



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2020 – 02:45 PM BST

PDB ID : 6WVG
Title : human CD53
Authors : Yang, Y.; Liu, S.; Li, W.
Deposited on : 2020-05-06
Resolution : 2.90 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 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 : 2.14.4.dev1
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) : 2.14.4.dev1

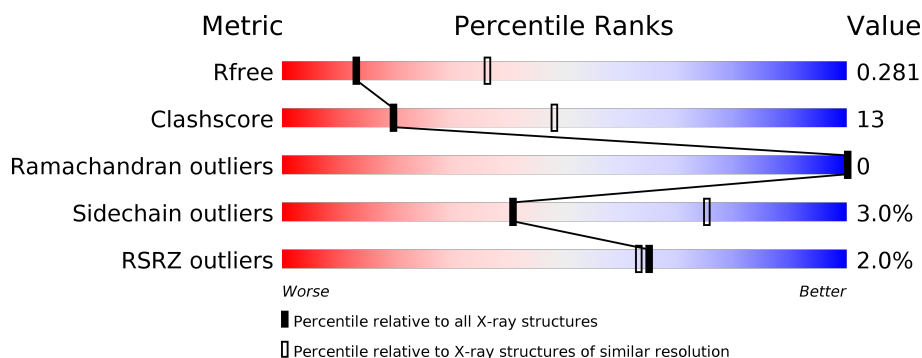
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 ≥ 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	457	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>24%</div> <div>• •</div> </div> </div>
1	B	457	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7073 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 Green fluorescent protein, Leukocyte surface antigen CD53 chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3480	2248	573	638	21			
1	B	441	Total	C	N	O	S	0	0	0
			3468	2241	572	634	21			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	ARG	SER	conflict	UNP P42212
A	39	ASN	TYR	conflict	UNP P42212
A	64	LEU	PHE	conflict	UNP P42212
A	66	CRO	SER	chromophore	UNP P42212
A	66	CRO	TYR	chromophore	UNP P42212
A	66	CRO	GLY	chromophore	UNP P42212
A	80	ARG	GLN	conflict	UNP P42212
A	99	SER	PHE	conflict	UNP P42212
A	105	THR	ASN	conflict	UNP P42212
A	224	SER	CYS	conflict	UNP P19397
A	292	ALA	ASN	conflict	UNP P19397
A	352	SER	CYS	conflict	UNP P19397
A	364	PHE	TYR	conflict	UNP P42212
A	372	THR	MET	conflict	UNP P42212
A	382	ALA	VAL	conflict	UNP P42212
A	390	VAL	ILE	conflict	UNP P42212
A	425	VAL	ALA	conflict	UNP P42212
A	450	HIS	-	expression tag	UNP P42212
A	451	HIS	-	expression tag	UNP P42212
A	452	HIS	-	expression tag	UNP P42212
A	453	HIS	-	expression tag	UNP P42212
A	454	HIS	-	expression tag	UNP P42212
A	455	HIS	-	expression tag	UNP P42212
A	456	HIS	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
A	457	HIS	-	expression tag	UNP P42212
A	458	HIS	-	expression tag	UNP P42212
A	459	HIS	-	expression tag	UNP P42212
B	30	ARG	SER	conflict	UNP P42212
B	39	ASN	TYR	conflict	UNP P42212
B	64	LEU	PHE	conflict	UNP P42212
B	66	CRO	SER	chromophore	UNP P42212
B	66	CRO	TYR	chromophore	UNP P42212
B	66	CRO	GLY	chromophore	UNP P42212
B	80	ARG	GLN	conflict	UNP P42212
B	99	SER	PHE	conflict	UNP P42212
B	105	THR	ASN	conflict	UNP P42212
B	224	SER	CYS	conflict	UNP P19397
B	292	ALA	ASN	conflict	UNP P19397
B	352	SER	CYS	conflict	UNP P19397
B	364	PHE	TYR	conflict	UNP P42212
B	372	THR	MET	conflict	UNP P42212
B	382	ALA	VAL	conflict	UNP P42212
B	390	VAL	ILE	conflict	UNP P42212
B	425	VAL	ALA	conflict	UNP P42212
B	450	HIS	-	expression tag	UNP P42212
B	451	HIS	-	expression tag	UNP P42212
B	452	HIS	-	expression tag	UNP P42212
B	453	HIS	-	expression tag	UNP P42212
B	454	HIS	-	expression tag	UNP P42212
B	455	HIS	-	expression tag	UNP P42212
B	456	HIS	-	expression tag	UNP P42212
B	457	HIS	-	expression tag	UNP P42212
B	458	HIS	-	expression tag	UNP P42212
B	459	HIS	-	expression tag	UNP P42212

- Molecule 2 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 17 17	0	0
2	A	1	Total C 9 9	0	0
2	A	1	Total C 11 11	0	0
2	A	1	Total C O 25 21 4	0	0
2	B	1	Total C 17 17	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

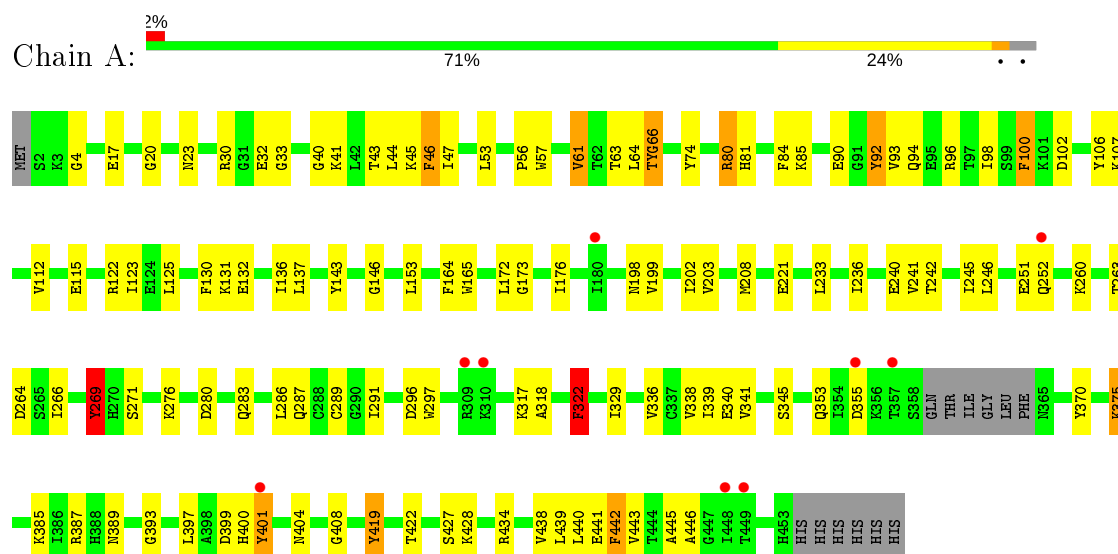
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total	O	0	0
			12	12		
4	B	6	Total	O	0	0
			6	6		

