

Full wwPDB X-ray Structure Validation Report (i)

Apr 20, 2022 - 07:05 pm BST

PDB ID : 7Q37

Title : Crystal structure of proton pump MAR rhodopsin pressurized with krypton Authors : Melnikov, I.; Rulev, M.; Astashkin, R.; Kovalev, K.; Carpentier, P.; Gordeliy,

V.; Popov, A.

Deposited on : 2021-10-27

Resolution : 2.25 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*A user guide is available at

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

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 : 2.27 buster-report : 1.1.7 (2018)

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

 $Refmac \quad : \quad 5.8.0267$

CCP4 : 7.1.010 (Gargrove)

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

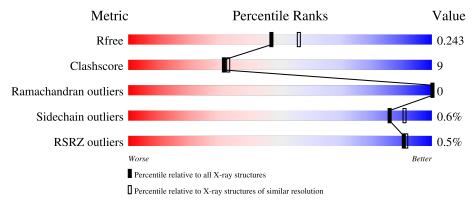
Validation Pipeline (wwPDB-VP) : 2.27

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 2.25 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	$(\# ext{Entries})$	$(\# ext{Entries}, ext{ resolution range}(\AA))$
R_{free}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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		
1	A	220	88%	10%	•

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
5	KR	A	321	-	-	X	-





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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	KR	A	325	-	-	X	-



2 Entry composition (i)

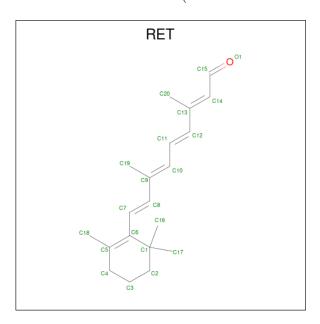
There are 6 unique types of molecules in this entry. The entry contains 1983 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bacteriorhodopsin.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	217	Total	С	N	O	S	0	1	0
1	Α	211	1683	1098	275	299	11	0	1	

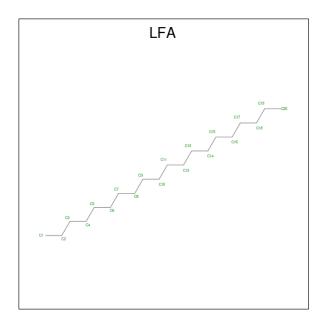
• Molecule 2 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 20 20	0	0

 \bullet Molecule 3 is EICOSANE (three-letter code: LFA) (formula: $\mathrm{C}_{20}\mathrm{H}_{42}).$

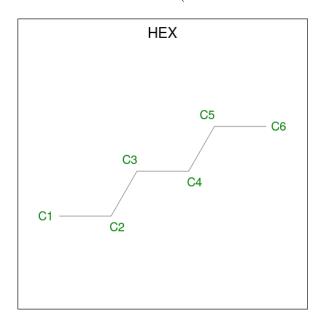




Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 7 7	0	0
3	A	1	Total C 7 7	0	0
3	A	1	Total C 4 4	0	0
3	A	1	Total C 9 9	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 20 20	0	0
3	A	1	Total C 12 12	0	0
3	A	1	Total C 17 17	0	0
3	A	1	Total C 7 7	0	0
3	A	1	Total C 12 12	0	0
3	A	1	Total C 9 9	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C 12 12	0	0
3	A	1	Total C 7 7	0	0



 \bullet Molecule 4 is HEXANE (three-letter code: HEX) (formula: $\mathrm{C_6H_{14}}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 6 6	0	0
4	A	1	Total C 4 4	0	0
4	A	1	Total C 5 5	0	0
4	A	1	Total C 4 4	0	0
4	A	1	Total C 6 6	0	0

• Molecule 5 is KRYPTON (three-letter code: KR) (formula: Kr) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	19	Total Kr 19 19	0	0

• Molecule 6 is water.

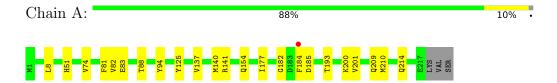
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	99	Total O 99 99	0	0



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: Bacteriorhodopsin





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants	50.90Å 40.38Å 60.62Å	Depositor
a, b, c, α , β , γ	90.00° 101.36° 90.00°	Depositor
Resolution (Å)	59.43 - 2.25	Depositor
resolution (A)	59.43 - 2.25	EDS
% Data completeness	99.7 (59.43-2.25)	Depositor
(in resolution range)	99.8 (59.43-2.25)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.31 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
P. P.	0.178 , 0.245	Depositor
R, R_{free}	0.189 , 0.243	DCC
R_{free} test set	570 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$ < L > = 0.52, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	1983	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 9.76% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities 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: HEX, RET, KR, LFA, FME

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	$\mathbf{lengths}$	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.73	0/1705	0.79	0/2322	

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 (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	1683	0	1678	23	0
2	A	20	0	27	4	0
3	A	137	0	248	5	1
4	A	25	0	51	2	0
5	A	19	0	0	16	0
6	A	99	0	0	9	0
All	All	1983	0	2004	35	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 9.

