.20	0.41
1:D:175:PRO:HB2	1:D:179:LEU:HD12	2.03	0.41
1:B:128:VAL:N	1:B:129:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:ARG:HD3	6:B:611:HOH:O	2.21	0.41
1:B:162:GLU:O	1:B:165:HIS:HB2	2.21	0.41
1:C:110:ILE:CG2	1:C:232:LEU:HD13	2.50	0.41
1:A:147:ARG:HD3	1:B:167:MET:HE2	2.02	0.40
1:C:54:VAL:HG22	1:C:242:VAL:HA	2.03	0.40
1:C:80:PRO:CB	1:C:85:ASP:HB3	2.51	0.40
1:A:93:ARG:HA	1:A:93:ARG:HD2	1.94	0.40
1:D:172:LEU:HD22	1:D:236:LYS:HB3	2.03	0.40
1:D:54:VAL:HG11	1:D:245:VAL:HG13	2.03	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	262/329 (80%)	240 (92%)	17 (6%)	5 (2%)	8	18
1	B	261/329 (79%)	230 (88%)	30 (12%)	1 (0%)	34	58
1	C	264/329 (80%)	247 (94%)	14 (5%)	3 (1%)	14	32
1	D	263/329 (80%)	235 (89%)	22 (8%)	6 (2%)	6	14
All	All	1050/1316 (80%)	952 (91%)	83 (8%)	15 (1%)	11	26

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	ASN
1	A	294	LEU
1	D	54	VAL
1	C	44	LEU
1	A	281	GLU
1	C	234	PRO

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Mol	Chain	Res	Type
1	D	59	SER
1	D	61	ASP
1	D	253	ALA
1	A	152	ILE
1	B	126	ALA
1	C	195	LEU
1	D	210	GLY
1	D	234	PRO
1	A	242	VAL

### 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	239/292 (82%)	211 (88%)	28 (12%)	5 12
1	B	238/292 (82%)	213 (90%)	25 (10%)	7 15
1	C	241/292 (82%)	216 (90%)	25 (10%)	7 15
1	D	240/292 (82%)	217 (90%)	23 (10%)	8 19
All	All	958/1168 (82%)	857 (90%)	101 (10%)	7 15

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	44	LEU
1	A	47	VAL
1	A	54	VAL
1	A	66	SER
1	A	72	ASN
1	A	86	THR
1	A	98	LEU
1	A	101	THR
1	A	106	ARG
1	A	112	GLU
1	A	136	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	145	MET
1	A	156	LEU
1	A	157	VAL
1	A	166	LEU
1	A	170	ILE
1	A	179	LEU
1	A	182	SER
1	A	196	VAL
1	A	233	ARG
1	A	242	VAL
1	A	258	LEU
1	A	263	ARG
1	A	271	VAL
1	A	284	LEU
1	A	285	GLN
1	A	288	VAL
1	B	40	ARG
1	B	44	LEU
1	B	45	GLU
1	B	52	LEU
1	B	60	GLU
1	B	81	ASN
1	B	87	LEU
1	B	106	ARG
1	B	107	PHE
1	B	136	LEU
1	B	156	LEU
1	B	166	LEU
1	B	170	ILE
1	B	179	LEU
1	B	185	ILE
1	B	196	VAL
1	B	221	THR
1	B	225	ARG
1	B	233	ARG
1	B	242	VAL
1	B	260	ASN
1	B	263	ARG
1	B	271	VAL
1	B	284	LEU
1	B	285	GLN
1	C	47	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	50	VAL
1	C	52	LEU
1	C	54	VAL
1	C	90	ARG
1	C	106	ARG
1	C	110	ILE
1	C	132	VAL
1	C	156	LEU
1	C	166	LEU
1	C	179	LEU
1	C	185	ILE
1	C	186	THR
1	C	192	LEU
1	C	196	VAL
1	C	233	ARG
1	C	242	VAL
1	C	250	SER
1	C	260	ASN
1	C	263	ARG
1	C	271	VAL
1	C	281	GLU
1	C	284	LEU
1	C	285	GLN
1	C	288	VAL
1	D	44	LEU
1	D	45	GLU
1	D	47	VAL
1	D	61	ASP
1	D	81	ASN
1	D	106	ARG
1	D	107	PHE
1	D	110	ILE
1	D	118	ARG
1	D	132	VAL
1	D	136	LEU
1	D	156	LEU
1	D	166	LEU
1	D	170	ILE
1	D	221	THR
1	D	225	ARG
1	D	233	ARG
1	D	237	ASN