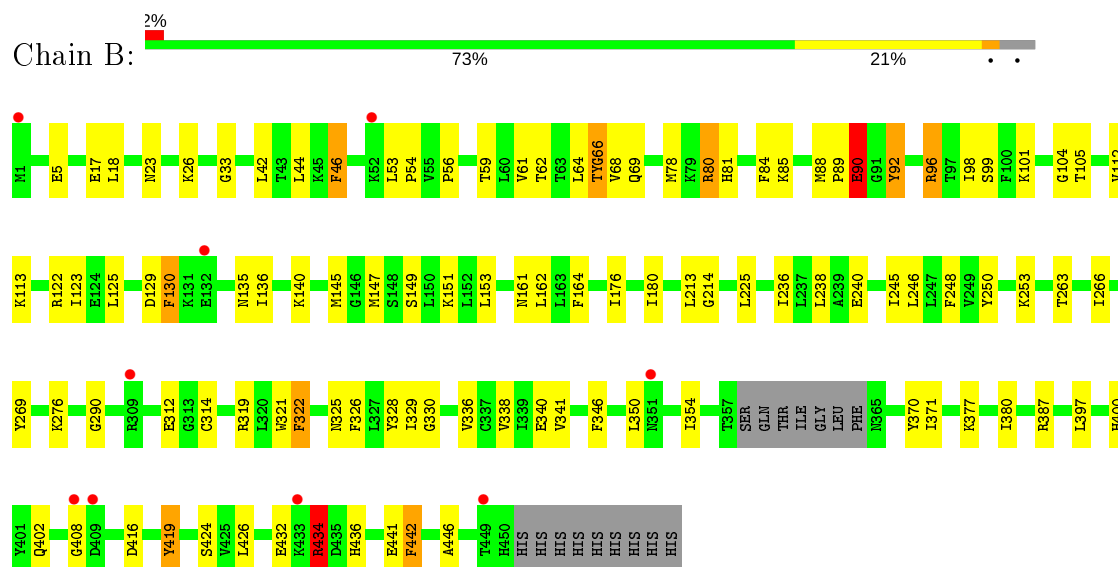
3 Residue-property plots [i](#)

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: Green fluorescent protein, Leukocyte surface antigen CD53 chimera



- Molecule 1: Green fluorescent protein, Leukocyte surface antigen CD53 chimera



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.31 Å 209.77 Å 73.28 Å 90.00° 100.29° 90.00°	Depositor
Resolution (Å)	35.61 – 2.90 35.61 – 2.88	Depositor EDS
% Data completeness (in resolution range)	75.2 (35.61-2.90) 91.7 (35.61-2.88)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.90 Å)	Xtriage
Refinement program	PHENIX 1.18_3845	Depositor
R, R_{free}	0.216 , 0.269 0.231 , 0.281	Depositor DCC
R_{free} test set	1536 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.749	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7073	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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: OLC, NAG, 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	0.41	3/3533 (0.1%)	0.70	5/4782 (0.1%)
1	B	0.36	0/3522	0.72	8/4766 (0.2%)
All	All	0.38	3/7055 (0.0%)	0.71	13/9548 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	375	LYS	CE-NZ	-8.00	1.29	1.49
1	A	375	LYS	CB-CG	6.67	1.70	1.52
1	A	107	LYS	CE-NZ	-5.25	1.35	1.49

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	434	ARG	CG-CD-NE	9.12	130.94	111.80
1	B	26	LYS	CD-CE-NZ	-7.12	95.32	111.70
1	B	319	ARG	NE-CZ-NH1	-6.58	117.01	120.30
1	B	319	ARG	NE-CZ-NH2	6.58	123.59	120.30
1	B	90	GLU	CA-CB-CG	6.40	127.47	113.40
1	A	375	LYS	CD-CE-NZ	-5.53	98.99	111.70
1	A	107	LYS	CD-CE-NZ	-5.51	99.02	111.70
1	A	322	PHE	CB-CG-CD2	-5.47	116.97	120.80
1	A	269	TYR	CB-CG-CD2	-5.46	117.72	121.00
1	B	96	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	A	355	ASP	CB-CG-OD1	5.33	123.09	118.30
1	B	322	PHE	CB-CG-CD2	-5.31	117.08	120.80
1	B	96	ARG	NE-CZ-NH1	-5.00	117.80	120.30

