

# Full wwPDB X-ray Structure Validation Report (i)

Dec 9, 2023 - 08:14 am GMT

PDB ID : 8CL8

Title: Krokinobacter eikastus rhodopsin 2 (KR2) extrapolated map 1 us after light

activation

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Deposited on : 2023-02-16

Resolution : 2.40 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.orgA user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity: 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

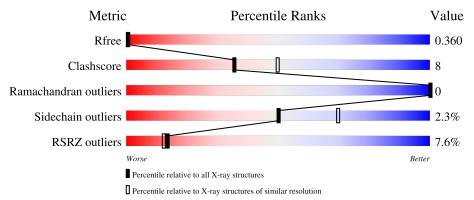
Validation Pipeline (wwPDB-VP) : 2.36

## 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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	Similar resolution
Metric	$(\#  ext{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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		
			8%		_
1	A	264	80%	19%	•

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LFA	A	302	-	-	-	X





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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LFA	A	307	-	-	-	X
2	LFA	A	308	-	-	-	X
2	LFA	A	309	-	-	-	X
2	LFA	A	311	-	-	-	X
2	LFA	A	312	-	-	-	X
2	LFA	A	313	-	-	-	X
2	LFA	A	314	-	-	-	X
2	LFA	A	316	-	-	-	X
2	LFA	A	319	-	-	-	X
2	LFA	A	320	-	-	-	X
2	LFA	A	322	-	-	-	X
2	LFA	A	324	-	-	-	X



# 2 Entry composition (i)

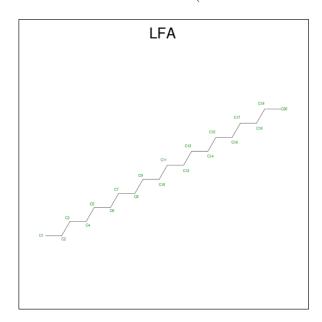
There are 4 unique types of molecules in this entry. The entry contains 2448 atoms, of which 55 are hydrogens and 0 are deuteriums.

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 Sodium pumping rhodopsin.

Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	Trace
1	Λ	264	Total	С	N	О	S	0	2	0
1	Λ	204	2095	1399	318	369	9	0	3	

• Molecule 2 is EICOSANE (three-letter code: LFA) (formula:  $C_{20}H_{42}$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 16 16	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 6 6	0	0
2	A	1	Total C 6 6	0	0
2	A	1	Total C 13 13	0	0

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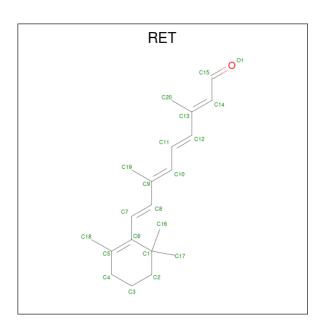


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Mol	Chain	$oxed{ \mathbf{Residues} }$	Atoms	ZeroOcc	AltConf
2	A	1	Total C 10 10	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C 11 11	0	0
2	A	1	Total C 5 5	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C 5 5	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C 9 9	0	0
2	A	1	Total C 9 9	0	0
2	A	1	Total C 6 6	0	0
2	A	1	Total C 5 5	0	0
2	A	1	Total C 4 4	0	0
2	A	1	Total C 6 6	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C 3 3	0	0
2	A	1	Total C 9 9	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C H 40 13 27	0	0

• Molecule 3 is RETINAL (three-letter code: RET) (formula:  $C_{20}H_{28}O$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	$\mathbf{At}$	oms		ZeroOcc	AltConf
3	A	1	Total 48	C 20	H 28	0	0

### • Molecule 4 is water.

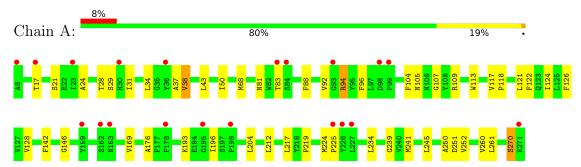
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	62	Total O 62 62	0	0



# 3 Residue-property plots (i)

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

• Molecule 1: Sodium pumping rhodopsin





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants	41.46Å 84.89Å 234.95Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.83 - 2.40	Depositor
resolution (A)	14.83 - 2.40	EDS
% Data completeness	94.0 (14.83-2.40)	Depositor
(in resolution range)	94.0 (14.83-2.40)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	0.88  (at  2.39Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
$R, R_{free}$	0.327 , $0.358$	Depositor
It, It free	0.327 , $0.360$	DCC
$R_{free}$ test set	780 reflections $(4.96\%)$	wwPDB-VP
Wilson B-factor $(\mathring{A}^2)$	28.9	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.33, 93.6	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.54, < L^2>=0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	2448	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.37% of the height of the origin peak. No significant pseudotranslation is detected.

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



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: LFA, RET

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).

Mal	Chain	Bo	nd lengths	Bond	angles
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z >5
1	A	0.40	$1/2159 \ (0.0\%)$	0.52	0/2940

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 maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

### All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	Observed(A)	Ideal(A)
1	A	270	SER	CA-CB	-5.59	1.44	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	94	ARG	Sidechain

