



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 06:26 am BST

PDB ID : 2R8A  
Title : Crystal structure of the long-chain fatty acid transporter FadL mutant delta N8  
Authors : Hearn, E.M.; Patel, D.R.; Lepore, B.W.; Indic, M.; van den Berg, B.  
Deposited on : 2007-09-10  
Resolution : 3.00 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

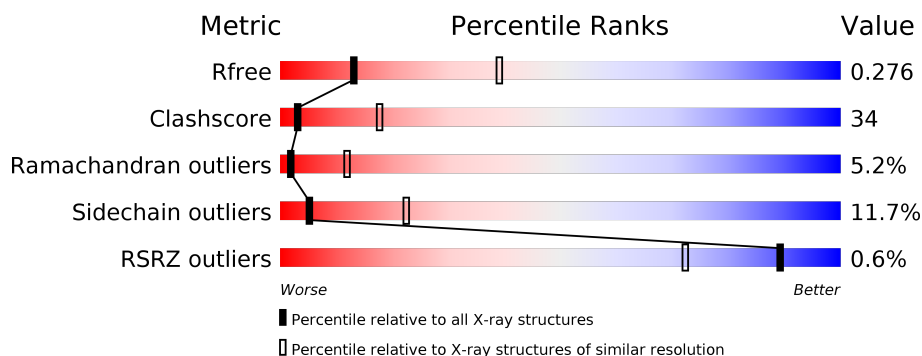
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	419	
1	B	419	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	C8E	B	502	-	-	-	X
2	C8E	B	503	-	-	-	X

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5642 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 Long-chain fatty acid transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	360	Total	C	N	O	S	0	0	0
			2779	1759	472	542	6			
1	B	360	Total	C	N	O	S	0	0	0
			2779	1759	472	542	6			

There are 30 discrepancies between the modelled and reference sequences:

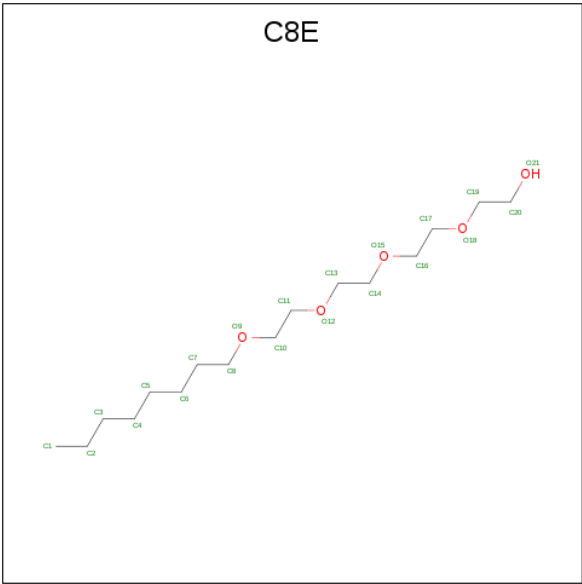
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PHE	DELETION	UNP P10384
A	?	-	GLN	DELETION	UNP P10384
A	?	-	LEU	DELETION	UNP P10384
A	?	-	ASN	DELETION	UNP P10384
A	?	-	GLU	DELETION	UNP P10384
A	?	-	PHE	DELETION	UNP P10384
A	?	-	SER	DELETION	UNP P10384
A	?	-	SER	DELETION	UNP P10384
A	197	THR	ILE	CONFLICT	UNP P10384
A	422	HIS	-	EXPRESSION TAG	UNP P10384
A	423	HIS	-	EXPRESSION TAG	UNP P10384
A	424	HIS	-	EXPRESSION TAG	UNP P10384
A	425	HIS	-	EXPRESSION TAG	UNP P10384
A	426	HIS	-	EXPRESSION TAG	UNP P10384
A	427	HIS	-	EXPRESSION TAG	UNP P10384
B	?	-	PHE	DELETION	UNP P10384
B	?	-	GLN	DELETION	UNP P10384
B	?	-	LEU	DELETION	UNP P10384
B	?	-	ASN	DELETION	UNP P10384
B	?	-	GLU	DELETION	UNP P10384
B	?	-	PHE	DELETION	UNP P10384
B	?	-	SER	DELETION	UNP P10384
B	?	-	SER	DELETION	UNP P10384
B	197	THR	ILE	CONFLICT	UNP P10384
B	422	HIS	-	EXPRESSION TAG	UNP P10384

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Chain	Residue	Modelled	Actual	Comment	Reference
B	423	HIS	-	EXPRESSION TAG	UNP P10384
B	424	HIS	-	EXPRESSION TAG	UNP P10384
B	425	HIS	-	EXPRESSION TAG	UNP P10384
B	426	HIS	-	EXPRESSION TAG	UNP P10384
B	427	HIS	-	EXPRESSION TAG	UNP P10384

- Molecule 2 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C<sub>16</sub>H<sub>34</sub>O<sub>5</sub>).

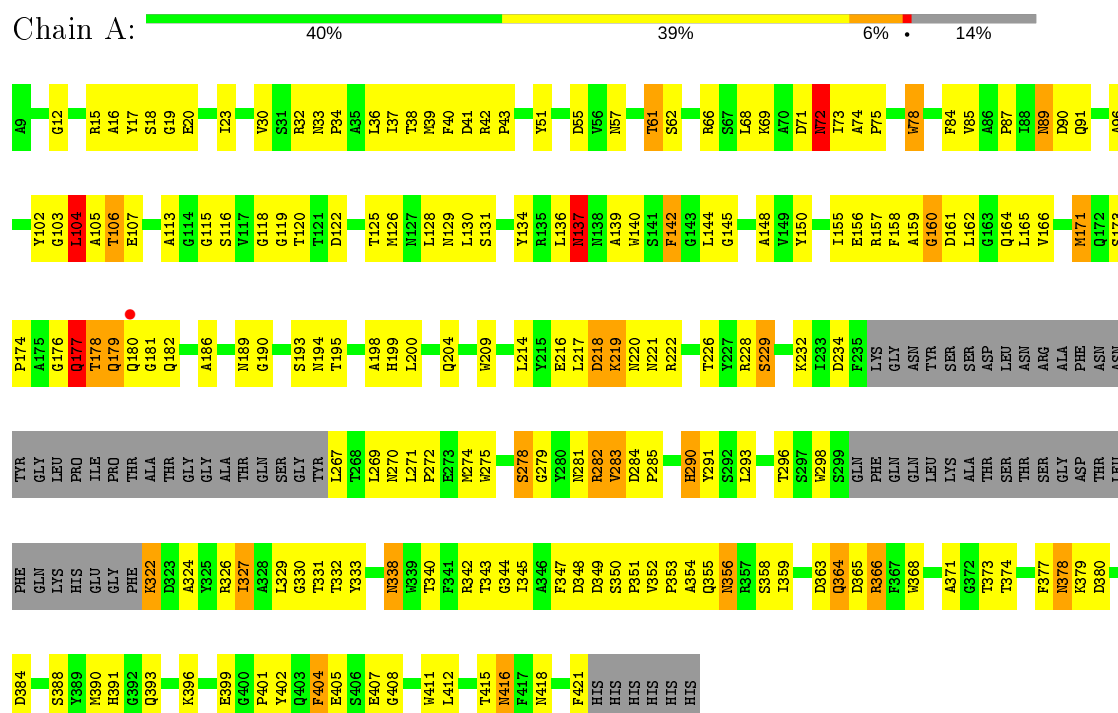


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			21	16	5		
2	A	1	Total	C	O	0	0
			21	16	5		
2	B	1	Total	C	O	0	0
			21	16	5		
2	B	1	Total	C	O	0	0
			21	16	5		