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	3480	0	3462	95	0
1	B	3468	0	3457	88	0
2	A	62	0	100	7	0
2	B	17	0	31	3	0
3	A	14	0	13	1	0
3	B	14	0	13	0	0
4	A	12	0	0	1	0
4	B	6	0	0	1	0
All	All	7073	0	7076	180	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 (180) 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:A:439:LEU:HD21	1:A:441:GLU:HG3	1.56	0.87
1:B:90:GLU:HA	1:B:113:LYS:HE3	1.63	0.80
1:A:90:GLU:HG3	1:A:408:GLY:HA3	1.67	0.76
1:A:271:SER:HA	3:A:505:NAG:H81	1.70	0.74
1:A:269:TYR:CE1	1:A:276:LYS:HG3	2.23	0.73
1:B:99:SER:HA	1:B:105:THR:HG22	1.71	0.73
1:A:419:TYR:HE1	1:A:446:ALA:HB3	1.56	0.71
1:B:92:TYR:CE1	1:B:112:VAL:HB	2.26	0.70
1:A:84:PHE:HD1	1:A:92:TYR:CE2	2.09	0.70
1:B:419:TYR:HE1	1:B:446:ALA:HB3	1.57	0.70
1:A:146:GLY:O	1:A:389:ASN:ND2	2.23	0.70
1:A:283:GLN:NE2	1:A:289:CYS:O	2.25	0.70
1:A:30:ARG:NH1	1:A:32:GLU:OE2	2.25	0.69
1:A:45:LYS:HE2	1:A:47:ILE:HD11	1.76	0.67
1:B:145:MET:HG2	1:B:426:LEU:HD11	1.76	0.67
1:B:419:TYR:CE1	1:B:446:ALA:HB3	2.29	0.67
1:A:33:GLY:HA3	1:A:44:LEU:HD23	1.77	0.67
1:B:104:GLY:HA3	1:B:130:PHE:CD1	2.30	0.66
1:A:260:LYS:NZ	1:A:264:ASP:OD2	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:PHE:HD1	1:B:92:TYR:CE2	2.16	0.64
1:B:432:GLU:OE2	1:B:434:ARG:HD2	1.99	0.62
1:A:102:ASP:O	1:A:131:LYS:NZ	2.33	0.61
1:B:96:ARG:HE	1:B:402:GLN:HE21	1.49	0.60
1:B:370:TYR:CE1	1:B:419:TYR:HD2	2.20	0.59
1:A:233:LEU:HD22	1:A:340:GLU:HG3	1.85	0.58
1:A:92:TYR:CE1	1:A:112:VAL:HB	2.40	0.57
1:B:18:LEU:HD11	1:B:125:LEU:HB2	1.87	0.57
1:B:213:LEU:HD22	1:B:225:LEU:HD22	1.86	0.57
1:A:173:GLY:O	1:A:176:ILE:HG22	2.04	0.57
1:A:338:VAL:HA	1:A:341:VAL:HG12	1.87	0.57
1:B:113:LYS:NZ	4:B:603:HOH:O	2.35	0.57
1:A:46:PHE:CD2	1:A:64:LEU:HD13	2.40	0.56
1:A:94:GLN:HB2	1:A:404:ASN:HD21	1.70	0.56
1:B:269:TYR:CE1	1:B:276:LYS:HG3	2.41	0.56
1:B:338:VAL:HA	1:B:341:VAL:HG12	1.87	0.56
1:A:23:ASN:ND2	1:A:130:PHE:HB2	2.20	0.55
1:B:250:TYR:HD1	1:B:253:LYS:HE2	1.72	0.55
2:A:504:OLC:H4	1:B:328:TYR:HD2	1.71	0.55
1:A:84:PHE:HD1	1:A:92:TYR:HE2	1.51	0.55
1:A:387:ARG:HE	1:A:397:LEU:HD21	1.71	0.55
1:B:161:ASN:ND2	1:B:214:GLY:HA3	2.21	0.55
1:B:62:THR:O	1:B:96:ARG:NH1	2.40	0.55
1:B:84:PHE:HD1	1:B:92:TYR:HE2	1.55	0.55
1:A:199:VAL:O	1:A:203:VAL:HG12	2.07	0.54
1:A:43:THR:HG22	1:A:440:LEU:HG	1.90	0.54
1:A:46:PHE:N	1:A:46:PHE:CD1	2.76	0.54
1:A:94:GLN:HB2	1:A:404:ASN:ND2	2.24	0.53
1:A:427:SER:HB2	1:A:438:VAL:HB	1.89	0.53
1:A:291:ILE:N	1:A:296:ASP:OD2	2.41	0.53
1:A:318:ALA:HA	2:A:502:OLC:H7	1.91	0.53
1:A:387:ARG:NH2	4:A:602:HOH:O	2.41	0.53
1:B:46:PHE:CE2	1:B:64:LEU:HB3	2.44	0.53
1:B:90:GLU:HG2	1:B:408:GLY:HA3	1.90	0.52
1:B:161:ASN:HD22	1:B:214:GLY:HA3	1.73	0.52
1:A:322:PHE:HD1	1:A:322:PHE:O	1.90	0.52
1:B:18:LEU:HD13	1:B:123:ILE:HB	1.92	0.52
1:B:290:GLY:O	1:B:314:CYS:N	2.43	0.52
1:A:385:LYS:HG2	1:A:399:ASP:OD1	2.10	0.51
1:B:96:ARG:NE	1:B:402:GLN:HE21	2.07	0.51
1:B:59:THR:HG21	1:B:136:ILE:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:LYS:HB2	1:B:397:LEU:HB3	1.92	0.51
1:A:23:ASN:HD21	1:A:130:PHE:H	1.57	0.51
1:A:276:LYS:NZ	1:A:280:ASP:OD2	2.40	0.51
1:B:145:MET:HG2	1:B:426:LEU:CD1	2.40	0.51
1:A:132:GLU:OE2	1:A:137:LEU:HD23	2.10	0.50
1:A:221:GLU:OE1	1:A:393:GLY:HA3	2.11	0.50
1:A:66:CRO:N2	1:A:66:CRO:HD1	2.26	0.50
1:B:424:SER:HB3	1:B:441:GLU:HG2	1.94	0.50
1:B:53:LEU:HD12	1:B:54:PRO:HD2	1.92	0.50
1:B:46:PHE:CD1	1:B:46:PHE:N	2.80	0.50
1:A:4:GLY:HA3	1:A:85:LYS:O	2.11	0.50
1:B:96:ARG:HG2	1:B:402:GLN:HG3	1.92	0.50
1:A:93:VAL:O	1:A:404:ASN:HA	2.10	0.50
1:A:46:PHE:CE2	1:A:64:LEU:HB3	2.47	0.49
1:A:322:PHE:CE1	1:A:329:ILE:HD11	2.47	0.49
1:A:61:VAL:O	1:A:66:CRO:N1	2.45	0.49
1:B:442:PHE:N	1:B:442:PHE:CD1	2.80	0.49
1:B:80:ARG:O	1:B:80:ARG:HD2	2.13	0.49
1:A:56:PRO:HD3	1:A:136:ILE:O	2.13	0.49
1:A:287:GLN:OE1	1:B:149:SER:HA	2.12	0.49
1:A:345:SER:OG	1:B:328:TYR:OH	2.29	0.49
1:B:5:GLU:HA	1:B:85:LYS:HD3	1.94	0.49
1:B:371:ILE:HD12	1:B:380:ILE:HD12	1.93	0.49
1:B:92:TYR:HE1	1:B:112:VAL:HB	1.75	0.49
1:B:263:THR:O	1:B:266:ILE:HG22	2.12	0.48
1:A:66:CRO:O2	1:A:96:ARG:NH2	2.46	0.48
1:A:236:ILE:O	1:A:240:GLU:HG3	2.13	0.48
1:B:236:ILE:O	1:B:240:GLU:HB2	2.13	0.48
1:B:46:PHE:CD2	1:B:64:LEU:HD13	2.49	0.48
1:A:80:ARG:HE	1:A:81:HIS:CE1	2.32	0.48