## 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	2095	0	2065	33	1
2	A	216	27	389	13	1
3	A	20	28	27	4	0
4	A	62	0	0	0	0
All	All	2393	55	2481	39	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (39) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1         Atom-2         distance (Å)         overlap (Å)           2:A:305:LFA:H13         2:A:305:LFA:H51         1.71         0.72           1:A:34:LEU:O         1:A:38:VAL:HG13         1.93         0.67           2:A:320:LFA:H42         2:A:320:LFA:H82         1.83         0.60           3:A:326:RET:H161         3:A:326:RET:C8         2.34         0.57           3:A:326:RET:H161         3:A:326:RET:H8         1.86         0.56           1:A:RSN:HD21         1:A:105:ASN:H         1.58         0.52           1:A:81:ASN:ND2         1:A:105:ASN:H         2.07         0.52           1:A:117:VAL:N         1:A:118:PRO:HD2         2.24         0.52           1:A:212:LEU:HD22         2:A:322:LFA:H31         1.91         0.52           1:A:21:SER:HB3         1:A:94:ARG:NH2         2.27         0.50           1:A:21:SER:HB3         1:A:94:ARG:NH2         2.27         0.50           1:A:21:SER:HB3         1:A:494:ARG:NH2         2.27         0.50           1:A:215:EPH:HG11         2:A:304:LFA:H51         1.94         0.48           1:A:17:THR:HG22         2:A:325:LFA:H171         1.95         0.47           1:A:24:ALA:HA         1:A:124:HEH:HS1         1.80         0.46	Atom-1	Atom-2	Interatomic	Clash
1:A:34:LEU:O       1:A:38:VAL:HG13       1.93       0.67         2:A:320:LFA:H42       2:A:320:LFA:H82       1.83       0.60         3:A:326:RET:H161       3:A:326:RET:C8       2.34       0.57         3:A:326:RET:H161       3:A:326:RET:H8       1.86       0.56         1:A:81:ASN:HD21       1:A:105:ASN:H       1.58       0.52         1:A:81:ASN:ND2       1:A:105:ASN:H       2.07       0.52         1:A:117:VAL:N       1:A:118:PRO:HD2       2.24       0.52         1:A:212:LEU:HD22       2:A:322:LFA:H31       1.91       0.52         1:A:21:SER:HB3       1:A:94:ARG:NH2       2.27       0.50         1:A:25:VAL:HG11       2:A:304:LFA:H51       1.94       0.48         1:A:17:THR:HG22       2:A:325:LFA:H171       1.95       0.47         1:A:24:ALA:HA       1:A:241:MET:SD       2.55       0.46         1:A:126:PHE:HE1       2:A:315:LFA:H51       1.80       0.46         1:A:117:VAL:HG11       1:A:104:PHE:HA       1.81       0.46         1:A:117:VAL:HG11       1:A:146:GLY:HA3       1.98       0.45         1:A:28:VAL:HG11       1:A:296:PHE:HZ       1.82       0.45         1:A:128:VAL:HG11       1:A:296:PHE:HZ       1.82       0.45	Atom-1	Atom-2	${\rm distance}(\mathring{\rm A})$	overlap (Å)
2:A:320:LFA:H42       2:A:320:LFA:H82       1.83       0.60         3:A:326:RET:H161       3:A:326:RET:C8       2.34       0.57         3:A:326:RET:H161       3:A:326:RET:H8       1.86       0.56         1:A:81:ASN:HD21       1:A:105:ASN:H       1.58       0.52         1:A:81:ASN:ND2       1:A:105:ASN:H       2.07       0.52         1:A:117:VAL:N       1:A:118:PRO:HD2       2.24       0.52         1:A:212:LEU:HD22       2:A:322:LFA:H31       1.91       0.52         1:A:21:SER:HB3       1:A:94:ARG:NH2       2.27       0.50         1:A:25:VAL:HG11       2:A:304:LFA:H51       1.94       0.48         1:A:17:THR:HG22       2:A:325:LFA:H171       1.95       0.47         1:A:24:ALA:HA       1:A:241:MET:SD       2.55       0.46         1:A:126:PHE:HE1       2:A:315:LFA:H51       1.80       0.46         1:A:117:VAL:HG11       1:A:104:PHE:HA       1.81       0.46         1:A:117:VAL:HG11       1:A:146:GLY:HA3       1.98       0.46         1:A:128:VAL:HG11       1:A:204:LEU:HD21       1.98       0.45         1:A:29:VAL:HG11       1:A:290:PHE:HZ       1.82       0.45         1:A:217:LEU:HB2       1:A:250:ALA:HB2       1.99       0.45<	2:A:305:LFA:H13	2:A:305:LFA:H51	1.71	0.72
3:A:326:RET:H161       3:A:326:RET:C8       2.34       0.57         3:A:326:RET:H161       3:A:326:RET:H8       1.86       0.56         1:A:81:ASN:HD21       1:A:105:ASN:H       1.58       0.52         1:A:81:ASN:ND2       1:A:105:ASN:H       2.07       0.52         1:A:117:VAL:N       1:A:118:PRO:HD2       2.24       0.52         1:A:212:LEU:HD22       2:A:322:LFA:H31       1.91       0.52         1:A:21:SER:HB3       1:A:94:ARG:NH2       2.27       0.50         1:A:21:SER:HB3       1:A:94:ARG:NH2       2.27       0.50         1:A:252:VAL:HG11       2:A:304:LFA:H51       1.94       0.48         1:A:17:THR:HG22       2:A:325:LFA:H171       1.95       0.47         1:A:24:ALA:HA       1:A:241:MET:SD       2.55       0.46         1:A:126:PHE:HE1       2:A:315:LFA:H51       1.80       0.46         1:A:117:VAL:HG11       1:A:104:PHE:HA       1.81       0.46         1:A:113:TRP:O       1:A:117:VAL:HG23       2.15       0.45         1:A:128:VAL:HG11       1:A:204:LEU:HD21       1.98       0.45         1:A:118:PRO:O       1:A:122:PHE:HB2       2.17       0.45         1:A:224:MET:N       1:A:225:PRO:HD2       2.32       0.44	1:A:34:LEU:O	1:A:38:VAL:HG13	1.93	0.67
3:A:326:RET:H161       3:A:326:RET:H8       1.86       0.56         1:A:81:ASN:HD21       1:A:105:ASN:H       1.58       0.52         1:A:81:ASN:ND2       1:A:105:ASN:H       2.07       0.52         1:A:117:VAL:N       1:A:118:PRO:HD2       2.24       0.52         1:A:21:SER:HB3       1:A:494:ARG:NH2       2.27       0.50         1:A:252:VAL:HG11       2:A:304:LFA:H51       1.94       0.48         1:A:17:THR:HG22       2:A:325:LFA:H171       1.95       0.47         1:A:24:ALA:HA       1:A:241:MET:SD       2.55       0.46         1:A:126:PHE:HE1       2:A:315:LFA:H51       1.80       0.46         1:A:117:VAL:HG11       1:A:104:PHE:HA       1.81       0.46         1:A:117:VAL:HG11       1:A:146:GLY:HA3       1.98       0.46         1:A:113:TRP:O       1:A:117:VAL:HG23       2.15       0.45         1:A:128:VAL:HG11       1:A:204:LEU:HD21       1.98       0.45         1:A:18:PRO:O       1:A:122:PHE:HB2       1.7       0.45         1:A:217:LEU:HB2       1:A:250:ALA:HB2       1.99       0.45         1:A:224:MET:N       1:A:225:PRO:HD2       2.32       0.44         1:A:37:ALA:HB1       2:A:312:LFA:H51       1.99       0.44	2:A:320:LFA:H42	2:A:320:LFA:H82	1.83	0.60
1:A:81:ASN:HD21       1:A:105:ASN:H       1.58       0.52         1:A:81:ASN:ND2       1:A:105:ASN:H       2.07       0.52         1:A:117:VAL:N       1:A:118:PRO:HD2       2.24       0.52         1:A:212:LEU:HD22       2:A:322:LFA:H31       1.91       0.52         1:A:21:SER:HB3       1:A:94:ARG:NH2       2.27       0.50         1:A:252:VAL:HG11       2:A:304:LFA:H51       1.94       0.48         1:A:17:THR:HG22       2:A:325:LFA:H171       1.95       0.47         1:A:24:ALA:HA       1:A:241:MET:SD       2.55       0.46         1:A:126:PHE:HE1       2:A:315:LFA:H51       1.80       0.46         1:A:17:VAL:HG11       1:A:104:PHE:HA       1.81       0.46         1:A:117:VAL:HG11       1:A:146:GLY:HA3       1.98       0.46         1:A:113:TRP:O       1:A:117:VAL:HG23       2.15       0.45         1:A:128:VAL:HG11       1:A:204:LEU:HD21       1.98       0.45         1:A:19:VAL:HG11       1:A:26:PHE:HZ       1.82       0.45         1:A:118:PRO:O       1:A:122:PHE:HB2       2.17       0.45         1:A:217:LEU:HB2       1:A:250:ALA:HB2       1.98       0.45         1:A:224:MET:N       1:A:225:PRO:HD2       2.32       0.44	3:A:326:RET:H161	3:A:326:RET:C8	2.34	0.57
1:A:81:ASN:ND2       1:A:105:ASN:H       2.07       0.52         1:A:117:VAL:N       1:A:118:PRO:HD2       2.24       0.52         1:A:212:LEU:HD22       2:A:322:LFA:H31       1.91       0.52         1:A:21:SER:HB3       1:A:94:ARG:NH2       2.27       0.50         1:A:252:VAL:HG11       2:A:304:LFA:H51       1.94       0.48         1:A:17:THR:HG22       2:A:325:LFA:H171       1.95       0.47         1:A:24:ALA:HA       1:A:241:MET:SD       2.55       0.46         1:A:126:PHE:HE1       2:A:315:LFA:H51       1.80       0.46         1:A:16:PHE:HE1       2:A:315:LFA:H51       1.80       0.46         1:A:17:VAL:HG11       1:A:104:PHE:HA       1.81       0.46         1:A:113:TRP:O       1:A:117:VAL:HG23       2.15       0.45         1:A:128:VAL:HG11       1:A:204:LEU:HD21       1.98       0.45         1:A:19:2:VAL:HG11       1:A:96:PHE:HZ       1.82       0.45         1:A:217:LEU:HB2       1:A:250:ALA:HB2       1.98       0.45         1:A:224:MET:N       1:A:250:ALA:HB2       1.99       0.45         1:A:224:MET:N       1:A:225:PRO:HD2       2.32       0.44         1:A:37:ALA:HB1       2:A:305:LFA:H81       2.00       0.44	3:A:326:RET:H161	3:A:326:RET:H8	1.86	0.56
1:A:117:VAL:N       1:A:118:PRO:HD2       2.24       0.52         1:A:212:LEU:HD22       2:A:322:LFA:H31       1.91       0.52         1:A:21:SER:HB3       1:A:94:ARG:NH2       2.27       0.50         1:A:252:VAL:HG11       2:A:304:LFA:H51       1.94       0.48         1:A:17:THR:HG22       2:A:325:LFA:H171       1.95       0.47         1:A:24:ALA:HA       1:A:241:MET:SD       2.55       0.46         1:A:126:PHE:HE1       2:A:315:LFA:H51       1.80       0.46         1:A:81:ASN:HD21       1:A:104:PHE:HA       1.81       0.46         1:A:117:VAL:HG11       1:A:146:GLY:HA3       1.98       0.46         1:A:113:TRP:O       1:A:117:VAL:HG23       2.15       0.45         1:A:128:VAL:HG11       1:A:204:LEU:HD21       1.98       0.45         1:A:92:VAL:HG11       1:A:96:PHE:HZ       1.82       0.45         1:A:118:PRO:O       1:A:122:PHE:HB2       2.17       0.45         1:A:217:LEU:HB2       1:A:250:ALA:HB2       1.98       0.45         1:A:224:MET:N       1:A:225:PRO:HD2       2.32       0.44         1:A:37:ALA:HB1       2:A:312:LFA:H51       1.99       0.44         1:A:107:GLY:HA3       2:A:305:LFA:H81       2.00       0.44 <td>1:A:81:ASN:HD21</td> <td>1:A:105:ASN:H</td> <td>1.58</td> <td>0.52</td>	1:A:81:ASN:HD21	1:A:105:ASN:H	1.58	0.52
1:A:212:LEU:HD22       2:A:322:LFA:H31       1.91       0.52         1:A:21:SER:HB3       1:A:94:ARG:NH2       2.27       0.50         1:A:252:VAL:HG11       2:A:304:LFA:H51       1.94       0.48         1:A:17:THR:HG22       2:A:325:LFA:H171       1.95       0.47         1:A:24:ALA:HA       1:A:241:MET:SD       2.55       0.46         1:A:126:PHE:HE1       2:A:315:LFA:H51       1.80       0.46         1:A:81:ASN:HD21       1:A:104:PHE:HA       1.81       0.46         1:A:117:VAL:HG11       1:A:146:GLY:HA3       1.98       0.46         1:A:113:TRP:O       1:A:117:VAL:HG23       2.15       0.45         1:A:128:VAL:HG11       1:A:204:LEU:HD21       1.98       0.45         1:A:92:VAL:HG11       1:A:96:PHE:HZ       1.82       0.45         1:A:118:PRO:O       1:A:122:PHE:HB2       2.17       0.45         1:A:217:LEU:HB2       1:A:250:ALA:HB2       1.98       0.45         1:A:224:MET:N       1:A:225:PRO:HD2       2.32       0.44         1:A:37:ALA:HB1       2:A:312:LFA:H51       1.99       0.44         1:A:107:GLY:HA3       2:A:305:LFA:H81       2.00       0.44         1:A:234:LEU:O       1:A:239:GLY:HA3       2.19       0.43 <td>1:A:81:ASN:ND2</td> <td>1:A:105:ASN:H</td> <td>2.07</td> <td>0.52</td>	1:A:81:ASN:ND2	1:A:105:ASN:H	2.07	0.52