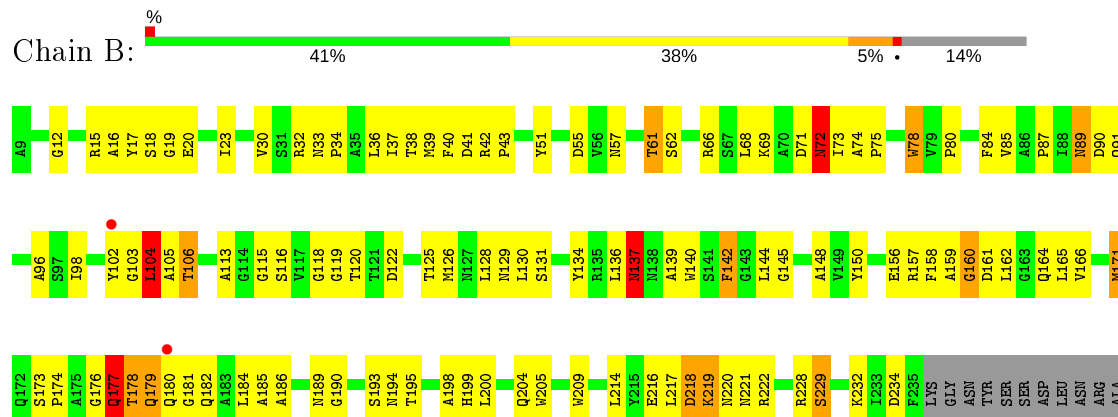
### 3 Residue-property plots

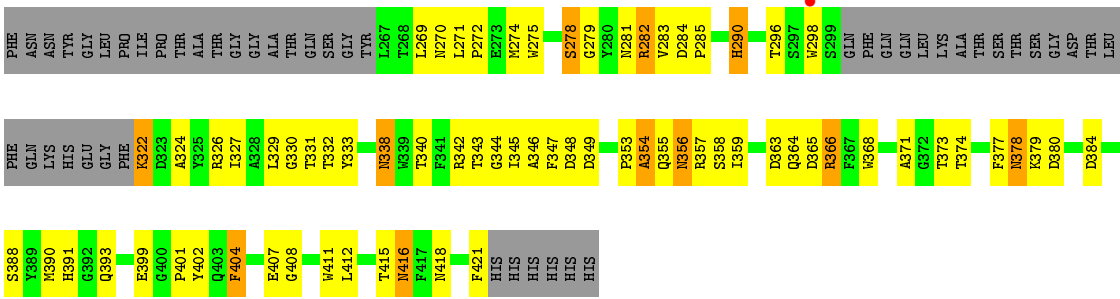
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Long-chain fatty acid transport protein



#### • Molecule 1: Long-chain fatty acid transport protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.77Å 64.77Å 270.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00 37.93 – 3.00	Depositor EDS
% Data completeness (in resolution range)	80.4 (10.00-3.00) 80.8 (37.93-3.00)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.06 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.248 , 0.294 0.236 , 0.276	Depositor DCC
$R_{free}$ test set	1398 reflections (7.79%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.3	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 12.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.479 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	5642	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: C8E

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	0.48	0/2854	0.71	0/3888
1	B	0.48	0/2854	0.71	0/3888
All	All	0.48	0/5708	0.71	0/7776

There are no bond length outliers.

There are no bond angle outliers.

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	2779	0	2588	186	0
1	B	2779	0	2588	180	0
2	A	42	0	68	13	0
2	B	42	0	68	8	0
All	All	5642	0	5312	369	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 34.