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Mol	Chain	Res	Type
1	D	238	ASP
1	D	245	VAL
1	D	271	VAL
1	D	284	LEU
1	D	285	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	187	GLN
1	A	273	ASN
1	A	274	HIS
1	B	161	ASN
1	B	187	GLN
1	B	269	HIS
1	B	273	ASN
1	B	274	HIS
1	C	72	ASN
1	C	248	ASN
1	C	260	ASN
1	C	273	ASN
1	C	285	GLN
1	C	286	ASN
1	D	248	ASN
1	D	260	ASN
1	D	269	HIS
1	D	273	ASN
1	D	274	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 8 are monoatomic and 4 are modelled with single atom - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	OXY	A	504	-	1,1,1	0.05	0	-		
4	OXY	C	504	2	1,1,1	0.11	0	-		
5	9AU	D	505	-	28,28,28	1.22	3 (10%)	34,37,37	1.68	8 (23%)
4	OXY	B	504	-	1,1,1	0.07	0	-		
4	OXY	D	504	-	1,1,1	0.09	0	-		
5	9AU	A	505	-	28,28,28	1.42	4 (14%)	34,37,37	1.82	7 (20%)
5	9AU	B	505	-	28,28,28	1.42	4 (14%)	34,37,37	2.27	6 (17%)
5	9AU	C	505	-	28,28,28	1.27	2 (7%)	34,37,37	1.82	8 (23%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	9AU	B	505	-	-	4/17/17/17	0/2/2/2
5	9AU	D	505	-	-	4/17/17/17	0/2/2/2
5	9AU	A	505	-	-	4/17/17/17	0/2/2/2
5	9AU	C	505	-	-	3/17/17/17	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	505	9AU	CAP-CAI	-4.64	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	505	9AU	CAP-CAI	-4.14	1.44	1.50
5	D	505	9AU	CBA-CAW	-3.87	1.39	1.45
5	C	505	9AU	CAP-CAI	-3.74	1.45	1.50
5	A	505	9AU	CBA-CAW	-3.69	1.39	1.45
5	C	505	9AU	CBA-CAW	-3.47	1.40	1.45
5	D	505	9AU	CAP-CAI	-2.73	1.46	1.50
5	B	505	9AU	CBA-CAW	-2.61	1.41	1.45
5	A	505	9AU	CAP-CAX	-2.29	1.47	1.51
5	B	505	9AU	CAP-CAX	-2.18	1.48	1.51
5	B	505	9AU	CAY-CAX	-2.13	1.39	1.45
5	A	505	9AU	CAY-CAX	-2.11	1.39	1.45
5	D	505	9AU	CAY-CAX	-2.05	1.39	1.45