1:A:21:SER:HB3       1:A:94:ARG:NH2       2.27       0.50         1:A:252:VAL:HG11       2:A:304:LFA:H51       1.94       0.48         1:A:17:THR:HG22       2:A:325:LFA:H171       1.95       0.47         1:A:24:ALA:HA       1:A:241:MET:SD       2.55       0.46         1:A:126:PHE:HE1       2:A:315:LFA:H51       1.80       0.46         1:A:81:ASN:HD21       1:A:104:PHE:HA       1.81       0.46         1:A:117:VAL:HG11       1:A:146:GLY:HA3       1.98       0.46         1:A:113:TRP:O       1:A:117:VAL:HG23       2.15       0.45         1:A:128:VAL:HG11       1:A:204:LEU:HD21       1.98       0.45         1:A:92:VAL:HG11       1:A:96:PHE:HZ       1.82       0.45         1:A:118:PRO:O       1:A:122:PHE:HB2       2.17       0.45         1:A:217:LEU:HB2       1:A:250:ALA:HB2       1.98       0.45         1:A:224:MET:N       1:A:225:PRO:HD2       2.32       0.44         1:A:37:ALA:HB1       2:A:312:LFA:H51       1.99       0.44         1:A:107:GLY:HA3       2:A:305:LFA:H81       2.00       0.44         1:A:234:LEU:O       1:A:239:GLY:HA3       2.19       0.43         1:A:121:LE:HG12       1:A:124:ILE:HG22       2.19       0.41 <td>1:A:117:VAL:N</td> <td>1:A:118:PRO:HD2</td> <td>2.24</td> <td>0.52</td>	1:A:117:VAL:N	1:A:118:PRO:HD2	2.24	0.52
1:A:252:VAL:HG11       2:A:304:LFA:H51       1.94       0.48         1:A:17:THR:HG22       2:A:325:LFA:H171       1.95       0.47         1:A:24:ALA:HA       1:A:241:MET:SD       2.55       0.46         1:A:126:PHE:HE1       2:A:315:LFA:H51       1.80       0.46         1:A:81:ASN:HD21       1:A:104:PHE:HA       1.81       0.46         1:A:117:VAL:HG11       1:A:146:GLY:HA3       1.98       0.46         1:A:113:TRP:O       1:A:117:VAL:HG23       2.15       0.45         1:A:128:VAL:HG11       1:A:204:LEU:HD21       1.98       0.45         1:A:92:VAL:HG11       1:A:96:PHE:HZ       1.82       0.45         1:A:118:PRO:O       1:A:122:PHE:HB2       2.17       0.45         1:A:217:LEU:HB2       1:A:250:ALA:HB2       1.98       0.45         1:A:261:LEU:HD21       2:A:320:LFA:H62       1.99       0.45         1:A:224:MET:N       1:A:225:PRO:HD2       2.32       0.44         1:A:37:ALA:HB1       2:A:312:LFA:H51       1.99       0.44         1:A:107:GLY:HA3       2:A:305:LFA:H81       2.00       0.44         1:A:234:LEU:O       1:A:239:GLY:HA3       2.19       0.43         1:A:31:ILE:HG12       1:A:124:ILE:HG22       2.19       0.41	1:A:212:LEU:HD22	2:A:322:LFA:H31	1.91	0.52
1:A:17:THR:HG22       2:A:325:LFA:H171       1.95       0.47         1:A:24:ALA:HA       1:A:241:MET:SD       2.55       0.46         1:A:126:PHE:HE1       2:A:315:LFA:H51       1.80       0.46         1:A:81:ASN:HD21       1:A:104:PHE:HA       1.81       0.46         1:A:117:VAL:HG11       1:A:146:GLY:HA3       1.98       0.46         1:A:113:TRP:O       1:A:117:VAL:HG23       2.15       0.45         1:A:128:VAL:HG11       1:A:204:LEU:HD21       1.98       0.45         1:A:92:VAL:HG11       1:A:96:PHE:HZ       1.82       0.45         1:A:118:PRO:O       1:A:122:PHE:HB2       2.17       0.45         1:A:217:LEU:HB2       1:A:250:ALA:HB2       1.98       0.45         1:A:261:LEU:HD21       2:A:320:LFA:H62       1.99       0.45         1:A:224:MET:N       1:A:225:PRO:HD2       2.32       0.44         1:A:37:ALA:HB1       2:A:312:LFA:H51       1.99       0.44         1:A:107:GLY:HA3       2:A:305:LFA:H81       2.00       0.44         3:A:326:RET:H7       3:A:326:RET:H181       1.87       0.44         1:A:234:LEU:O       1:A:245:LEU:HD23       2.01       0.42         1:A:121:LEU:O       1:A:124:ILE:HG22       2.19       0.41 </td <td>1:A:21:SER:HB3</td> <td>1:A:94:ARG:NH2</td> <td>2.27</td> <td>0.50</td>	1:A:21:SER:HB3	1:A:94:ARG:NH2	2.27	0.50
1:A:24:ALA:HA       1:A:241:MET:SD       2.55       0.46         1:A:126:PHE:HE1       2:A:315:LFA:H51       1.80       0.46         1:A:81:ASN:HD21       1:A:104:PHE:HA       1.81       0.46         1:A:117:VAL:HG11       1:A:146:GLY:HA3       1.98       0.46         1:A:113:TRP:O       1:A:117:VAL:HG23       2.15       0.45         1:A:128:VAL:HG11       1:A:204:LEU:HD21       1.98       0.45         1:A:92:VAL:HG11       1:A:96:PHE:HZ       1.82       0.45         1:A:118:PRO:O       1:A:122:PHE:HB2       2.17       0.45         1:A:217:LEU:HB2       1:A:250:ALA:HB2       1.98       0.45         1:A:261:LEU:HD21       2:A:320:LFA:H62       1.99       0.45         1:A:224:MET:N       1:A:225:PRO:HD2       2.32       0.44         1:A:37:ALA:HB1       2:A:312:LFA:H51       1.99       0.44         1:A:107:GLY:HA3       2:A:305:LFA:H81       2.00       0.44         3:A:326:RET:H7       3:A:326:RET:H181       1.87       0.44         1:A:234:LEU:O       1:A:245:LEU:HD23       2.01       0.42         1:A:121:LEU:O       1:A:124:ILE:HG22       2.19       0.41	1:A:252:VAL:HG11	2:A:304:LFA:H51	1.94	0.48
1:A:126:PHE:HE1       2:A:315:LFA:H51       1.80       0.46         1:A:81:ASN:HD21       1:A:104:PHE:HA       1.81       0.46         1:A:117:VAL:HG11       1:A:146:GLY:HA3       1.98       0.46         1:A:113:TRP:O       1:A:117:VAL:HG23       2.15       0.45         1:A:128:VAL:HG11       1:A:204:LEU:HD21       1.98       0.45         1:A:92:VAL:HG11       1:A:96:PHE:HZ       1.82       0.45         1:A:118:PRO:O       1:A:122:PHE:HB2       2.17       0.45         1:A:217:LEU:HB2       1:A:250:ALA:HB2       1.98       0.45         1:A:261:LEU:HD21       2:A:320:LFA:H62       1.99       0.45         1:A:224:MET:N       1:A:225:PRO:HD2       2.32       0.44         1:A:37:ALA:HB1       2:A:312:LFA:H51       1.99       0.44         1:A:107:GLY:HA3       2:A:305:LFA:H81       2.00       0.44         3:A:326:RET:H7       3:A:326:RET:H181       1.87       0.44         1:A:234:LEU:O       1:A:239:GLY:HA3       2.19       0.43         1:A:121:LEU:O       1:A:124:ILE:HG22       2.19       0.41	1:A:17:THR:HG22	2:A:325:LFA:H171	1.95	0.47
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1:A:128:VAL:HG11       1:A:204:LEU:HD21       1.98       0.45         1:A:92:VAL:HG11       1:A:96:PHE:HZ       1.82       0.45         1:A:118:PRO:O       1:A:122:PHE:HB2       2.17       0.45         1:A:217:LEU:HB2       1:A:250:ALA:HB2       1.98       0.45         1:A:261:LEU:HD21       2:A:320:LFA:H62       1.99       0.45         1:A:224:MET:N       1:A:225:PRO:HD2       2.32       0.44         1:A:37:ALA:HB1       2:A:312:LFA:H51       1.99       0.44         1:A:107:GLY:HA3       2:A:305:LFA:H81       2.00       0.44         3:A:326:RET:H7       3:A:326:RET:H181       1.87       0.44         1:A:234:LEU:O       1:A:239:GLY:HA3       2.19       0.43         1:A:31:ILE:HG12       1:A:245:LEU:HD23       2.01       0.42         1:A:121:LEU:O       1:A:124:ILE:HG22       2.19       0.41	1:A:117:VAL:HG11	1:A:146:GLY:HA3	1.98	0.46
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1:A:118:PRO:O       1:A:122:PHE:HB2       2.17       0.45         1:A:217:LEU:HB2       1:A:250:ALA:HB2       1.98       0.45         1:A:261:LEU:HD21       2:A:320:LFA:H62       1.99       0.45         1:A:224:MET:N       1:A:225:PRO:HD2       2.32       0.44         1:A:37:ALA:HB1       2:A:312:LFA:H51       1.99       0.44         1:A:107:GLY:HA3       2:A:305:LFA:H81       2.00       0.44         3:A:326:RET:H7       3:A:326:RET:H181       1.87       0.44         1:A:234:LEU:O       1:A:239:GLY:HA3       2.19       0.43         1:A:31:ILE:HG12       1:A:245:LEU:HD23       2.01       0.42         1:A:121:LEU:O       1:A:124:ILE:HG22       2.19       0.41	1:A:128:VAL:HG11	1:A:204:LEU:HD21	1.98	0.45
1:A:217:LEU:HB2       1:A:250:ALA:HB2       1.98       0.45         1:A:261:LEU:HD21       2:A:320:LFA:H62       1.99       0.45         1:A:224:MET:N       1:A:225:PRO:HD2       2.32       0.44         1:A:37:ALA:HB1       2:A:312:LFA:H51       1.99       0.44         1:A:107:GLY:HA3       2:A:305:LFA:H81       2.00       0.44         3:A:326:RET:H7       3:A:326:RET:H181       1.87       0.44         1:A:234:LEU:O       1:A:239:GLY:HA3       2.19       0.43         1:A:31:ILE:HG12       1:A:245:LEU:HD23       2.01       0.42         1:A:121:LEU:O       1:A:124:ILE:HG22       2.19       0.41	1:A:92:VAL:HG11	1:A:96:PHE:HZ	1.82	0.45
1:A:261:LEU:HD21       2:A:320:LFA:H62       1.99       0.45         1:A:224:MET:N       1:A:225:PRO:HD2       2.32       0.44         1:A:37:ALA:HB1       2:A:312:LFA:H51       1.99       0.44         1:A:107:GLY:HA3       2:A:305:LFA:H81       2.00       0.44         3:A:326:RET:H7       3:A:326:RET:H181       1.87       0.44         1:A:234:LEU:O       1:A:239:GLY:HA3       2.19       0.43         1:A:31:ILE:HG12       1:A:245:LEU:HD23       2.01       0.42         1:A:121:LEU:O       1:A:124:ILE:HG22       2.19       0.41	1:A:118:PRO:O	1:A:122:PHE:HB2	2.17	0.45
1:A:224:MET:N       1:A:225:PRO:HD2       2.32       0.44         1:A:37:ALA:HB1       2:A:312:LFA:H51       1.99       0.44         1:A:107:GLY:HA3       2:A:305:LFA:H81       2.00       0.44         3:A:326:RET:H7       3:A:326:RET:H181       1.87       0.44         1:A:234:LEU:O       1:A:239:GLY:HA3       2.19       0.43         1:A:31:ILE:HG12       1:A:245:LEU:HD23       2.01       0.42         1:A:121:LEU:O       1:A:124:ILE:HG22       2.19       0.41	1:A:217:LEU:HB2	1:A:250:ALA:HB2	1.98	0.45
1:A:37:ALA:HB1       2:A:312:LFA:H51       1.99       0.44         1:A:107:GLY:HA3       2:A:305:LFA:H81       2.00       0.44         3:A:326:RET:H7       3:A:326:RET:H181       1.87       0.44         1:A:234:LEU:O       1:A:239:GLY:HA3       2.19       0.43         1:A:31:ILE:HG12       1:A:245:LEU:HD23       2.01       0.42         1:A:121:LEU:O       1:A:124:ILE:HG22       2.19       0.41	1:A:261:LEU:HD21	2:A:320:LFA:H62	1.99	0.45
1:A:107:GLY:HA3       2:A:305:LFA:H81       2.00       0.44         3:A:326:RET:H7       3:A:326:RET:H181       1.87       0.44         1:A:234:LEU:O       1:A:239:GLY:HA3       2.19       0.43         1:A:31:ILE:HG12       1:A:245:LEU:HD23       2.01       0.42         1:A:121:LEU:O       1:A:124:ILE:HG22       2.19       0.41	1:A:224:MET:N	1:A:225:PRO:HD2	2.32	0.44
3:A:326:RET:H7       3:A:326:RET:H181       1.87       0.44         1:A:234:LEU:O       1:A:239:GLY:HA3       2.19       0.43         1:A:31:ILE:HG12       1:A:245:LEU:HD23       2.01       0.42         1:A:121:LEU:O       1:A:124:ILE:HG22       2.19       0.41	1:A:37:ALA:HB1	2:A:312:LFA:H51	1.99	0.44
1:A:234:LEU:O       1:A:239:GLY:HA3       2.19       0.43         1:A:31:ILE:HG12       1:A:245:LEU:HD23       2.01       0.42         1:A:121:LEU:O       1:A:124:ILE:HG22       2.19       0.41	1:A:107:GLY:HA3	2:A:305:LFA:H81	2.00	0.44
1:A:31:ILE:HG12       1:A:245:LEU:HD23       2.01       0.42         1:A:121:LEU:O       1:A:124:ILE:HG22       2.19       0.41	3:A:326:RET:H7	3:A:326:RET:H181	1.87	0.44
1:A:121:LEU:O 1:A:124:ILE:HG22 2.19 0.41	1:A:234:LEU:O	1:A:239:GLY:HA3	2.19	0.43
	1:A:31:ILE:HG12	1:A:245:LEU:HD23	2.01	0.42
1:A:260:VAL:HG21 2:A:301:LFA:H51 2.03 0.41	1:A:121:LEU:O	1:A:124:ILE:HG22	2.19	0.41
	1:A:260:VAL:HG21	2:A:301:LFA:H51	2.03	0.41