All (35) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
1:A:140:MET:HE1	5:A:321:KR:KR	1.95	1.26
3:A:313:LFA:C8	5:A:331:KR:KR	2.53	1.18
1:A:140:MET:CE	5:A:321:KR:KR	2.64	1.06
5:A:337:KR:KR	6:A:401:HOH:O	2.38	1.01
4:A:317:HEX:C4	5:A:327:KR:KR	2.92	0.78
1:A:74:VAL:HG11	3:A:312:LFA:H41	1.68	0.76
1:A:83:GLU:OE1	6:A:401:HOH:O	2.11	0.69
2:A:301:RET:H8	2:A:301:RET:H161	1.76	0.68
1:A:209:GLN:NE2	6:A:403:HOH:O	2.28	0.66
1:A:51:HIS:NE2	3:A:307:LFA:H203	2.17	0.60
5:A:336:KR:KR	6:A:447:HOH:O	2.82	0.58
1:A:88:THR:O	6:A:402:HOH:O	2.17	0.57
1:A:125:TYR:OH	1:A:177:ILE:HA	2.05	0.56
3:A:307:LFA:H202	6:A:454:HOH:O	2.05	0.55
1:A:140:MET:HE2	5:A:325:KR:KR	2.67	0.55
1:A:81:PHE:HB2	5:A:322:KR:KR	2.68	0.55
1:A:140:MET:CE	5:A:325:KR:KR	3.17	0.54
1:A:82:VAL:HG13	1:A:94:TYR:OH	2.07	0.54
5:A:338:KR:KR	6:A:447:HOH:O	2.87	0.54
2:A:301:RET:H161	2:A:301:RET:C8	2.37	0.53
1:A:193:THR:OG1	5:A:324:KR:KR	2.89	0.52
1:A:201:VAL:HG13	5:A:323:KR:KR	2.74	0.49
1:A:182:GLY:HA3	1:A:184:PHE:CE2	2.49	0.47
1:A:137:VAL:O	1:A:141:ARG:HG2	2.14	0.47
1:A:200:LYS:NZ	6:A:406:HOH:O	2.48	0.47
4:A:316:HEX:H52	5:A:334:KR:KR	2.75	0.47
1:A:182:GLY:HA3	1:A:184:PHE:CD2	2.49	0.47
1:A:184:PHE:CD2	5:A:326:KR:KR	3.31	0.45
1:A:8:LEU:HD22	5:A:332:KR:KR	2.78	0.45
1:A:140:MET:HE3	5:A:325:KR:KR	2.78	0.45
3:A:312:LFA:C10	6:A:481:HOH:O	2.65	0.45
1:A:154:GLN:NE2	1:A:214:GLN:HE21	2.15	0.44
2:A:301:RET:H181	2:A:301:RET:H7	1.84	0.42
2:A:301:RET:H11	2:A:301:RET:H191	1.92	0.42
1:A:154:GLN:HA	1:A:210:MET:HE1	2.01	0.41

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	Interatomic distance (Å)	Clash overlap (Å)
3:A:309:LFA:C1	3:A:309:LFA:C1[2_656]	1.97	0.23



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	215/220 (98%)	212 (99%)	3 (1%)	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	165/172 (96%)	164 (99%)	1 (1%)	86 91		

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	ASP

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	214	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.



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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol Type	Chain	Res	Timle	Bond lengths			Bond angles			
IVIOI	туре	Chain	nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	FME	A	1[A]	-	8,9,10	0.42	0	7,9,11	0.85	0
1	FME	A	1[B]	-	8,9,10	0.48	0	7,9,11	0.84	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
1	FME	A	1[A]	-	-	4/7/9/11	_
1	FME	A	1[B]	-	-	3/7/9/11	_

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1[A]	FME	O1-CN-N-CA
1	A	1[A]	FME	N-CA-CB-CG
1	A	1[A]	FME	C-CA-CB-CG
1	A	1[B]	FME	N-CA-CB-CG
1	A	1[B]	FME	C-CA-CB-CG
1	A	1[B]	FME	CB-CG-SD-CE
1	A	1[A]	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.



5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 39 ligands modelled in this entry, 19 are monoatomic - leaving 20 for Mogul analysis.

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

Mol	Trino	Chain	Dag	T inle	Во	ond leng	ths	В	ond ang	les
IVIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LFA	A	302	-	6,6,19	0.25	0	5,5,18	0.19	0
4	HEX	A	318	-	4,4,5	0.22	0	3,3,4	0.19	0
3	LFA	A	313	-	5,5,19	0.17	0	4,4,18	0.18	0
3	LFA	A	304	-	3,3,19	0.20	0	2,2,18	0.52	0
3	LFA	A	311	-	11,11,19	0.20	0	10,10,18	0.12	0
3	LFA	A	306	-	7,7,19	0.13	0	6,6,18	0.07	0
3	LFA	A	309	ı	16,16,19	0.24	0	15,15,18	0.26	0
3	LFA	A	312	-	8,8,19	0.23	0	7,7,18	0.10	0
2	RET	A	301	1	20,20,21	2.24	5 (25%)	27,27,28	1.32	3 (11%)
4	HEX	A	317	-	3,3,5	0.26	0	2,2,4	0.48	0
3	LFA	A	314	-	11,11,19	0.29	0	10,10,18	0.25	0
3	LFA	A	308	-	11,11,19	0.19	0	10,10,18	0.16	0
3	LFA	A	305	-	8,8,19	0.22	0	7,7,18	0.13	0
4	HEX	A	319	-	3,3,5	0.34	0	2,2,4	0.32	0
4	HEX	A	320	-	5,5,5	0.18	0	4,4,4	0.17	0
3	LFA	A	307	-	19,19,19	0.19	0	18,18,18	0.11	0
3	LFA	A	310	-	6,6,19	0.10	0	5,5,18	0.20	0
3	LFA	A	315	-	6,6,19	0.20	0	5,5,18	0.13	0
3	LFA	A	303	-	6,6,19	0.21	0	5,5,18	0.17	0
4	HEX	A	316	-	5,5,5	0.18	0	4,4,4	0.18	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
3	LFA	A	302	-	-	4/4/4/17	-
4	HEX	A	318	-	-	0/2/2/3	-
3	LFA	A	313	_	-	3/3/3/17	-
3	LFA	A	304	-	-	1/1/1/17	-
3	LFA	A	311	-	-	5/9/9/17	-
3	LFA	A	306	-	-	2/5/5/17	-
3	LFA	A	309	-	-	8/14/14/17	-
3	LFA	A	312	-	-	3/6/6/17	-
2	RET	A	301	1	-	0/13/30/31	0/1/1/1
4	HEX	A	317	_	-	0/1/1/3	-
3	LFA	A	314	_	-	5/9/9/17	-
3	LFA	A	308	-	-	6/9/9/17	-
3	LFA	A	305	-	-	4/6/6/17	-
4	HEX	A	319	-	-	1/1/1/3	-
4	HEX	A	320	-	-	2/3/3/3	-
3	LFA	A	307	-	-	8/17/17/17	-
3	LFA	A	310	-	-	2/4/4/17	-
3	LFA	A	315	-	-	0/4/4/17	-
3	LFA	A	303	-	-	2/4/4/17	
4	HEX	A	316	-	-	1/3/3/3	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(Å)	$\operatorname{Ideal}(\text{\AA})$
2	A	301	RET	C14-C13	5.78	1.38	1.33
2	A	301	RET	C10-C9	5.62	1.43	1.35
2	A	301	RET	C12-C13	-3.27	1.38	1.45
2	A	301	RET	C8-C9	-2.33	1.40	1.45
2	A	301	RET	C2-C3	-2.19	1.47	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
2	A	301	RET	C19-C9-C10	-4.32	116.88	122.92
2	A	301	RET	C8-C9-C10	2.73	123.13	118.94
2	A	301	RET	C1-C6-C5	-2.40	119.24	122.61

There are no chirality outliers.