1:A:98:ILE:HG12	1:A:400:HIS:CD2	2.48	0.48
1:B:84:PHE:CD1	1:B:92:TYR:HE2	2.32	0.48
1:A:46:PHE:HD1	1:A:46:PHE:N	2.12	0.48
1:A:143:TYR:CZ	1:A:428:LYS:HD3	2.49	0.47
1:B:66:CRO:HD1	1:B:66:CRO:N2	2.29	0.47
1:B:176:ILE:O	1:B:180:ILE:HG22	2.15	0.47
1:A:100:PHE:N	1:A:100:PHE:CD1	2.83	0.47
1:A:269:TYR:CD2	1:A:297:TRP:CH2	3.02	0.47
1:A:419:TYR:CE1	1:A:446:ALA:HB3	2.43	0.47
1:B:33:GLY:HA3	1:B:44:LEU:HD23	1.94	0.47
1:B:98:ILE:HG12	1:B:400:HIS:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:LYS:HE2	1:B:354:ILE:HA	1.96	0.47
1:A:442:PHE:N	1:A:442:PHE:CD1	2.83	0.47
1:A:98:ILE:HB	1:A:106:TYR:HB2	1.97	0.47
1:A:20:GLY:HA2	1:A:125:LEU:O	2.15	0.47
1:A:164:PHE:HE2	2:A:501:OLC:H11	1.80	0.47
1:A:153:LEU:HD21	2:A:504:OLC:H4A	1.97	0.46
1:B:78:MET:HE1	1:B:446:ALA:HA	1.96	0.46
1:A:241:VAL:O	1:A:245:ILE:HG12	2.15	0.46
1:A:269:TYR:HD1	1:A:269:TYR:C	2.19	0.46
1:A:84:PHE:CD1	1:A:92:TYR:HE2	2.33	0.46
1:A:345:SER:HG	1:B:328:TYR:HH	1.55	0.46
1:A:74:TYR:CD1	1:A:445:ALA:HB2	2.50	0.46
1:B:46:PHE:HE2	1:B:64:LEU:HB3	1.81	0.46
1:B:66:CRO:O2	1:B:69:GLN:NE2	2.50	0.45
1:B:434:ARG:H	1:B:434:ARG:HG3	1.33	0.45
1:A:339:ILE:HG23	2:A:501:OLC:H8A	1.99	0.45
1:B:164:PHE:CD2	2:B:501:OLC:H14A	2.52	0.45
1:B:336:VAL:O	1:B:340:GLU:HB2	2.17	0.44
1:A:40:GLY:O	1:A:442:PHE:HA	2.18	0.44
1:A:130:PHE:HB3	1:A:137:LEU:HD13	1.99	0.44
1:B:147:MET:HE1	1:B:387:ARG:HD2	1.98	0.44
1:B:441:GLU:C	1:B:442:PHE:CD1	2.91	0.44
1:A:322:PHE:CD1	1:A:322:PHE:C	2.91	0.44
1:B:62:THR:C	1:B:96:ARG:HH12	2.20	0.44
1:A:336:VAL:O	1:A:340:GLU:HB2	2.18	0.44
1:B:23:ASN:HD21	1:B:129:ASP:N	2.16	0.43
1:B:442:PHE:HD1	1:B:442:PHE:N	2.16	0.43
1:B:88:MET:HB3	1:B:89:PRO:HA	1.99	0.43
1:A:66:CRO:OG1	1:A:441:GLU:OE2	2.28	0.43
1:B:81:HIS:CE1	1:B:416:ASP:H	2.37	0.43
1:B:161:ASN:OD1	2:B:501:OLC:H12	2.18	0.43
1:A:17:GLU:OE1	1:A:122:ARG:NH1	2.51	0.43
1:A:422:THR:HG23	1:A:443:VAL:HG22	1.99	0.43
1:B:164:PHE:HE2	2:B:501:OLC:H11A	1.83	0.43
1:A:251:GLU:HG3	1:A:252:GLN:N	2.33	0.43
1:B:432:GLU:HB3	1:B:436:HIS:CE1	2.53	0.43
1:B:17:GLU:OE1	1:B:122:ARG:NH1	2.51	0.43
1:B:153:LEU:HD11	1:B:346:PHE:CD1	2.53	0.43
1:A:286:LEU:O	1:A:317:LYS:HE2	2.18	0.43
1:B:329:ILE:HG13	1:B:330:GLY:N	2.33	0.43
1:B:350:LEU:O	1:B:354:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:THR:O	1:A:246:LEU:HB2	2.19	0.43
1:A:263:THR:O	1:A:266:ILE:HG22	2.19	0.43
2:A:504:OLC:H3	1:B:325:ASN:CG	2.38	0.43
1:B:153:LEU:HD12	1:B:153:LEU:HA	1.84	0.43
1:B:238:LEU:HA	1:B:238:LEU:HD23	1.88	0.43
1:A:92:TYR:HD1	1:A:92:TYR:O	2.02	0.42
1:A:269:TYR:CD1	1:A:269:TYR:C	2.92	0.42
2:A:504:OLC:H2A	1:B:321:TRP:HE1	1.83	0.42
1:B:42:LEU:HB2	1:B:441:GLU:HB2	2.02	0.42
1:B:245:ILE:HG13	1:B:246:LEU:N	2.35	0.42
1:A:41:LYS:HZ3	1:A:442:PHE:HE2	1.65	0.42
1:A:172:LEU:HD22	1:A:208:MET:CE	2.50	0.42
1:A:100:PHE:N	1:A:100:PHE:HD1	2.18	0.42
1:B:46:PHE:HD1	1:B:46:PHE:N	2.18	0.42
1:A:401:TYR:N	1:A:401:TYR:CD1	2.88	0.41
1:A:63:THR:CG2	1:A:123:ILE:HG21	2.50	0.41
1:A:23:ASN:HD21	1:A:130:PHE:N	2.17	0.41
1:B:419:TYR:CD1	1:B:419:TYR:C	2.93	0.41
1:A:269:TYR:HE1	1:A:276:LYS:HE2	1.85	0.41
1:A:283:GLN:HE22	1:A:297:TRP:HZ2	1.65	0.41
1:B:248:PHE:HZ	1:B:326:PHE:CE1	2.37	0.41
1:A:269:TYR:HD1	1:A:269:TYR:O	2.04	0.41
1:B:162:LEU:HD12	1:B:162:LEU:HA	1.85	0.41
1:B:92:TYR:HD1	1:B:92:TYR:O	2.03	0.41
1:A:115:GLU:OE1	1:A:122:ARG:NH2	2.45	0.41
1:A:370:TYR:CE1	1:A:419:TYR:HD2	2.39	0.41
1:B:56:PRO:O	1:B:59:THR:OG1	2.35	0.41
1:B:61:VAL:O	1:B:66:CRO:OG1	2.31	0.41
1:A:47:ILE:HD13	1:A:434:ARG:NH1	2.35	0.41
1:B:68:VAL:HG23	1:B:68:VAL:O	2.21	0.41
1:A:401:TYR:HD1	1:A:401:TYR:N	2.19	0.40
1:A:53:LEU:HD22	1:A:57:TRP:CD2	2.56	0.40
1:B:269:TYR:CZ	1:B:276:LYS:HG3	2.56	0.40
1:B:56:PRO:HD3	1:B:136:ILE:O	2.20	0.40
1:A:165:TRP:CZ3	1:A:208:MET:HB3	2.57	0.40
1:A:441:GLU:C	1:A:442:PHE:CD1	2.94	0.40
1:A:198:ASN:O	1:A:202:ILE:HG12	2.22	0.40
1:B:135:ASN:HA	1:B:140:LYS:HB2	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	437/457 (96%)	425 (97%)	12 (3%)	0	100	100
1	B	434/457 (95%)	424 (98%)	10 (2%)	0	100	100
All	All	871/914 (95%)	849 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	382/400 (96%)	370 (97%)	12 (3%)	40	74
1	B	382/400 (96%)	371 (97%)	11 (3%)	42	76
All	All	764/800 (96%)	741 (97%)	23 (3%)	41	75

