



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 6, 2026 – 02:53 pm BST

PDB ID : 9RSE / pdb_00009rse
Title : Human CD1d with lipid antigen bound
Authors : Burns, D.; Maly, M.; Tews, I.; Mansour, S.
Deposited on : 2025-07-01
Resolution : 1.76 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

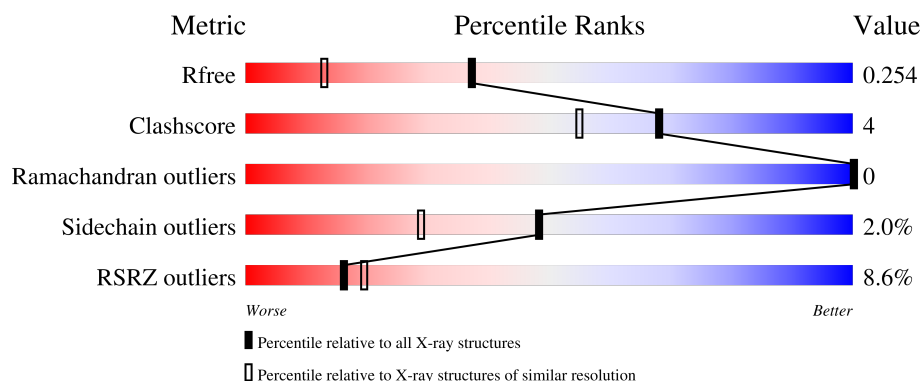
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	296	
1	C	296	
2	B	100	
2	D	100	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13466 atoms, of which 6259 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 Antigen-presenting glycoprotein CD1d.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	273	Total	C	H	N	O	S	0	20	0
			4527	1472	2222	408	418	7			
1	C	273	Total	C	H	N	O	S	0	26	0
			4533	1475	2216	408	427	7			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MET	-	initiating methionine	UNP P15813
A	279	PRO	-	expression tag	UNP P15813
A	280	GLY	-	expression tag	UNP P15813
A	281	SER	-	expression tag	UNP P15813
A	282	GLY	-	expression tag	UNP P15813
A	283	GLY	-	expression tag	UNP P15813
A	284	GLY	-	expression tag	UNP P15813
A	285	LEU	-	expression tag	UNP P15813
A	286	ASN	-	expression tag	UNP P15813
A	287	ASP	-	expression tag	UNP P15813
A	288	ILE	-	expression tag	UNP P15813
A	289	PHE	-	expression tag	UNP P15813
A	290	GLU	-	expression tag	UNP P15813
A	291	ALA	-	expression tag	UNP P15813
A	292	GLN	-	expression tag	UNP P15813
A	293	LYS	-	expression tag	UNP P15813
A	294	ILE	-	expression tag	UNP P15813
A	295	GLU	-	expression tag	UNP P15813
A	296	TRP	-	expression tag	UNP P15813
A	297	HIS	-	expression tag	UNP P15813
C	2	MET	-	initiating methionine	UNP P15813
C	279	PRO	-	expression tag	UNP P15813
C	280	GLY	-	expression tag	UNP P15813
C	281	SER	-	expression tag	UNP P15813
C	282	GLY	-	expression tag	UNP P15813

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Chain	Residue	Modelled	Actual	Comment	Reference
C	283	GLY	-	expression tag	UNP P15813
C	284	GLY	-	expression tag	UNP P15813
C	285	LEU	-	expression tag	UNP P15813
C	286	ASN	-	expression tag	UNP P15813
C	287	ASP	-	expression tag	UNP P15813
C	288	ILE	-	expression tag	UNP P15813
C	289	PHE	-	expression tag	UNP P15813
C	290	GLU	-	expression tag	UNP P15813
C	291	ALA	-	expression tag	UNP P15813
C	292	GLN	-	expression tag	UNP P15813
C	293	LYS	-	expression tag	UNP P15813
C	294	ILE	-	expression tag	UNP P15813
C	295	GLU	-	expression tag	UNP P15813
C	296	TRP	-	expression tag	UNP P15813
C	297	HIS	-	expression tag	UNP P15813

