



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 12:25 am BST

PDB ID : 5A3J  
Title : Crystal structure of the chloroplastic gamma-ketol reductase from Arabidopsis thaliana bound to 13-Oxo-9(Z),11(E),15(Z)- octadecatrienoic acid.  
Authors : Mas-y-mas, S.; Curien, G.; Giustini, C.; Rolland, N.; Ferrer, J.L.; Cobessi, D.  
Deposited on : 2015-06-01  
Resolution : 2.78 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

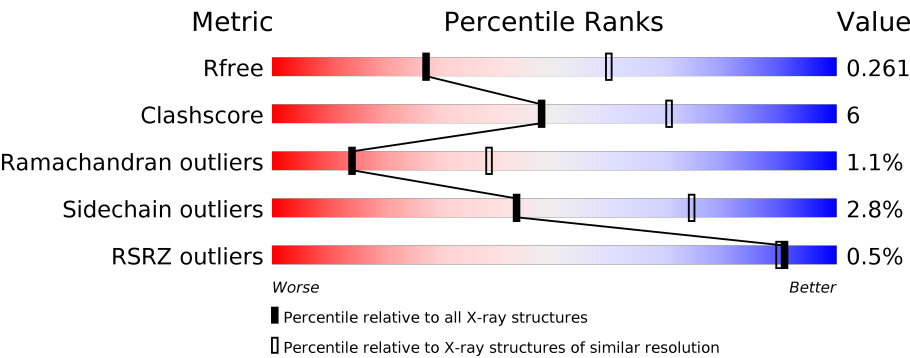
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.78 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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

Mol	Chain	Length	Quality of chain
1	A	329	<div><div></div><div>86%12%..</div></div>
1	B	329	<div><div>%</div><div>84%12%...</div></div>
1	C	329	<div><div></div><div>85%12%..</div></div>
1	D	329	<div><div></div><div>83%15%..</div></div>
1	E	329	<div><div>%</div><div>82%16%..</div></div>
1	F	329	<div><div></div><div>87%11%..</div></div>

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Mol	Chain	Length	Quality of chain
1	G	329	<div><div>%</div><div><div></div><div>83%</div><div>14%</div><div>..</div></div></div>
1	H	329	<div><div></div><div><div>88%</div><div>10%</div><div>..</div></div></div>
1	I	329	<div><div></div><div><div>85%</div><div>12%</div><div>..</div></div></div>
1	J	329	<div><div></div><div><div>86%</div><div>12%</div><div>..</div></div></div>
1	K	329	<div><div>4%</div><div><div></div><div>84%</div><div>13%</div><div>..</div></div></div>
1	L	329	<div><div></div><div><div>85%</div><div>13%</div><div>..</div></div></div>

## 2 Entry composition

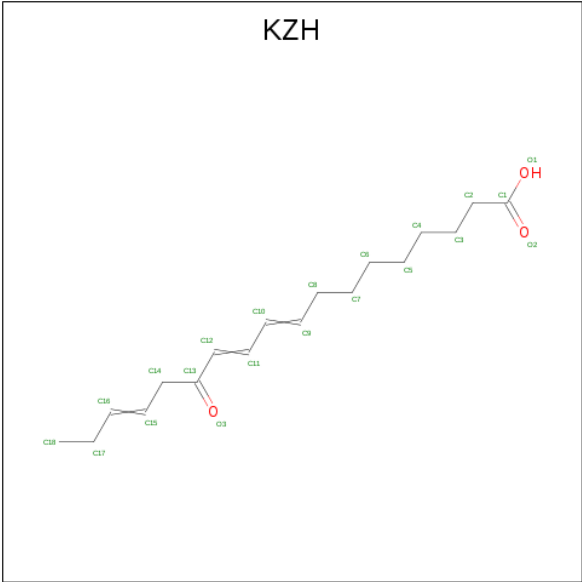
There are 2 unique types of molecules in this entry. The entry contains 28366 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PUTATIVE QUINONE-OXIDOREDUCTASE HOMOLOG, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	1	0
			2337	1494	392	441	10			
1	B	325	Total	C	N	O	S	0	0	0
			2344	1499	395	441	9			
1	C	327	Total	C	N	O	S	0	1	0
			2349	1501	395	443	10			
1	D	326	Total	C	N	O	S	0	0	0
			2341	1494	397	441	9			
1	E	327	Total	C	N	O	S	0	1	0
			2357	1506	397	444	10			
1	F	327	Total	C	N	O	S	0	0	0
			2362	1509	400	444	9			
1	G	325	Total	C	N	O	S	0	0	0
			2336	1493	394	440	9			
1	H	327	Total	C	N	O	S	0	1	0
			2346	1497	395	444	10			
1	I	325	Total	C	N	O	S	0	1	0
			2336	1492	392	442	10			
1	J	327	Total	C	N	O	S	0	1	0
			2369	1516	400	443	10			
1	K	324	Total	C	N	O	S	0	0	0
			2320	1482	390	439	9			
1	L	327	Total	C	N	O	S	0	1	0
			2360	1508	398	444	10			

- Molecule 2 is (13-oxo-9(Z),11(E),15(Z)-octadecatrienoic acid) (three-letter code: KZH) (formula: C<sub>18</sub>H<sub>28</sub>O<sub>3</sub>).




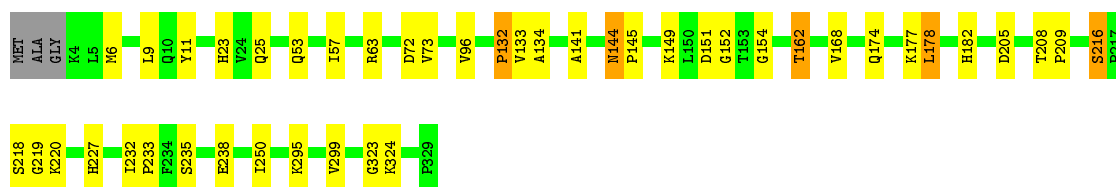
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			14	12	2		
2	B	1	Total	C	O	0	0
			21	18	3		
2	C	1	Total	C	O	0	0
			21	18	3		
2	D	1	Total	C	O	0	0
			16	13	3		
2	E	1	Total	C	O	0	0
			20	17	3		
2	F	1	Total	C	O	0	0
			18	15	3		
2	G	1	Total	C	O	0	0
			17	14	3		
2	H	1	Total	C	O	0	0
			21	18	3		
2	I	1	Total	C	O	0	0
			16	13	3		
2	J	1	Total	C	O	0	0
			13	11	2		
2	K	1	Total	C	O	0	0
			13	11	2		
2	L	1	Total	C	O	0	0
			19	16	3		

### 3 Residue-property plots


These plots are drawn for all protein, RNA and DNA 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.

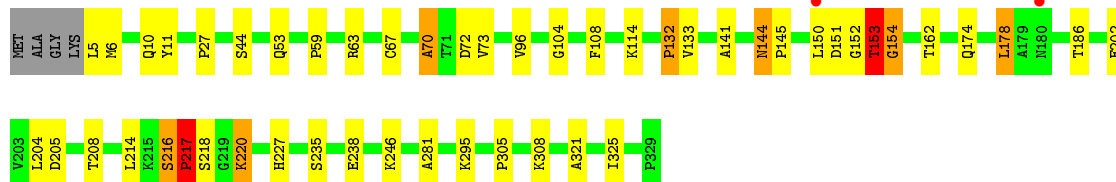
- Molecule 1: PUTATIVE QUINONE-OXIDOREDUCTASE HOMOLOG, CHLOROPLASTIC

Chain A: 




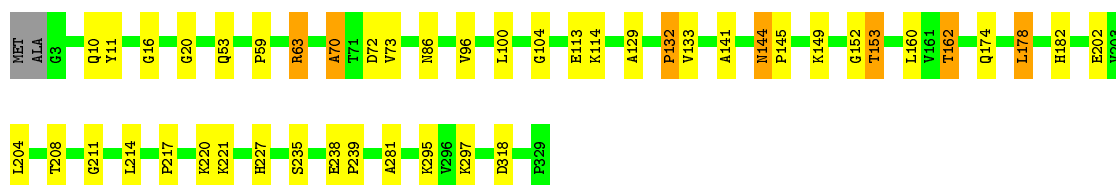
- Molecule 1: PUTATIVE QUINONE-OXIDOREDUCTASE HOMOLOG, CHLOROPLASTIC

Chain B: 



- Molecule 1: PUTATIVE QUINONE-OXIDOREDUCTASE HOMOLOG, CHLOROPLASTIC

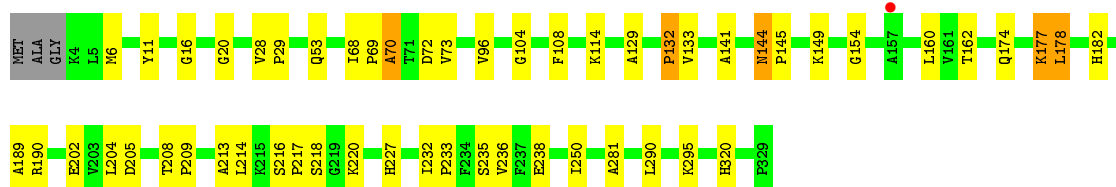
Chain C: 



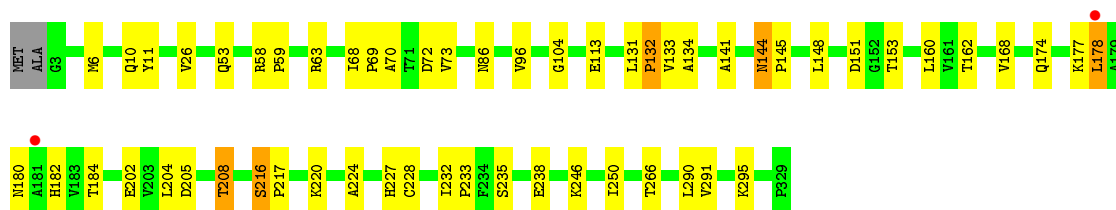
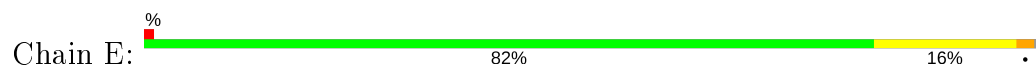
- Molecule 1: PUTATIVE QUINONE-OXIDOREDUCTASE HOMOLOG, CHLOROPLASTIC

Chain D: 

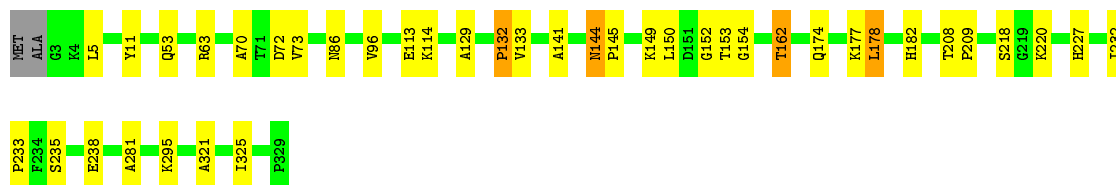
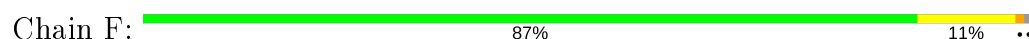




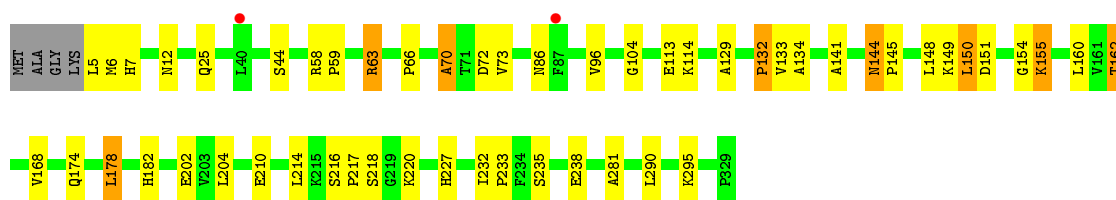
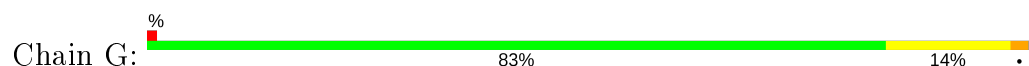
- Molecule 1: PUTATIVE QUINONE-OXIDOREDUCTASE HOMOLOG, CHLOROPLASTIC



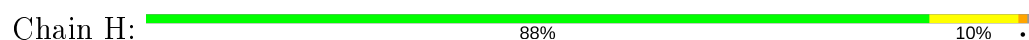
- Molecule 1: PUTATIVE QUINONE-OXIDOREDUCTASE HOMOLOG, CHLOROPLASTIC



- Molecule 1: PUTATIVE QUINONE-OXIDOREDUCTASE HOMOLOG, CHLOROPLASTIC



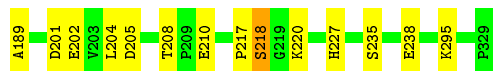
- Molecule 1: PUTATIVE QUINONE-OXIDOREDUCTASE HOMOLOG, CHLOROPLASTIC





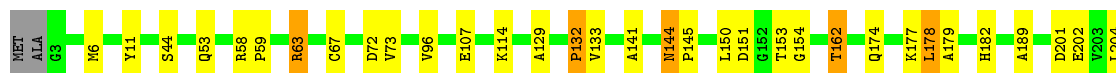
- Molecule 1: PUTATIVE QUINONE-OXIDOREDUCTASE HOMOLOG, CHLOROPLASTIC

Chain I: 85% 12% ..