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	PHE
1	A	61	VAL
1	A	80	ARG
1	A	92	TYR
1	A	100	PHE
1	A	269	TYR
1	A	322	PHE
1	A	353	GLN

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Mol	Chain	Res	Type
1	A	375	LYS
1	A	401	TYR
1	A	419	TYR
1	A	442	PHE
1	B	46	PHE
1	B	80	ARG
1	B	90	GLU
1	B	92	TYR
1	B	130	PHE
1	B	312	GLU
1	B	322	PHE
1	B	377	LYS
1	B	419	TYR
1	B	434	ARG
1	B	442	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	267	HIS
1	A	365	ASN
1	B	94	GLN
1	B	402	GLN

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	2.79	7 (30%)	30,32,34	2.60	10 (33%)
1	CRO	B	66	1	23,23,24	2.80	7 (30%)	30,32,34	2.37	11 (36%)

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	-	0/12/31/32	0/2/2/2
1	CRO	B	66	1	-	1/12/31/32	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	CRO	CA2-C2	7.49	1.56	1.48
1	A	66	CRO	C1-N2	7.26	1.42	1.32
1	B	66	CRO	C1-N2	7.06	1.42	1.32
1	A	66	CRO	CA2-C2	7.03	1.55	1.48
1	A	66	CRO	C1-N3	4.80	1.45	1.37
1	B	66	CRO	C1-N3	4.56	1.44	1.37
1	B	66	CRO	C2-N3	4.12	1.49	1.39
1	A	66	CRO	C2-N3	3.87	1.49	1.39
1	B	66	CRO	CG2-CB2	3.83	1.54	1.46
1	A	66	CRO	CG2-CB2	3.80	1.54	1.46
1	B	66	CRO	CB2-CA2	-2.59	1.33	1.35
1	A	66	CRO	CA2-N2	2.38	1.43	1.38
1	A	66	CRO	CB2-CA2	-2.29	1.33	1.35
1	B	66	CRO	CA2-N2	2.02	1.42	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	CRO	CA2-C2-N3	7.55	106.94	103.37
1	B	66	CRO	O2-C2-CA2	-7.26	126.88	130.96
1	A	66	CRO	O2-C2-CA2	-6.01	127.59	130.96
1	A	66	CRO	CA2-N2-C1	4.97	109.44	105.77
1	B	66	CRO	CA2-C2-N3	4.68	105.58	103.37
1	B	66	CRO	CA2-N2-C1	4.41	109.02	105.77
1	A	66	CRO	C2-N3-C1	-4.40	105.74	107.97
1	A	66	CRO	C2-CA2-N2	-4.14	106.03	108.93
1	A	66	CRO	CG2-CB2-CA2	-3.78	125.31	129.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	CRO	C2-N3-C1	-3.29	106.30	107.97
1	B	66	CRO	CA3-N3-C1	-3.11	123.44	127.16
1	B	66	CRO	O3-C3-CA3	-2.92	117.56	126.39
1	B	66	CRO	CG2-CB2-CA2	-2.89	126.41	129.94
1	A	66	CRO	O3-C3-CA3	-2.84	117.82	126.39
1	B	66	CRO	CA3-N3-C2	2.80	130.21	123.80
1	A	66	CRO	CB2-CA2-C2	2.77	125.58	122.28
1	B	66	CRO	C2-CA2-N2	-2.65	107.08	108.93
1	B	66	CRO	CB2-CA2-C2	2.63	125.42	122.28
1	A	66	CRO	CA1-C1-N3	-2.39	121.88	124.75
1	B	66	CRO	CA1-C1-N3	-2.06	122.28	124.75
1	A	66	CRO	CA3-N3-C2	2.03	128.45	123.80

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	66	CRO	N2-C1-CA1-CB1

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	66	CRO	4	0
1	B	66	CRO	3	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	OLC	A	504	-	24,24,24	0.83	1 (4%)	25,25,25	0.95	1 (4%)
2	OLC	A	503	-	10,10,24	0.40	0	8,9,25	0.70	0
3	NAG	A	505	1	14,14,15	1.66	2 (14%)	17,19,21	2.43	4 (23%)
3	NAG	B	502	1	14,14,15	1.87	4 (28%)	17,19,21	1.83	4 (23%)
2	OLC	A	502	-	8,8,24	0.42	0	7,7,25	0.86	0
2	OLC	A	501	-	16,16,24	0.36	0	15,15,25	0.66	0
2	OLC	B	501	-	16,16,24	0.34	0	15,15,25	0.74	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	A	504	-	-	8/24/24/24	-
2	OLC	A	503	-	-	1/8/8/24	-
3	NAG	A	505	1	-	2/6/23/26	0/1/1/1
3	NAG	B	502	1	-	2/6/23/26	0/1/1/1
2	OLC	A	502	-	-	3/6/6/24	-
2	OLC	A	501	-	-	8/14/14/24	-
2	OLC	B	501	-	-	11/14/14/24	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	NAG	O5-C1	4.12	1.50	1.43
3	A	505	NAG	O5-C1	4.08	1.50	1.43
3	B	502	NAG	C7-N2	3.29	1.45	1.34
3	A	505	NAG	C7-N2	2.94	1.44	1.34
2	A	504	OLC	O20-C1	2.55	1.40	1.33
3	B	502	NAG	O5-C5	2.31	1.48	1.43
3	B	502	NAG	C2-N2	2.11	1.49	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	505	NAG	C1-C2-N2	-7.05	98.44	110.49
3	A	505	NAG	C1-O5-C5	-4.60	105.96	112.19
3	A	505	NAG	C4-C3-C2	4.14	117.08	111.02
3	B	502	NAG	C1-O5-C5	-3.81	107.03	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	NAG	C3-C4-C5	3.11	115.78	110.24
3	B	502	NAG	C2-N2-C7	-3.05	118.56	122.90
2	A	504	OLC	O20-C1-C2	2.73	120.46	111.91
3	B	502	NAG	C8-C7-N2	2.68	120.64	116.10
3	A	505	NAG	O5-C5-C6	2.34	110.87	107.20

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	503	OLC	C9-C10-C11-C12
3	B	502	NAG	C4-C5-C6-O6
3	B	502	NAG	O5-C5-C6-O6
2	A	504	OLC	C2-C1-O20-C21
3	A	505	NAG	O5-C5-C6-O6
2	A	504	OLC	O19-C1-O20-C21
3	A	505	NAG	C4-C5-C6-O6
2	A	501	OLC	C6-C7-C8-C9
2	A	502	OLC	C4-C5-C6-C7
2	A	504	OLC	C5-C6-C7-C8
2	B	501	OLC	C3-C4-C5-C6
2	B	501	OLC	C5-C6-C7-C8
2	B	501	OLC	C11-C12-C13-C14
2	B	501	OLC	C6-C7-C8-C9
2	A	504	OLC	C6-C7-C8-C9
2	A	501	OLC	C5-C6-C7-C8
2	A	501	OLC	C2-C3-C4-C5
2	B	501	OLC	C15-C16-C17-C18
2	A	502	OLC	C3-C4-C5-C6
2	A	501	OLC	C11-C12-C13-C14
2	B	501	OLC	C12-C13-C14-C15
2	B	501	OLC	C14-C15-C16-C17
2	A	504	OLC	C4-C5-C6-C7
2	A	504	OLC	C14-C15-C16-C17
2	A	504	OLC	C1-C2-C3-C4
2	A	501	OLC	C12-C13-C14-C15
2	B	501	OLC	C7-C8-C9-C10
2	B	501	OLC	C9-C10-C11-C12
2	B	501	OLC	C4-C5-C6-C7
2	A	502	OLC	C7-C8-C9-C10
2	A	501	OLC	C7-C8-C9-C10
2	A	501	OLC	C13-C14-C15-C16