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	505	9AU	CAP-CAI-CAV	-9.91	110.29	126.79
5	C	505	9AU	CAP-CAI-CAV	-6.30	116.31	126.79
5	A	505	9AU	CAP-CAI-CAV	-6.23	116.42	126.79
5	B	505	9AU	OAF-CAW-CBA	3.92	122.37	115.53
5	D	505	9AU	OAS-CAZ-CAL	3.77	121.26	116.26
5	C	505	9AU	OAS-CAY-CAX	3.17	121.31	118.01
5	D	505	9AU	CAP-CAI-CAV	-3.10	121.63	126.79
5	D	505	9AU	CAI-CAP-CAX	3.02	120.18	112.05
5	C	505	9AU	CAZ-CBA-CAW	2.92	120.48	117.79
5	A	505	9AU	CAO-CAR-CAV	-2.88	103.52	112.98
5	B	505	9AU	CAI-CAP-CAX	2.84	119.69	112.05
5	C	505	9AU	OAS-CAZ-CAL	2.74	119.89	116.26
5	A	505	9AU	OAS-CAY-CAX	2.73	120.86	118.01
5	A	505	9AU	CAZ-CBA-CAW	2.66	120.24	117.79
5	D	505	9AU	OAS-CAY-OAE	2.57	119.61	116.22
5	B	505	9AU	OAS-CAY-CAX	2.54	120.65	118.01
5	C	505	9AU	OAS-CAZ-CBA	-2.53	119.15	121.56
5	D	505	9AU	CAD-CAV-CAR	2.53	119.52	115.27
5	D	505	9AU	OAE-CAY-CAX	-2.47	119.84	125.30
5	D	505	9AU	OAS-CAY-CAX	2.43	120.54	118.01
5	A	505	9AU	OAF-CAW-CBA	2.38	119.69	115.53
5	B	505	9AU	CAO-CAR-CAV	-2.32	105.34	112.98
5	B	505	9AU	CAZ-CBA-CAW	2.32	119.93	117.79
5	A	505	9AU	OAS-CAZ-CAL	2.22	119.20	116.26
5	C	505	9AU	CAI-CAP-CAX	2.18	117.93	112.05
5	C	505	9AU	OAF-CAW-CBA	2.08	119.17	115.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	505	9AU	OAE-CAY-CAX	-2.02	120.84	125.30
5	D	505	9AU	CAZ-CBA-CAW	2.01	119.64	117.79
5	A	505	9AU	CAC-CAU-CAQ	2.00	118.64	115.27

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	505	9AU	CAI-CAP-CAX-CAY
5	A	505	9AU	CAI-CAP-CAX-CAW
5	B	505	9AU	CAI-CAP-CAX-CAY
5	B	505	9AU	CAI-CAP-CAX-CAW
5	C	505	9AU	CAI-CAP-CAX-CAY
5	C	505	9AU	CAI-CAP-CAX-CAW
5	D	505	9AU	CAI-CAP-CAX-CAY
5	D	505	9AU	CAI-CAP-CAX-CAW
5	B	505	9AU	CAH-CAO-CAR-CAV
5	B	505	9AU	CAG-CAN-CAQ-CAU
5	A	505	9AU	CAH-CAO-CAR-CAV
5	C	505	9AU	CAH-CAO-CAR-CAV
5	D	505	9AU	CAH-CAO-CAR-CAV
5	A	505	9AU	CAG-CAN-CAQ-CAU
5	D	505	9AU	CAO-CAR-CAV-CAD

There are no ring outliers.