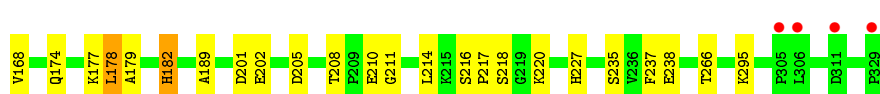
- Molecule 1: PUTATIVE QUINONE-OXIDOREDUCTASE HOMOLOG, CHLOROPLASTIC

Chain J: 86% 12% ..



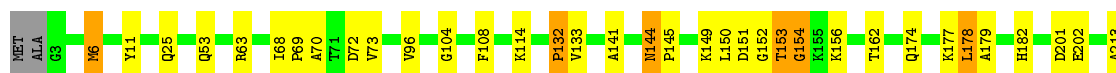
- Molecule 1: PUTATIVE QUINONE-OXIDOREDUCTASE HOMOLOG, CHLOROPLASTIC

Chain K: 4% 84% 13% ..



- Molecule 1: PUTATIVE QUINONE-OXIDOREDUCTASE HOMOLOG, CHLOROPLASTIC

Chain L: 85% 13% ..





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.87Å 121.01Å 122.94Å 66.73° 79.10° 79.99°	Depositor
Resolution (Å)	40.21 – 2.78 49.19 – 2.78	Depositor EDS
% Data completeness (in resolution range)	95.0 (40.21-2.78) 95.0 (49.19-2.78)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 2.77Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.200 , 0.258 0.215 , 0.261	Depositor DCC
$R_{free}$ test set	5127 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.8	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 26.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.043 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	28366	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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: KZH

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	0.51	0/2388	0.62	0/3263
1	B	0.51	2/2392 (0.1%)	0.63	1/3264 (0.0%)
1	C	0.48	0/2400	0.61	1/3277 (0.0%)
1	D	0.45	0/2389	0.59	0/3263
1	E	0.53	2/2408 (0.1%)	0.60	0/3286
1	F	0.52	0/2410	0.62	1/3286 (0.0%)
1	G	0.48	0/2384	0.62	0/3256
1	H	0.48	0/2397	0.59	0/3273
1	I	0.51	0/2387	0.60	0/3261
1	J	0.53	2/2420 (0.1%)	0.62	1/3297 (0.0%)
1	K	0.47	0/2368	0.60	1/3237 (0.0%)
1	L	0.53	0/2411	0.63	0/3289
All	All	0.50	6/28754 (0.0%)	0.61	5/39252 (0.0%)

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	B	0	3
1	G	0	1
1	L	0	1
All	All	0	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	180	ASN	CG-ND2	7.58	1.51	1.32
1	B	217	PRO	CB-CG	7.14	1.85	1.50
1	E	180	ASN	CG-OD1	6.37	1.38	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	220	LYS	CE-NZ	-5.46	1.35	1.49
1	J	67[A]	CYS	CB-SG	5.22	1.91	1.82
1	J	67[B]	CYS	CB-SG	5.22	1.91	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	150	LEU	CA-CB-CG	6.19	129.54	115.30
1	B	153	THR	N-CA-C	6.13	127.55	111.00
1	F	5	LEU	CA-CB-CG	5.58	128.14	115.30
1	J	154	GLY	N-CA-C	5.06	125.75	113.10
1	C	152	GLY	N-CA-C	-5.00	100.59	113.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	150	LEU	Peptide
1	B	152	GLY	Peptide
1	B	216	SER	Peptide
1	G	150	LEU	Peptide
1	L	154	GLY	Peptide

## 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	2337	0	2327	27	0
1	B	2344	0	2357	28	0
1	C	2349	0	2347	27	0
1	D	2341	0	2332	38	0
1	E	2357	0	2364	33	0
1	F	2362	0	2384	24	0
1	G	2336	0	2337	32	0
1	H	2346	0	2339	21	0
1	I	2336	0	2332	30	0
1	J	2369	0	2402	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	2320	0	2301	39	0
1	L	2360	0	2373	33	0
2	A	14	0	0	0	0
2	B	21	0	0	0	0
2	C	21	0	0	1	0
2	D	16	0	0	0	0
2	E	20	0	0	0	0
2	F	18	0	0	0	0
2	G	17	0	0	0	0
2	H	21	0	0	1	0
2	I	16	0	0	1	0
2	J	13	0	0	0	0
2	K	13	0	0	0	0
2	L	19	0	0	0	0
All	All	28366	0	28195	343	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 6.