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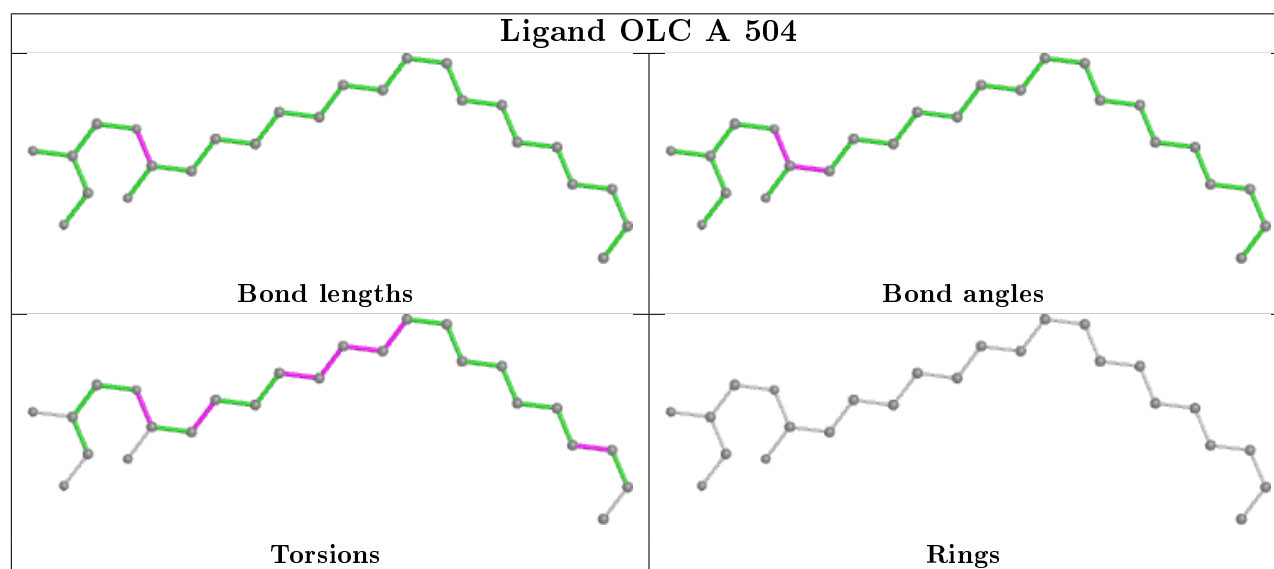
Mol	Chain	Res	Type	Atoms
2	B	501	OLC	C13-C14-C15-C16
2	A	501	OLC	C10-C11-C12-C13
2	A	504	OLC	C7-C8-C9-C10

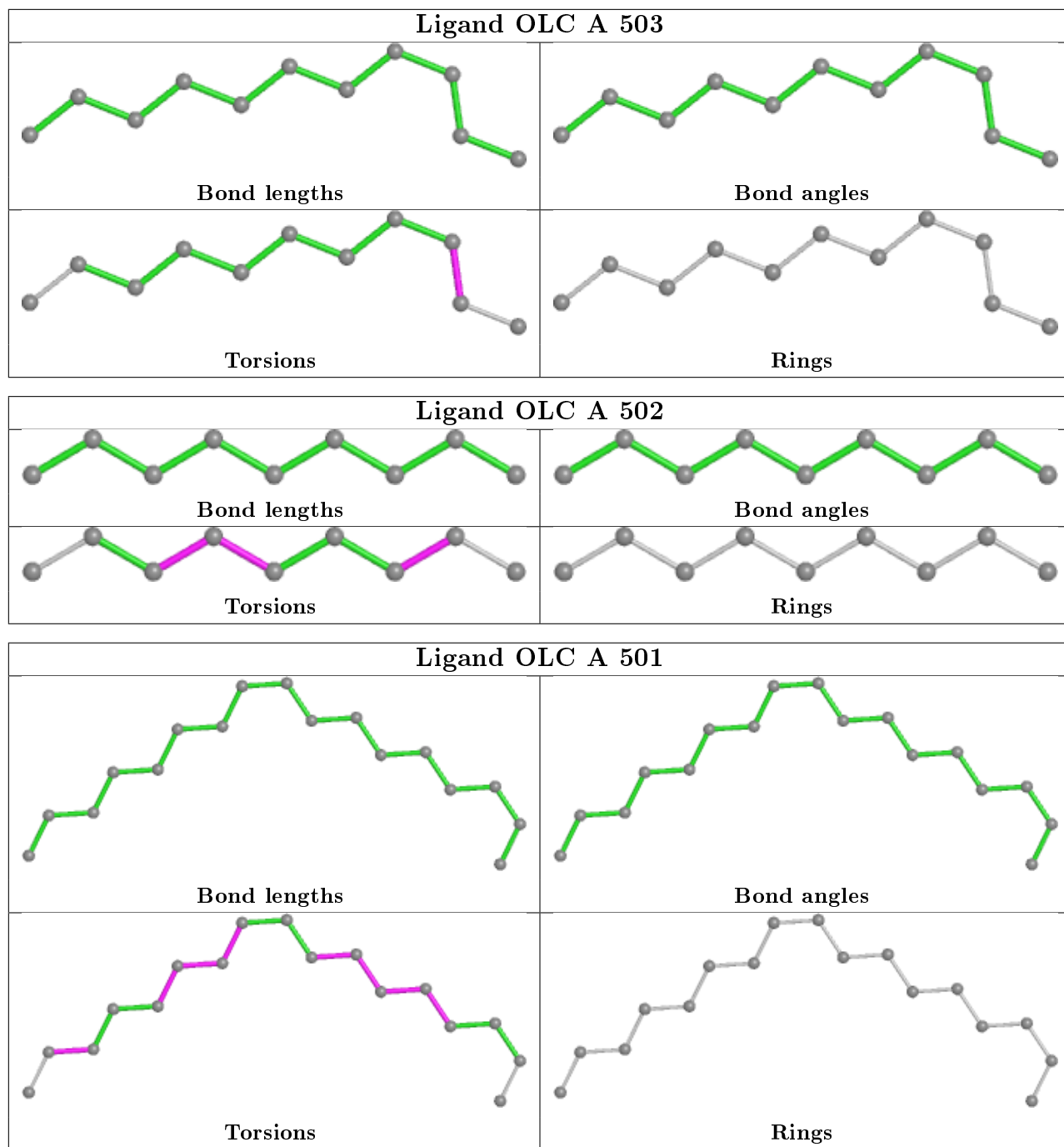
There are no ring outliers.