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Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${ m distance} \; ({ m \AA})$	overlap (Å)
1:A:29:SER:HB3	1:A:83:THR:HG22	2.02	0.41
1:A:109:ARG:NH1	1:A:251:ASP:OD2	2.54	0.41
1:A:28:THR:O	1:A:31:ILE:HG22	2.21	0.41
1:A:193:LYS:O	1:A:196:ILE:HG12	2.21	0.41
1:A:219:PRO:HB3	3:A:326:RET:H183	2.02	0.41
1:A:176:ALA:HB1	2:A:316:LFA:H52	2.03	0.40
2:A:320:LFA:H42	2:A:320:LFA:C8	2.51	0.40
1:A:43:LEU:N	1:A:68:MET:HG3	2.36	0.40
1:A:169:VAL:HG11	2:A:303:LFA:H31	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1 Atom-2		$egin{aligned} &  ext{Interatomic} \ &  ext{distance} \ &  ext{(Å)} \end{aligned}$	$egin{aligned} \operatorname{Clash} \ \operatorname{overlap}\ (\mathring{\mathbf{A}}) \end{aligned}$
1:A:17:THR:CG2	2:A:325:LFA:H131[3_857]	1.41	0.19

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	265/264 (100%)	256 (97%)	9 (3%)	0	100 100	

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains (i)

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

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



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	221/226 (98%)	216 (98%)	5 (2%)	50 70	

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	VAL
1	A	50	ILE
1	A	88	PHE
1	A	142	PHE
1	A	270	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

26 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).