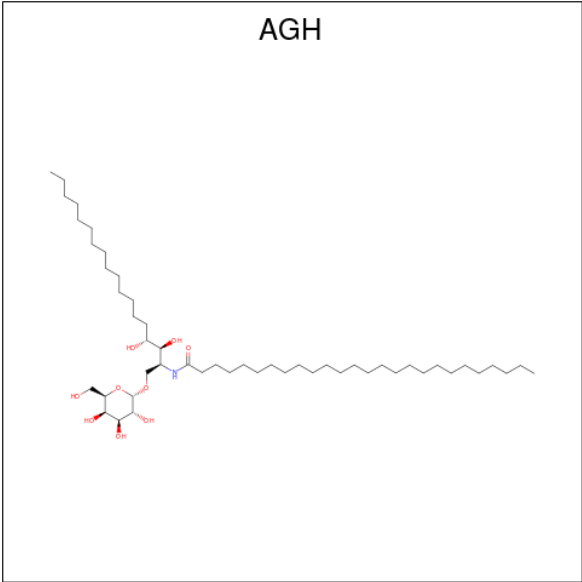
- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	99	Total	C	H	N	O	S	0	7	0
			1660	550	798	143	166	3			
2	D	99	Total	C	H	N	O	S	0	6	0
			1658	550	797	141	167	3			

There are 2 discrepancies between the modelled and reference sequences:

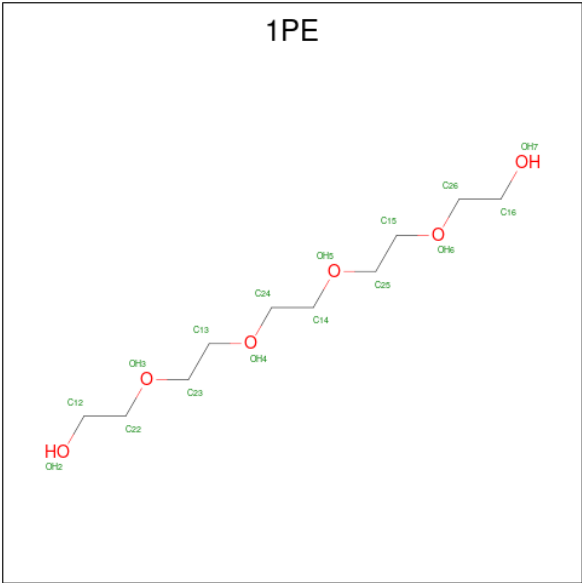
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P61769
D	1	MET	-	initiating methionine	UNP P61769

- Molecule 3 is N-{(1S,2R,3S)-1-[(ALPHA-D-GALACTOPYRANOSYLOXY)METHYL]-2,3-DIHYDROXYHEPTADECYL}HEXACOSANAMIDE (CCD ID: AGH) (formula: C₅₀H₉₉NO₉) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			153	50	93	1	9		
3	C	1	Total	C	H	N	O	0	0
			153	50	93	1	9		

- Molecule 4 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			36	10	20	6		
4	C	1	Total	C	H	O	0	0
			36	10	20	6		

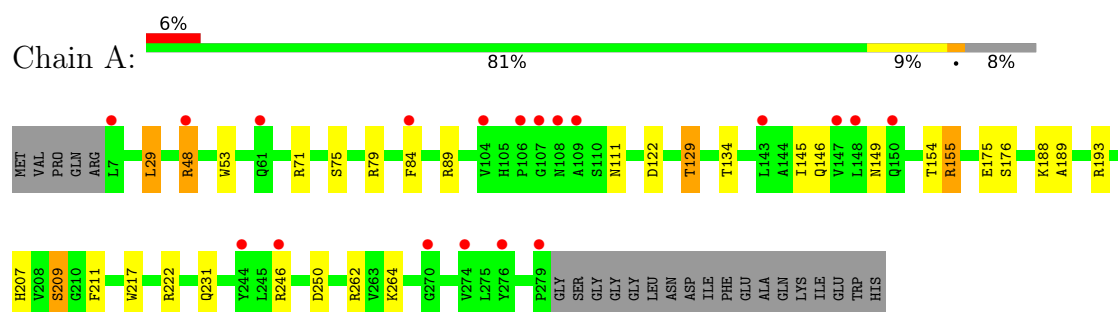
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	235	Total 237	O 237	0	7
5	B	127	Total 130	O 130	0	3
5	C	214	Total 219	O 219	0	8
5	D	123	Total 124	O 124	0	3