All (343) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:PRO:CB	1:B:217:PRO:CG	1.85	1.44
1:K:182:HIS:HD2	1:K:220:LYS:HE3	1.26	0.96
1:K:182:HIS:CD2	1:K:220:LYS:HE3	2.07	0.88
1:E:58:ARG:NH2	2:H:501:KZH:O2	2.08	0.86
1:I:202:GLU:OE2	1:I:218:SER:OG	1.98	0.81
1:K:150:LEU:HA	1:K:179:ALA:HA	1.64	0.80
1:C:149:LYS:HD2	1:C:153:THR:HG21	1.64	0.78
1:L:150:LEU:HD12	1:L:179:ALA:HB2	1.66	0.78
1:J:182:HIS:CD2	1:J:220:LYS:HE3	2.19	0.77
1:G:5:LEU:HD21	1:G:25:GLN:HB3	1.67	0.76
1:L:218:SER:HB3	1:L:220:LYS:HG2	1.66	0.76
1:F:218:SER:HB2	1:F:220:LYS:HG2	1.67	0.74
1:G:202:GLU:OE2	1:G:218:SER:HB2	1.86	0.74
1:F:63:ARG:NH2	1:G:59:PRO:O	2.17	0.74
1:K:205:ASP:O	1:K:208:THR:HG22	1.89	0.71
1:K:182:HIS:CD2	1:K:220:LYS:CE	2.74	0.69
1:H:96:VAL:HG22	1:H:132:PRO:HB3	1.75	0.69
1:B:96:VAL:HG22	1:B:132:PRO:HB3	1.75	0.69
1:G:218:SER:HB3	1:G:220:LYS:HG2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:GLU:CD	1:D:217:PRO:HD2	2.12	0.69
1:K:59:PRO:O	1:L:63:ARG:NH2	2.21	0.69
1:A:162:THR:OG1	1:A:227:HIS:HA	1.95	0.67
1:K:162:THR:OG1	1:K:227:HIS:HA	1.95	0.67
1:H:162:THR:OG1	1:H:227:HIS:HA	1.95	0.66
1:C:297:LYS:NZ	1:K:82:SER:O	2.26	0.66
1:F:96:VAL:HG22	1:F:132:PRO:HB3	1.77	0.66
1:I:96:VAL:HG22	1:I:132:PRO:HB3	1.77	0.66
1:A:144:ASN:HB2	1:A:145:PRO:HD3	1.77	0.66
1:D:6:MET:SD	1:D:28:VAL:HG22	2.36	0.65
1:L:151:ASP:OD1	1:L:153:THR:OG1	2.12	0.65
1:B:205:ASP:HB3	1:B:208:THR:HG23	1.76	0.65
1:B:144:ASN:HB2	1:B:145:PRO:HD3	1.79	0.65
1:D:144:ASN:HB2	1:D:145:PRO:HD3	1.76	0.65
1:J:144:ASN:HB2	1:J:145:PRO:HD3	1.79	0.65
1:K:96:VAL:HG22	1:K:132:PRO:HB3	1.78	0.65
1:E:144:ASN:HB2	1:E:145:PRO:HD3	1.77	0.65
1:K:208:THR:CG2	1:K:210:GLU:HG2	2.27	0.64
1:B:216:SER:OG	1:B:220:LYS:N	2.30	0.64
1:L:144:ASN:HB2	1:L:145:PRO:HD3	1.80	0.64
1:I:144:ASN:HB2	1:I:145:PRO:HD3	1.79	0.64
1:C:182:HIS:CD2	1:C:220:LYS:HE3	2.33	0.64
1:J:150:LEU:HD23	1:J:179:ALA:HB2	1.78	0.64
1:C:144:ASN:HB2	1:C:145:PRO:HD3	1.80	0.64
1:C:96:VAL:HG22	1:C:132:PRO:HB3	1.79	0.64
1:D:96:VAL:HG22	1:D:132:PRO:HB3	1.80	0.63
1:K:144:ASN:HB2	1:K:145:PRO:HD3	1.80	0.63
1:G:162:THR:OG1	1:G:227:HIS:HA	1.98	0.63
1:F:162:THR:OG1	1:F:227:HIS:HA	1.98	0.63
1:G:144:ASN:HB2	1:G:145:PRO:HD3	1.81	0.63
1:H:144:ASN:HB2	1:H:145:PRO:HD3	1.80	0.63
1:E:162:THR:OG1	1:E:227:HIS:HA	1.99	0.62
1:D:202:GLU:OE1	1:D:217:PRO:HD2	1.98	0.62
1:J:96:VAL:HG22	1:J:132:PRO:HB3	1.80	0.62
1:A:218:SER:HB2	1:A:220:LYS:HG2	1.80	0.62
1:H:214:LEU:HD12	1:H:236:VAL:HG12	1.82	0.62
1:L:96:VAL:HG22	1:L:132:PRO:HB3	1.81	0.62
1:E:96:VAL:HG22	1:E:132:PRO:HB3	1.81	0.62
1:G:96:VAL:HG22	1:G:132:PRO:HB3	1.81	0.61
1:F:144:ASN:HB2	1:F:145:PRO:HD3	1.80	0.61
1:A:96:VAL:HG22	1:A:132:PRO:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:LYS:HB2	1:C:153:THR:HB	1.82	0.60
1:I:182:HIS:HD2	1:I:220:LYS:HD2	1.67	0.60
1:D:160:LEU:HD21	1:D:214:LEU:HD22	1.84	0.60
1:I:182:HIS:CD2	1:I:220:LYS:HE3	2.37	0.60
1:D:218:SER:O	1:D:218:SER:OG	2.20	0.59
1:E:59:PRO:O	1:H:63:ARG:NH2	2.34	0.59
1:G:204:LEU:HD21	1:G:217:PRO:HD3	1.84	0.59
1:D:214:LEU:HD12	1:D:236:VAL:HG12	1.84	0.58
1:D:6:MET:SD	1:D:108:PHE:HB2	2.44	0.58
1:L:11:TYR:CD1	1:L:53:GLN:HG3	2.39	0.58
1:K:202:GLU:OE2	1:K:217:PRO:HD2	2.04	0.58
1:J:162:THR:OG1	1:J:227:HIS:HA	2.04	0.57
1:C:221:LYS:HE2	1:C:239:PRO:O	2.04	0.57
1:D:202:GLU:HB3	1:D:217:PRO:HG2	1.87	0.57
1:J:182:HIS:CD2	1:J:220:LYS:CE	2.88	0.57
1:K:182:HIS:HD2	1:K:220:LYS:CE	2.04	0.57
1:D:204:LEU:HD21	1:D:217:PRO:HG3	1.86	0.57
1:F:152:GLY:C	1:F:154:GLY:H	2.09	0.56
1:L:182:HIS:HD2	1:L:220:LYS:HD2	1.70	0.56
1:I:63:ARG:NH2	1:J:59:PRO:O	2.32	0.56
1:B:72:ASP:OD1	1:B:133:VAL:HG23	2.06	0.56
1:I:63:ARG:HD3	1:J:63:ARG:O	2.06	0.56
1:K:208:THR:HG23	1:K:211:GLY:H	1.71	0.56
1:E:182:HIS:CD2	1:E:220:LYS:HE3	2.41	0.56
1:D:190:ARG:NH2	1:D:320:HIS:HB3	2.21	0.56
1:E:72:ASP:OD1	1:E:133:VAL:HG23	2.06	0.56
1:K:202:GLU:CD	1:K:217:PRO:HD2	2.27	0.55
1:B:162:THR:OG1	1:B:227:HIS:HA	2.06	0.55
1:K:141:ALA:O	1:K:145:PRO:HD2	2.07	0.55
1:I:182:HIS:CE1	1:I:201:ASP:HB2	2.42	0.55
1:L:174:GLN:O	1:L:178:LEU:HD12	2.07	0.55
1:F:72:ASP:OD1	1:F:133:VAL:HG23	2.05	0.55
1:G:72:ASP:OD1	1:G:133:VAL:HG23	2.06	0.55
1:G:7:HIS:CD2	1:G:25:GLN:HE21	2.25	0.55
1:E:266:THR:HB	1:G:58:ARG:NH2	2.22	0.55
1:L:202:GLU:OE2	1:L:217:PRO:HD2	2.06	0.55
1:J:182:HIS:HD2	1:J:220:LYS:HD2	1.72	0.54
1:L:6:MET:HG3	1:L:108:PHE:HD2	1.72	0.54
1:J:72:ASP:OD1	1:J:133:VAL:HG23	2.07	0.54
1:K:208:THR:HG23	1:K:210:GLU:HG2	1.90	0.54
1:C:202:GLU:OE2	1:C:217:PRO:HD2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:204:LEU:HD21	1:I:217:PRO:HD3	1.90	0.54
1:C:162:THR:OG1	1:C:227:HIS:HA	2.08	0.54
1:E:141:ALA:O	1:E:145:PRO:HD2	2.08	0.53
1:C:160:LEU:HD21	1:C:214:LEU:HD22	1.91	0.53
1:D:182:HIS:CD2	1:D:220:LYS:HE3	2.43	0.53
1:I:162:THR:OG1	1:I:227:HIS:HA	2.08	0.53
1:E:205:ASP:HB3	1:E:208:THR:HG23	1.91	0.53
1:C:208:THR:O	1:C:211:GLY:N	2.42	0.53
1:F:178:LEU:HD21	1:F:295:LYS:HB3	1.91	0.53
1:D:208:THR:HB	1:D:209:PRO:HD2	1.89	0.53
1:K:182:HIS:CE1	1:K:201:ASP:HB2	2.44	0.53
1:A:72:ASP:OD1	1:A:133:VAL:HG23	2.09	0.53
1:A:141:ALA:O	1:A:145:PRO:HD2	2.09	0.53
1:B:204:LEU:HD21	1:B:217:PRO:HG3	1.91	0.53
1:C:141:ALA:O	1:C:145:PRO:HD2	2.09	0.53
1:G:174:GLN:O	1:G:178:LEU:HD12	2.09	0.53
1:E:63:ARG:O	1:H:63:ARG:HD3	2.08	0.53
1:C:178:LEU:HD21	1:C:295:LYS:HB3	1.90	0.52
1:J:182:HIS:CE1	1:J:201:ASP:HB2	2.45	0.52
1:I:72:ASP:OD1	1:I:133:VAL:HG23	2.09	0.52
1:J:202:GLU:OE2	1:J:218:SER:HB3	2.09	0.52
1:L:178:LEU:HD21	1:L:295:LYS:HB3	1.92	0.52
1:L:72:ASP:OD1	1:L:133:VAL:HG23	2.10	0.52
1:D:174:GLN:O	1:D:178:LEU:HD12	2.10	0.52
1:G:12:ASN:ND2	1:G:66:PRO:HB3	2.25	0.52
1:D:162:THR:OG1	1:D:227:HIS:HA	2.10	0.52
1:A:9:LEU:HG	1:A:23:HIS:CD2	2.45	0.51
1:F:218:SER:CB	1:F:220:LYS:HE2	2.41	0.51
1:L:182:HIS:CD2	1:L:220:LYS:HE3	2.46	0.51
1:D:178:LEU:HD21	1:D:295:LYS:HB3	1.93	0.51
1:G:154:GLY:O	1:G:155:LYS:HB2	2.11	0.51
1:K:178:LEU:HD21	1:K:295:LYS:HB3	1.92	0.51
1:A:9:LEU:HG	1:A:23:HIS:HD2	1.74	0.51
1:B:305:PRO:HG2	1:B:308:LYS:HB2	1.92	0.51
1:L:149:LYS:HD3	1:L:153:THR:HB	1.93	0.51
1:E:6:MET:HB3	1:E:26:VAL:O	2.11	0.51
1:E:174:GLN:O	1:E:178:LEU:HD12	2.11	0.51
1:G:218:SER:OG	1:G:220:LYS:HE2	2.11	0.51
1:A:182:HIS:CD2	1:A:220:LYS:HE3	2.46	0.50
1:D:6:MET:SD	1:D:108:PHE:HD2	2.34	0.50
1:D:72:ASP:OD1	1:D:133:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:ARG:HH22	1:D:320:HIS:HB3	1.77	0.50
1:B:178:LEU:HD21	1:B:295:LYS:HB3	1.92	0.50
1:L:162:THR:OG1	1:L:227:HIS:HA	2.11	0.50
1:A:178:LEU:HD21	1:A:295:LYS:HB3	1.93	0.50
1:D:141:ALA:O	1:D:145:PRO:HD2	2.12	0.49
1:F:182:HIS:CD2	1:F:220:LYS:HE3	2.47	0.49
1:J:178:LEU:HD21	1:J:295:LYS:HB3	1.93	0.49
1:K:11:TYR:CD2	1:K:53:GLN:HG3	2.47	0.49
1:K:208:THR:HG21	1:K:210:GLU:CG	2.43	0.49
1:K:174:GLN:O	1:K:178:LEU:HD12	2.13	0.49
1:K:72:ASP:OD1	1:K:133:VAL:HG23	2.11	0.49
1:D:149:LYS:HD2	1:D:154:GLY:HA2	1.94	0.49
1:L:141:ALA:O	1:L:145:PRO:HD2	2.13	0.49
1:A:151:ASP:OD1	1:A:152:GLY:N	2.46	0.49
1:E:178:LEU:HD21	1:E:295:LYS:HB3	1.95	0.49
1:F:141:ALA:O	1:F:145:PRO:HD2	2.13	0.49
1:F:63:ARG:O	1:G:63:ARG:HD3	2.12	0.49
1:I:178:LEU:HD21	1:I:295:LYS:HB3	1.95	0.49
1:I:100:LEU:HD21	2:I:501:KZH:C4	2.43	0.48
1:H:72:ASP:OD1	1:H:133:VAL:HG23	2.11	0.48
1:K:182:HIS:HE1	1:K:202:GLU:HG3	1.77	0.48
1:I:62:PRO:HB2	1:I:67[B]:CYS:SG	2.53	0.48
1:L:182:HIS:CD2	1:L:220:LYS:HD2	2.48	0.48
1:A:174:GLN:O	1:A:178:LEU:HD12	2.12	0.48
1:I:11:TYR:CD2	1:I:53:GLN:HG3	2.48	0.48
1:I:63:ARG:O	1:J:63:ARG:HD3	2.14	0.48
1:J:205:ASP:HB3	1:J:208:THR:OG1	2.13	0.48
1:E:204:LEU:HD21	1:E:217:PRO:HD3	1.96	0.48
1:F:11:TYR:CD2	1:F:53:GLN:HG3	2.49	0.48
1:G:141:ALA:O	1:G:145:PRO:HD2	2.13	0.48
1:K:160:LEU:HD21	1:K:214:LEU:HD22	1.95	0.48
1:L:202:GLU:OE2	1:L:218:SER:HB2	2.13	0.48
1:F:208:THR:HB	1:F:209:PRO:HD2	1.96	0.48
1:G:178:LEU:HD21	1:G:295:LYS:HB3	1.95	0.48
1:I:141:ALA:O	1:I:145:PRO:HD2	2.14	0.48
1:D:205:ASP:HB3	1:D:208:THR:HG23	1.94	0.48
1:I:210:GLU:CD	1:I:210:GLU:H	2.17	0.48
1:K:177:LYS:HA	1:K:177:LYS:HD2	1.58	0.48
1:B:186:THR:HG21	1:B:214:LEU:HD23	1.95	0.47
1:B:5:LEU:HD12	1:B:27:PRO:HA	1.95	0.47
1:C:72:ASP:OD1	1:C:133:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:208:THR:HG21	1:K:210:GLU:HG2	1.94	0.47
1:A:205:ASP:HB3	1:A:208:THR:HG23	1.97	0.47
1:H:178:LEU:HD21	1:H:295:LYS:HB3	1.96	0.47
1:I:174:GLN:O	1:I:178:LEU:HD12	2.14	0.47
1:E:11:TYR:CD2	1:E:53:GLN:HG3	2.49	0.47
1:F:174:GLN:O	1:F:178:LEU:HD12	2.14	0.47
1:I:177:LYS:HA	1:I:177:LYS:HD2	1.60	0.47
1:L:182:HIS:CE1	1:L:201:ASP:HB2	2.49	0.47
1:B:153:THR:O	1:B:154:GLY:O	2.32	0.47
1:J:11:TYR:CD2	1:J:53:GLN:HG3	2.50	0.46
1:D:114:LYS:O	1:D:281:ALA:HB2	2.15	0.46
1:D:6:MET:CE	1:D:29:PRO:HD3	2.46	0.46
1:G:202:GLU:OE1	1:G:216:SER:HB2	2.15	0.46
1:H:145:PRO:O	1:H:246:LYS:NZ	2.32	0.46
1:G:232:ILE:HA	1:G:233:PRO:HD3	1.84	0.46
1:K:63:ARG:HD3	1:L:63:ARG:O	2.15	0.46
1:H:204:LEU:HD21	1:H:217:PRO:HG3	1.97	0.46
1:C:86:ASN:ND2	1:C:113:GLU:OE2	2.41	0.46
1:A:208:THR:HB	1:A:209:PRO:CD	2.45	0.46
1:C:11:TYR:CD2	1:C:53:GLN:HG3	2.51	0.46
1:I:86:ASN:ND2	1:I:113:GLU:OE2	2.41	0.46
1:D:6:MET:HE2	1:D:29:PRO:HD3	1.98	0.46
1:F:218:SER:HB2	1:F:220:LYS:HE2	1.97	0.46
1:G:160:LEU:HD21	1:G:214:LEU:HD22	1.97	0.46
1:C:100:LEU:HD21	2:C:501:KZH:C4	2.46	0.46
1:D:177:LYS:HA	1:D:177:LYS:HD2	1.55	0.46
1:A:216:SER:O	1:A:219:GLY:N	2.36	0.45
1:L:232:ILE:HA	1:L:233:PRO:HD3	1.83	0.45
1:K:208:THR:CG2	1:K:210:GLU:CG	2.94	0.45
1:B:59:PRO:O	1:C:63:ARG:NH2	2.46	0.45
1:H:182:HIS:CD2	1:H:220:LYS:HE3	2.51	0.45
1:B:63:ARG:NH2	1:C:59:PRO:O	2.43	0.45
1:E:177:LYS:HD2	1:E:177:LYS:HA	1.57	0.45
1:F:149:LYS:O	1:F:150:LEU:HB2	2.15	0.45
1:G:86:ASN:ND2	1:G:113:GLU:OE2	2.42	0.45
1:G:114:LYS:O	1:G:281:ALA:HB2	2.17	0.45
1:F:86:ASN:ND2	1:F:113:GLU:OE2	2.42	0.45
1:J:177:LYS:HD2	1:J:177:LYS:HA	1.58	0.45
1:J:174:GLN:O	1:J:178:LEU:HD12	2.16	0.45
1:A:232:ILE:HA	1:A:233:PRO:HD3	1.83	0.45
1:E:151:ASP:OD1	1:E:153:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:152:GLY:O	1:F:154:GLY:N	2.48	0.45
1:I:72:ASP:HB3	1:I:129:ALA:O	2.17	0.45
1:L:213:ALA:O	1:L:240:ASN:ND2	2.50	0.45
1:J:182:HIS:HD2	1:J:220:LYS:CD	2.30	0.44
1:E:63:ARG:NH2	1:H:59:PRO:O	2.42	0.44
1:I:6:MET:HB3	1:I:28:VAL:HG22	1.99	0.44
1:K:134:ALA:HA	1:K:168:VAL:HG22	1.99	0.44
1:F:114:LYS:O	1:F:281:ALA:HB2	2.18	0.44
1:J:305:PRO:HG2	1:J:308:LYS:HB2	1.99	0.44
1:B:218:SER:OG	1:B:220:LYS:HG2	2.17	0.44
1:E:162:THR:O	1:E:228:CYS:HB2	2.18	0.44
1:G:182:HIS:CD2	1:G:220:LYS:HE3	2.53	0.44
1:I:70:ALA:HB3	1:I:104:GLY:HA3	1.99	0.44
1:A:299:VAL:HG23	1:A:323:GLY:HA3	2.00	0.44
1:D:70:ALA:HB3	1:D:104:GLY:HA3	1.99	0.44
1:B:11:TYR:CD2	1:B:53:GLN:HG3	2.53	0.44
1:J:151:ASP:HB3	1:J:153:THR:H	1.83	0.44
1:L:216:SER:HA	1:L:217:PRO:HD3	1.75	0.44
1:D:232:ILE:HA	1:D:233:PRO:HD3	1.83	0.43
1:K:150:LEU:HA	1:K:179:ALA:CA	2.43	0.43
1:F:232:ILE:HA	1:F:233:PRO:HD3	1.87	0.43
1:A:134:ALA:HA	1:A:168:VAL:HG22	2.00	0.43
1:A:57:ILE:HG22	1:A:57:ILE:O	2.18	0.43
1:K:227:HIS:ND1	1:K:237:PHE:HZ	2.16	0.43
1:L:152:GLY:O	1:L:154:GLY:N	2.51	0.43
1:C:204:LEU:HD21	1:C:217:PRO:HD3	2.00	0.43
1:D:213:ALA:O	1:D:214:LEU:HB2	2.18	0.43
1:H:11:TYR:CD2	1:H:53:GLN:HG3	2.53	0.43
1:A:11:TYR:CD2	1:A:53:GLN:HG3	2.52	0.43
1:B:5:LEU:HD12	1:B:5:LEU:HA	1.68	0.43
1:C:114:LYS:O	1:C:281:ALA:HB2	2.19	0.43
1:H:134:ALA:HA	1:H:168:VAL:HG22	2.01	0.43
1:H:321:ALA:HB2	1:H:325:ILE:HD11	2.00	0.43
1:L:68:ILE:HA	1:L:69:PRO:HD3	1.84	0.43
1:B:6:MET:SD	1:B:108:PHE:HB2	2.58	0.43
1:C:318:ASP:OD2	1:L:25:GLN:N	2.47	0.43
1:E:160:LEU:HD12	1:E:184:THR:O	2.19	0.43
1:H:218:SER:O	1:H:218:SER:OG	2.34	0.43
1:K:72:ASP:HB3	1:K:129:ALA:O	2.19	0.43
1:J:204:LEU:HD21	1:J:217:PRO:HD3	2.01	0.43
1:A:6:MET:O	1:A:25:GLN:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:GLY:HA3	1:C:20:GLY:HA3	2.01	0.42
1:D:216:SER:HA	1:D:217:PRO:HD3	1.81	0.42
1:G:134:ALA:HA	1:G:168:VAL:HG22	2.01	0.42
1:D:68:ILE:HA	1:D:69:PRO:HD3	1.81	0.42
1:E:202:GLU:OE1	1:E:216:SER:HB2	2.19	0.42
1:J:72:ASP:HB3	1:J:129:ALA:O	2.19	0.42
1:J:58:ARG:NH2	1:K:266:THR:HB	2.34	0.42
1:B:174:GLN:O	1:B:178:LEU:HD12	2.18	0.42
1:C:70:ALA:HB3	1:C:104:GLY:HA3	2.01	0.42
1:C:174:GLN:O	1:C:178:LEU:HD12	2.19	0.42
1:G:290:LEU:HA	1:G:290:LEU:HD23	1.83	0.42
1:E:134:ALA:HA	1:E:168:VAL:HG22	2.00	0.42
1:J:114:LYS:O	1:J:281:ALA:HB2	2.20	0.42
1:E:232:ILE:HA	1:E:233:PRO:HD3	1.84	0.42
1:D:11:TYR:CD2	1:D:53:GLN:HG3	2.55	0.42
1:H:174:GLN:O	1:H:178:LEU:HD12	2.19	0.42
1:I:147:GLY:O	1:I:155:LYS:HE3	2.20	0.42
1:K:16:GLY:HA3	1:K:20:GLY:HA3	2.02	0.42
1:L:70:ALA:HB3	1:L:104:GLY:HA3	2.01	0.42
1:L:182:HIS:CD2	1:L:220:LYS:CD	3.02	0.42
1:J:6:MET:HG3	1:J:107:GLU:HB2	2.01	0.42
1:A:151:ASP:CG	1:A:152:GLY:H	2.23	0.42
1:L:114:LYS:O	1:L:281:ALA:HB2	2.20	0.42
1:D:189:ALA:HB2	1:D:205:ASP:OD2	2.19	0.41
1:E:68:ILE:HA	1:E:69:PRO:HD3	1.87	0.41
1:L:177:LYS:HD2	1:L:177:LYS:HA	1.59	0.41
1:E:86:ASN:ND2	1:E:113:GLU:OE2	2.41	0.41
1:E:148:LEU:HA	1:E:148:LEU:HD23	1.66	0.41
1:K:68:ILE:HA	1:K:69:PRO:HD3	1.82	0.41
1:B:216:SER:HA	1:B:217:PRO:HD2	1.48	0.41
1:F:152:GLY:C	1:F:154:GLY:N	2.73	0.41
1:H:131:LEU:HD23	1:H:171:TYR:CZ	2.54	0.41
1:A:149:LYS:HB2	1:A:154:GLY:CA	2.50	0.41
1:B:141:ALA:O	1:B:145:PRO:HD2	2.21	0.41
1:D:250:ILE:H	1:D:250:ILE:HG13	1.76	0.41
1:K:63:ARG:O	1:L:63:ARG:HD3	2.20	0.41
1:B:202:GLU:OE1	1:B:216:SER:HB2	2.20	0.41
1:B:205:ASP:HB3	1:B:208:THR:CG2	2.46	0.41
1:A:299:VAL:CG2	1:A:323:GLY:HA3	2.51	0.41
1:E:290:LEU:HA	1:E:290:LEU:HD23	1.89	0.41
1:H:16:GLY:HA3	1:H:20:GLY:HA3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:141:ALA:O	1:H:145:PRO:HD2	2.20	0.41
1:A:149:LYS:HD3	1:A:154:GLY:HA2	2.03	0.41
1:A:324:LYS:HB3	1:A:324:LYS:HE2	1.87	0.41
1:E:70:ALA:HB3	1:E:104:GLY:HA3	2.03	0.41
1:B:70:ALA:HB3	1:B:104:GLY:HA3	2.03	0.41
1:F:129:ALA:O	1:F:132:PRO:HD2	2.21	0.41
1:G:72:ASP:HB3	1:G:129:ALA:O	2.20	0.41
1:G:149:LYS:HE3	1:G:149:LYS:HB2	1.82	0.41
1:G:216:SER:C	1:G:218:SER:H	2.23	0.41
1:I:189:ALA:HB2	1:I:205:ASP:OD2	2.21	0.41
1:J:141:ALA:O	1:J:145:PRO:HD2	2.21	0.41
1:D:72:ASP:HB3	1:D:129:ALA:O	2.21	0.41
1:E:227:HIS:O	1:E:250:ILE:HG13	2.21	0.41
1:I:205:ASP:HB3	1:I:208:THR:HG23	2.03	0.41
1:D:16:GLY:HA3	1:D:20:GLY:HA3	2.03	0.40
1:D:290:LEU:HA	1:D:290:LEU:HD23	1.86	0.40
1:E:131:LEU:HD11	1:E:291:VAL:HG21	2.03	0.40
1:G:70:ALA:HB3	1:G:104:GLY:HA3	2.04	0.40
1:I:134:ALA:HA	1:I:168:VAL:HG22	2.03	0.40
1:I:205:ASP:O	1:I:208:THR:OG1	2.27	0.40
1:K:189:ALA:HB2	1:K:205:ASP:OD2	2.21	0.40
1:B:321:ALA:HB2	1:B:325:ILE:HD11	2.02	0.40
1:K:218:SER:HB3	1:K:220:LYS:HG2	2.02	0.40
1:L:227:HIS:O	1:L:250:ILE:HG13	2.21	0.40
1:A:250:ILE:HG13	1:A:250:ILE:H	1.80	0.40
1:B:10:GLN:HA	1:B:67:CYS:O	2.22	0.40
1:C:72:ASP:HB3	1:C:129:ALA:O	2.21	0.40
1:E:224:ALA:HA	1:E:246:LYS:O	2.22	0.40
1:F:321:ALA:HB2	1:F:325:ILE:HD11	2.03	0.40
1:G:148:LEU:N	1:G:148:LEU:HD23	2.36	0.40
1:G:5:LEU:HD23	1:G:6:MET:N	2.35	0.40
1:H:114:LYS:O	1:H:281:ALA:HB2	2.21	0.40
1:J:189:ALA:HB2	1:J:205:ASP:OD2	2.20	0.40
1:B:114:LYS:O	1:B:281:ALA:HB2	2.21	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	325/329 (99%)	314 (97%)	9 (3%)	2 (1%)	25	54
1	B	323/329 (98%)	313 (97%)	4 (1%)	6 (2%)	8	23
1	C	326/329 (99%)	318 (98%)	5 (2%)	3 (1%)	17	44
1	D	324/329 (98%)	312 (96%)	9 (3%)	3 (1%)	17	44
1	E	326/329 (99%)	316 (97%)	8 (2%)	2 (1%)	25	54
1	F	325/329 (99%)	313 (96%)	8 (2%)	4 (1%)	13	36
1	G	323/329 (98%)	310 (96%)	9 (3%)	4 (1%)	13	36
1	H	326/329 (99%)	318 (98%)	5 (2%)	3 (1%)	17	44
1	I	324/329 (98%)	317 (98%)	4 (1%)	3 (1%)	17	44
1	J	326/329 (99%)	319 (98%)	5 (2%)	2 (1%)	25	54
1	K	322/329 (98%)	313 (97%)	4 (1%)	5 (2%)	9	28
1	L	326/329 (99%)	317 (97%)	5 (2%)	4 (1%)	13	36
All	All	3896/3948 (99%)	3780 (97%)	75 (2%)	41 (1%)	14	38