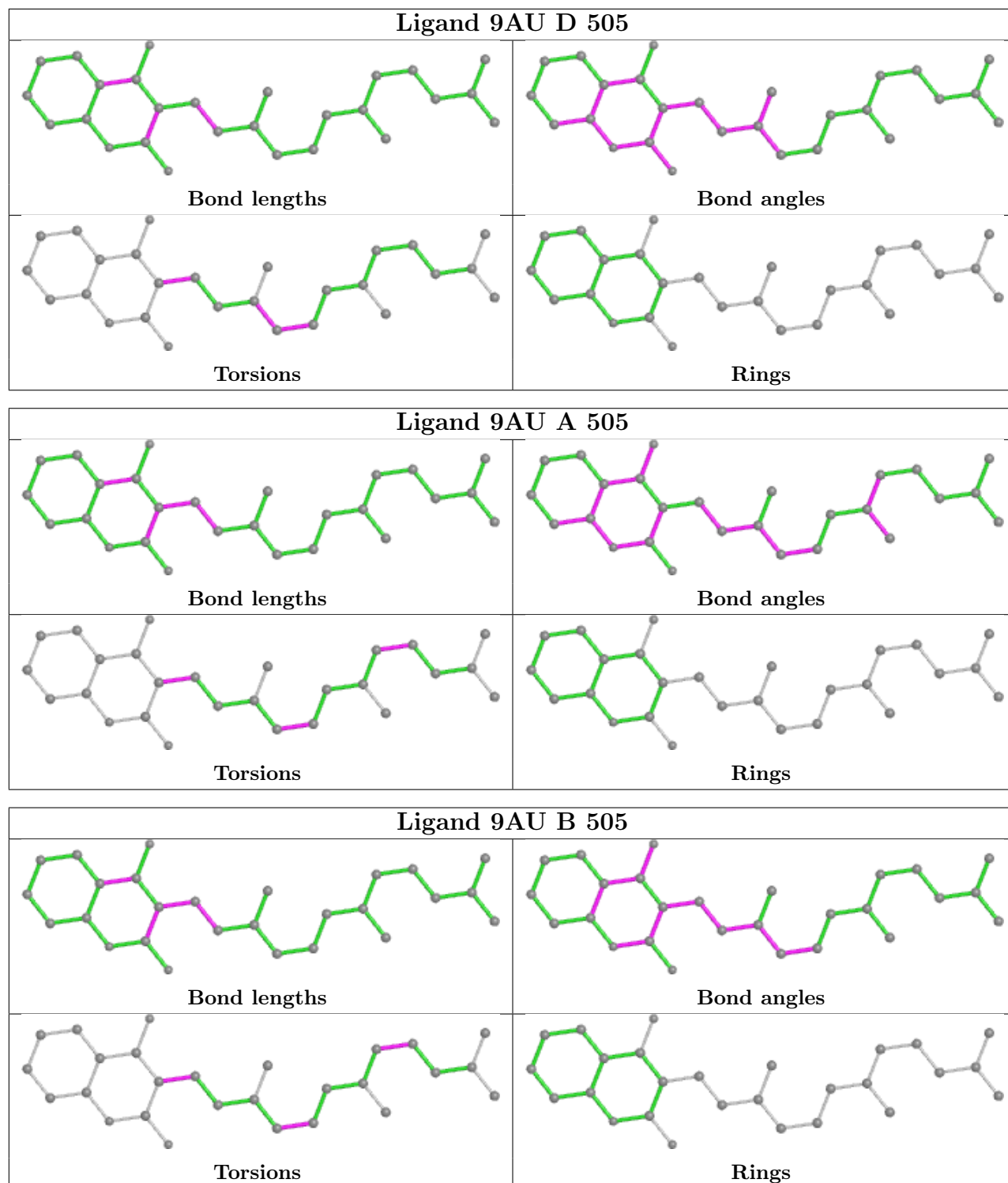
4 monomers are involved in 14 short contacts:

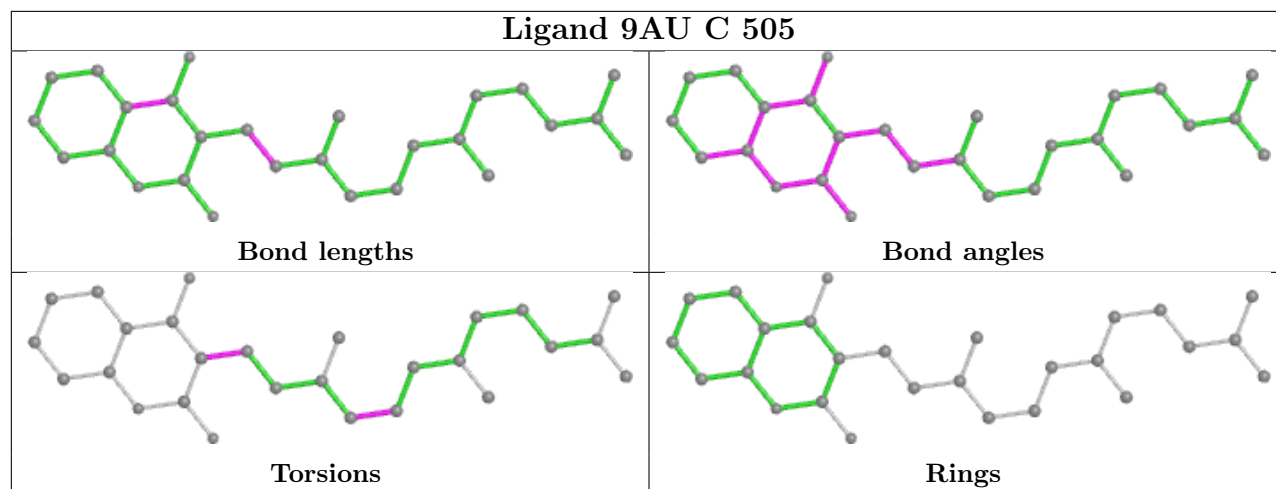
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	505	9AU	2	0
5	A	505	9AU	4	0
5	B	505	9AU	2	0
5	C	505	9AU	6	0