All (57) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
3	A	309	LFA	C9-C10-C11-C12
3	A	302	LFA	C4-C5-C6-C7
3	A	305	LFA	C3-C4-C5-C6
3	A	307	LFA	C6-C7-C8-C9
3	A	311	LFA	C11-C10-C9-C8
3	A	309	LFA	C5-C6-C7-C8
3	A	309	LFA	C11-C12-C13-C14
3	A	309	LFA	C12-C13-C14-C15
3	A	308	LFA	C4-C5-C6-C7
3	A	314	LFA	C3-C4-C5-C6
3	A	312	LFA	C5-C6-C7-C8
3	A	314	LFA	C11-C10-C9-C8
4	A	320	HEX	C3-C4-C5-C6
4	A	316	HEX	C1-C2-C3-C4
3	A	307	LFA	C7-C8-C9-C10
3	A	312	LFA	C6-C7-C8-C9
3	A	309	LFA	C7-C8-C9-C10
3	A	308	LFA	C10-C11-C12-C13
3	A	307	LFA	C17-C18-C19-C20
3	A	310	LFA	C1-C2-C3-C4
3	A	303	LFA	C4-C5-C6-C7
3	A	308	LFA	C3-C4-C5-C6
3	A	306	LFA	C5-C6-C7-C8
3	A	313	LFA	C3-C4-C5-C6
3	A	311	LFA	C5-C6-C7-C8
3	A	302	LFA	C6-C7-C8-C9
3	A	313	LFA	C4-C5-C6-C7
3	A	303	LFA	C1-C2-C3-C4
4	A	320	HEX	C1-C2-C3-C4
3	A	307	LFA	C5-C6-C7-C8
3	A	310	LFA	C3-C4-C5-C6
3	A	305	LFA	C5-C6-C7-C8
3	A	313	LFA	C5-C6-C7-C8
3	A	312	LFA	C2-C3-C4-C5
3	A	308	LFA	C11-C12-C13-C14
3	A	304	LFA	C1-C2-C3-C4
4	A	319	HEX	C3-C4-C5-C6
3	A	314	LFA	C4 C5 C6 C7
3	A	305	LFA	C4-C5-C6-C7
3	A	306	LFA	C4-C5-C6-C7
3	A	302	LFA	C3-C4-C5-C6
3	A	311	LFA	C2-C3-C4-C5
3	A	305	LFA	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	A	311	LFA	C7-C8-C9-C10
3	A	314	LFA	C7-C8-C9-C10
3	A	309	LFA	C3-C4-C5-C6
3	A	302	LFA	C5-C6-C7-C8
3	A	308	LFA	C7-C8-C9-C10
3	A	309	LFA	C6-C7-C8-C9
3	A	307	LFA	C16-C17-C18-C19
3	A	307	LFA	C11-C10-C9-C8
3	A	311	LFA	C4-C5-C6-C7
3	A	307	LFA	C9-C10-C11-C12
3	A	307	LFA	C13-C14-C15-C16
3	A	308	LFA	C5-C6-C7-C8
3	A	309	LFA	C2-C3-C4-C5
3	A	314	LFA	C5-C6-C7-C8

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	313	LFA	1	0
3	A	309	LFA	0	1
3	A	312	LFA	2	0
2	A	301	RET	4	0
4	A	317	HEX	1	0
3	A	307	LFA	2	0
4	A	316	HEX	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.



Ligand L	FA A 302
Bond lengths	Bond angles
Torsions	Rings
Ligand L	FA A 313
Bond lengths	Bond angles
Torsions	Rings
Ligand L	FA A 304
Bond lengths	Bond angles
Torsions	Rings
Ligand L	FA A 311
~~~~	~~~~
Bond lengths	Bond angles
<b>~~~</b>	
Torsions	Rings

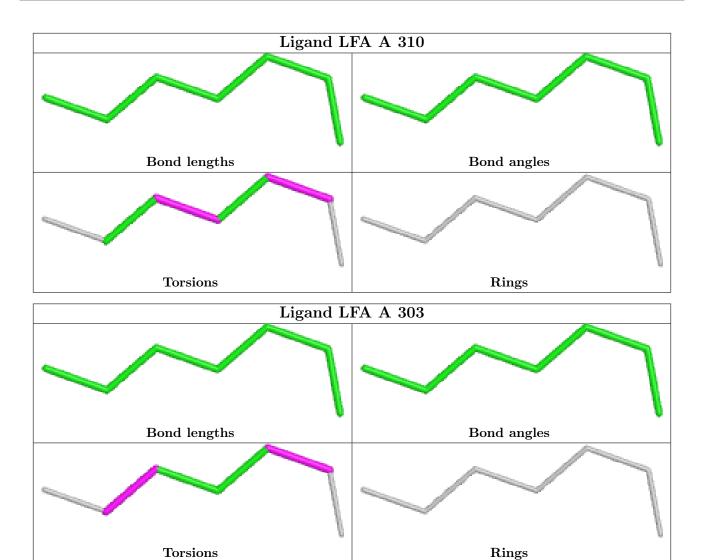


Ligand I	JFA A 306
Bond lengths	Bond angles
Torsions	Rings
	FA A 309
~~~~~	<b>~~~~</b>
Bond lengths	Bond angles
Doild lengths	Doild angles
Torsions	Dings
	Rings
Ligand 1	FA A 312
D 11 4	
Bond lengths	Bond angles
Torsions	Rings
Ligand F	ET A 301
7	The
Bond lengths	Bond angles
7	
Torsions	Rings



Ligand LFA A 314								
~~~~	~~~~							
Bond lengths	Bond angles							
<b>\\\\</b>								
Torsions	Rings							
Ligand L	FA A 308							
<b>~~~~</b>								
Bond lengths	Bond angles							
<b>/////</b>								
Torsions	Rings							
Ligand L	FA A 305							
<b>\\\</b>	<b>✓</b>							
Bond lengths	Bond angles							
<b>✓</b>								
Torsions	Rings							
Ligand L	FA A 307							
~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	~~~~~							
Bond lengths	Bond angles							
~~~~								
Torsions	Rings							





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	<rsrz></rsrz>	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	216/220 (98%)	-0.35	1 (0%) 91 91	23, 31, 54, 82	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	184	PHE	3.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	FME	A	1[A]	10/11	0.93	0.27	54,58,68,68	7
1	FME	A	1[B]	10/11	0.93	0.27	47,55,68,68	7

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.