All (369) 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:176:GLY:O	1:A:182:GLN:HG3	1.70	0.92
1:B:176:GLY:O	1:B:182:GLN:HG3	1.70	0.91
1:B:128:LEU:HB2	1:B:148:ALA:HB3	1.58	0.85
1:A:128:LEU:HB2	1:A:148:ALA:HB3	1.59	0.84
1:B:378:ASN:O	1:B:380:ASP:N	2.09	0.84
1:B:353:PRO:HB2	1:B:355:GLN:HE21	1.43	0.84
1:A:378:ASN:O	1:A:380:ASP:N	2.10	0.84
1:A:353:PRO:HB2	1:A:355:GLN:HE21	1.43	0.83
1:A:18:SER:O	1:A:290:HIS:HB2	1.79	0.83
1:A:329:LEU:HD12	2:A:501:C8E:H192	1.60	0.81
1:B:18:SER:O	1:B:290:HIS:HB2	1.80	0.81
1:A:57:ASN:ND2	1:A:72:ASN:H	1.79	0.80
1:B:272:PRO:HG3	1:B:298:TRP:CE3	2.17	0.80
1:B:15:ARG:HD2	1:B:20:GLU:OE1	1.81	0.79
1:B:171:MET:HA	1:B:171:MET:HE3	1.64	0.79
1:B:57:ASN:ND2	1:B:72:ASN:H	1.80	0.79
1:A:15:ARG:HD2	1:A:20:GLU:OE1	1.82	0.79
1:B:144:LEU:HD23	1:B:145:GLY:N	1.98	0.79
1:A:272:PRO:HG3	1:A:298:TRP:CE3	2.17	0.79
1:A:144:LEU:HD23	1:A:145:GLY:N	1.98	0.78
1:A:119:GLY:H	1:A:157:ARG:HE	1.31	0.78
1:A:41:ASP:O	1:A:87:PRO:HG2	1.82	0.78
1:B:119:GLY:H	1:B:157:ARG:HE	1.32	0.77
1:B:161:ASP:O	1:B:165:LEU:HG	1.85	0.77
1:B:41:ASP:O	1:B:87:PRO:HG2	1.84	0.77
1:A:232:LYS:HG2	1:A:270:ASN:ND2	2.01	0.76
1:B:232:LYS:HG2	1:B:270:ASN:ND2	2.01	0.76
1:A:161:ASP:O	1:A:165:LEU:HG	1.85	0.76
1:B:162:LEU:HD23	1:B:165:LEU:HD12	1.69	0.74
1:A:171:MET:HE3	1:A:171:MET:HA	1.69	0.74
1:B:19:GLY:HA2	1:B:278:SER:HB3	1.70	0.73
1:B:329:LEU:HD23	1:B:330:GLY:N	2.03	0.73
1:A:162:LEU:HD23	1:A:165:LEU:HD12	1.70	0.72
1:A:33:ASN:ND2	1:A:36:LEU:HG	2.04	0.72
1:B:33:ASN:ND2	1:B:36:LEU:HG	2.04	0.72
1:A:19:GLY:HA2	1:A:278:SER:HB3	1.69	0.72
1:A:329:LEU:HD23	1:A:330:GLY:N	2.05	0.71
1:B:116:SER:O	1:B:157:ARG:HD2	1.91	0.71
1:A:116:SER:O	1:A:157:ARG:HD2	1.91	0.70
1:A:293:LEU:HB2	2:A:501:C8E:H142	1.71	0.70
1:B:89:ASN:ND2	1:B:91:GLN:H	1.91	0.68
1:A:232:LYS:HG2	1:A:270:ASN:HD21	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:GLN:HE22	1:A:356:ASN:HB2	1.59	0.68
1:A:89:ASN:ND2	1:A:91:GLN:H	1.91	0.67
1:A:355:GLN:NE2	1:A:356:ASN:HB2	2.09	0.67
1:B:355:GLN:NE2	1:B:356:ASN:HB2	2.10	0.67
1:A:157:ARG:HB2	1:A:198:ALA:HB3	1.76	0.67
1:A:209:TRP:O	1:A:229:SER:HB3	1.95	0.67
1:B:157:ARG:HB2	1:B:198:ALA:HB3	1.76	0.67
1:B:232:LYS:HG2	1:B:270:ASN:HD21	1.58	0.67
1:B:80:PRO:HG3	2:B:502:C8E:H52	1.77	0.67
1:A:164:GLN:HG2	1:A:189:ASN:ND2	2.10	0.67
1:B:164:GLN:HG2	1:B:189:ASN:ND2	2.10	0.66
1:A:177:GLN:OE1	1:A:177:GLN:N	2.28	0.66
2:A:504:C8E:H101	2:A:504:C8E:H142	1.76	0.66
1:B:209:TRP:O	1:B:229:SER:HB3	1.96	0.66
1:B:177:GLN:N	1:B:177:GLN:OE1	2.28	0.66
1:A:232:LYS:HA	1:A:270:ASN:ND2	2.11	0.66
1:B:232:LYS:HA	1:B:270:ASN:ND2	2.11	0.65
1:A:178:THR:OG1	1:A:179:GLN:N	2.30	0.65
1:B:324:ALA:HB1	1:B:349:ASP:O	1.96	0.65
1:B:355:GLN:HE22	1:B:356:ASN:HB2	1.60	0.65
1:A:324:ALA:HB1	1:A:349:ASP:O	1.96	0.65
1:A:37:ILE:C	1:A:39:MET:H	2.00	0.65
1:B:282:ARG:HG3	1:B:282:ARG:HH11	1.62	0.65
1:A:137:ASN:HD21	1:A:140:TRP:H	1.45	0.64
1:B:179:GLN:O	1:B:181:GLY:N	2.31	0.64
1:B:37:ILE:C	1:B:39:MET:H	2.01	0.64
1:A:179:GLN:O	1:A:181:GLY:N	2.30	0.64
1:A:282:ARG:HG3	1:A:282:ARG:HH11	1.63	0.63
1:B:137:ASN:HD21	1:B:140:TRP:H	1.44	0.63
1:A:327:ILE:HD11	2:A:501:C8E:O18	1.99	0.63
1:B:178:THR:OG1	1:B:179:GLN:N	2.30	0.62
1:B:36:LEU:HD23	1:B:214:LEU:HD22	1.81	0.62
1:A:348:ASP:OD2	1:A:366:ARG:HG3	1.99	0.62
1:B:126:MET:CE	2:B:502:C8E:H42	2.30	0.62
1:B:348:ASP:OD2	1:B:366:ARG:HG3	1.98	0.62
1:B:216:GLU:HB3	1:B:222:ARG:HB3	1.82	0.61
1:A:178:THR:O	1:A:179:GLN:HB3	2.00	0.61
1:B:178:THR:O	1:B:179:GLN:HB3	2.00	0.61
1:B:126:MET:HE3	2:B:502:C8E:H42	1.80	0.61
1:A:216:GLU:HB3	1:A:222:ARG:HB3	1.82	0.61
1:B:204:GLN:HG2	1:B:234:ASP:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:GLN:O	1:A:366:ARG:HG2	2.01	0.61
1:B:364:GLN:O	1:B:366:ARG:HG2	2.01	0.61
1:A:204:GLN:HG2	1:A:234:ASP:O	2.01	0.61
1:A:57:ASN:HD22	1:A:71:ASP:HA	1.67	0.60
1:A:137:ASN:C	1:A:137:ASN:HD22	2.03	0.60
2:A:504:C8E:H142	2:A:504:C8E:C10	2.31	0.60
1:A:36:LEU:HD23	1:A:214:LEU:HD22	1.82	0.59
1:B:43:PRO:HB2	1:B:421:PHE:CD2	2.38	0.59
1:B:57:ASN:HD22	1:B:71:ASP:HA	1.67	0.59
1:A:179:GLN:C	1:A:181:GLY:H	2.06	0.59
1:B:388:SER:HB3	1:B:412:LEU:HB2	1.85	0.59
1:A:130:LEU:HD23	1:A:131:SER:N	2.18	0.59
1:B:171:MET:HA	1:B:171:MET:CE	2.32	0.59
1:B:137:ASN:HD22	1:B:137:ASN:C	2.04	0.58
1:A:344:GLY:C	1:A:345:ILE:HD12	2.24	0.58
1:B:120:THR:HB	1:B:156:GLU:HB2	1.86	0.58
1:A:120:THR:HB	1:A:156:GLU:HB2	1.86	0.58
1:A:43:PRO:HB2	1:A:421:PHE:CD2	2.38	0.58
1:B:179:GLN:C	1:B:181:GLY:H	2.06	0.58
1:B:344:GLY:C	1:B:345:ILE:HD12	2.24	0.58
1:B:130:LEU:HD23	1:B:131:SER:N	2.18	0.58
1:A:89:ASN:O	1:A:91:GLN:N	2.37	0.57
1:B:89:ASN:O	1:B:91:GLN:N	2.37	0.57
1:A:171:MET:HA	1:A:171:MET:CE	2.33	0.57
1:A:179:GLN:O	1:A:179:GLN:HG3	2.05	0.57
1:A:388:SER:HB3	1:A:412:LEU:HB2	1.85	0.57
1:B:179:GLN:C	1:B:181:GLY:N	2.57	0.56
1:A:179:GLN:C	1:A:181:GLY:N	2.57	0.56
1:A:40:PHE:O	1:A:87:PRO:HG3	2.05	0.56
1:A:136:LEU:O	1:A:137:ASN:HB3	2.04	0.56
1:B:174:PRO:C	1:B:176:GLY:N	2.59	0.56
1:B:40:PHE:O	1:B:87:PRO:HG3	2.05	0.56
1:B:179:GLN:HG3	1:B:179:GLN:O	2.05	0.56
1:A:131:SER:HB3	1:A:145:GLY:HA2	1.87	0.56
1:B:113:ALA:O	1:B:160:GLY:HA3	2.06	0.56
1:B:282:ARG:NH1	1:B:282:ARG:HG3	2.21	0.56
1:B:272:PRO:HG3	1:B:298:TRP:CD2	2.41	0.56
1:A:142:PHE:CD1	1:A:142:PHE:N	2.74	0.56
1:B:353:PRO:O	1:B:355:GLN:N	2.38	0.56
1:A:353:PRO:O	1:A:355:GLN:N	2.39	0.56