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.





## 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	264/329 (80%)	-0.26	3 (1%) 80 82	23, 39, 58, 91	0
1	B	263/329 (79%)	-0.13	8 (3%) 50 51	19, 38, 60, 94	0
1	C	266/329 (80%)	0.31	27 (10%) 6 5	27, 46, 97, 163	0
1	D	265/329 (80%)	0.58	34 (12%) 3 3	34, 55, 118, 159	0
All	All	1058/1316 (80%)	0.13	72 (6%) 17 16	19, 44, 84, 163	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	109	SER	13.1
1	C	107	PHE	10.4
1	D	110	ILE	10.0
1	D	235	THR	9.8
1	D	106	ARG	7.9
1	C	110	ILE	7.6
1	D	108	GLY	7.1
1	C	106	ARG	6.9
1	D	102	PHE	6.8
1	C	108	GLY	6.5
1	C	105	TYR	6.5
1	C	109	SER	6.4
1	D	107	PHE	6.1
1	D	97	TRP	6.1
1	D	233	ARG	5.4
1	D	101	THR	4.8
1	D	234	PRO	4.6
1	D	104	LEU	4.4
1	D	48	PRO	3.9
1	C	177	LEU	3.8
1	C	52	LEU	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	105	TYR	3.7
1	C	102	PHE	3.6
1	B	238	ASP	3.5
1	D	231	ARG	3.5
1	B	293	VAL	3.3
1	C	97	TRP	3.3
1	C	48	PRO	3.3
1	D	52	LEU	3.2
1	D	87	LEU	3.1
1	D	283	ARG	3.0
1	C	235	THR	3.0
1	D	103	SER	3.0
1	D	83	LEU	3.0
1	D	232	LEU	2.9
1	D	81	ASN	2.9
1	C	236	LYS	2.9
1	C	49	VAL	2.8
1	D	111	THR	2.8
1	C	115	VAL	2.8
1	C	111	THR	2.8
1	B	107	PHE	2.8
1	D	177	LEU	2.7
1	B	294	LEU	2.6
1	D	252	ASN	2.6
1	C	174	GLN	2.6
1	C	238	ASP	2.6
1	D	178	PRO	2.5
1	D	98	LEU	2.5
1	A	106	ARG	2.5
1	D	32	VAL	2.5
1	B	283	ARG	2.4
1	C	251	LYS	2.3
1	D	90	ARG	2.3
1	A	251	LYS	2.3
1	B	200	ILE	2.3
1	C	181	VAL	2.3
1	C	244	ARG	2.2
1	C	296	LYS	2.2
1	D	50	VAL	2.2
1	D	174	GLN	2.2
1	C	204	PHE	2.2
1	A	233	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	31	PRO	2.2
1	B	32	VAL	2.2
1	C	252	ASN	2.2
1	B	46	THR	2.1
1	D	200	ILE	2.1
1	D	94	THR	2.1
1	C	32	VAL	2.0
1	D	216	ALA	2.0
1	C	103	SER	2.0