Mal	Trens	Chain	Dag	T inle	Во	nd leng	ths	Bond angles			
Mol	Type	Chain	Res	Link	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
2	LFA	A	311	-	9,9,19	0.31	0	8,8,18	0.78	0	
2	LFA	A	308	-	11,11,19	0.30	0	10,10,18	0.83	0	
2	LFA	A	309	-	10,10,19	0.30	0	9,9,18	0.81	0	
2	LFA	A	313	-	9,9,19	0.30	0	8,8,18	0.78	0	
2	LFA	A	325	-	12,12,19	0.30	0	11,11,18	0.91	0	
2	LFA	A	321	-	2,2,19	0.34	0	0,1,18	-	-	
2	LFA	A	319	-	5,5,19	0.32	0	4,4,18	0.54	0	
2	LFA	A	301	-	15,15,19	0.30	0	14,14,18	0.87	0	
2	LFA	A	317	-	4,4,19	0.32	0	3,3,18	0.56	0	
2	LFA	A	316	-	5,5,19	0.32	0	4,4,18	0.57	0	
2	LFA	A	304	-	5,5,19	0.32	0	4,4,18	0.57	0	
2	LFA	A	312	-	4,4,19	0.33	0	3,3,18	0.54	0	
2	LFA	A	324	-	11,11,19	0.30	0	10,10,18	0.83	0	
2	LFA	A	318	-	3,3,19	0.41	0	2,2,18	0.74	0	
2	LFA	A	310	_	4,4,19	0.33	0	3,3,18	0.53	0	
2	LFA	A	306	_	9,9,19	0.30	0	8,8,18	0.81	0	
2	LFA	A	323	_	9,9,19	0.30	0	8,8,18	0.79	0	
2	LFA	A	303	_	5,5,19	0.31	0	4,4,18	0.57	0	
2	LFA	A	307	-	7,7,19	0.32	0	6,6,18	0.68	0	
2	LFA	A	302	_	7,7,19	0.30	0	6,6,18	0.74	0	
2	LFA	A	315	-	8,8,19	0.31	0	7,7,18	0.74	0	
2	LFA	A	320	-	9,9,19	0.32	0	8,8,18	0.75	0	
2	LFA	A	305	-	12,12,19	0.31	0	11,11,18	0.81	0	
3	RET	A	326	1	20,20,21	0.81	1 (5%)	27,27,28	0.43	0	
2	LFA	A	314	-	8,8,19	0.31	0	7,7,18	0.74	0	
2	LFA	A	322	-	8,8,19	0.32	0	7,7,18	0.73	0	

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	A	311	-	-	0/7/7/17	-
2	LFA	A	308	-	-	1/9/9/17	-
2	LFA	A	309	-	-	1/8/8/17	-
2	LFA	A	313	-	-	1/7/7/17	-
2	LFA	A	325	-	-	7/10/10/17	-
2	LFA	A	319	-	-	0/3/3/17	-
2	LFA	A	301	-	-	1/13/13/17	-
2	LFA	A	317	-	-	0/2/2/17	-
2	LFA	A	316	-	-	0/3/3/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	A	304	-	-	0/3/3/17	-
2	LFA	A	312	-	-	0/2/2/17	-
2	LFA	A	324	-	-	0/9/9/17	-
2	LFA	A	318	-	-	1/1/1/17	-
2	LFA	A	310	-	-	0/2/2/17	-
2	LFA	A	306	-	-	0/7/7/17	-
2	LFA	A	323	-	-	2/7/7/17	-
2	LFA	A	303	-	-	0/3/3/17	-
2	LFA	A	307	-	-	1/5/5/17	-
2	LFA	A	302	ı	-	0/5/5/17	-
2	LFA	A	315	-	-	3/6/6/17	-
2	LFA	A	320	-	-	2/7/7/17	-
2	LFA	A	305	-	-	3/10/10/17	-
3	RET	A	326	1	-	0/13/30/31	0/1/1/1
2	LFA	A	314	_	-	1/6/6/17	_
2	LFA	A	322	-	-	0/6/6/17	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(A)
3	A	326	RET	C14-C13	2.97	1.36	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	318	LFA	C3-C4-C5-C6
2	A	325	LFA	C12-C13-C14-C15
2	A	325	LFA	C14-C15-C16-C17
2	A	314	LFA	C6-C7-C8-C9
2	A	305	LFA	C9-C10-C11-C12
2	A	315	LFA	C3-C4-C5-C6
2	A	320	LFA	C5-C6-C7-C8
2	A	320	LFA	C3-C4-C5-C6
2	A	305	LFA	C4-C5-C6-C7
2	A	325	LFA	C11-C12-C13-C14
2	A	325	LFA	C17-C18-C19-C20
2	A	325	LFA	C11-C10-C9-C8
2	A	305	LFA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	A	301	LFA	C11-C12-C13-C14
2	A	325	LFA	C10-C11-C12-C13
2	A	315	LFA	C1-C2-C3-C4
2	A	323	LFA	C6-C7-C8-C9
2	A	313	LFA	C5-C6-C7-C8
2	A	307	LFA	C3-C4-C5-C6
2	A	315	LFA	C4-C5-C6-C7
2	A	308	LFA	C6-C7-C8-C9
2	A	325	LFA	C9-C10-C11-C12
2	A	323	LFA	C3-C4-C5-C6
2	A	309	LFA	C11-C10-C9-C8

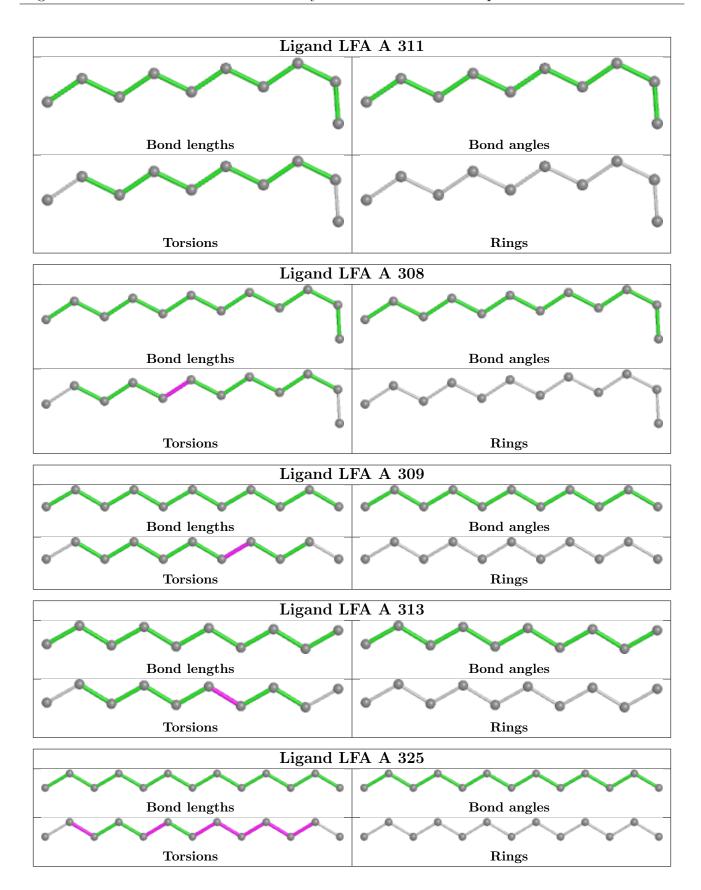
There are no ring outliers.

11 monomers are involved in 18 short contacts:

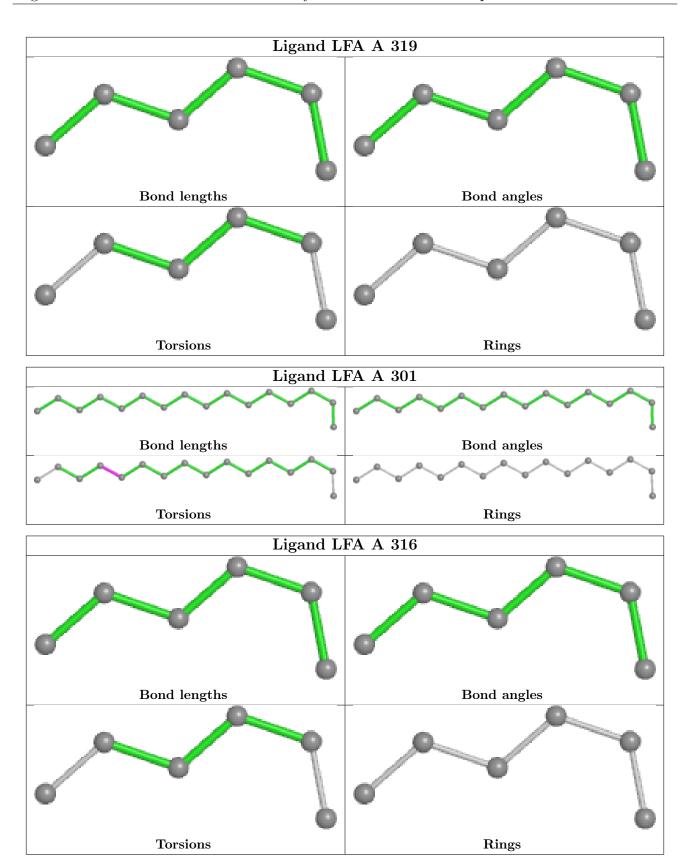
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	325	LFA	1	1
2	A	301	LFA	1	0
2	A	316	LFA	1	0
2	A	304	LFA	1	0
2	A	312	LFA	1	0
2	A	303	LFA	1	0
2	A	315	LFA	1	0
2	A	320	LFA	3	0
2	A	305	LFA	2	0
3	A	326	RET	4	0
2	A	322	LFA	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