1:B:126:MET:CE	2:B:502:C8E:H61	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:LEU:O	1:B:137:ASN:HB3	2.04	0.55
1:A:113:ALA:O	1:A:160:GLY:HA3	2.06	0.55
1:B:142:PHE:N	1:B:142:PHE:CD1	2.74	0.55
1:B:364:GLN:O	1:B:365:ASP:C	2.44	0.55
1:B:30:VAL:HG21	1:B:85:VAL:HG21	1.88	0.55
1:A:364:GLN:O	1:A:365:ASP:C	2.45	0.55
1:A:282:ARG:NH1	1:A:282:ARG:HG3	2.21	0.55
1:B:355:GLN:HE22	1:B:356:ASN:CB	2.20	0.55
1:A:272:PRO:HG3	1:A:298:TRP:CD2	2.41	0.55
1:B:131:SER:HB3	1:B:145:GLY:HA2	1.87	0.54
1:A:174:PRO:C	1:A:176:GLY:N	2.59	0.54
1:B:68:LEU:HD23	1:B:113:ALA:HB3	1.90	0.54
1:A:390:MET:CE	2:A:504:C8E:H51	2.38	0.54
1:B:57:ASN:HD21	1:B:72:ASN:H	1.53	0.53
1:A:17:TYR:HB2	1:A:326:ARG:HH21	1.72	0.53
1:B:75:PRO:HD2	1:B:105:ALA:CB	2.39	0.53
1:A:173:SER:OG	1:A:174:PRO:HD2	2.09	0.53
1:A:355:GLN:HE22	1:A:356:ASN:CB	2.20	0.53
1:B:174:PRO:C	1:B:176:GLY:H	2.12	0.53
1:A:174:PRO:C	1:A:176:GLY:H	2.12	0.53
1:A:57:ASN:HD21	1:A:72:ASN:H	1.52	0.53
1:B:113:ALA:O	1:B:161:ASP:OD1	2.27	0.53
1:B:66:ARG:HH11	1:B:164:GLN:HE22	1.56	0.53
1:A:66:ARG:HH11	1:A:164:GLN:HE22	1.55	0.53
1:A:30:VAL:HG21	1:A:85:VAL:HG21	1.90	0.53
1:B:159:ALA:O	1:B:160:GLY:O	2.27	0.53
1:B:17:TYR:HB2	1:B:326:ARG:HH21	1.72	0.53
1:A:113:ALA:O	1:A:161:ASP:OD1	2.27	0.52
1:B:33:ASN:HD22	1:B:36:LEU:HG	1.74	0.52
1:A:20:GLU:HB3	1:A:32:ARG:HG2	1.92	0.52
1:A:68:LEU:HD23	1:A:113:ALA:HB3	1.90	0.52
1:B:322:LYS:HG2	1:B:353:PRO:HD3	1.91	0.52
1:A:199:HIS:O	1:A:200:LEU:HD12	2.10	0.52
1:A:358:SER:HA	1:A:399:GLU:OE2	2.10	0.52
1:B:199:HIS:O	1:B:200:LEU:HD12	2.10	0.52
1:A:75:PRO:HD2	1:A:105:ALA:CB	2.39	0.52
1:A:137:ASN:C	1:A:137:ASN:ND2	2.63	0.52
1:B:329:LEU:C	1:B:329:LEU:HD23	2.29	0.52
1:B:73:ILE:O	1:B:106:THR:HA	2.10	0.52
1:B:20:GLU:HB3	1:B:32:ARG:HG2	1.92	0.52
1:A:322:LYS:HG2	1:A:353:PRO:HD3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:LEU:HD23	1:A:329:LEU:C	2.30	0.52
1:B:16:ALA:O	1:B:326:ARG:NH2	2.43	0.52
1:B:358:SER:HA	1:B:399:GLU:OE2	2.10	0.52
1:A:73:ILE:O	1:A:106:THR:HA	2.09	0.52
1:B:55:ASP:O	1:B:408:GLY:HA2	2.09	0.52
1:A:164:GLN:HG2	1:A:189:ASN:HD21	1.74	0.51
1:A:272:PRO:HB2	1:A:296:THR:HG23	1.93	0.51
1:B:340:THR:HB	1:B:374:THR:HB	1.92	0.51
1:B:105:ALA:H	2:B:503:C8E:H202	1.74	0.51
1:A:159:ALA:O	1:A:160:GLY:O	2.28	0.51
1:A:55:ASP:O	1:A:408:GLY:HA2	2.10	0.51
1:A:411:TRP:C	1:A:412:LEU:HD22	2.31	0.51
1:B:411:TRP:C	1:B:412:LEU:HD22	2.31	0.51
1:A:16:ALA:O	1:A:326:ARG:NH2	2.43	0.51
1:B:144:LEU:C	1:B:144:LEU:HD23	2.30	0.51
1:B:137:ASN:ND2	1:B:137:ASN:C	2.63	0.51
1:A:218:ASP:C	1:A:220:ASN:H	2.13	0.51
1:A:284:ASP:CG	1:A:285:PRO:HD2	2.31	0.51
1:A:218:ASP:O	1:A:220:ASN:N	2.44	0.51
1:B:96:ALA:HA	1:B:129:ASN:O	2.10	0.51
1:B:173:SER:OG	1:B:174:PRO:HD2	2.09	0.51
1:A:144:LEU:C	1:A:144:LEU:HD23	2.30	0.51
1:B:164:GLN:HG2	1:B:189:ASN:HD21	1.75	0.51
1:B:284:ASP:CG	1:B:285:PRO:HD2	2.31	0.51
1:B:332:THR:HG22	1:B:333:TYR:N	2.26	0.51
1:A:134:TYR:CE1	1:A:136:LEU:HA	2.46	0.51
1:A:353:PRO:C	1:A:355:GLN:H	2.13	0.51
1:B:103:GLY:O	1:B:104:LEU:CB	2.59	0.51
1:A:33:ASN:HD22	1:A:36:LEU:HG	1.74	0.50
1:A:401:PRO:HD2	1:A:402:TYR:CD1	2.46	0.50
1:B:401:PRO:HD2	1:B:402:TYR:CD1	2.45	0.50
1:A:338:ASN:HD22	1:A:338:ASN:N	2.09	0.50
1:A:51:TYR:HD1	1:A:78:TRP:HD1	1.59	0.50
1:A:269:LEU:HD12	1:A:270:ASN:N	2.26	0.50
1:A:291:TYR:CE1	2:A:501:C8E:H72	2.46	0.50
1:B:51:TYR:HD1	1:B:78:TRP:HD1	1.59	0.50
1:A:103:GLY:O	1:A:104:LEU:CB	2.59	0.50
1:B:272:PRO:HB2	1:B:296:THR:HG23	1.93	0.50
1:B:269:LEU:HD12	1:B:270:ASN:N	2.27	0.50
1:B:134:TYR:CE1	1:B:136:LEU:HA	2.46	0.50
1:B:218:ASP:C	1:B:220:ASN:H	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ALA:HA	1:A:129:ASN:O	2.11	0.50
1:B:34:PRO:O	1:B:37:ILE:HG13	2.12	0.50
1:A:162:LEU:HA	1:A:165:LEU:HD12	1.94	0.49
1:A:332:THR:HG22	1:A:333:TYR:N	2.26	0.49
1:A:34:PRO:O	1:A:37:ILE:HG13	2.12	0.49
1:B:342:ARG:O	1:B:371:ALA:HA	2.12	0.49
1:B:353:PRO:C	1:B:355:GLN:H	2.13	0.49
2:B:503:C8E:H51	2:B:503:C8E:H101	1.94	0.49
2:A:504:C8E:H101	2:A:504:C8E:H61	1.93	0.49
1:B:218:ASP:O	1:B:220:ASN:N	2.45	0.49
1:B:415:THR:HG22	1:B:416:ASN:N	2.26	0.49
1:A:232:LYS:HG2	1:A:270:ASN:CG	2.33	0.49
1:A:340:THR:HB	1:A:374:THR:HB	1.93	0.49
1:B:338:ASN:HD22	1:B:338:ASN:N	2.09	0.49
1:B:43:PRO:HA	1:B:85:VAL:O	2.13	0.49
1:A:103:GLY:HA3	2:A:504:C8E:H162	1.95	0.49
1:B:221:ASN:OD1	1:B:281:ASN:HA	2.13	0.49
1:A:232:LYS:CG	1:A:270:ASN:HD21	2.25	0.49
1:A:342:ARG:O	1:A:371:ALA:HA	2.13	0.49
1:A:43:PRO:HA	1:A:85:VAL:O	2.12	0.49
1:A:221:ASN:OD1	1:A:281:ASN:HA	2.13	0.49
1:B:162:LEU:HA	1:B:165:LEU:HD12	1.93	0.49
1:B:232:LYS:HG2	1:B:270:ASN:CG	2.33	0.49
1:B:384:ASP:O	1:B:415:THR:HA	2.13	0.49
1:B:377:PHE:O	1:B:378:ASN:HB3	2.13	0.49
2:A:501:C8E:H102	1:B:98:ILE:HD11	1.94	0.48
1:A:116:SER:HA	1:A:158:PHE:O	2.13	0.48
1:A:404:PHE:CD1	1:A:404:PHE:N	2.81	0.48
1:A:377:PHE:O	1:A:378:ASN:HB3	2.13	0.48
1:A:279:GLY:O	1:A:290:HIS:HA	2.13	0.48
1:A:364:GLN:NE2	1:A:393:GLN:O	2.47	0.48
1:A:415:THR:HG22	1:A:416:ASN:N	2.28	0.48
1:B:174:PRO:O	1:B:176:GLY:N	2.46	0.48
1:A:126:MET:HB3	1:A:150:TYR:HB3	1.96	0.48
1:B:228:ARG:HB3	1:B:274:MET:HB3	1.96	0.48
1:B:364:GLN:NE2	1:B:393:GLN:O	2.46	0.48
1:B:162:LEU:HA	1:B:162:LEU:HD23	1.68	0.48
1:B:390:MET:SD	2:B:503:C8E:H32	2.54	0.48
1:A:384:ASP:O	1:A:415:THR:HA	2.13	0.48
1:B:116:SER:HA	1:B:158:PHE:O	2.14	0.48
1:A:37:ILE:C	1:A:39:MET:N	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:LYS:CG	1:B:270:ASN:HD21	2.25	0.47