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	154	GLY
1	F	153	THR
1	G	155	LYS
1	K	150	LEU
1	A	132	PRO
1	B	151	ASP
1	F	132	PRO
1	G	132	PRO
1	K	153	THR
1	L	153	THR
1	B	132	PRO
1	B	217	PRO

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Mol	Chain	Res	Type
1	C	132	PRO
1	D	132	PRO
1	E	132	PRO
1	H	132	PRO
1	I	132	PRO
1	J	132	PRO
1	K	132	PRO
1	L	132	PRO
1	J	144	ASN
1	L	156	LYS
1	A	144	ASN
1	B	70	ALA
1	B	144	ASN
1	C	144	ASN
1	D	70	ALA
1	D	144	ASN
1	E	144	ASN
1	F	70	ALA
1	F	144	ASN
1	G	70	ALA
1	G	144	ASN
1	H	70	ALA
1	H	144	ASN
1	I	70	ALA
1	K	70	ALA
1	L	144	ASN
1	C	70	ALA
1	I	144	ASN
1	K	144	ASN

### 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	237/255 (93%)	229 (97%)	8 (3%)	37 68
1	B	240/255 (94%)	233 (97%)	7 (3%)	42 73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	239/255 (94%)	232 (97%)	7 (3%)	42	73
1	D	237/255 (93%)	232 (98%)	5 (2%)	53	81
1	E	241/255 (94%)	235 (98%)	6 (2%)	47	77
1	F	243/255 (95%)	237 (98%)	6 (2%)	47	77
1	G	238/255 (93%)	228 (96%)	10 (4%)	30	60
1	H	239/255 (94%)	234 (98%)	5 (2%)	53	81
1	I	239/255 (94%)	233 (98%)	6 (2%)	47	77
1	J	244/255 (96%)	236 (97%)	8 (3%)	38	69
1	K	234/255 (92%)	226 (97%)	8 (3%)	37	68
1	L	242/255 (95%)	237 (98%)	5 (2%)	53	81
All	All	2873/3060 (94%)	2792 (97%)	81 (3%)	43	74

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ARG
1	A	73	VAL
1	A	162	THR
1	A	177	LYS
1	A	178	LEU
1	A	216	SER
1	A	235	SER
1	A	238	GLU
1	B	44	SER
1	B	73	VAL
1	B	153	THR
1	B	178	LEU
1	B	235	SER
1	B	238	GLU
1	B	246	LYS
1	C	63	ARG
1	C	73	VAL
1	C	153	THR
1	C	162	THR
1	C	178	LEU
1	C	235	SER
1	C	238	GLU
1	D	73	VAL

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Mol	Chain	Res	Type
1	D	177	LYS
1	D	178	LEU
1	D	235	SER
1	D	238	GLU
1	E	73	VAL
1	E	178	LEU
1	E	208	THR
1	E	216	SER
1	E	235	SER
1	E	238	GLU
1	F	73	VAL
1	F	162	THR
1	F	177	LYS
1	F	178	LEU
1	F	235	SER
1	F	238	GLU
1	G	44	SER
1	G	63	ARG
1	G	73	VAL
1	G	150	LEU
1	G	151	ASP
1	G	162	THR
1	G	178	LEU
1	G	210	GLU
1	G	235	SER
1	G	238	GLU
1	H	73	VAL
1	H	162	THR
1	H	178	LEU
1	H	235	SER
1	H	238	GLU
1	I	73	VAL
1	I	162	THR
1	I	178	LEU
1	I	218	SER
1	I	235	SER
1	I	238	GLU
1	J	44	SER
1	J	63	ARG
1	J	73	VAL
1	J	162	THR
1	J	178	LEU

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Mol	Chain	Res	Type
1	J	218	SER
1	J	235	SER
1	J	238	GLU
1	K	73	VAL
1	K	150	LEU
1	K	162	THR
1	K	178	LEU
1	K	182	HIS
1	K	216	SER
1	K	235	SER
1	K	238	GLU
1	L	6	MET
1	L	73	VAL
1	L	178	LEU
1	L	235	SER
1	L	238	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	F	23	HIS
1	G	7	HIS
1	G	12	ASN
1	G	23	HIS
1	G	25	GLN
1	I	182	HIS
1	J	12	ASN
1	J	182	HIS
1	J	271	GLN
1	K	182	HIS
1	L	182	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