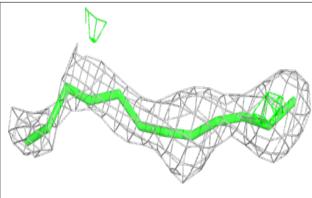
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\AA^2)$	Q < 0.9
4	HEX	A	320	6/6	0.54	0.29	82,85,85,87	0
4	HEX	A	319	4/6	0.56	0.34	58,63,65,66	0
3	LFA	A	311	12/20	0.63	0.28	58,67,71,72	0
3	LFA	A	306	8/20	0.68	0.29	75,79,82,82	0
3	LFA	A	308	12/20	0.73	0.21	50,58,61,66	0
4	HEX	A	318	5/6	0.78	0.25	58,58,62,62	0
3	LFA	A	302	7/20	0.79	0.26	70,70,73,73	0
3	LFA	A	315	7/20	0.81	0.23	66,70,71,74	0
3	LFA	A	314	12/20	0.81	0.20	41,48,51,51	0
5	KR	A	332	1/1	0.81	0.27	37,37,37,37	1
4	HEX	A	317	4/6	0.82	0.21	52,53,56,56	0
3	LFA	A	307	20/20	0.83	0.23	50,60,66,66	0
3	LFA	A	303	7/20	0.83	0.19	49,52,55,57	0
3	LFA	A	305	9/20	0.84	0.26	62,65,68,69	0
5	KR	A	334	1/1	0.84	0.59	28,28,28,28	1
4	HEX	A	316	6/6	0.85	0.26	61,65,69,70	0
3	LFA	A	310	7/20	0.86	0.19	49,55,58,58	0
3	LFA	A	309	17/20	0.88	0.17	46,52,56,59	0
5	KR	A	339	1/1	0.90	0.20	44,44,44,44	1
5	KR	A	327	1/1	0.91	0.22	30,30,30,30	1
3	LFA	A	304	4/20	0.92	0.18	39,40,42,43	0
5	KR	A	333	1/1	0.92	0.25	30,30,30,30	1
3	LFA	A	313	6/20	0.92	0.16	41,46,48,48	0
5	KR	A	336	1/1	0.92	0.13	41,41,41,41	1
5	KR	A	330	1/1	0.92	0.34	32,32,32,32	1
5	KR	A	331	1/1	0.93	0.30	33,33,33,33	1
3	LFA	A	312	9/20	0.93	0.17	39,43,45,45	0
2	RET	A	301	20/21	0.94	0.13	23,25,27,28	0
5	KR	A	335	1/1	0.94	0.34	32,32,32,32	1
5	KR	A	323	1/1	0.95	0.10	32,32,32,32	1
5	KR	A	329	1/1	0.95	0.17	42,42,42,42	1
5	KR	A	338	1/1	0.97	0.17	33,33,33,33	1
5	KR	A	337	1/1	0.97	0.14	31,31,31,31	1
5	KR	A	326	1/1	0.98	0.11	63,63,63,63	1
5	KR	A	325	1/1	0.99	0.07	30,30,30,30	1
5	KR	A	322	1/1	0.99	0.08	30,30,30,30	1
5	KR	A	321	1/1	0.99	0.07	29,29,29,29	1
5	KR	A	328	1/1	0.99	0.41	33,33,33,33	1
5	KR	A	324	1/1	0.99	0.07	30,30,30,30	1

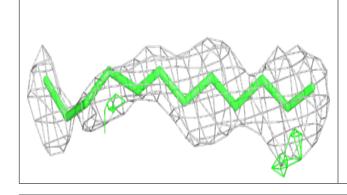
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

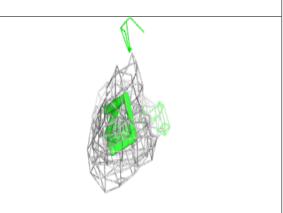


Electron density around LFA A 311:

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

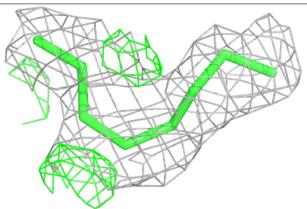


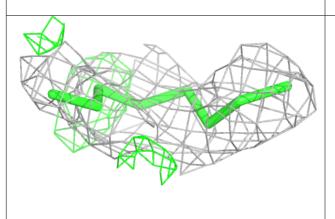


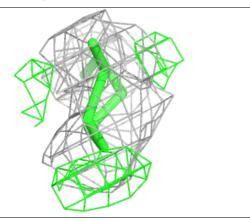


Electron density around LFA A 306:

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



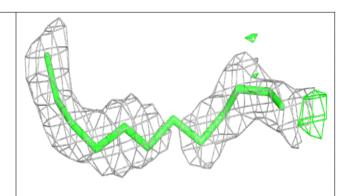




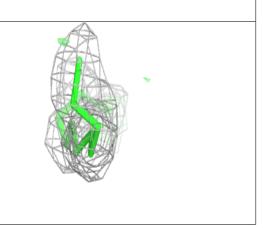


Electron density around LFA A 308:

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

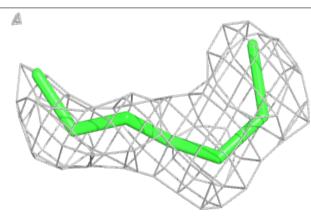


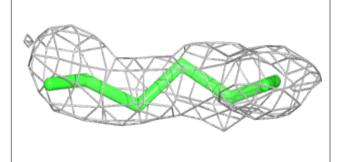


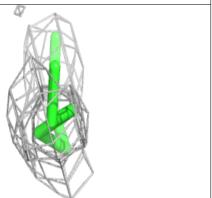


Electron density around LFA A 302:

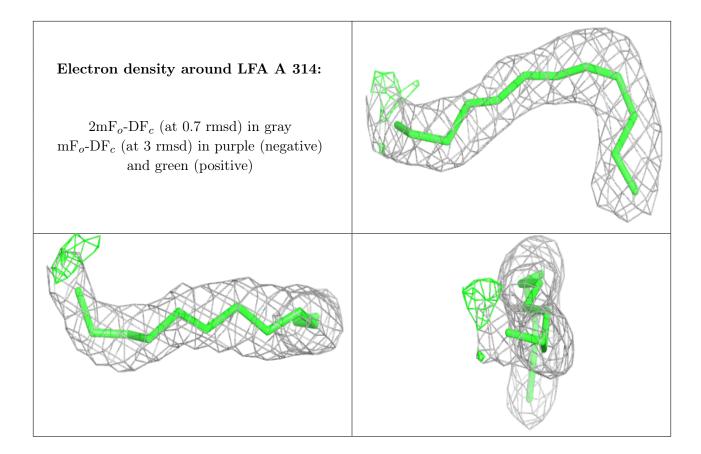
 $2 \text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray $\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)