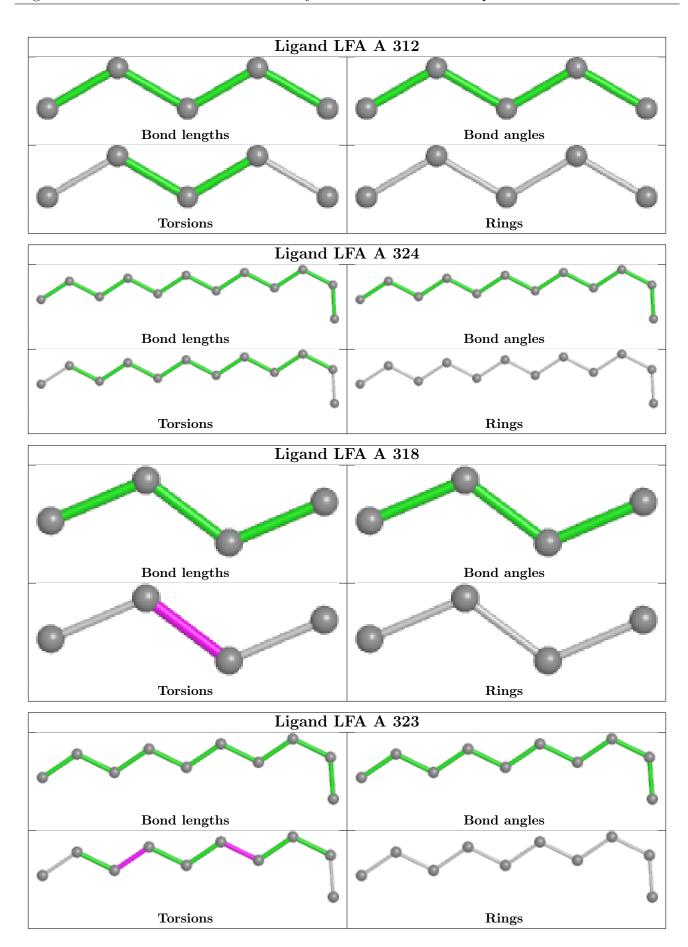




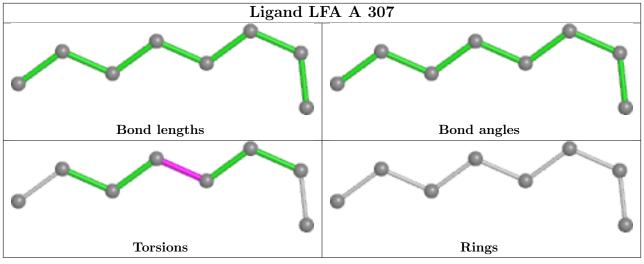


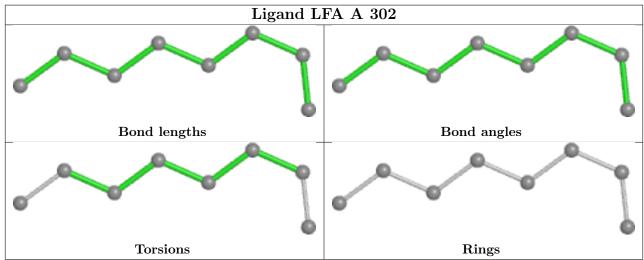


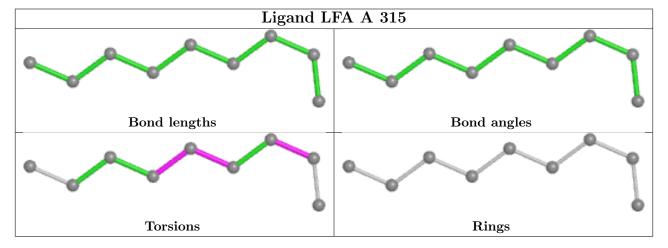




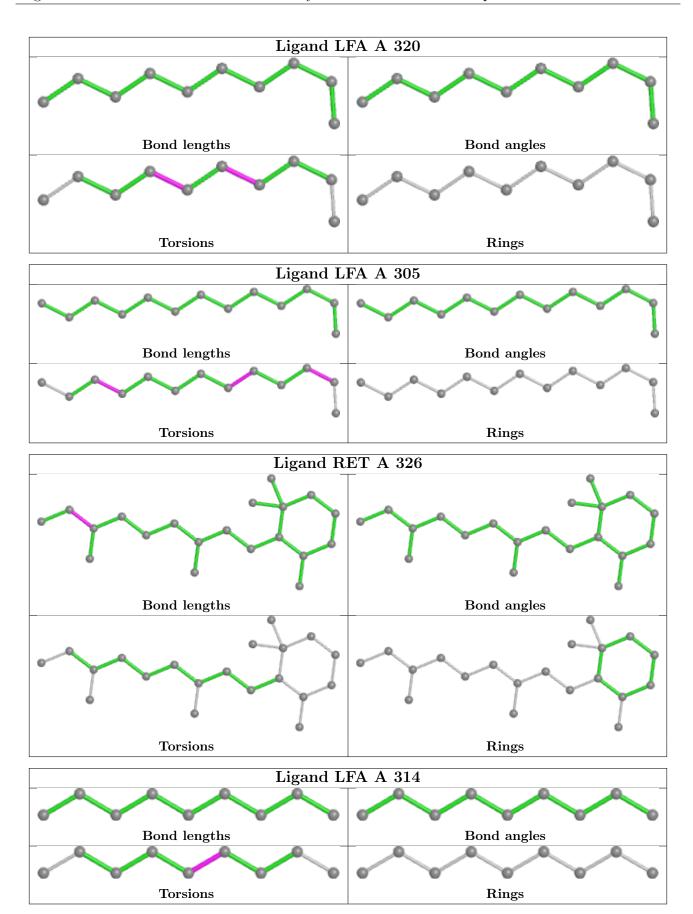




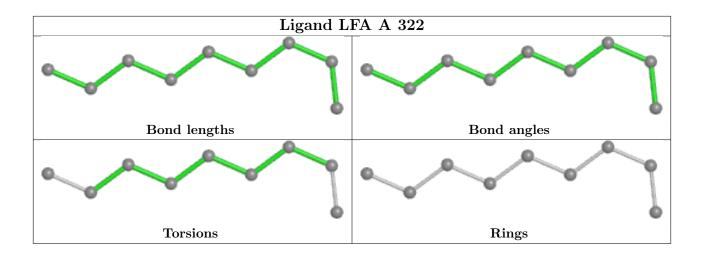












# 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 Fit of model and data (i)

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

In the following table, the column labelled '#RSRZ>2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median,  $95^{th}$  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	$\langle { m RSRZ} \rangle$	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q<0.9
1	A	264/264 (100%)	0.40	20 (7%) 13 12	15, 33, 69, 89	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	ASP	3.2
1	A	8	ALA	3.1
1	A	163	ASN	3.1
1	A	99	PRO	3.0
1	A	23	ILE	2.9
1	A	227	LEU	2.9
1	A	36	TYR	2.8
1	A	93	GLY	2.7
1	A	159	TYR	2.5
1	A	17	THR	2.4
1	A	225	PRO	2.4
1	A	195	GLY	2.3
1	A	84	SER	2.3
1	A	271	LYS	2.2
1	A	83	THR	2.2
1	A	30	HIS	2.1
1	A	198	PRO	2.1
1	A	162	SER	2.0
1	A	226	TYR	2.0
1	A	178	PHE	2.0