12 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	KZH	K	501	-	9,12,20	0.33	0	8,12,21	0.53	0
2	KZH	H	501	-	17,20,20	0.82	2 (11%)	15,21,21	0.86	1 (6%)
2	KZH	J	501	-	9,12,20	0.31	0	8,12,21	0.75	0
2	KZH	A	501	-	10,13,20	0.68	0	9,13,21	0.65	0
2	KZH	G	501	-	13,16,20	0.96	1 (7%)	13,17,21	1.06	1 (7%)
2	KZH	D	501	-	12,15,20	1.19	2 (16%)	11,15,21	0.67	0
2	KZH	I	501	-	12,15,20	1.16	2 (16%)	11,15,21	0.62	0
2	KZH	F	501	-	14,17,20	0.89	1 (7%)	14,18,21	1.11	2 (14%)
2	KZH	C	501	-	17,20,20	0.70	0	15,21,21	1.12	1 (6%)
2	KZH	E	501	-	16,19,20	0.83	1 (6%)	15,20,21	1.33	1 (6%)
2	KZH	B	501	-	17,20,20	0.82	1 (5%)	15,21,21	1.23	1 (6%)
2	KZH	L	501	-	15,18,20	0.88	1 (6%)	13,19,21	1.22	1 (7%)

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	KZH	K	501	-	-	5/8/10/19	-
2	KZH	H	501	-	-	8/17/19/19	-
2	KZH	J	501	-	-	1/8/10/19	-
2	KZH	A	501	-	-	8/9/11/19	-
2	KZH	G	501	-	-	7/12/14/19	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KZH	D	501	-	-	7/11/13/19	-
2	KZH	I	501	-	-	7/11/13/19	-
2	KZH	F	501	-	-	8/14/16/19	-
2	KZH	C	501	-	-	7/17/19/19	-
2	KZH	E	501	-	-	8/16/18/19	-
2	KZH	B	501	-	-	12/17/19/19	-
2	KZH	L	501	-	-	7/15/17/19	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	KZH	C10-C11	3.14	1.53	1.44
2	I	501	KZH	C10-C11	2.66	1.51	1.44
2	B	501	KZH	C10-C11	2.35	1.51	1.44
2	G	501	KZH	C12-C13	2.32	1.53	1.47
2	H	501	KZH	C10-C11	2.30	1.50	1.44
2	I	501	KZH	C12-C13	2.24	1.51	1.44
2	L	501	KZH	C12-C13	2.14	1.55	1.48
2	F	501	KZH	C10-C11	2.06	1.50	1.44
2	H	501	KZH	C12-C13	2.02	1.55	1.48
2	D	501	KZH	C12-C13	2.02	1.50	1.44
2	E	501	KZH	C12-C13	2.00	1.54	1.48

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	KZH	C10-C11-C12	-4.08	114.47	124.67
2	L	501	KZH	C10-C11-C12	-4.02	114.64	124.67
2	B	501	KZH	C14-C15-C16	-3.40	117.09	125.03
2	G	501	KZH	C10-C11-C12	-2.99	117.20	124.67
2	C	501	KZH	C10-C11-C12	-2.90	117.42	124.67
2	H	501	KZH	C10-C11-C12	-2.64	118.07	124.67
2	F	501	KZH	C10-C11-C12	-2.42	118.62	124.67
2	F	501	KZH	O3-C13-C14	-2.08	118.41	121.14

There are no chirality outliers.

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	501	KZH	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
2	H	501	KZH	C14-C15-C16-C17
2	H	501	KZH	C10-C11-C12-C13
2	A	501	KZH	C9-C10-C11-C12
2	A	501	KZH	C11-C10-C9-C8
2	A	501	KZH	C1-C2-C3-C4
2	G	501	KZH	C11-C12-C13-O3
2	G	501	KZH	C10-C11-C12-C13
2	G	501	KZH	C1-C2-C3-C4
2	D	501	KZH	C11-C12-C13-O3
2	D	501	KZH	C10-C11-C12-C13
2	D	501	KZH	C11-C10-C9-C8
2	I	501	KZH	C10-C11-C12-C13
2	I	501	KZH	C11-C10-C9-C8
2	I	501	KZH	C1-C2-C3-C4
2	F	501	KZH	C11-C10-C9-C8
2	C	501	KZH	C13-C14-C15-C16
2	E	501	KZH	C11-C12-C13-O3
2	E	501	KZH	C13-C14-C15-C16
2	B	501	KZH	C15-C16-C17-C18
2	B	501	KZH	C10-C11-C12-C13
2	B	501	KZH	C9-C10-C11-C12
2	B	501	KZH	C11-C10-C9-C8
2	B	501	KZH	C1-C2-C3-C4
2	L	501	KZH	C13-C14-C15-C16
2	L	501	KZH	C10-C11-C12-C13
2	L	501	KZH	C1-C2-C3-C4
2	F	501	KZH	C9-C10-C11-C12
2	G	501	KZH	C2-C3-C4-C5
2	H	501	KZH	C9-C10-C11-C12
2	E	501	KZH	C9-C10-C11-C12
2	L	501	KZH	C9-C10-C11-C12
2	H	501	KZH	C2-C3-C4-C5
2	A	501	KZH	C4-C5-C6-C7
2	D	501	KZH	C4-C5-C6-C7
2	I	501	KZH	C2-C3-C4-C5
2	I	501	KZH	C5-C6-C7-C8
2	H	501	KZH	C11-C10-C9-C8
2	L	501	KZH	C11-C10-C9-C8
2	H	501	KZH	C6-C7-C8-C9
2	K	501	KZH	C4-C5-C6-C7
2	B	501	KZH	C5-C6-C7-C8
2	F	501	KZH	C12-C13-C14-C15

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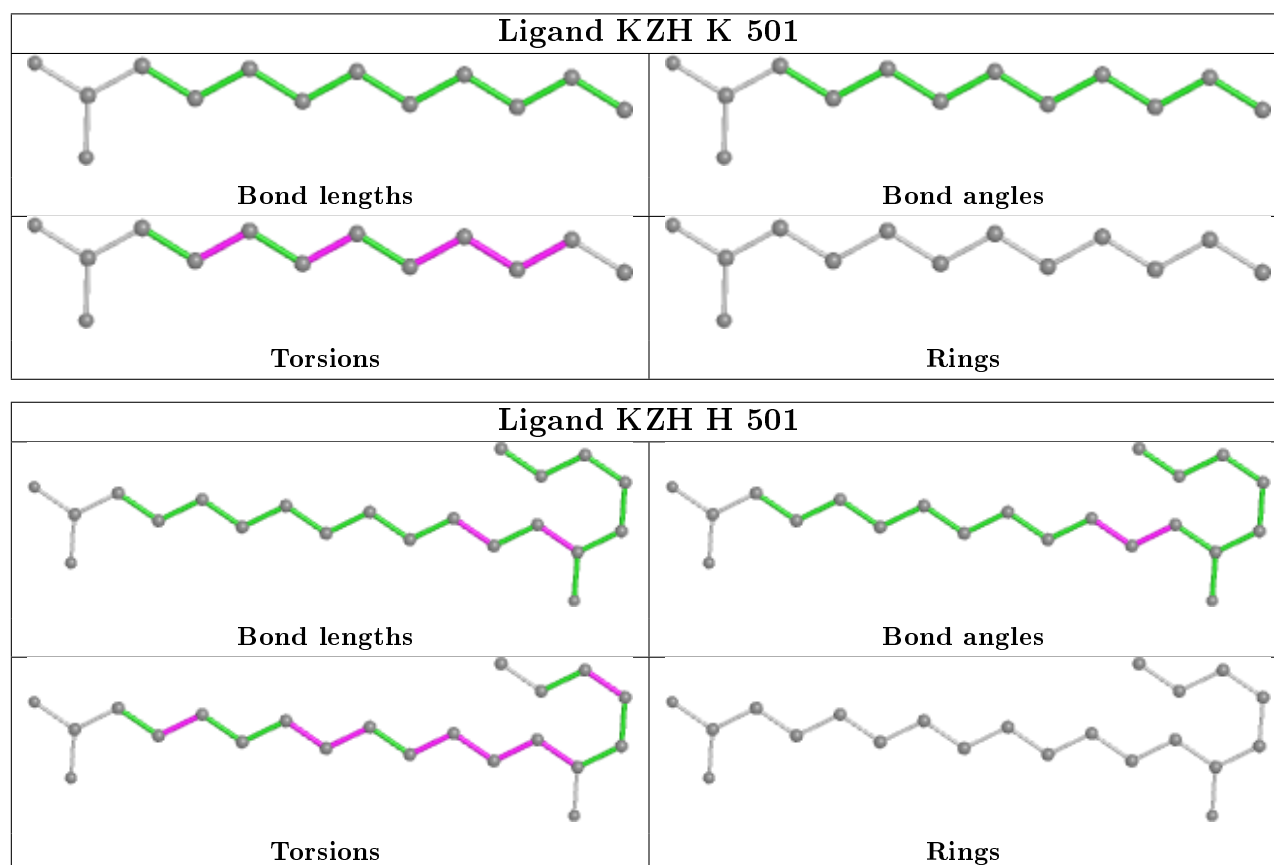
Mol	Chain	Res	Type	Atoms
2	B	501	KZH	C6-C7-C8-C9
2	G	501	KZH	C11-C12-C13-C14
2	F	501	KZH	C10-C11-C12-C13
2	A	501	KZH	C6-C7-C8-C9
2	C	501	KZH	C2-C3-C4-C5
2	H	501	KZH	C5-C6-C7-C8
2	E	501	KZH	C2-C3-C4-C5
2	B	501	KZH	C11-C12-C13-O3
2	B	501	KZH	C7-C8-C9-C10
2	K	501	KZH	C6-C7-C8-C9
2	L	501	KZH	C6-C7-C8-C9
2	F	501	KZH	C11-C12-C13-C14
2	E	501	KZH	C11-C12-C13-C14
2	B	501	KZH	C11-C12-C13-C14
2	F	501	KZH	C6-C7-C8-C9
2	C	501	KZH	C3-C4-C5-C6
2	C	501	KZH	C14-C15-C16-C17
2	B	501	KZH	C2-C3-C4-C5
2	C	501	KZH	C10-C11-C12-C13
2	D	501	KZH	C9-C10-C11-C12
2	D	501	KZH	C3-C4-C5-C6
2	A	501	KZH	C3-C4-C5-C6
2	F	501	KZH	O3-C13-C14-C15
2	C	501	KZH	C4-C5-C6-C7
2	A	501	KZH	C2-C3-C4-C5
2	E	501	KZH	C1-C2-C3-C4
2	C	501	KZH	O3-C13-C14-C15
2	K	501	KZH	C2-C3-C4-C5
2	E	501	KZH	C4-C5-C6-C7
2	B	501	KZH	C4-C5-C6-C7
2	K	501	KZH	C7-C8-C9-C10
2	L	501	KZH	C5-C6-C7-C8
2	E	501	KZH	C7-C8-C9-C10
2	D	501	KZH	C2-C3-C4-C5
2	A	501	KZH	C7-C8-C9-C10
2	I	501	KZH	C6-C7-C8-C9
2	J	501	KZH	C4-C5-C6-C7
2	F	501	KZH	C7-C8-C9-C10
2	I	501	KZH	C7-C8-C9-C10
2	H	501	KZH	C11-C12-C13-C14
2	G	501	KZH	C3-C4-C5-C6
2	G	501	KZH	C9-C10-C11-C12