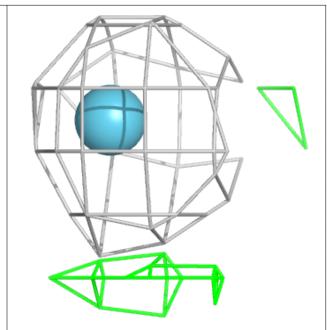


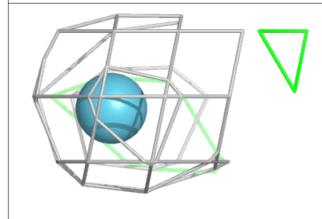


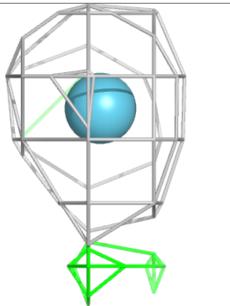




Electron density around KR A 332:



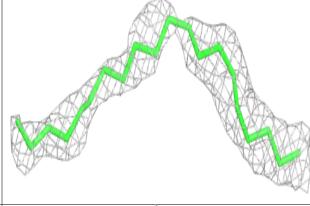


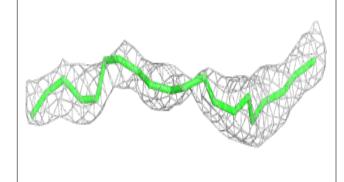


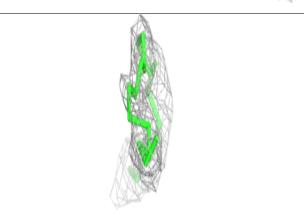


Electron density around LFA A 307:

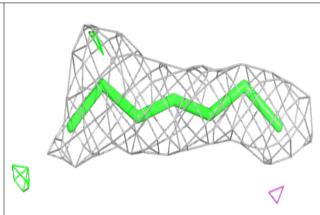
 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

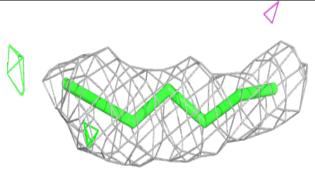


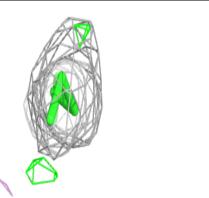




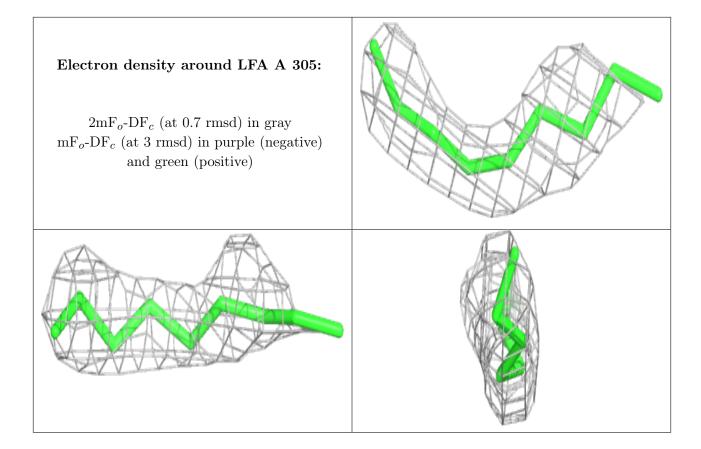
Electron density around LFA A 303:



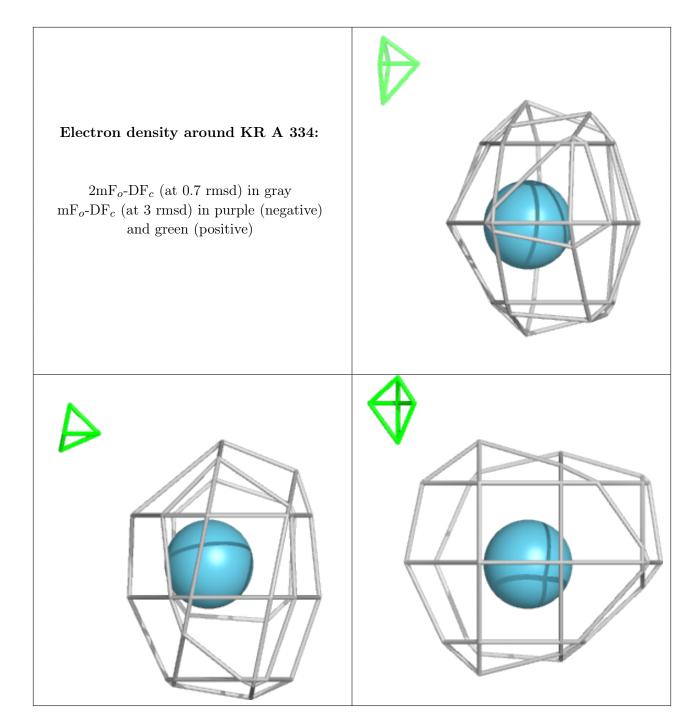








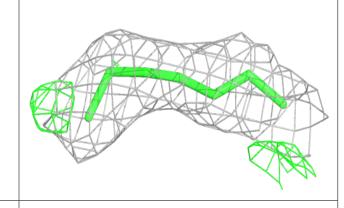


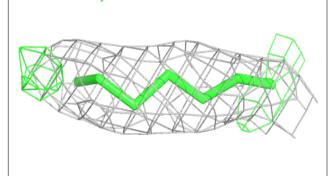


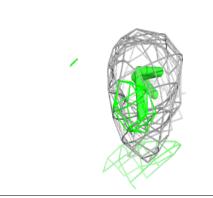


Electron density around LFA A 310:

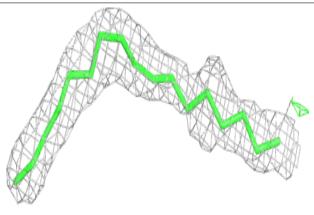
 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