## 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 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.

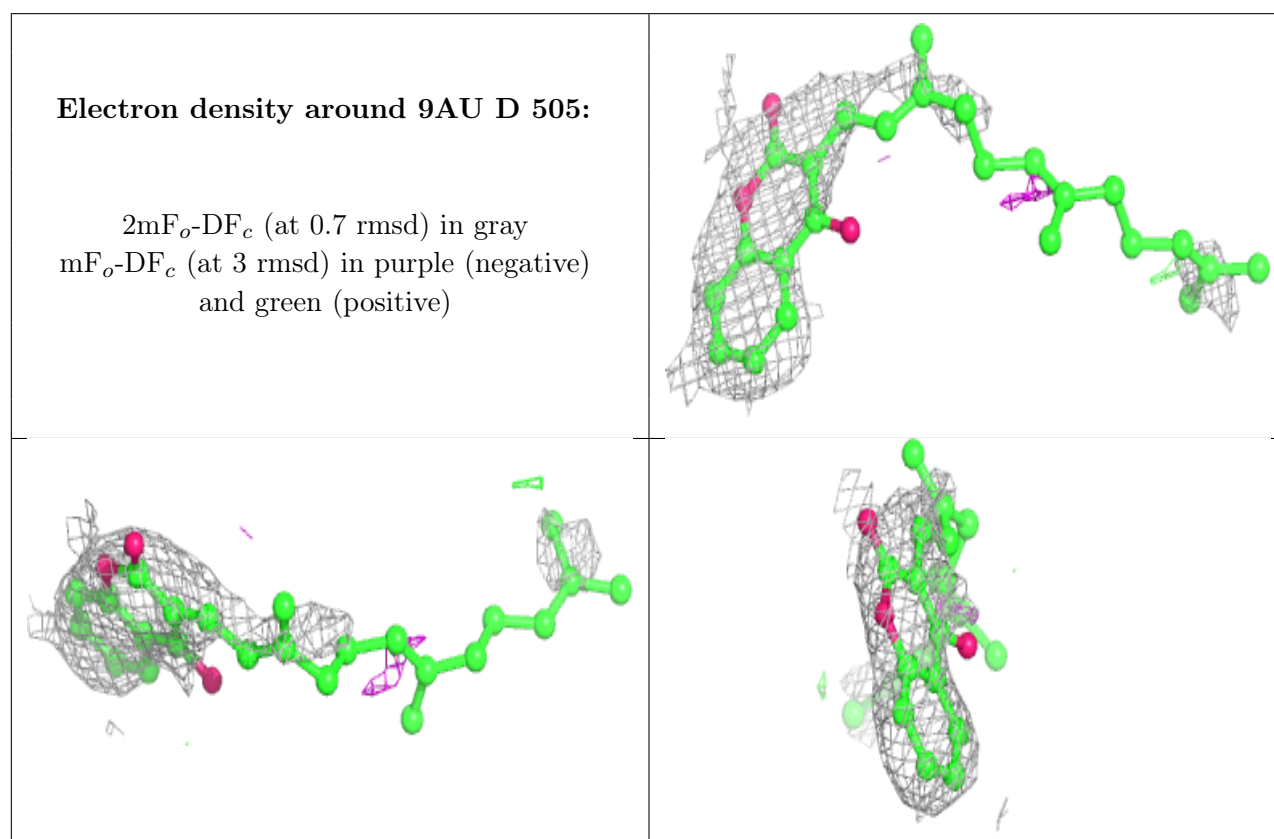
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	9AU	D	505	27/27	0.74	0.51	77,108,124,126	0
5	9AU	C	505	27/27	0.83	0.28	56,64,69,73	0
5	9AU	A	505	27/27	0.91	0.21	51,62,68,73	0
5	9AU	B	505	27/27	0.91	0.23	37,49,79,82	0
4	OXY	B	504	2/2	0.93	0.50	43,43,43,48	0
4	OXY	D	504	2/2	0.96	0.24	45,45,45,48	0
2	FE	C	501	1/1	0.97	0.15	49,49,49,49	0
4	OXY	C	504	2/2	0.98	0.26	48,48,48,50	0
4	OXY	A	504	2/2	0.98	0.43	29,29,29,30	0
2	FE	A	501	1/1	0.98	0.13	44,44,44,44	0
2	FE	B	502	1/1	0.99	0.13	27,27,27,27	0
2	FE	A	502	1/1	0.99	0.15	38,38,38,38	0
2	FE	D	501	1/1	0.99	0.13	51,51,51,51	0
2	FE	D	502	1/1	0.99	0.14	56,56,56,56	0