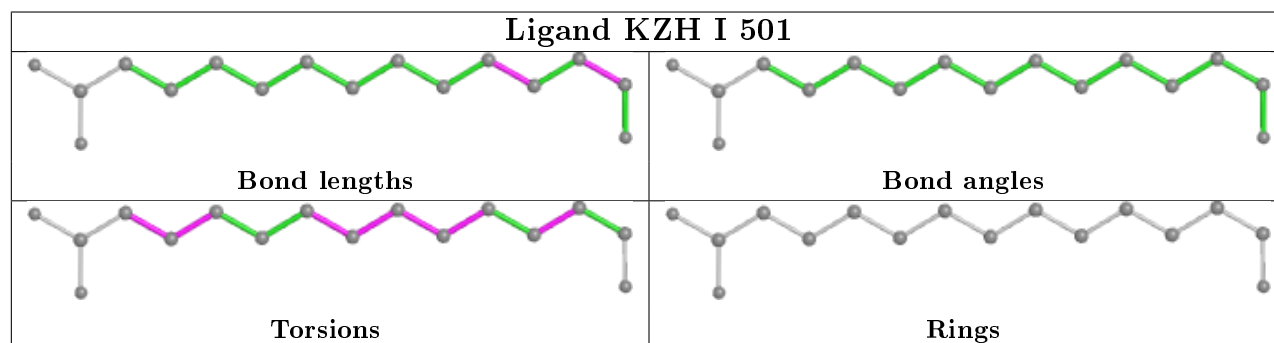
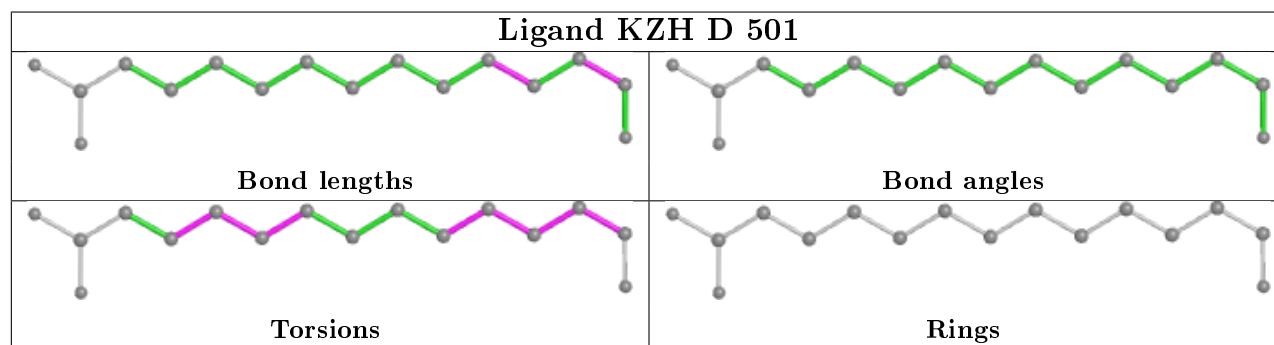
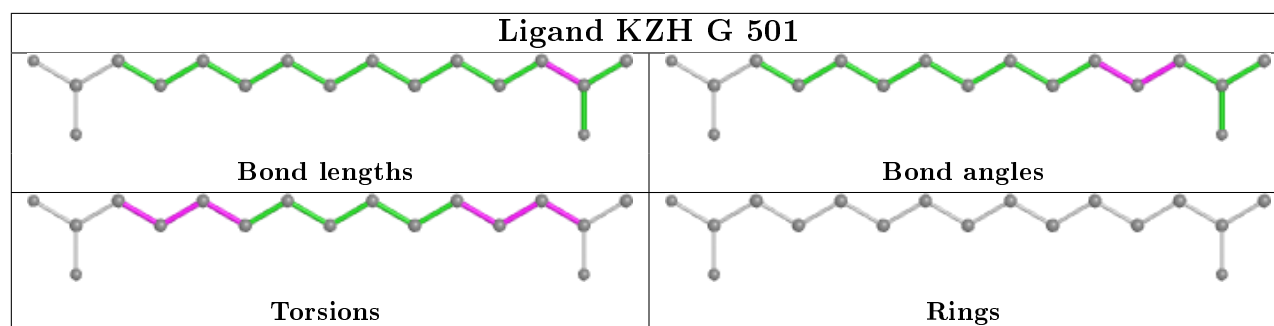
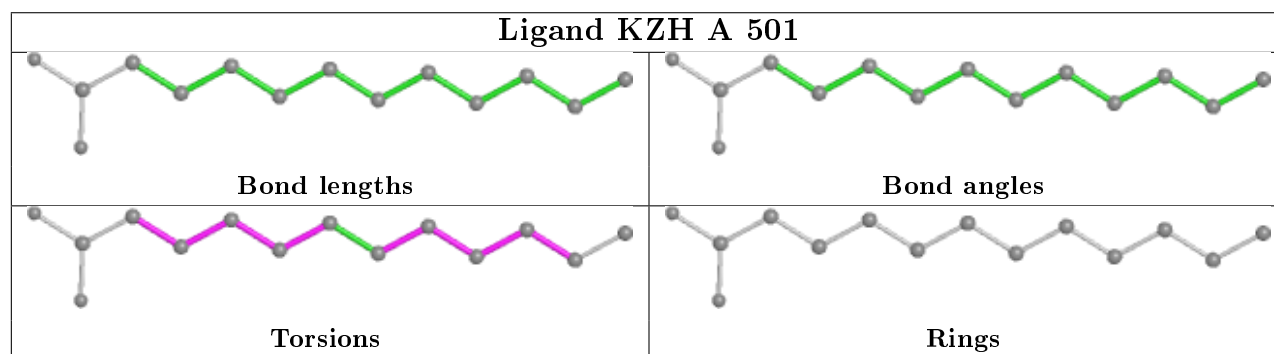
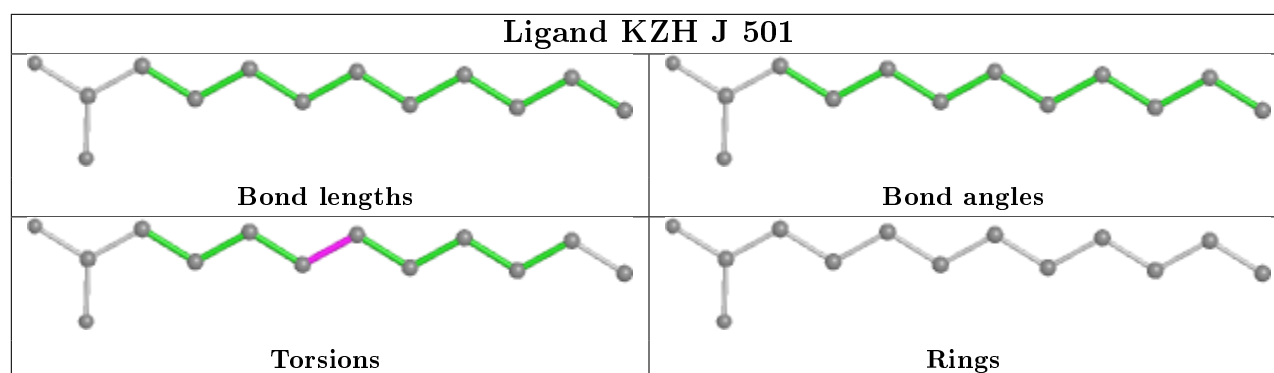
There are no ring outliers.

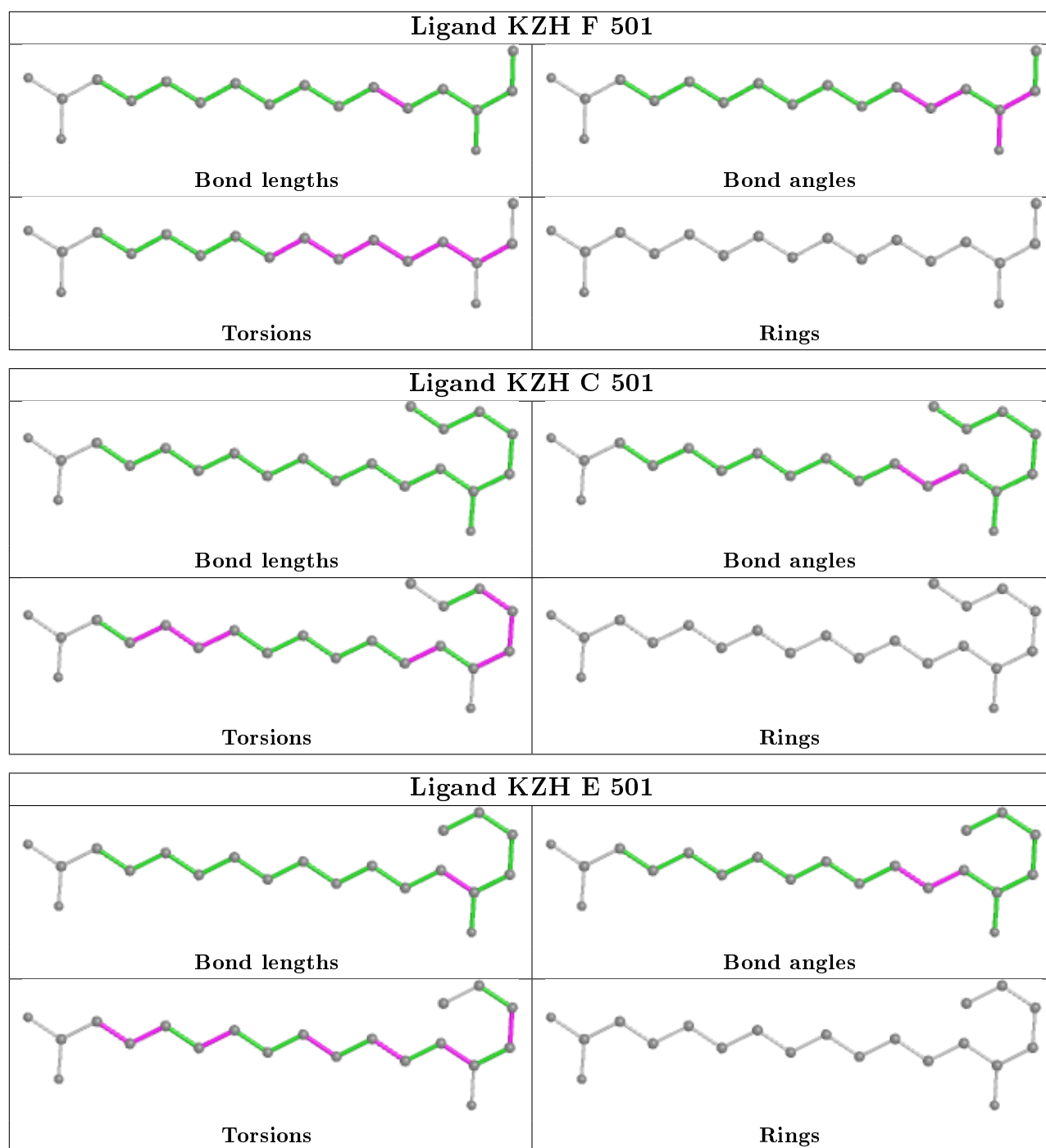
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	501	KZH	1	0
2	I	501	KZH	1	0
2	C	501	KZH	1	0

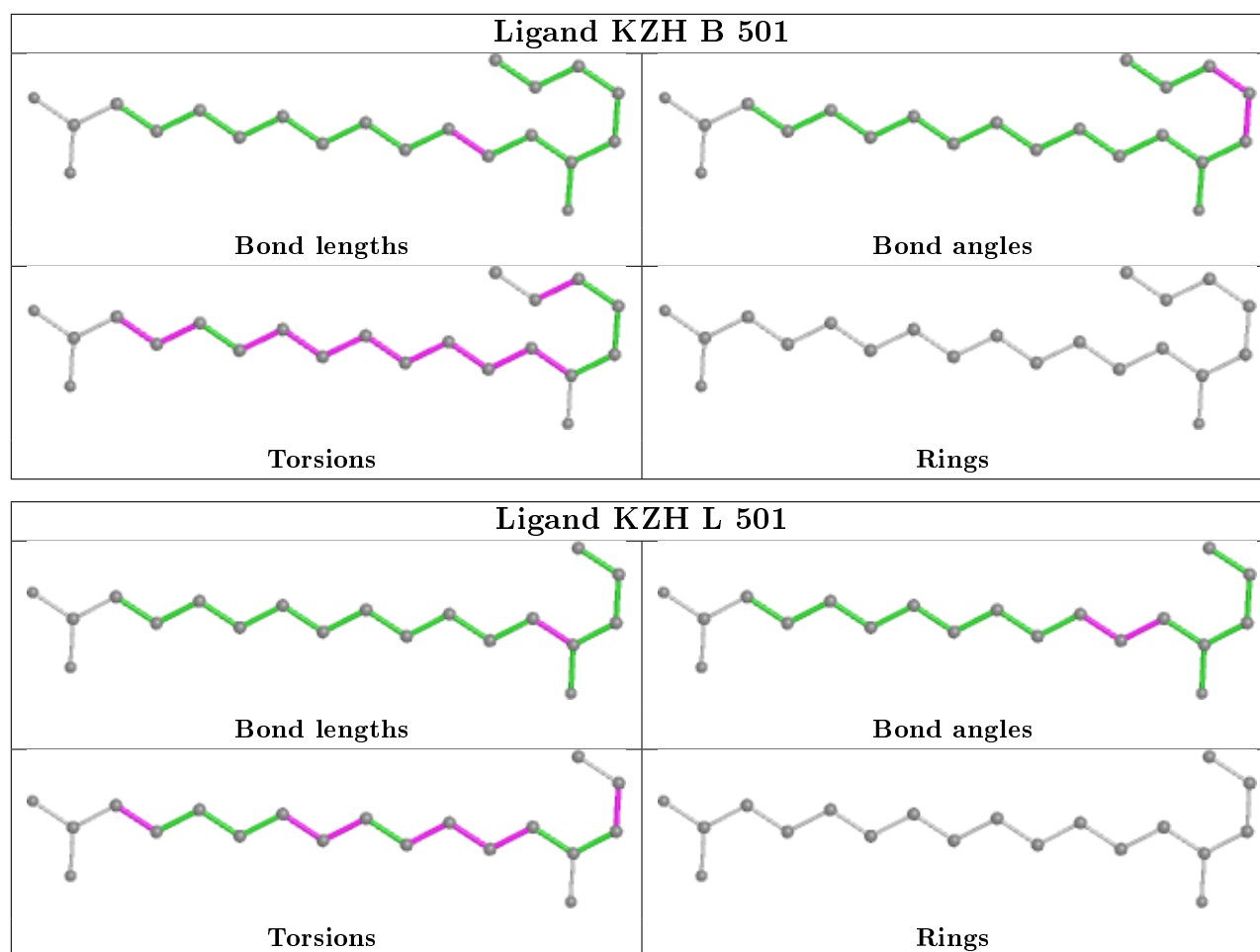
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	326/329 (99%)	-0.34	0 100 100	19, 34, 51, 68	0
1	B	325/329 (98%)	-0.08	2 (0%) 89 88	21, 49, 77, 95	0
1	C	327/329 (99%)	-0.18	0 100 100	21, 44, 66, 87	0
1	D	326/329 (99%)	-0.11	1 (0%) 94 94	31, 51, 70, 80	0
1	E	327/329 (99%)	-0.10	2 (0%) 89 88	23, 49, 72, 103	0
1	F	327/329 (99%)	-0.34	0 100 100	19, 34, 52, 75	0
1	G	325/329 (98%)	-0.11	2 (0%) 89 88	28, 48, 76, 88	0
1	H	327/329 (99%)	-0.32	0 100 100	20, 39, 57, 73	0
1	I	325/329 (98%)	-0.33	0 100 100	19, 38, 57, 71	0
1	J	327/329 (99%)	-0.32	0 100 100	18, 36, 55, 66	0
1	K	324/329 (98%)	0.38	14 (4%) 35 30	25, 75, 104, 117	0
1	L	327/329 (99%)	-0.31	0 100 100	20, 35, 60, 78	0
All	All	3913/3948 (99%)	-0.18	21 (0%) 91 90	18, 42, 77, 117	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	87	PHE	4.0
1	K	329	PRO	3.5
1	B	150	LEU	3.4
1	D	157	ALA	3.4
1	K	154	GLY	3.3
1	K	43	THR	3.2
1	K	128	ALA	3.1
1	K	311	ASP	3.1
1	K	306	LEU	3.0
1	K	130	ALA	2.9
1	E	178	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	40	LEU	2.8
1	K	38	LEU	2.6
1	E	181	ALA	2.5
1	K	305	PRO	2.5
1	K	96	VAL	2.4
1	K	95	ALA	2.3
1	K	20	GLY	2.2
1	K	40	LEU	2.1
1	K	37	CYS	2.1
1	B	180	ASN	2.1