1:A:174:PRO:O	1:A:176:GLY:N	2.46	0.47
1:B:126:MET:HB3	1:B:150:TYR:HB3	1.96	0.47
1:B:37:ILE:C	1:B:39:MET:N	2.67	0.47
1:B:404:PHE:N	1:B:404:PHE:CD1	2.81	0.47
1:B:279:GLY:O	1:B:290:HIS:HA	2.13	0.47
1:A:284:ASP:OD1	1:A:285:PRO:HD2	2.15	0.47
1:B:16:ALA:O	1:B:17:TYR:HB2	2.14	0.47
1:A:228:ARG:HB3	1:A:274:MET:HB3	1.96	0.46
1:A:102:TYR:CG	1:A:271:LEU:HD22	2.50	0.46
1:B:102:TYR:CG	1:B:271:LEU:HD22	2.50	0.46
1:B:177:GLN:O	1:B:178:THR:O	2.34	0.46
1:B:232:LYS:HA	1:B:270:ASN:HD22	1.80	0.46
1:B:284:ASP:OD1	1:B:285:PRO:HD2	2.15	0.46
1:A:363:ASP:O	1:A:364:GLN:HB3	2.16	0.46
1:A:16:ALA:O	1:A:17:TYR:HB2	2.15	0.46
1:B:363:ASP:O	1:B:364:GLN:HB3	2.16	0.46
1:A:176:GLY:O	1:A:178:THR:N	2.49	0.46
1:A:217:LEU:O	1:A:218:ASP:CB	2.63	0.46
1:B:131:SER:HB3	1:B:145:GLY:CA	2.46	0.46
1:A:102:TYR:O	1:A:125:THR:HB	2.16	0.46
1:A:355:GLN:NE2	1:A:356:ASN:CB	2.78	0.46
1:B:217:LEU:O	1:B:218:ASP:CB	2.64	0.46
1:A:12:GLY:HA2	1:A:15:ARG:HG2	1.98	0.46
1:A:350:SER:HA	1:A:351:PRO:HD3	1.72	0.46
1:B:102:TYR:O	1:B:125:THR:HB	2.16	0.46
1:A:217:LEU:O	1:A:218:ASP:HB3	2.16	0.46
1:A:343:THR:HG22	1:A:344:GLY:N	2.31	0.45
1:B:176:GLY:O	1:B:178:THR:N	2.48	0.45
1:B:33:ASN:HA	1:B:34:PRO:HD2	1.70	0.45
1:A:137:ASN:ND2	1:A:139:ALA:H	2.14	0.45
1:B:402:TYR:HB2	1:B:404:PHE:CE1	2.51	0.45
1:A:131:SER:HB3	1:A:145:GLY:CA	2.46	0.45
1:B:217:LEU:O	1:B:218:ASP:HB3	2.17	0.45
1:B:343:THR:HG22	1:B:344:GLY:N	2.31	0.45
1:A:178:THR:HG23	1:A:179:GLN:N	2.32	0.45
1:A:177:GLN:O	1:A:178:THR:O	2.34	0.45
1:A:68:LEU:HD11	1:A:402:TYR:HD2	1.81	0.45
1:B:68:LEU:HD11	1:B:402:TYR:HD2	1.82	0.44
1:A:402:TYR:HB2	1:A:404:PHE:CE1	2.51	0.44
1:B:119:GLY:H	1:B:157:ARG:NE	2.08	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:LYS:HA	1:A:270:ASN:HD22	1.80	0.44
1:A:326:ARG:HG3	1:A:348:ASP:HB3	1.98	0.44
1:B:137:ASN:ND2	1:B:139:ALA:H	2.14	0.44
1:B:178:THR:HG23	1:B:179:GLN:N	2.33	0.44
1:B:326:ARG:HG3	1:B:348:ASP:HB3	1.98	0.44
1:A:75:PRO:HD2	1:A:105:ALA:HB1	2.00	0.44
1:B:37:ILE:O	1:B:39:MET:N	2.48	0.44
1:A:15:ARG:HH11	1:A:20:GLU:CD	2.20	0.44
1:A:160:GLY:C	1:A:162:LEU:H	2.21	0.44
1:A:352:VAL:HA	1:A:353:PRO:HD3	1.84	0.44
1:A:347:PHE:HE1	1:A:365:ASP:HB3	1.83	0.44
1:A:37:ILE:O	1:A:39:MET:N	2.48	0.44
1:A:75:PRO:HD2	1:A:105:ALA:HB3	2.00	0.44
1:B:12:GLY:HA2	1:B:15:ARG:HG2	1.99	0.43
1:B:160:GLY:C	1:B:162:LEU:H	2.21	0.43
1:A:390:MET:HE1	2:A:504:C8E:H51	2.00	0.43
1:B:75:PRO:HD2	1:B:105:ALA:HB1	2.00	0.43
1:A:119:GLY:H	1:A:157:ARG:NE	2.08	0.43
1:A:353:PRO:HB2	1:A:355:GLN:NE2	2.24	0.43
1:B:75:PRO:HD2	1:B:105:ALA:HB3	2.00	0.43
1:B:218:ASP:C	1:B:220:ASN:N	2.72	0.43
1:A:102:TYR:CZ	1:A:272:PRO:HD2	2.54	0.43
1:B:15:ARG:HH11	1:B:20:GLU:CD	2.20	0.43
1:B:158:PHE:CD1	1:B:158:PHE:N	2.86	0.43
1:B:61:THR:HG22	1:B:62:SER:H	1.84	0.43
1:B:102:TYR:CZ	1:B:272:PRO:HD2	2.54	0.43
1:B:356:ASN:HA	1:B:356:ASN:HD22	1.62	0.43
1:B:140:TRP:N	1:B:140:TRP:CD1	2.87	0.42
1:B:353:PRO:C	1:B:355:GLN:N	2.72	0.42
1:B:355:GLN:NE2	1:B:356:ASN:CB	2.78	0.42
1:B:347:PHE:HE1	1:B:365:ASP:HB3	1.83	0.42
1:A:218:ASP:C	1:A:220:ASN:N	2.71	0.42
1:A:353:PRO:C	1:A:355:GLN:N	2.72	0.42
1:B:74:ALA:HA	1:B:75:PRO:HD3	1.77	0.42
1:B:84:PHE:HE1	1:B:421:PHE:CE2	2.38	0.42
1:A:140:TRP:N	1:A:140:TRP:CD1	2.87	0.42
1:A:272:PRO:HG3	1:A:298:TRP:CZ3	2.54	0.42
1:A:158:PHE:N	1:A:158:PHE:CD1	2.86	0.42
1:B:193:SER:O	1:B:195:THR:N	2.53	0.42
1:B:89:ASN:C	1:B:89:ASN:ND2	2.73	0.42
1:A:17:TYR:HB2	1:A:326:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ALA:O	1:A:190:GLY:N	2.53	0.42
1:B:272:PRO:HG3	1:B:298:TRP:CZ3	2.54	0.42
1:B:186:ALA:O	1:B:190:GLY:N	2.52	0.42
1:B:345:ILE:HA	1:B:368:TRP:O	2.20	0.42
1:A:155:ILE:O	1:A:155:ILE:HG22	2.20	0.41
1:A:359:ILE:HG21	1:A:404:PHE:CG	2.55	0.41
1:A:89:ASN:C	1:A:89:ASN:ND2	2.73	0.41
1:A:283:VAL:HG22	1:B:205:TRP:CE2	2.56	0.41
1:B:193:SER:C	1:B:195:THR:H	2.24	0.41
1:B:30:VAL:HG11	1:B:37:ILE:HG12	2.01	0.41
1:B:359:ILE:HD13	1:B:404:PHE:CE2	2.56	0.41
1:A:131:SER:CB	1:A:145:GLY:HA2	2.50	0.41
1:A:61:THR:HG22	1:A:62:SER:H	1.84	0.41
1:B:162:LEU:O	1:B:166:VAL:HG23	2.21	0.41
1:A:329:LEU:HD12	2:A:501:C8E:C19	2.40	0.41
1:A:327:ILE:CD1	2:A:501:C8E:O18	2.68	0.41
1:A:193:SER:O	1:A:195:THR:N	2.53	0.41
1:A:359:ILE:HD13	1:A:404:PHE:CE2	2.55	0.41
1:A:162:LEU:O	1:A:166:VAL:HG23	2.21	0.41
1:B:131:SER:CB	1:B:145:GLY:HA2	2.51	0.41
1:A:284:ASP:CG	1:A:285:PRO:CD	2.89	0.41
1:A:345:ILE:HA	1:A:368:TRP:O	2.20	0.41
1:A:193:SER:C	1:A:195:THR:H	2.24	0.41
1:B:284:ASP:CG	1:B:285:PRO:CD	2.89	0.41
1:B:359:ILE:HG21	1:B:404:PHE:CG	2.56	0.41
1:A:396:LYS:HE3	1:A:405:GLU:OE2	2.21	0.41
1:B:326:ARG:NH1	1:B:346:ALA:HB1	2.36	0.41
1:A:267:LEU:C	1:A:267:LEU:HD23	2.42	0.41
1:A:84:PHE:HE1	1:A:421:PHE:CE2	2.39	0.41
1:A:136:LEU:O	1:A:137:ASN:CB	2.70	0.40
1:A:30:VAL:HG11	1:A:37:ILE:HG12	2.02	0.40
1:A:74:ALA:HA	1:A:75:PRO:HD3	1.77	0.40
1:A:355:GLN:C	1:A:355:GLN:CD	2.80	0.40
1:A:73:ILE:O	1:A:107:GLU:N	2.50	0.40
1:B:354:ALA:HA	1:B:357:ARG:NE	2.37	0.40
1:B:126:MET:HE1	2:B:502:C8E:H42	2.02	0.40
1:A:162:LEU:HD23	1:A:162:LEU:HA	1.68	0.40
1:A:33:ASN:HB2	1:A:226:THR:HG21	2.04	0.40
1:B:184:LEU:O	1:B:185:ALA:C	2.60	0.40
1:B:363:ASP:C	1:B:363:ASP:OD1	2.60	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	354/419 (84%)	302 (85%)	33 (9%)	19 (5%)	2	11
1	B	354/419 (84%)	302 (85%)	34 (10%)	18 (5%)	2	12
All	All	708/838 (84%)	604 (85%)	67 (10%)	37 (5%)	2	12