*Continued on next page...*

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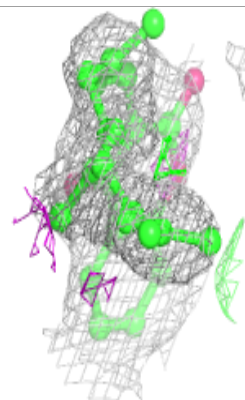
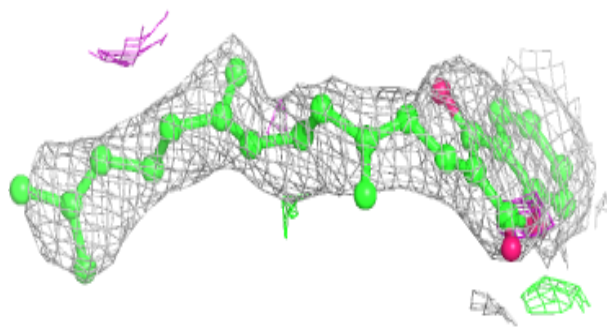
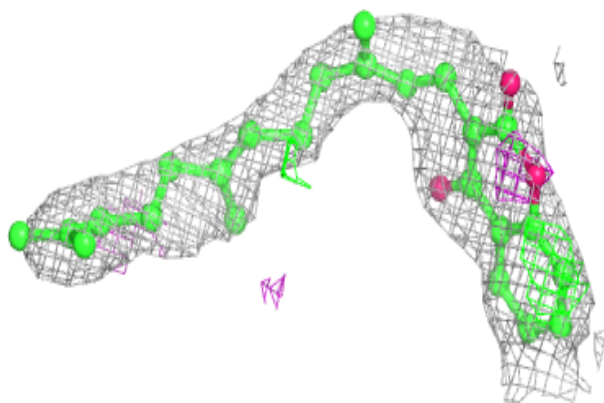
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	OH	A	503	1/1	0.99	0.17	16,16,16,16	0
3	OH	D	503	1/1	0.99	0.18	14,14,14,14	0
2	FE	B	501	1/1	0.99	0.11	28,28,28,28	0
2	FE	C	502	1/1	1.00	0.15	35,35,35,35	0
3	OH	B	503	1/1	1.00	0.11	40,40,40,40	0
3	OH	C	503	1/1	1.00	0.14	24,24,24,24	0

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.

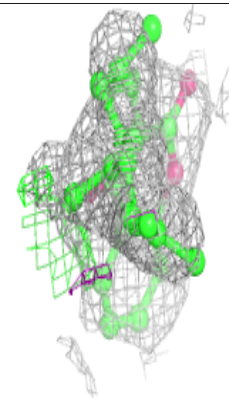
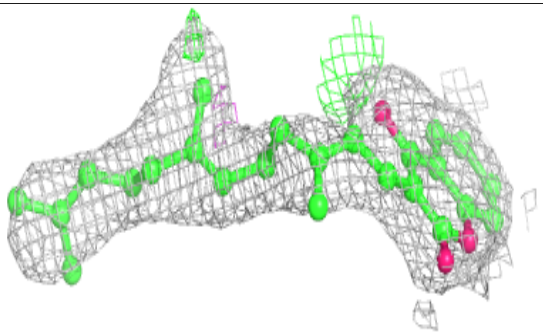
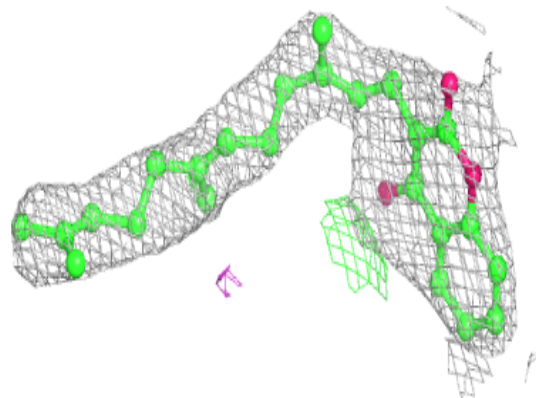