## 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](#)

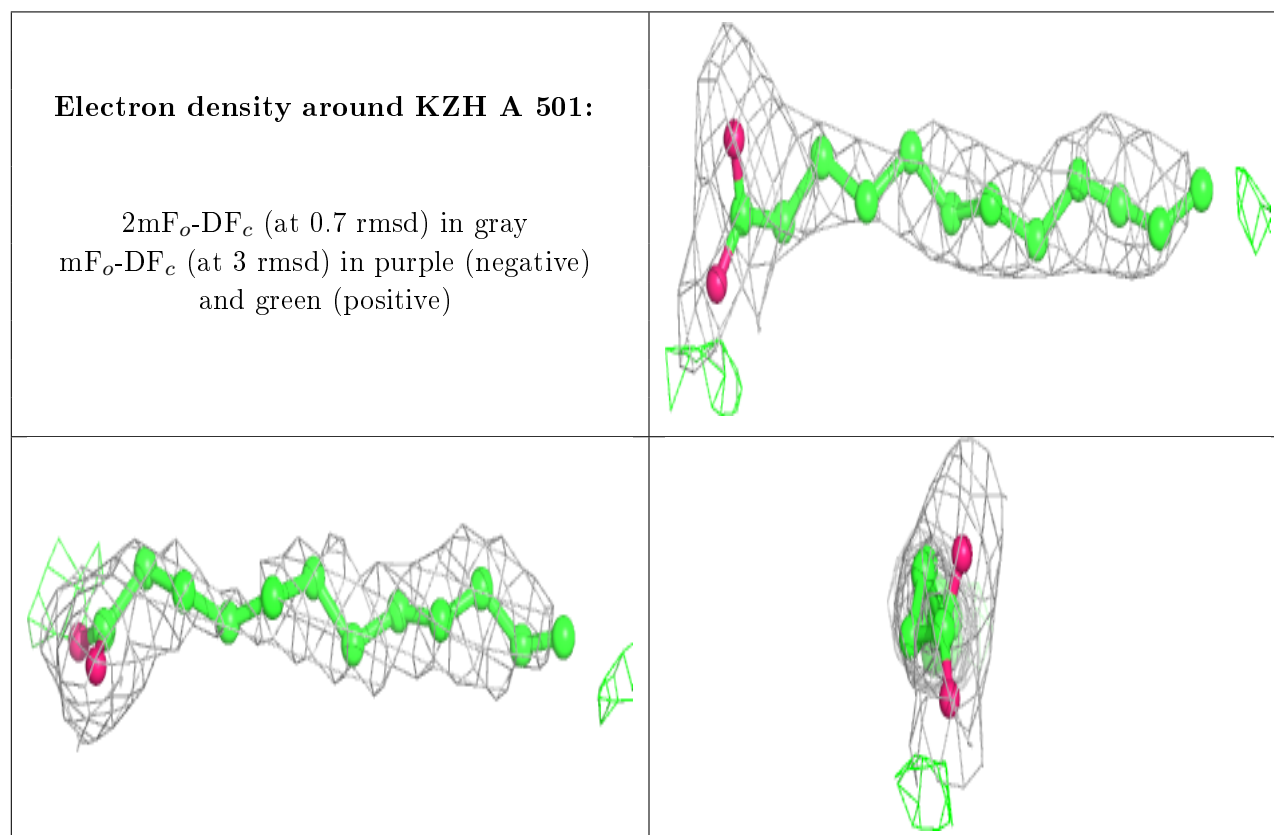
There are no carbohydrates in this entry.

## 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.

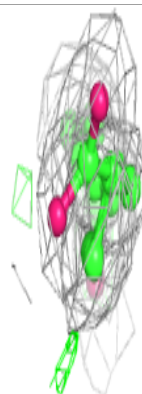
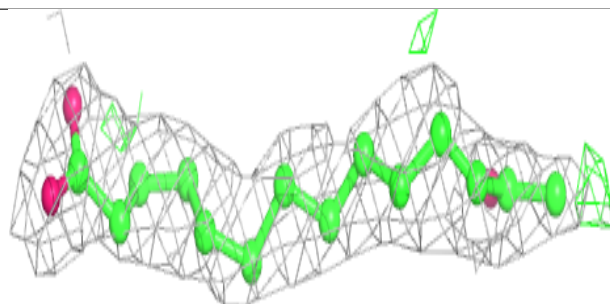
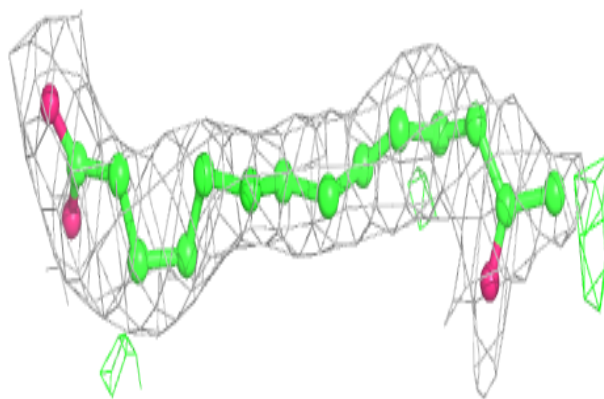
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	KZH	A	501	14/21	0.93	0.32	29,43,55,59	0
2	KZH	G	501	17/21	0.94	0.24	11,36,67,76	0
2	KZH	F	501	18/21	0.94	0.22	13,42,66,67	0
2	KZH	J	501	13/21	0.95	0.23	19,33,41,44	0
2	KZH	H	501	21/21	0.95	0.20	20,33,46,57	0
2	KZH	I	501	16/21	0.96	0.22	24,41,52,55	0
2	KZH	K	501	13/21	0.96	0.23	16,38,55,55	0
2	KZH	E	501	20/21	0.96	0.18	11,37,52,55	0
2	KZH	B	501	21/21	0.96	0.21	25,42,67,82	0
2	KZH	L	501	19/21	0.96	0.23	11,36,62,63	0
2	KZH	C	501	21/21	0.97	0.19	19,34,53,53	0
2	KZH	D	501	16/21	0.97	0.23	25,39,48,56	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.

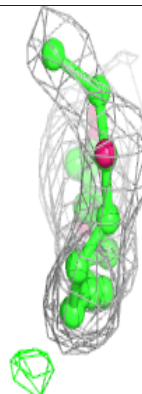
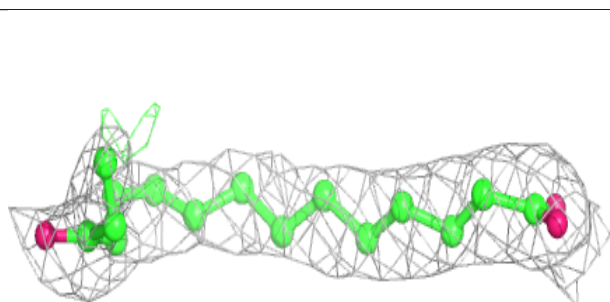
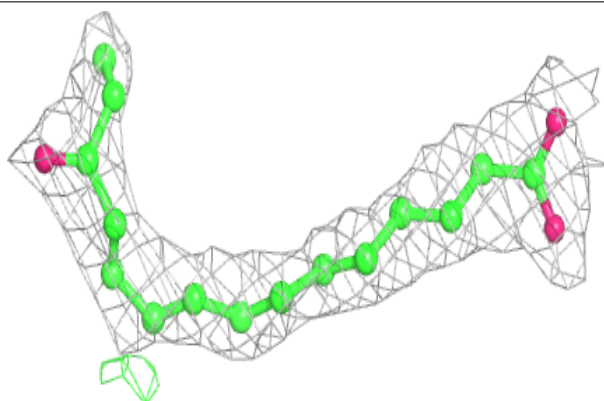


**Electron density around KZH G 501:**

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

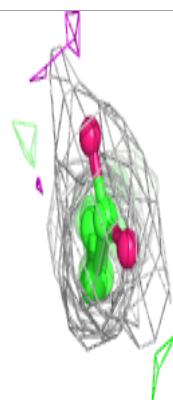
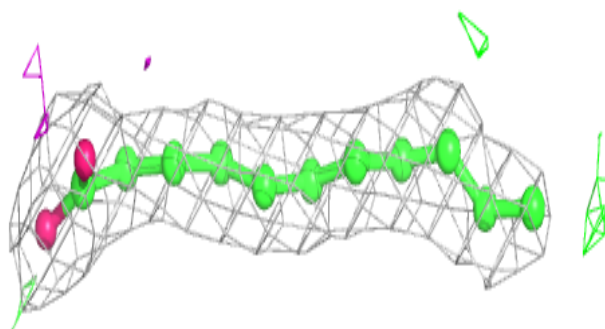
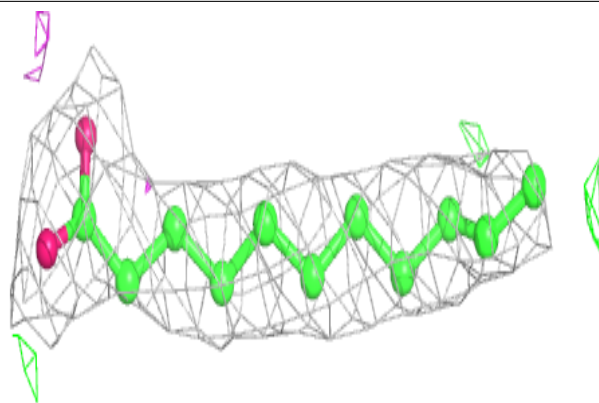
**Electron density around KZH F 501:**

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

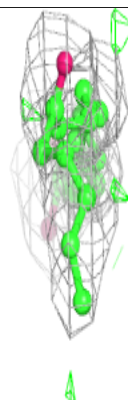
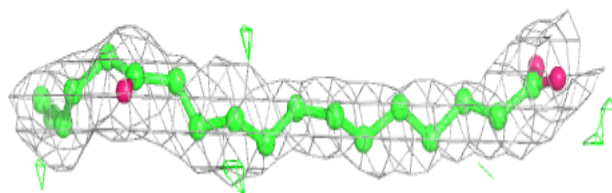
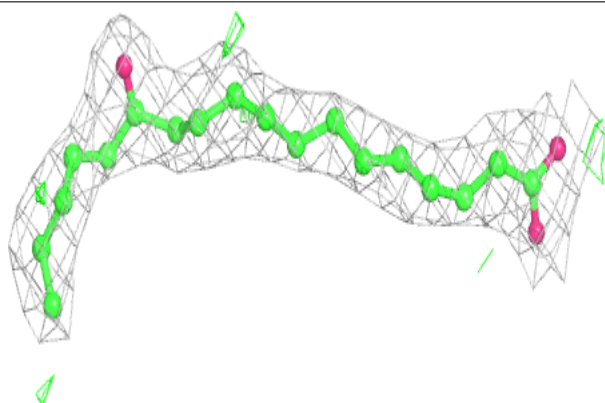