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

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



## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

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

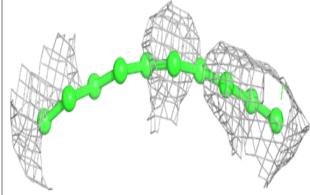
Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B ext{-}factors}({f \AA}^2)$	Q<0.9
2	LFA	A	311	10/20	0.17	0.54	53,76,95,100	0
2	LFA	A	309	11/20	0.24	0.50	53,61,70,73	0
2	LFA	A	321	3/20	0.25	0.35	57,57,57,68	0
2	LFA	A	319	6/20	0.26	0.55	50,66,73,78	0
2	LFA	A	324	12/20	0.36	0.48	36,56,64,66	0
2	LFA	A	302	8/20	0.48	0.48	34,35,39,39	8
2	LFA	A	314	9/20	0.51	0.55	57,71,77,83	0
2	LFA	A	312	5/20	0.53	0.42	34,36,47,51	0
2	LFA	A	313	10/20	0.53	0.40	48,50,57,58	0
2	LFA	A	310	5/20	0.55	0.40	46,49,58,61	0
2	LFA	A	307	8/20	0.55	0.43	40,43,48,56	0
2	LFA	A	308	12/20	0.59	0.49	52,58,60,70	0
2	LFA	A	320	10/20	0.59	0.40	41,46,53,56	0
2	LFA	A	315	9/20	0.60	0.26	37,47,50,51	0
2	LFA	A	305	13/20	0.63	0.28	36,42,52,53	0
2	LFA	A	325	13/20	0.64	0.26	65,79,82,83	40
2	LFA	A	317	5/20	0.66	0.23	39,44,51,55	0
2	LFA	A	323	10/20	0.66	0.32	44,48,57,58	0
2	LFA	A	322	9/20	0.67	0.56	41,54,76,79	0
2	LFA	A	304	6/20	0.70	0.24	47,52,56,58	0
2	LFA	A	316	6/20	0.73	0.47	38,45,57,58	0
2	LFA	A	303	6/20	0.75	0.20	41,45,51,51	0
2	LFA	A	318	4/20	0.76	0.36	35,36,44,49	0
2	LFA	A	306	10/20	0.79	0.31	32,37,44,46	0
2	LFA	A	301	16/20	0.80	0.18	30,39,46,46	0
3	RET	A	326	20/21	0.85	0.21	20,32,38,45	0

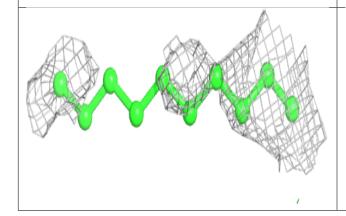
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

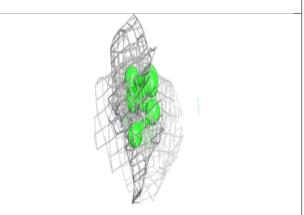


# Electron density around LFA A 311:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$  (at 0.7 rmsd) in gray  ${\rm mF}_o\text{-}{\rm DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)

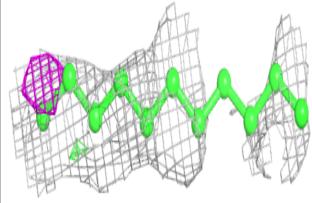


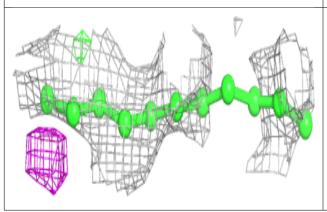


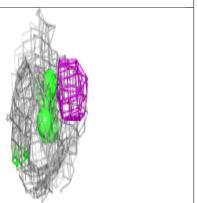


### Electron density around LFA A 309:

 $2 {
m mF}_o {
m -DF}_c$  (at 0.7 rmsd) in gray  ${
m mF}_o {
m -DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)



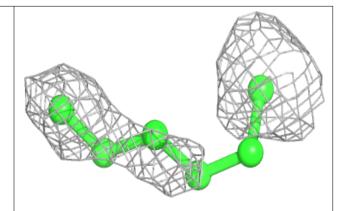


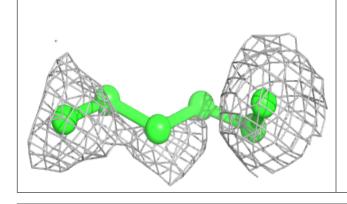


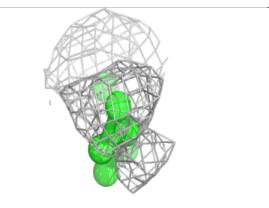


### Electron density around LFA A 319:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 0.7 rmsd) in gray  $\mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)

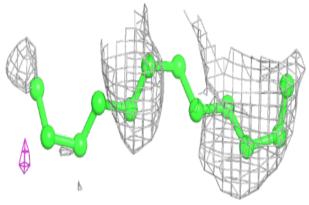


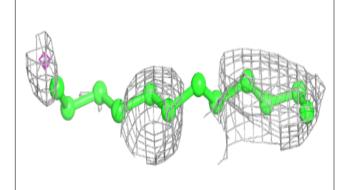


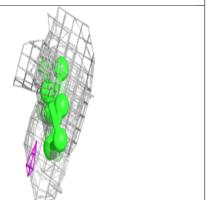


### Electron density around LFA A 324:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 0.7 rmsd) in gray  $\mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)



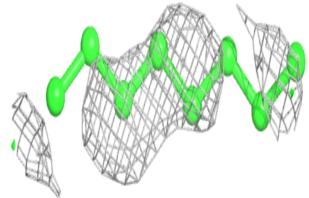


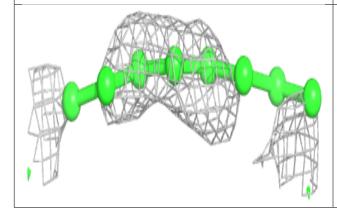


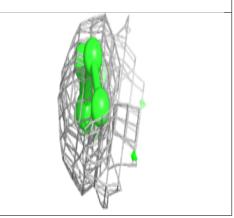


### Electron density around LFA A 302:

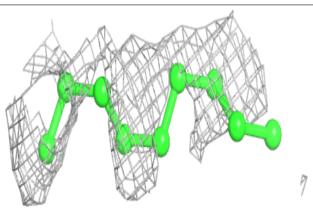
 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 0.7 rmsd) in gray  $\mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)

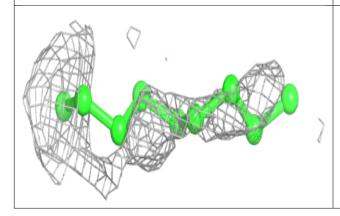


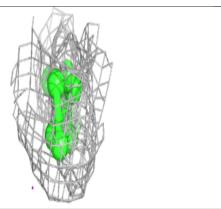




### Electron density around LFA A 314:



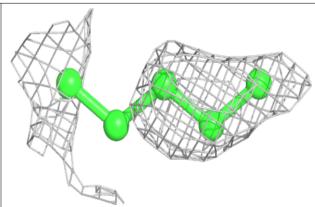


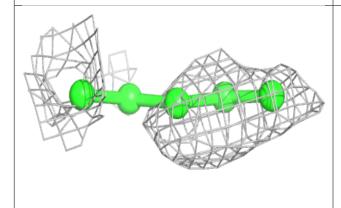


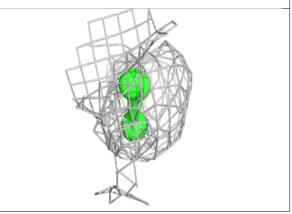


### Electron density around LFA A 312:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$  (at 0.7 rmsd) in gray  ${\rm mF}_o\text{-}{\rm DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)

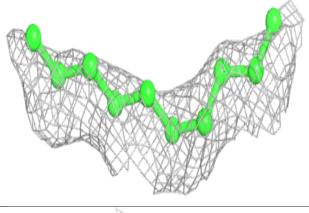


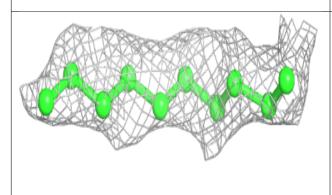


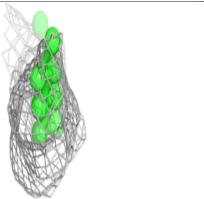


### Electron density around LFA A 313:

 $2 {
m mF}_o {
m -DF}_c$  (at 0.7 rmsd) in gray  ${
m mF}_o {
m -DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)



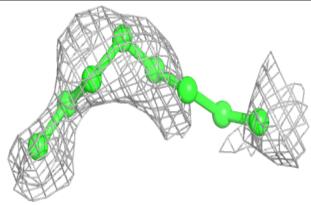


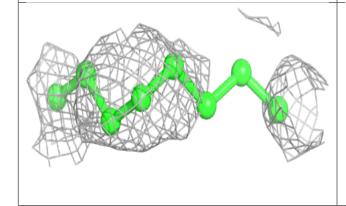


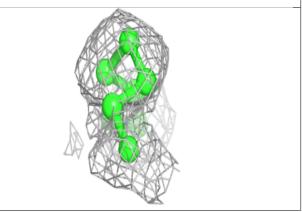


### Electron density around LFA A 307:

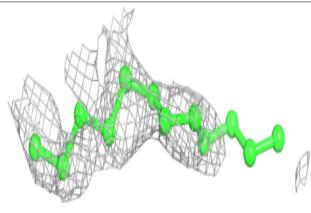
 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 0.7 rmsd) in gray  $\mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)