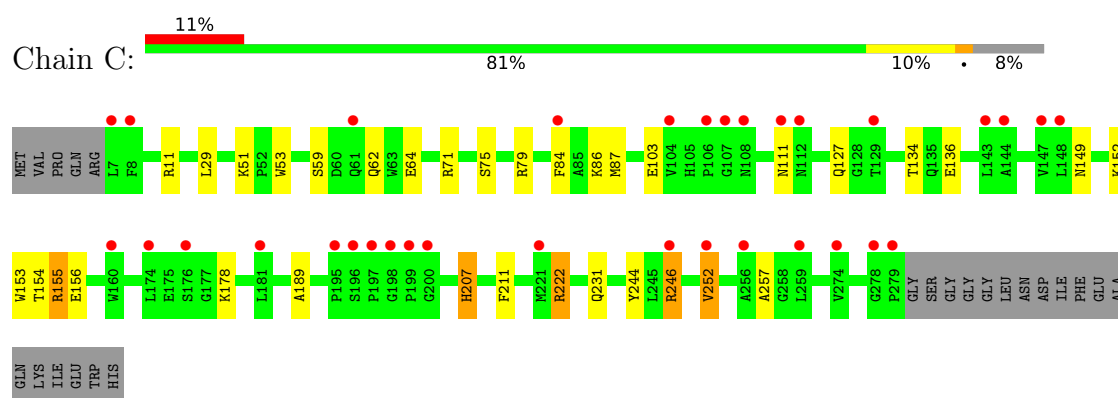
3 Residue-property plots [i](#)

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.

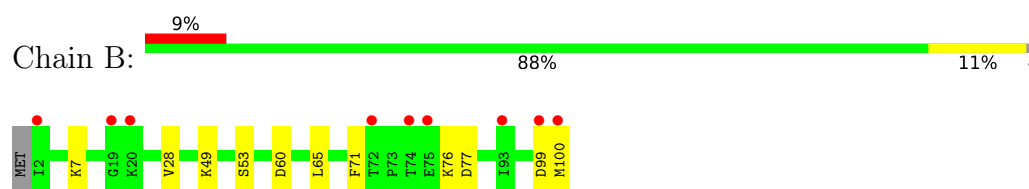
- Molecule 1: Antigen-presenting glycoprotein CD1d



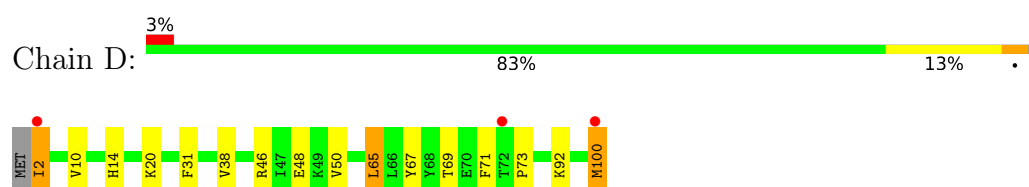
- Molecule 1: Antigen-presenting glycoprotein CD1d



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	117.62Å 156.37Å 51.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.27 – 1.76 49.27 – 1.76	Depositor EDS
% Data completeness (in resolution range)	96.4 (49.27-1.76) 96.4 (49.27-1.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 1.76Å)	Xtriage
Refinement program	Servalcat 0.4.113	Depositor
R, R_{free}	0.213 , 0.254 0.212 , 0.254	Depositor DCC
R_{free} test set	2020 reflections (2.18%)	wwPDB-VP
Wilson B-factor (Å ²)	28.3	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13466	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AGH, 1PE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.82	0/2428	1.32	8/3300 (0.2%)
1	C	0.77	0/2489	1.24	6/3386 (0.2%)
2	B	0.96	1/919 (0.1%)	1.32	4/1244 (0.3%)
2	D	0.88	0/905	1.28	4/1226 (0.3%)
All	All	0.83	1/6741 (0.0%)	1.29	22/9156 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	C	0	6
2	D	0	2
All	All	0	15