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	ASP
1	A	137	ASN
1	A	178	THR
1	A	180	GLN
1	A	379	LYS
1	B	90	ASP
1	B	137	ASN
1	B	178	THR
1	B	180	GLN
1	B	194	ASN
1	B	379	LYS
1	A	72	ASN
1	A	104	LEU
1	A	160	GLY
1	A	194	ASN
1	A	218	ASP
1	A	219	LYS
1	A	283	VAL
1	A	354	ALA
1	A	378	ASN
1	B	72	ASN
1	B	104	LEU
1	B	160	GLY
1	B	218	ASP
1	B	219	LYS

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Mol	Chain	Res	Type
1	B	283	VAL
1	B	354	ALA
1	B	378	ASN
1	A	38	THR
1	A	115	GLY
1	A	177	GLN
1	B	38	THR
1	B	115	GLY
1	B	177	GLN
1	A	364	GLN
1	A	118	GLY
1	B	118	GLY

### 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	281/329 (85%)	248 (88%)	33 (12%)	5	22
1	B	281/329 (85%)	248 (88%)	33 (12%)	5	22
All	All	562/658 (85%)	496 (88%)	66 (12%)	5	22

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ILE
1	A	42	ARG
1	A	61	THR
1	A	69	LYS
1	A	72	ASN
1	A	78	TRP
1	A	89	ASN
1	A	104	LEU
1	A	106	THR
1	A	122	ASP
1	A	137	ASN

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Mol	Chain	Res	Type
1	A	142	PHE
1	A	171	MET
1	A	177	GLN
1	A	179	GLN
1	A	219	LYS
1	A	229	SER
1	A	275	TRP
1	A	278	SER
1	A	282	ARG
1	A	290	HIS
1	A	322	LYS
1	A	327	ILE
1	A	331	THR
1	A	338	ASN
1	A	356	ASN
1	A	366	ARG
1	A	373	THR
1	A	391	HIS
1	A	404	PHE
1	A	407	GLU
1	A	416	ASN
1	A	418	ASN
1	B	23	ILE
1	B	42	ARG
1	B	61	THR
1	B	69	LYS
1	B	72	ASN
1	B	78	TRP
1	B	89	ASN
1	B	104	LEU
1	B	106	THR
1	B	122	ASP
1	B	137	ASN
1	B	142	PHE
1	B	171	MET
1	B	177	GLN
1	B	179	GLN
1	B	219	LYS
1	B	229	SER
1	B	275	TRP
1	B	278	SER
1	B	282	ARG

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Mol	Chain	Res	Type
1	B	290	HIS
1	B	322	LYS
1	B	327	ILE
1	B	331	THR
1	B	338	ASN
1	B	356	ASN
1	B	366	ARG
1	B	373	THR
1	B	391	HIS
1	B	404	PHE
1	B	407	GLU
1	B	416	ASN
1	B	418	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	72	ASN
1	A	89	ASN
1	A	137	ASN
1	A	164	GLN
1	A	172	GLN
1	A	179	GLN
1	A	182	GLN
1	A	189	ASN
1	A	199	HIS
1	A	270	ASN
1	A	281	ASN
1	A	290	HIS
1	A	338	ASN
1	A	355	GLN
1	A	356	ASN
1	A	364	GLN
1	A	403	GLN
1	B	57	ASN
1	B	72	ASN
1	B	89	ASN
1	B	137	ASN
1	B	164	GLN
1	B	172	GLN
1	B	182	GLN

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Mol	Chain	Res	Type
1	B	189	ASN
1	B	199	HIS
1	B	270	ASN
1	B	281	ASN
1	B	290	HIS
1	B	338	ASN
1	B	355	GLN
1	B	356	ASN
1	B	364	GLN
1	B	403	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 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	C8E	A	504	-	20,20,20	1.27	2 (10%)	19,19,19	2.27	7 (36%)
2	C8E	B	502	-	20,20,20	0.91	0	19,19,19	2.00	6 (31%)
2	C8E	B	503	-	20,20,20	0.75	0	19,19,19	1.96	6 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	C8E	A	501	-	20,20,20	0.92	0	19,19,19	2.19	6 (31%)

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	C8E	A	504	-	-	10/18/18/18	-
2	C8E	B	502	-	-	8/18/18/18	-
2	C8E	B	503	-	-	7/18/18/18	-
2	C8E	A	501	-	-	11/18/18/18	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	504	C8E	C19-C20	2.98	1.65	1.49
2	A	504	C8E	O18-C19	2.11	1.51	1.42

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	C8E	O15-C14-C13	4.81	132.07	110.39
2	A	504	C8E	O15-C14-C13	4.79	131.97	110.39
2	B	502	C8E	O15-C14-C13	4.57	131.00	110.39
2	B	503	C8E	O15-C14-C13	4.40	130.23	110.39
2	A	501	C8E	O12-C13-C14	4.07	128.76	110.39
2	A	504	C8E	O12-C13-C14	4.06	128.71	110.39
2	B	502	C8E	O12-C13-C14	3.68	126.98	110.39
2	A	504	C8E	O9-C8-C7	3.60	129.21	110.26
2	B	503	C8E	O12-C13-C14	3.31	125.33	110.39
2	A	501	C8E	O9-C8-C7	3.31	127.64	110.26
2	B	503	C8E	O18-C19-C20	3.29	124.51	110.07
2	A	501	C8E	O18-C19-C20	3.14	123.86	110.07
2	A	504	C8E	C7-C6-C5	-3.13	98.51	114.42
2	B	502	C8E	O9-C8-C7	3.08	126.46	110.26
2	B	503	C8E	O9-C8-C7	3.04	126.23	110.26
2	B	502	C8E	O18-C19-C20	2.95	123.02	110.07
2	A	504	C8E	O18-C19-C20	2.91	122.86	110.07
2	A	501	C8E	C7-C6-C5	-2.85	99.94	114.42
2	B	503	C8E	C7-C6-C5	-2.80	100.20	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	C8E	O18-C17-C16	2.79	122.96	110.39
2	B	502	C8E	C7-C6-C5	-2.79	100.28	114.42
2	A	501	C8E	O18-C17-C16	2.75	122.81	110.39
2	A	504	C8E	O18-C17-C16	2.67	122.45	110.39
2	B	503	C8E	O18-C17-C16	2.41	121.25	110.39
2	A	504	C8E	C13-O12-C11	2.11	122.44	113.29