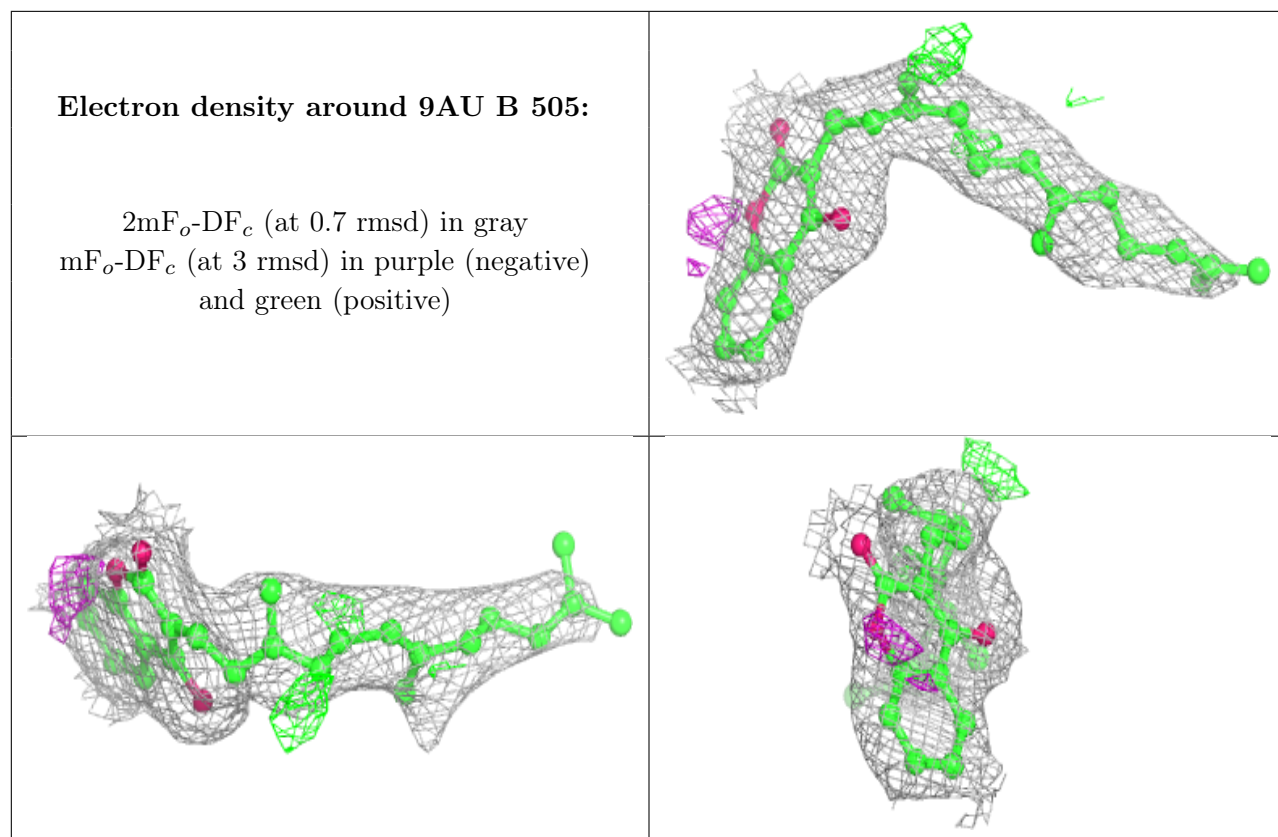
**Electron density around 9AU C 505:**

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

**Electron density around 9AU A 505:**

$2mF_o-DF_c$  (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.