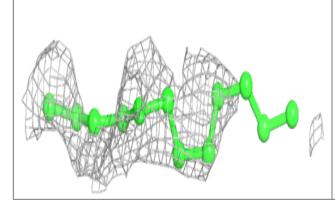


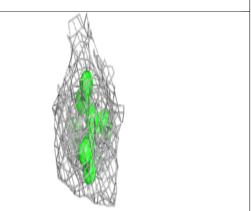




### Electron density around LFA A 308:



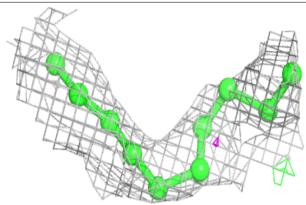


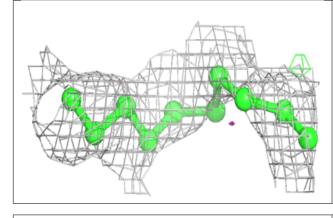


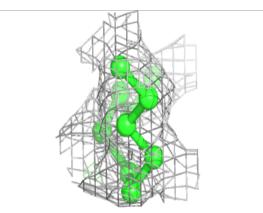


### Electron density around LFA A 320:

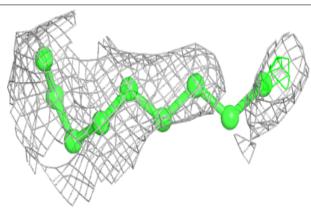
 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 0.7 rmsd) in gray  $\mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)

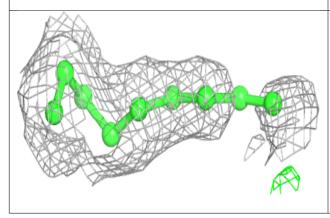


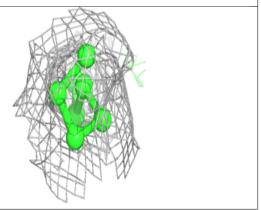




### Electron density around LFA A 315:



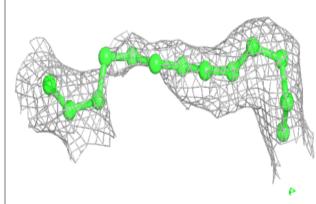


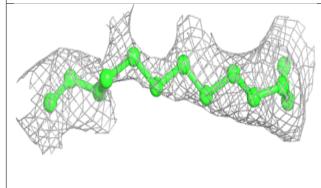


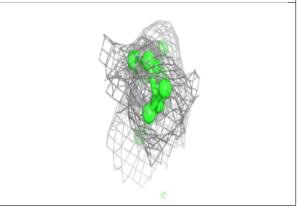


# Electron density around LFA A 305:

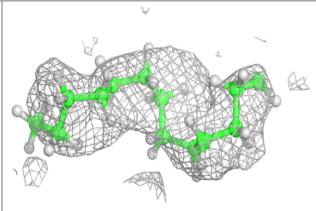
 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 0.7 rmsd) in gray  $\mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)

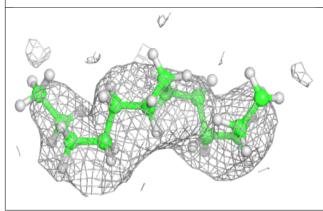


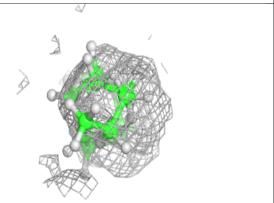




### Electron density around LFA A 325:



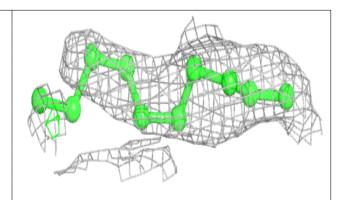


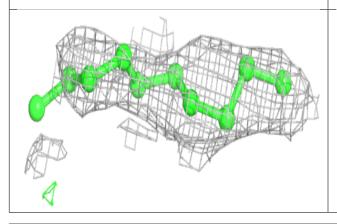


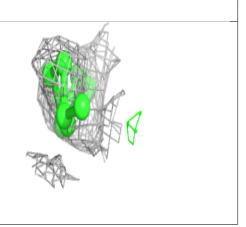


### Electron density around LFA A 323:

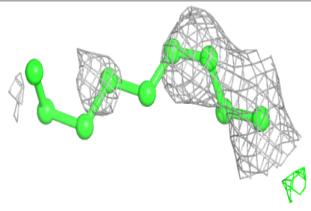
 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 0.7 rmsd) in gray  $\mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)

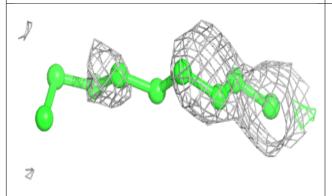


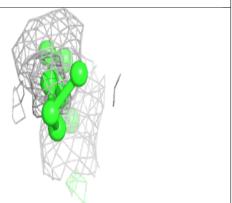




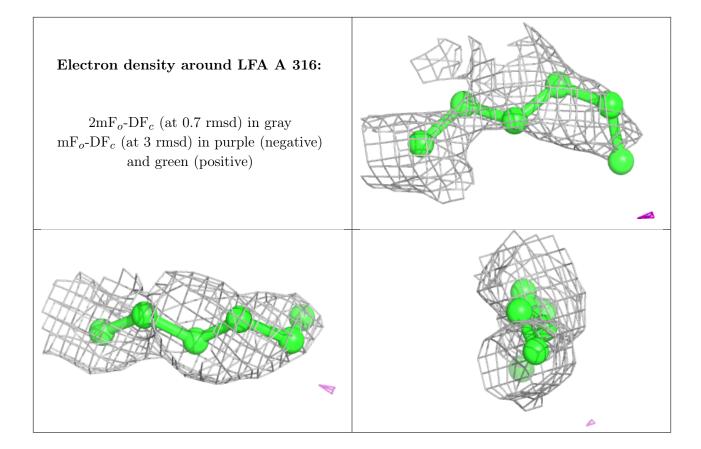
### Electron density around LFA A 322:





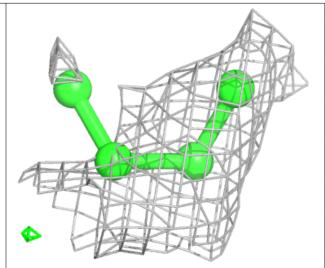


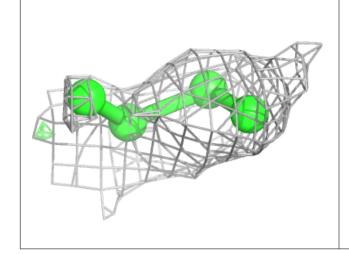


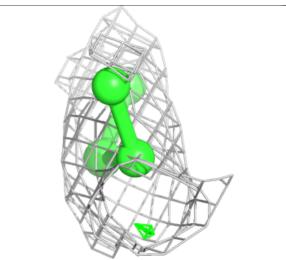




### Electron density around LFA A 318:



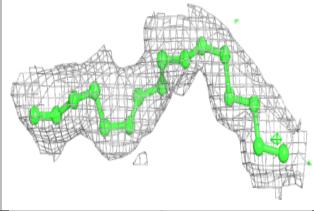


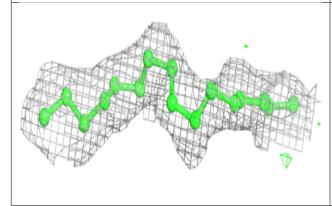


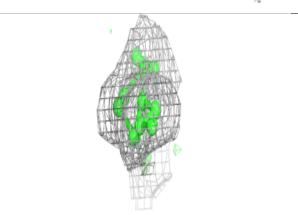


### Electron density around LFA A 301:

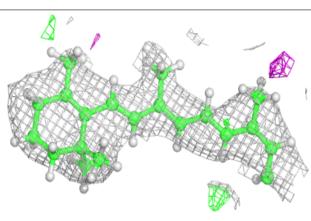
 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 0.7 rmsd) in gray  $\mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)

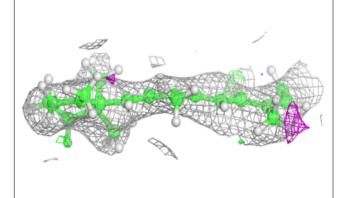


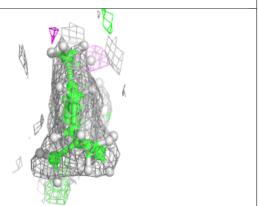




### Electron density around RET A 326:









# 6.5 Other polymers (i)

There are no such residues in this entry.