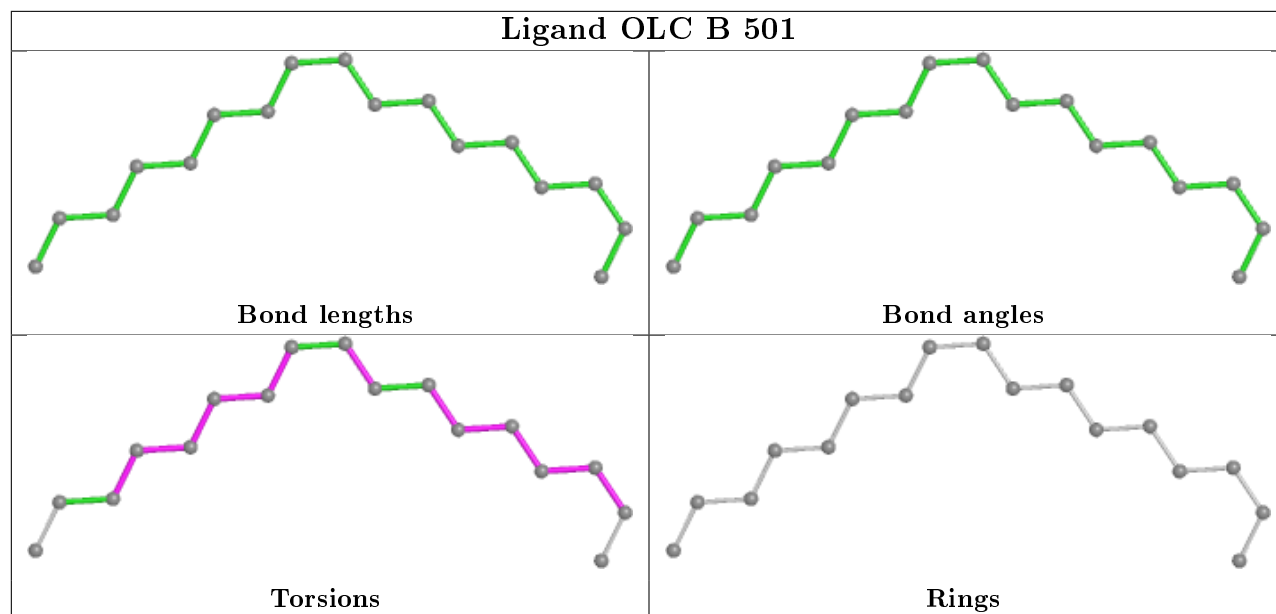
5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	504	OLC	4	0
3	A	505	NAG	1	0
2	A	502	OLC	1	0
2	A	501	OLC	2	0
2	B	501	OLC	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 [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	443/457 (96%)	-0.19	9 (2%) 65 63	36, 57, 89, 125	0
1	B	440/457 (96%)	-0.07	9 (2%) 65 63	40, 63, 91, 121	0
All	All	883/914 (96%)	-0.13	18 (2%) 65 63	36, 60, 90, 125	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	309	ARG	4.6
1	B	409	ASP	3.9
1	A	310	LYS	3.8
1	B	1	MET	3.6
1	B	309	ARG	3.3
1	A	355	ASP	3.2
1	A	448	ILE	3.0
1	A	252	GLN	2.9
1	B	132	GLU	2.7
1	B	52	LYS	2.6
1	A	357	THR	2.4
1	B	351	ASN	2.4
1	A	449	THR	2.3
1	B	408	GLY	2.3
1	B	449	THR	2.2
1	A	180	ILE	2.1
1	A	401	TYR	2.1
1	B	433	LYS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	CRO	B	66	22/23	0.92	0.25	51,61,73,78	0
1	CRO	A	66	22/23	0.95	0.20	28,47,58,63	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

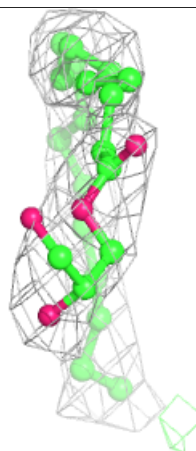
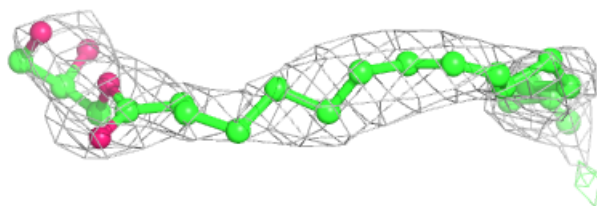
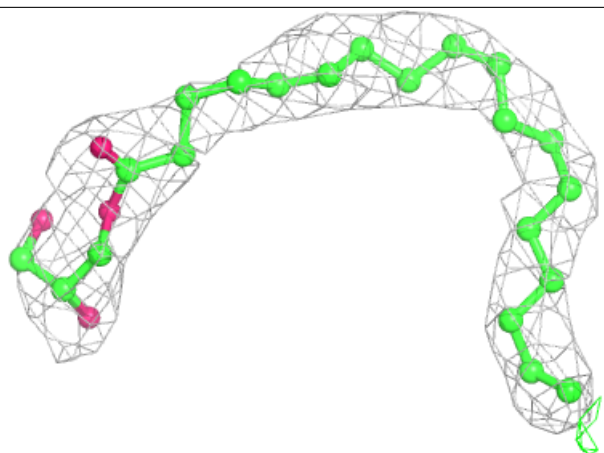
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	A	505	14/15	0.81	0.39	80,101,115,116	0
3	NAG	B	502	14/15	0.82	0.43	90,107,120,121	0
2	OLC	A	504	25/25	0.87	0.27	41,60,81,87	0
2	OLC	B	501	17/25	0.88	0.30	25,54,72,81	0
2	OLC	A	501	17/25	0.92	0.26	31,45,56,58	0
2	OLC	A	503	11/25	0.94	0.19	45,53,60,61	0
2	OLC	A	502	9/25	0.94	0.20	43,46,51,52	0

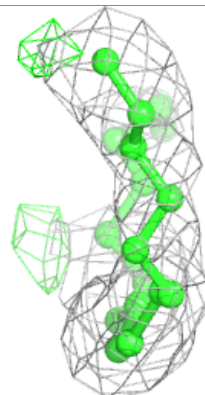
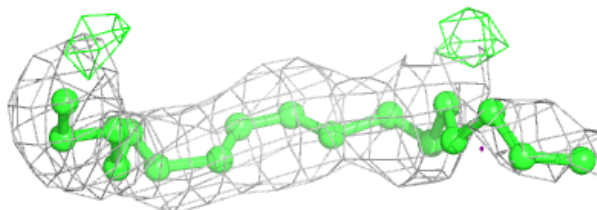
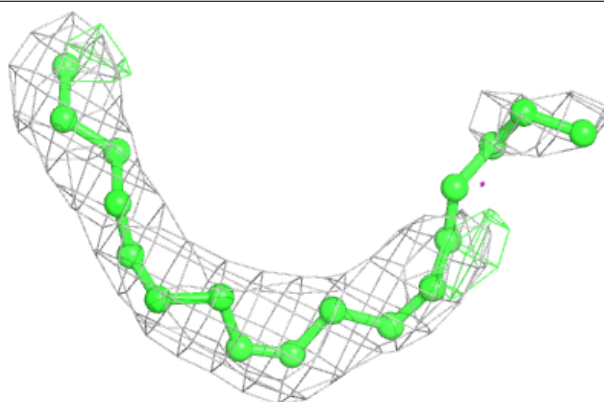
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 504:

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

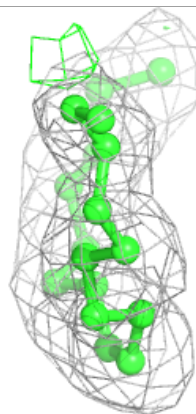
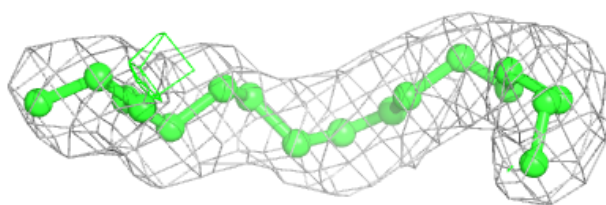
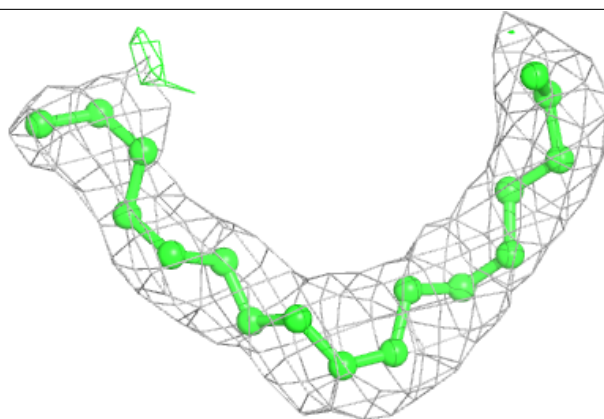
**Electron density around OLC B 501:**

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

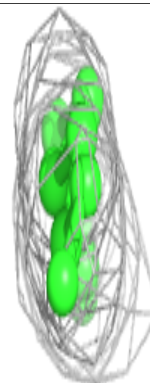
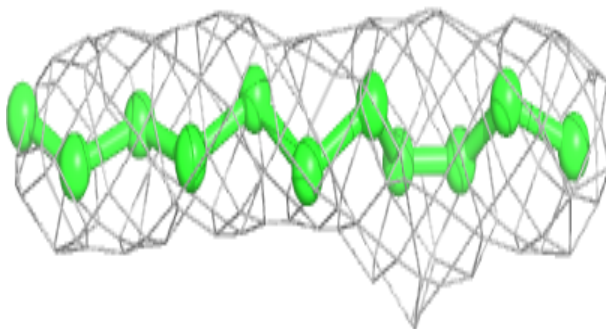
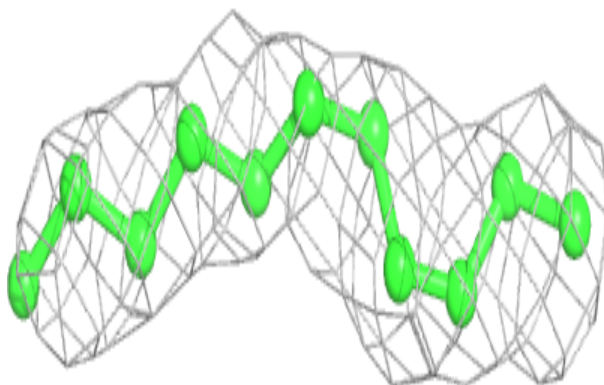


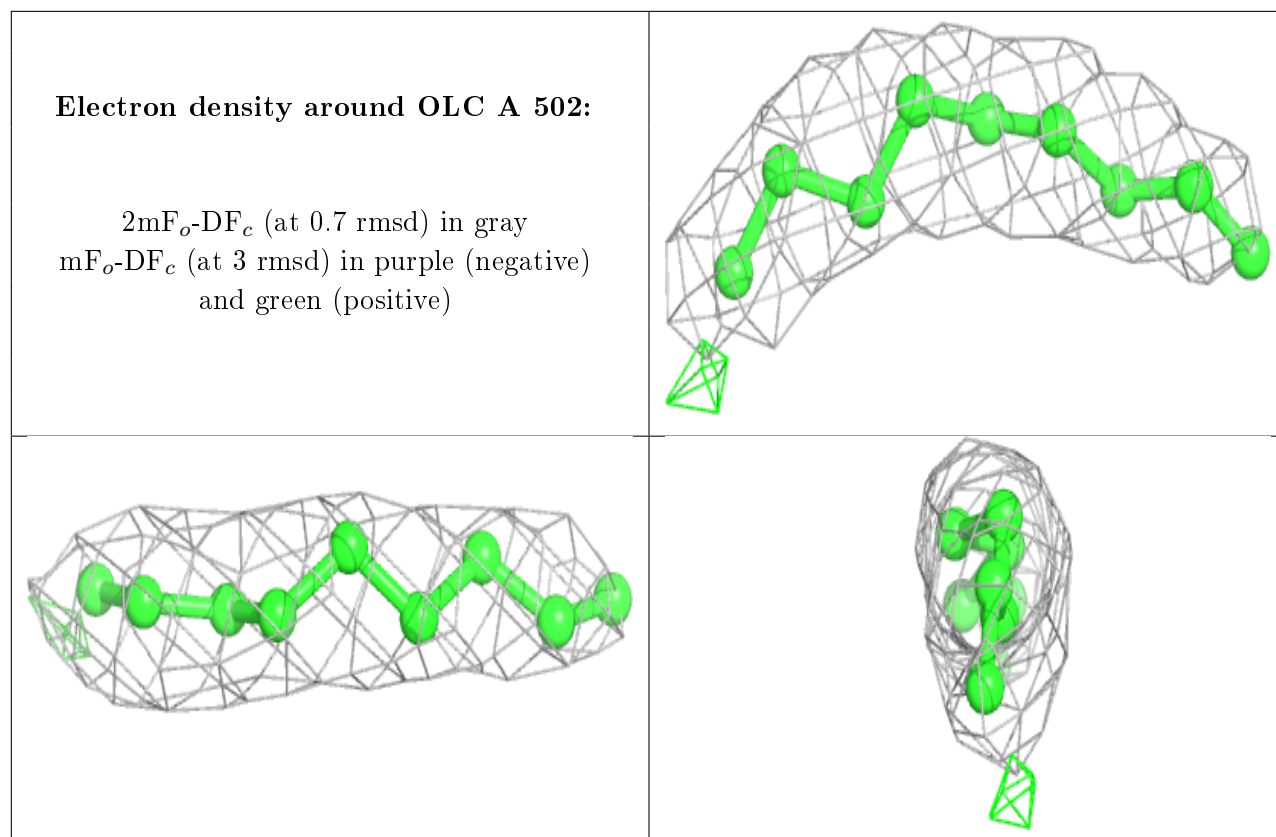
Electron density around OLC A 501:

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

**Electron density around OLC A 503:**

$2mF_o-DF_c$ (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.