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	504	C8E	C10-C11-O12-C13
2	A	504	C8E	C14-C13-O12-C11
2	A	504	C8E	O12-C13-C14-O15
2	B	502	C8E	O9-C10-C11-O12
2	A	501	C8E	C14-C13-O12-C11
2	B	503	C8E	O15-C16-C17-O18
2	B	502	C8E	C6-C7-C8-O9
2	A	501	C8E	O9-C10-C11-O12
2	A	504	C8E	O18-C19-C20-O21
2	B	503	C8E	O9-C10-C11-O12
2	B	503	C8E	C3-C4-C5-C6
2	A	501	C8E	C2-C3-C4-C5
2	B	502	C8E	C4-C5-C6-C7
2	A	501	C8E	C3-C4-C5-C6
2	B	502	C8E	O18-C19-C20-O21
2	A	504	C8E	C3-C4-C5-C6
2	B	503	C8E	C2-C3-C4-C5
2	B	503	C8E	C5-C6-C7-C8
2	A	501	C8E	O18-C19-C20-O21
2	A	501	C8E	C5-C6-C7-C8
2	A	501	C8E	C10-C11-O12-C13
2	A	501	C8E	O12-C13-C14-O15
2	A	501	C8E	C1-C2-C3-C4
2	A	501	C8E	C4-C5-C6-C7
2	A	504	C8E	C20-C19-O18-C17
2	B	502	C8E	C7-C8-O9-C10
2	A	501	C8E	C7-C8-O9-C10
2	B	503	C8E	C7-C8-O9-C10
2	A	504	C8E	C5-C6-C7-C8
2	A	504	C8E	C7-C8-O9-C10
2	B	502	C8E	C5-C6-C7-C8

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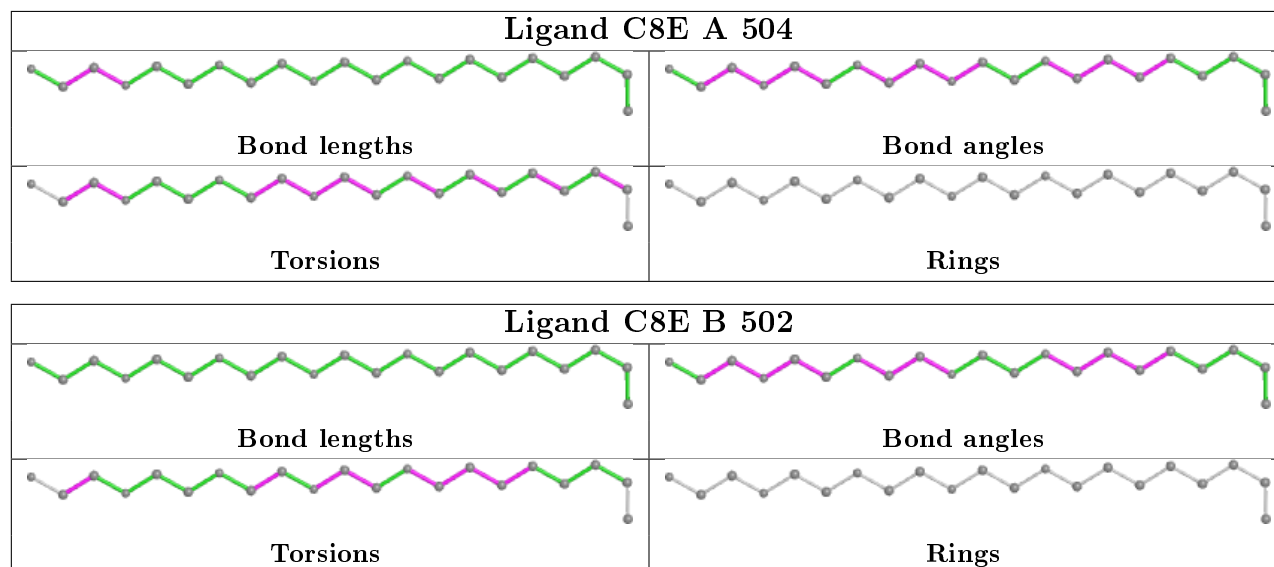
Mol	Chain	Res	Type	Atoms
2	B	502	C8E	O12-C13-C14-O15
2	A	504	C8E	C1-C2-C3-C4
2	B	502	C8E	C10-C11-O12-C13
2	A	504	C8E	O9-C10-C11-O12
2	B	503	C8E	O12-C13-C14-O15

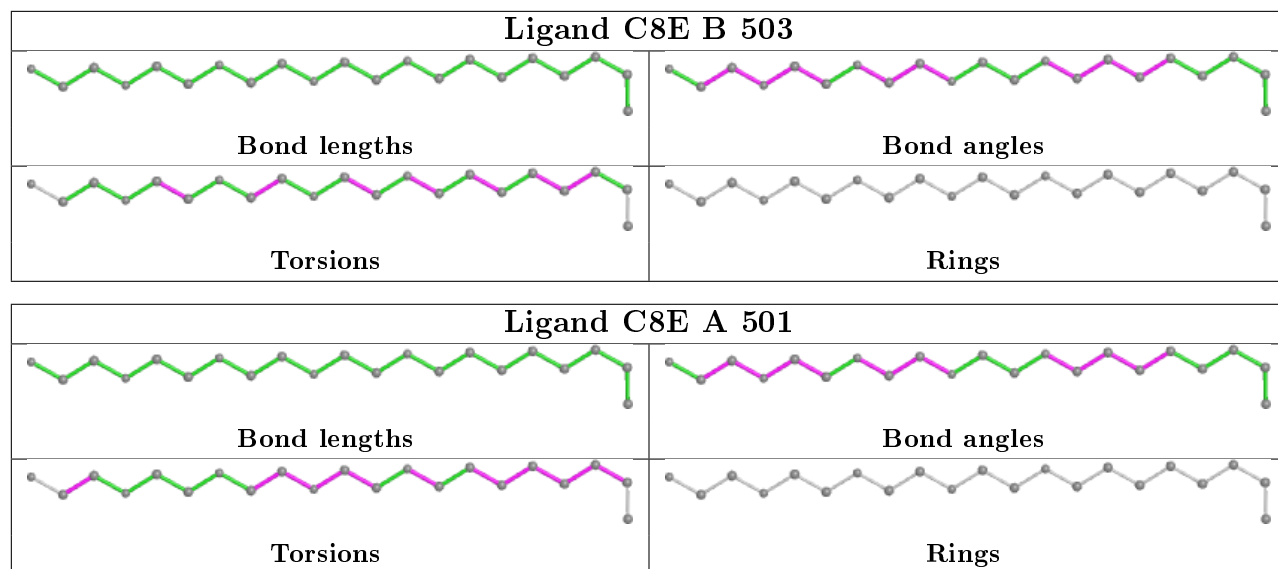
There are no ring outliers.