**Electron density around KZH J 501:**

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

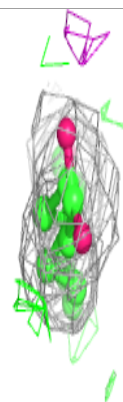
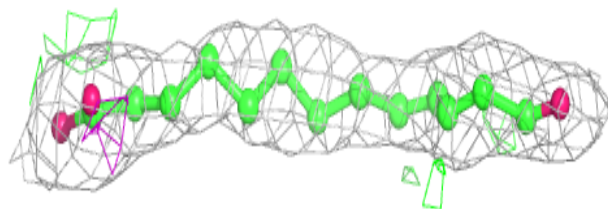
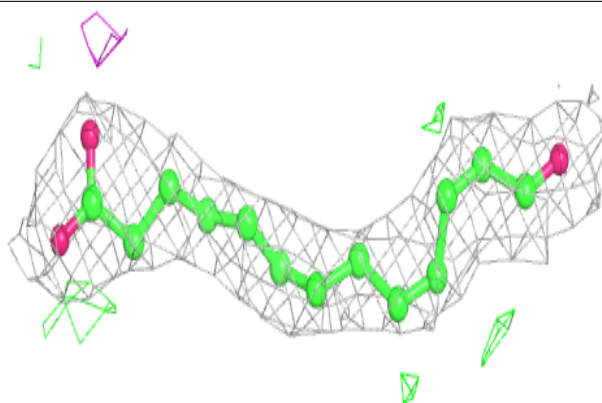
**Electron density around KZH H 501:**

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

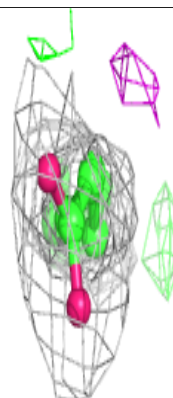
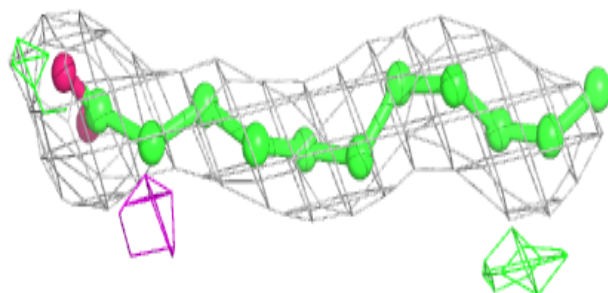
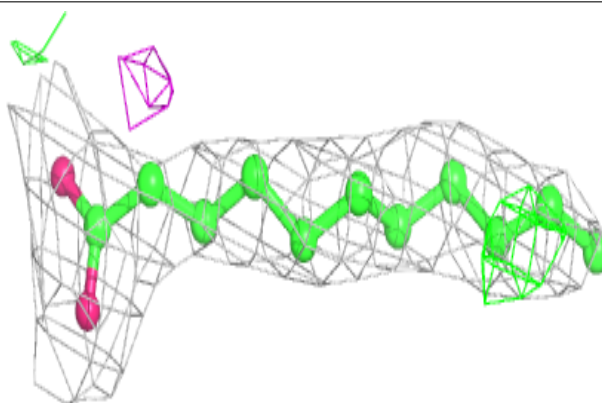


**Electron density around KZH I 501:**

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

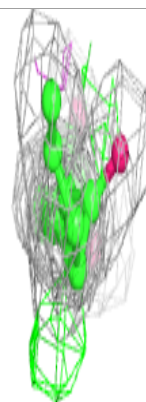
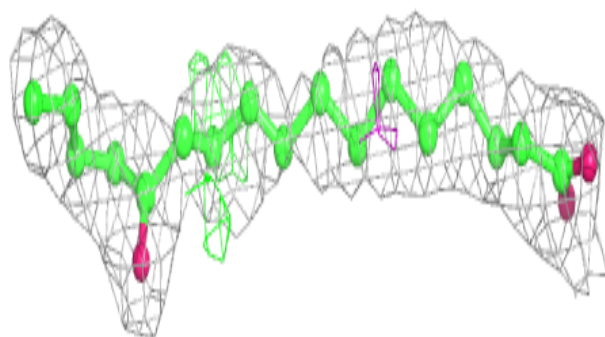
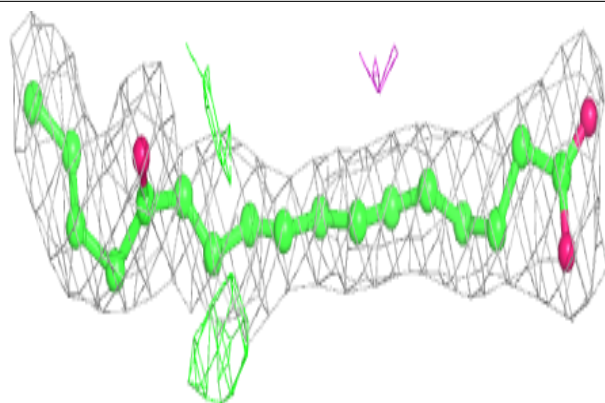
**Electron density around KZH K 501:**

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

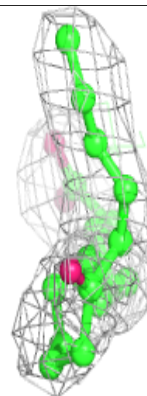
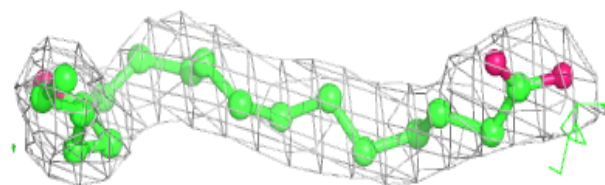
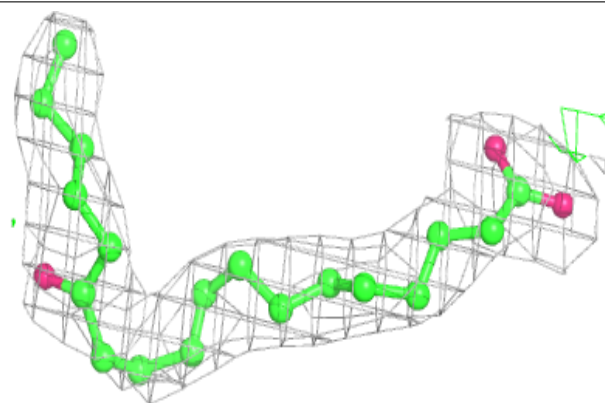


**Electron density around KZH E 501:**

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

**Electron density around KZH B 501:**

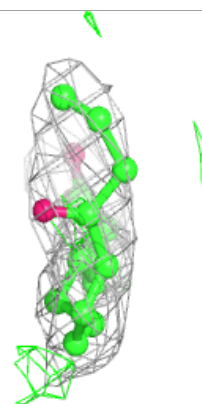
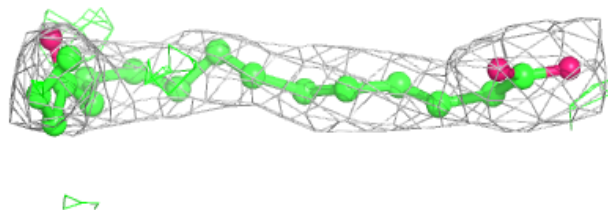
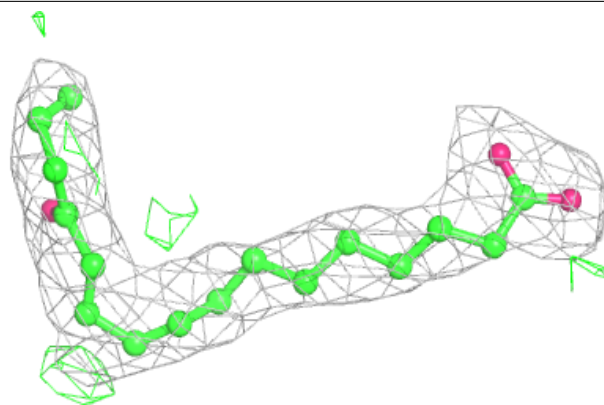
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



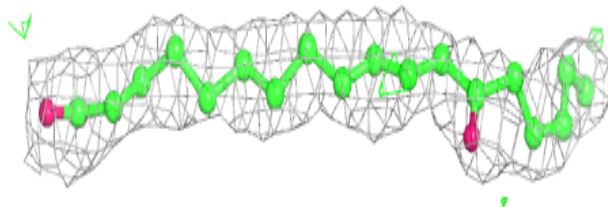
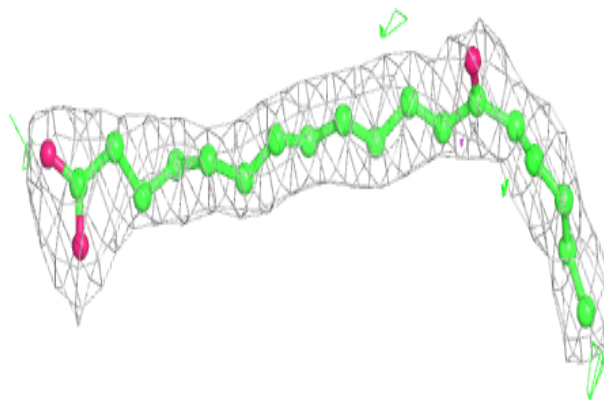


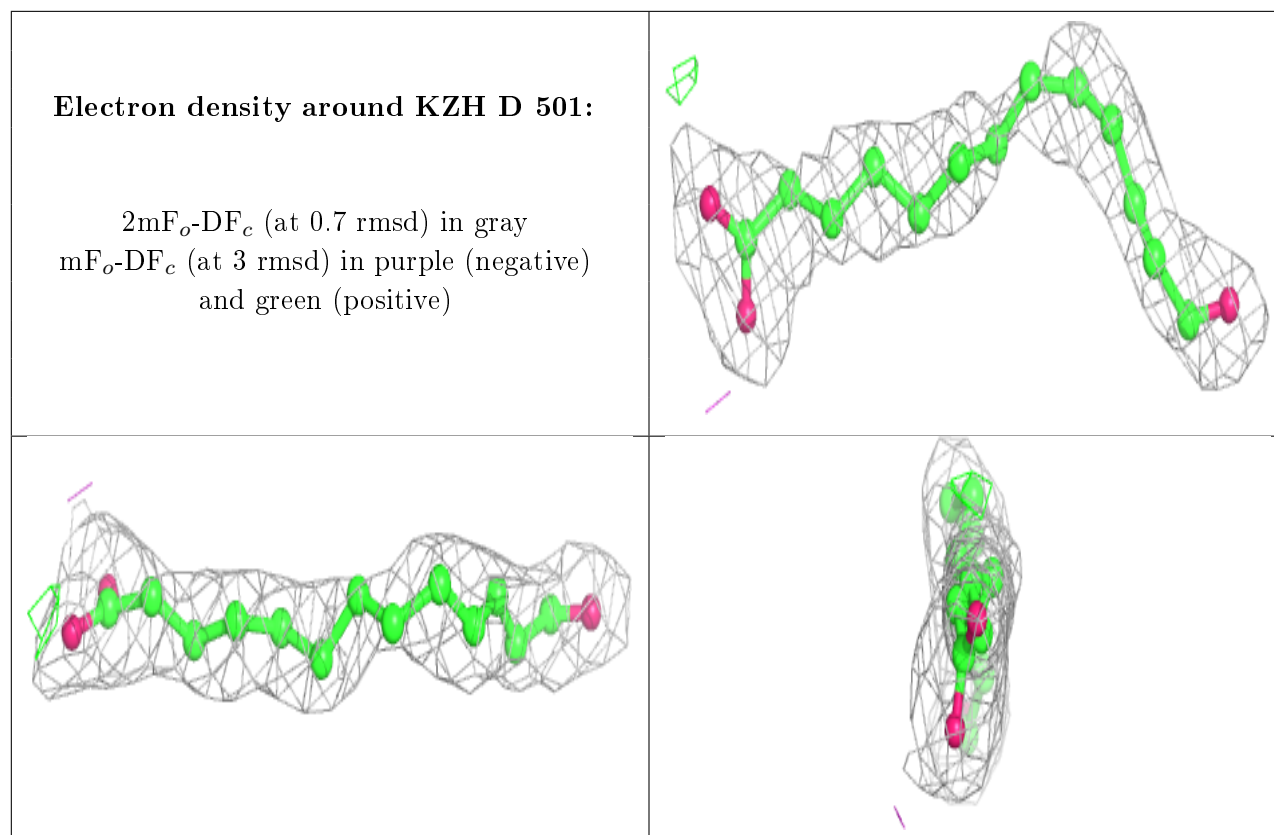
**Electron density around KZH L 501:**

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

**Electron density around KZH C 501:**

$2mF_o-DF_c$  (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.