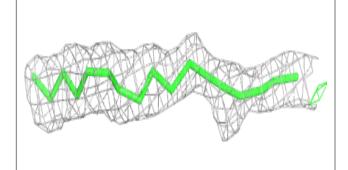


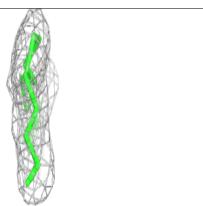




Electron density around LFA A 309:



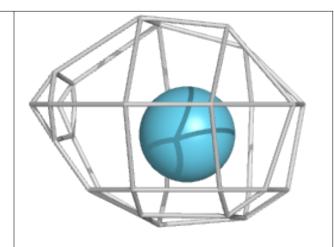


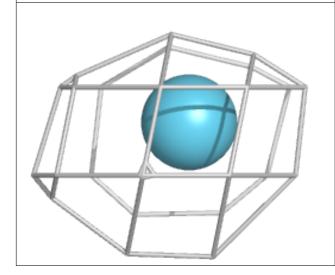


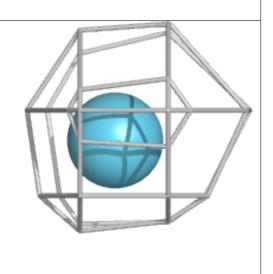


Electron density around KR A 339:

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

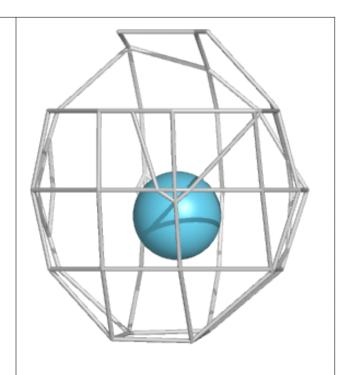


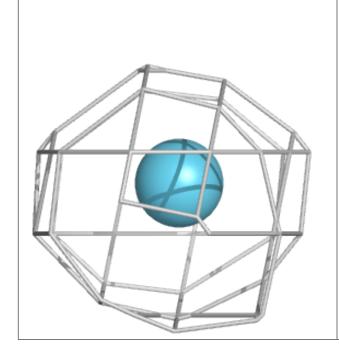


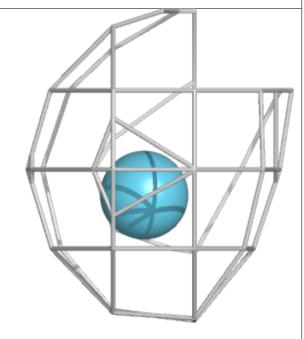




Electron density around KR A 327:

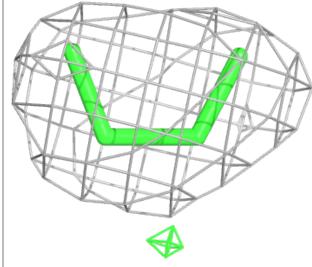


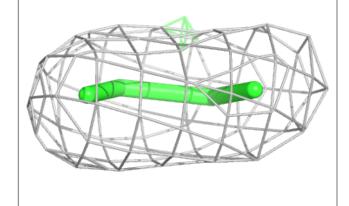


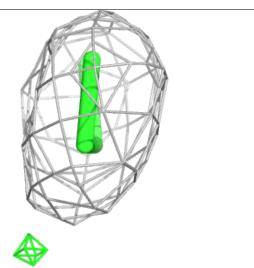


Electron density around LFA A 304:

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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)



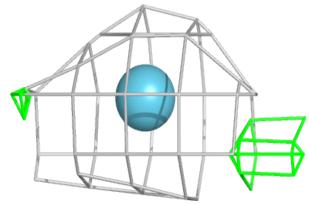


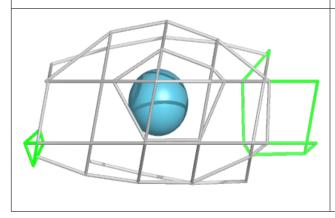


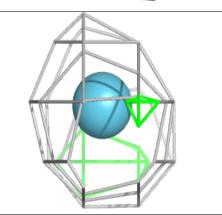


Electron density around KR A 333:

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

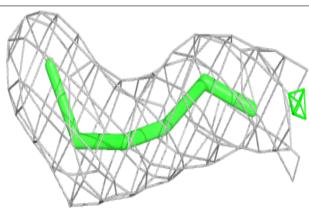


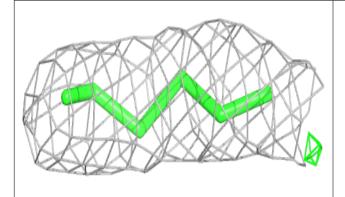


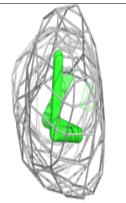


Electron density around LFA A 313:

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

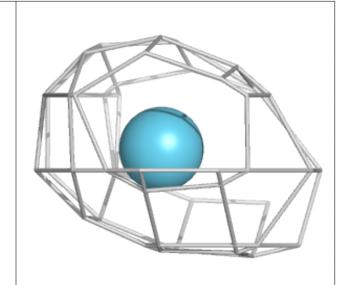


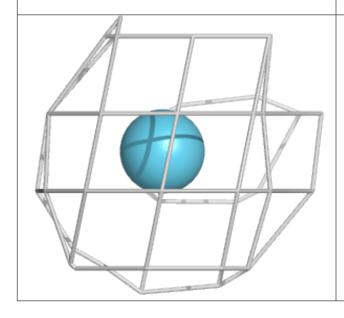


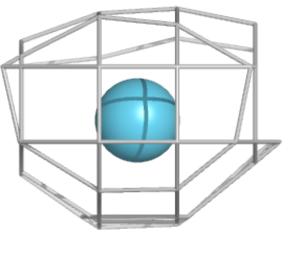




Electron density around KR A 336:

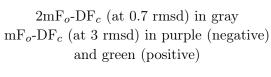


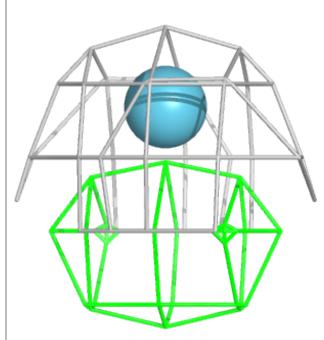


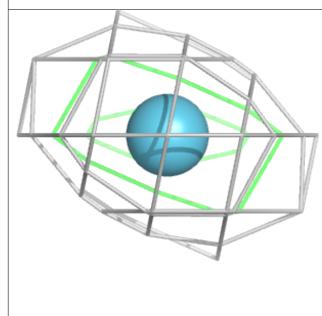


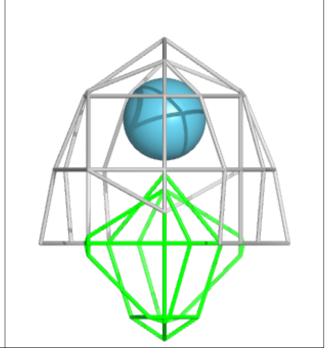


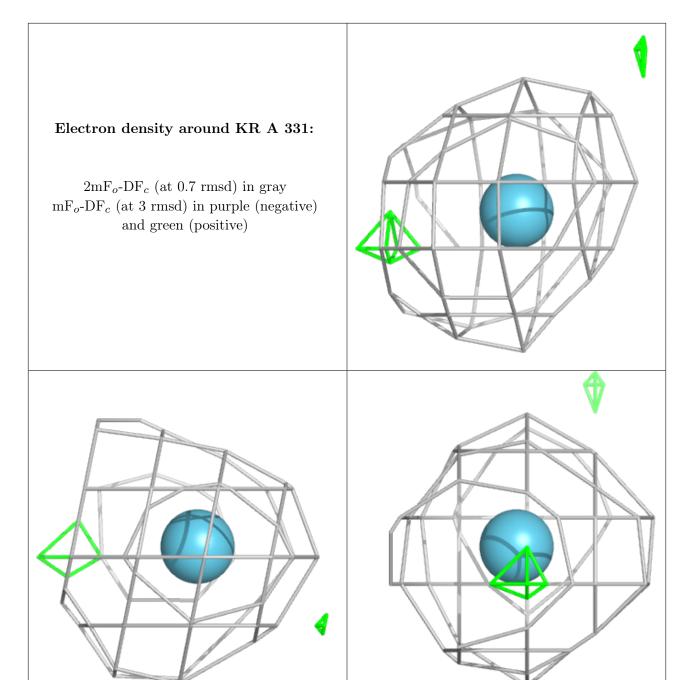
Electron density around KR A 330: $\,$







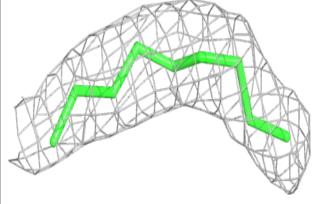


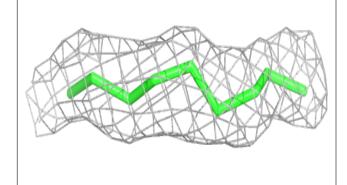


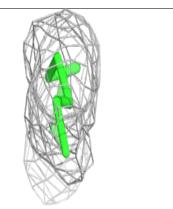


Electron density around LFA A 312:

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

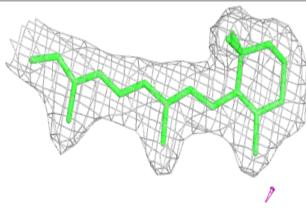


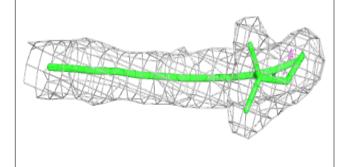


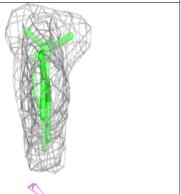


Electron density around RET A 301:

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



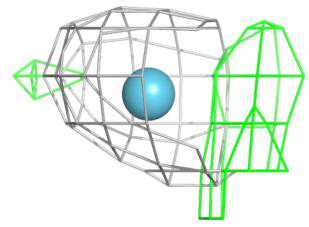


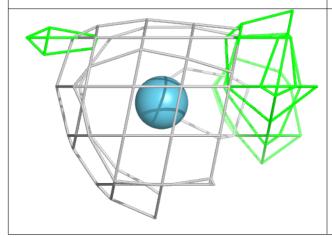


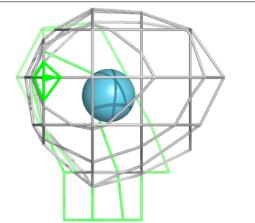


Electron density around KR A 335:

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



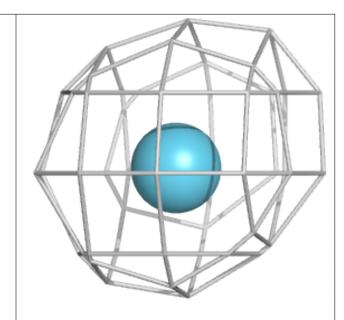


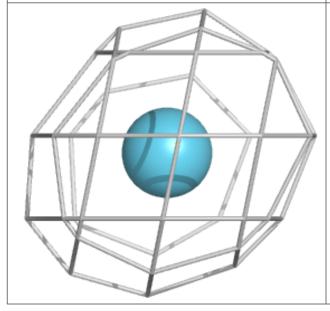


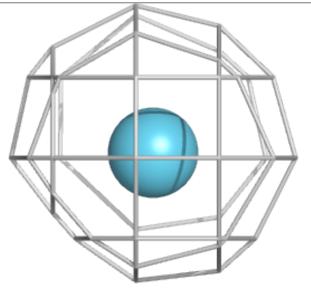


Electron density around KR A 323:

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



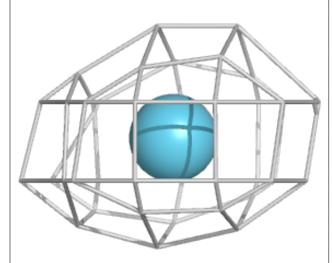


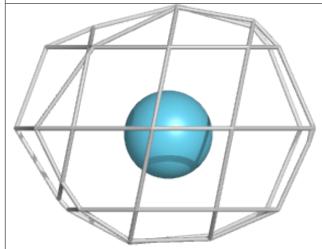


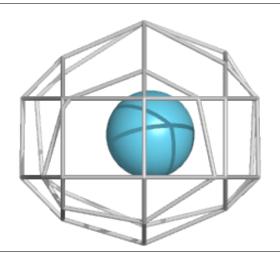


Electron density around KR A 329:

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

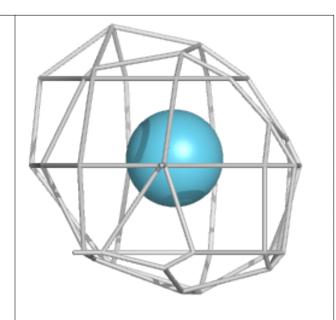


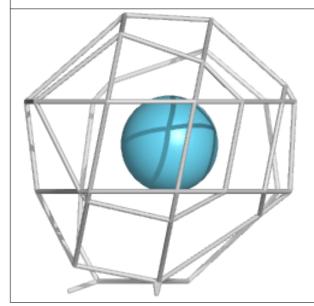


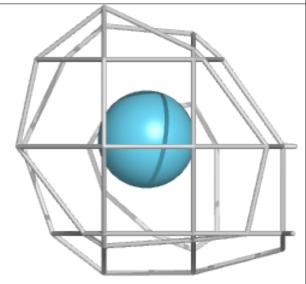


Electron density around KR A 338:

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





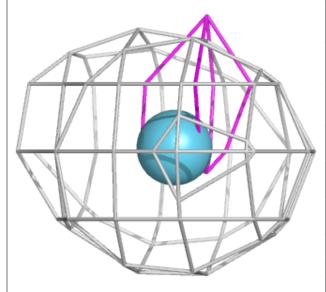


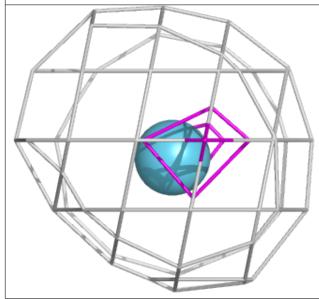


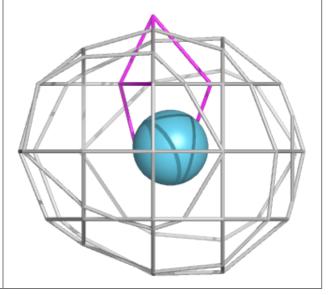


Electron density around KR A 326: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c \ (\mathrm{at}\ 0.7\ \mathrm{rmsd}) \ \mathrm{in}\ \mathrm{gray}$

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



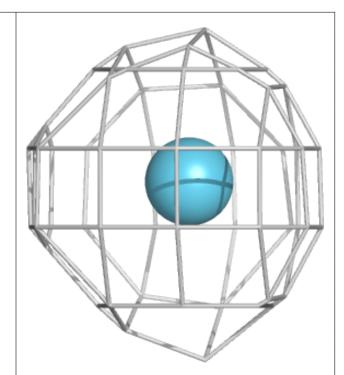


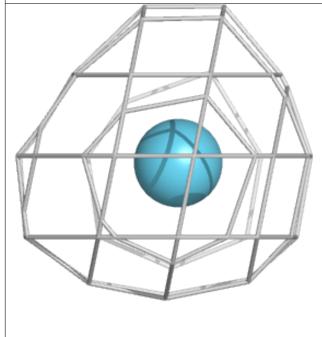


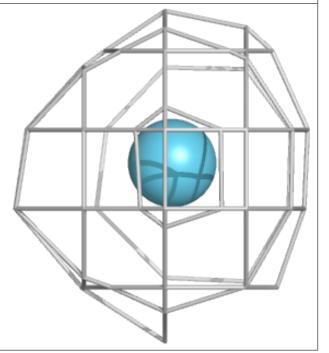


Electron density around KR A 325:

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





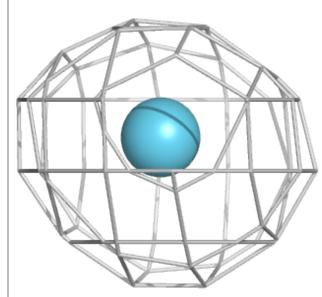


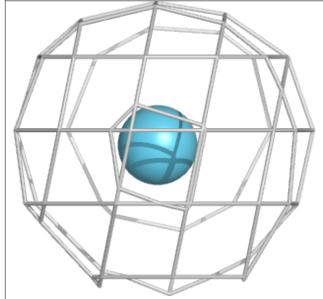
Electron density around KR A 322: 2mF_o-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

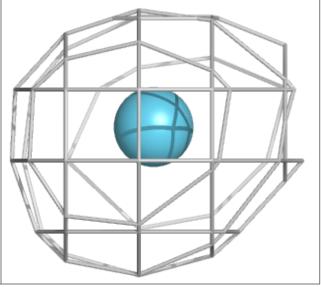


Electron density around KR A 321:

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

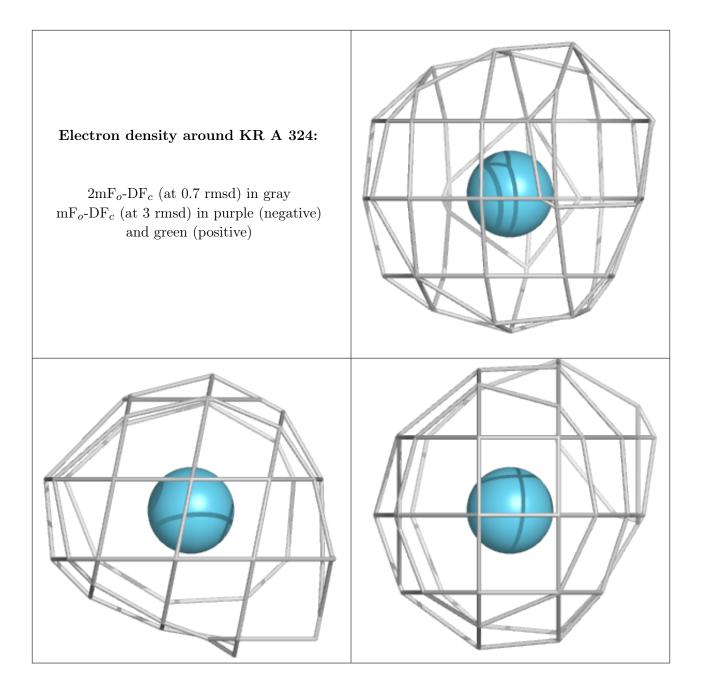






Electron density around KR A 328: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_{o}\text{-}\mathrm{DF}_{c}$ (at 3 rmsd) in purple (negative) and green (positive)





6.5 Other polymers (i)

There are no such residues in this entry.