4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	504	C8E	6	0
2	B	502	C8E	5	0
2	B	503	C8E	3	0
2	A	501	C8E	7	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	360/419 (85%)	-0.25	1 (0%) 94 84	25, 43, 75, 86	0
1	B	360/419 (85%)	-0.25	3 (0%) 86 65	24, 43, 74, 86	0
All	All	720/838 (85%)	-0.25	4 (0%) 89 72	24, 43, 75, 86	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	180	GLN	3.5
1	B	180	GLN	2.6
1	B	102	TYR	2.3
1	B	298	TRP	2.2

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	C8E	B	502	21/21	0.72	0.50	61,66,75,75	0

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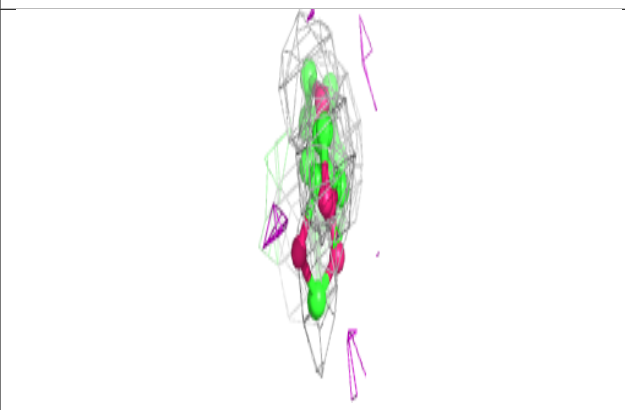
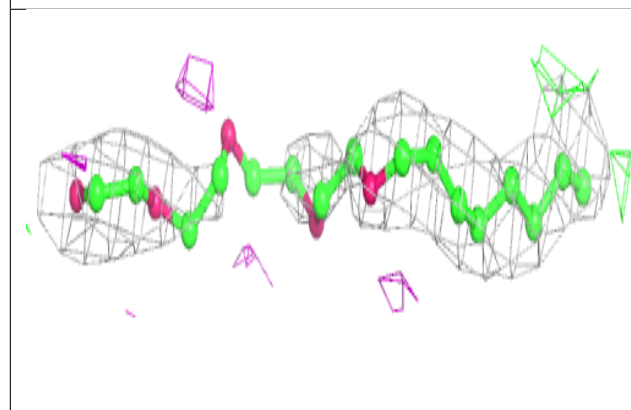
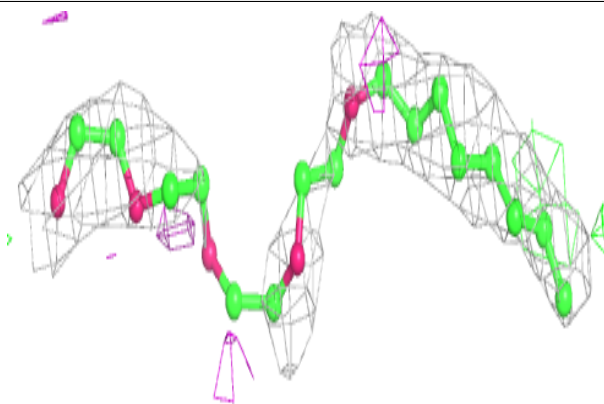
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	C8E	B	503	21/21	0.79	0.56	64,76,90,91	0
2	C8E	A	501	21/21	0.80	0.81	76,89,91,91	0
2	C8E	A	504	21/21	0.81	0.59	67,74,83,84	0

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.

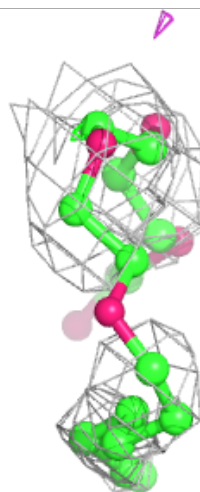
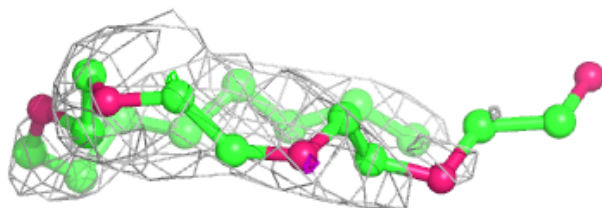
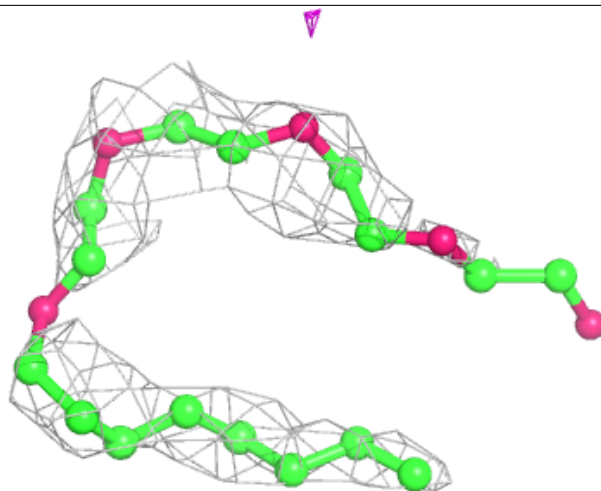
**Electron density around C8E B 502:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



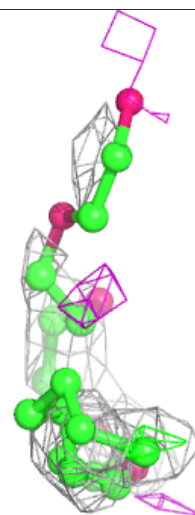
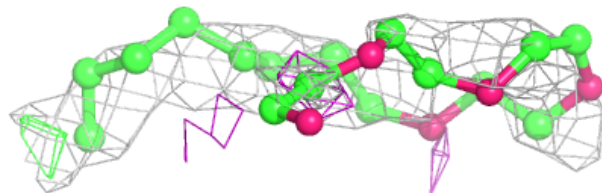
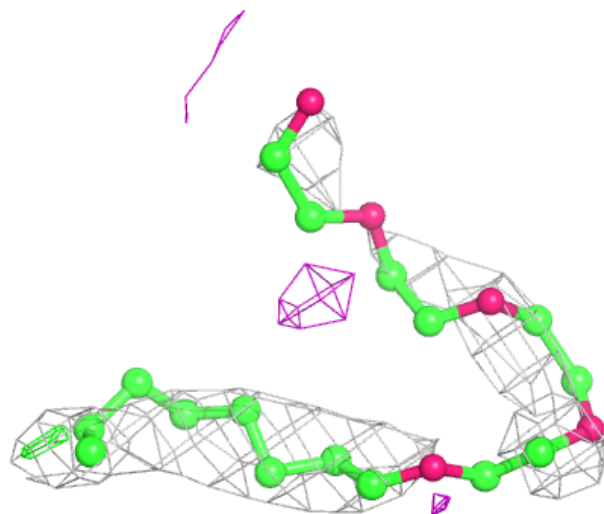
**Electron density around C8E B 503:**

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



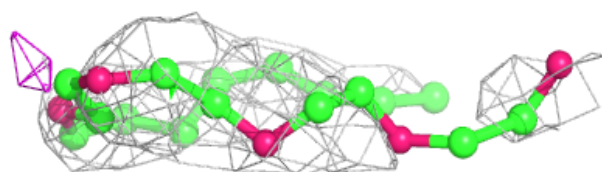
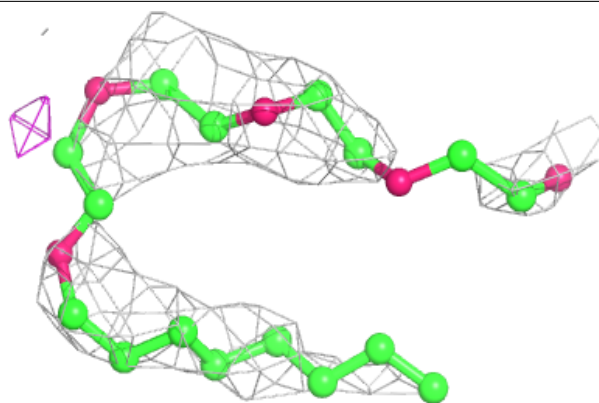
**Electron density around C8E A 501:**

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



**Electron density around C8E 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.