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	53	SER	CA-CB	-12.91	1.32	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	PHE	CA-CB-CG	10.77	124.57	113.80
1	C	84	PHE	CA-CB-CG	10.69	124.49	113.80
2	D	65	LEU	N-CA-CB	-8.56	95.84	110.99
1	C	84	PHE	N-CA-CB	8.05	121.68	110.01
1	C	211	PHE	CA-CB-CG	7.58	121.38	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	69	THR	CA-CB-OG1	-7.09	98.96	109.60
1	C	231	GLN	CB-CA-C	6.63	118.96	110.34
1	A	211	PHE	CA-CB-CG	6.57	120.37	113.80
2	B	49	LYS	CB-CA-C	-6.33	100.33	111.22
1	A	231	GLN	N-CA-CB	6.31	120.27	110.12
2	D	71	PHE	CA-CB-CG	6.22	120.02	113.80
1	A	231	GLN	CB-CA-C	-5.83	104.38	110.33
1	A	188	LYS	CB-CA-C	5.53	118.85	109.50
2	D	31	PHE	CA-CB-CG	5.53	119.33	113.80
2	B	60	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	250	ASP	CA-CB-CG	5.37	117.97	112.60
1	C	64	GLU	CB-CG-CD	5.35	121.69	112.60
1	C	207	HIS	CA-CB-CG	5.31	119.11	113.80
1	A	111	ASN	CB-CA-C	5.16	119.23	109.37
2	B	99	ASP	CB-CA-C	5.11	118.87	110.95
2	B	77	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	154	THR	CA-CB-OG1	-5.07	101.99	109.60

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	155[A]	ARG	Sidechain
1	A	222[A]	ARG	Sidechain
1	A	246[A]	ARG	Sidechain
1	A	262	ARG	Sidechain
1	A	48[A]	ARG	Sidechain
1	A	48[B]	ARG	Sidechain
1	A	48[C]	ARG	Sidechain
1	C	155[A]	ARG	Sidechain
1	C	155[B]	ARG	Sidechain
1	C	222[A]	ARG	Sidechain
1	C	222[B]	ARG	Sidechain
1	C	246[A]	ARG	Sidechain
1	C	246[B]	ARG	Sidechain
2	D	2	ILE	Peptide
2	D	46	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2305	2222	2262	15	0
1	C	2317	2216	2209	20	0
2	B	862	798	793	2	0
2	D	861	797	810	13	0
3	A	60	93	99	0	0
3	C	60	93	99	2	0
4	A	16	20	22	0	0
4	C	16	20	22	0	0
5	A	237	0	0	4	0
5	B	130	0	0	0	0
5	C	219	0	0	5	0
5	D	124	0	0	2	0
All	All	7207	6259	6316	47	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (47) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:SER:OG	1:C:79:ARG:NH1	2.01	0.94
1:A:75[A]:SER:OG	1:A:79:ARG:NH1	2.04	0.91
2:D:65:LEU:CD2	2:D:67[B]:TYR:HE1	1.92	0.81
1:C:134[A]:THR:HG22	1:C:136[A]:GLU:OE1	1.82	0.78
1:C:87:MET:HG2	5:C:579[A]:HOH:O	1.83	0.77
1:A:217:TRP:CE3	1:A:264:LYS:HD2	2.21	0.76
2:D:65:LEU:HD21	2:D:67[B]:TYR:HE1	1.54	0.73
2:D:65:LEU:HD21	2:D:67[B]:TYR:CE1	2.29	0.68
1:C:11[A]:ARG:NH1	5:C:401:HOH:O	2.21	0.67
1:C:222[A]:ARG:NH2	1:C:257:ALA:O	2.30	0.65
1:A:149:ASN:HA	1:A:155[A]:ARG:HD2	1.80	0.64
2:D:14:HIS:HE1	5:D:293:HOH:O	1.81	0.64
1:A:175:GLU:HG2	5:A:606:HOH:O	1.98	0.63
2:D:20:LYS:O	2:D:73:PRO:HD2	1.99	0.63
1:C:152:LYS:HG2	1:C:156:GLU:OE1	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:65:LEU:CD2	2:D:67[B]:TYR:CE1	2.80	0.60
1:C:59:SER:OG	1:C:62:GLN:HG3	2.02	0.59
1:A:193:ARG:HD2	5:A:540:HOH:O	2.04	0.57
1:C:154:THR:HG23	3:C:301:AGH:HAC2	1.86	0.57
2:D:10:VAL:O	2:D:100:MET:CE	2.54	0.55
1:A:89:ARG:NH1	2:D:48:GLU:OE1	2.39	0.55
1:C:246[B]:ARG:HH22	2:D:100:MET:C	2.16	0.54
1:C:244:TYR:OH	1:C:246[A]:ARG:HG2	2.08	0.53
1:A:48[C]:ARG:HD2	5:A:520:HOH:O	2.08	0.53
2:D:10:VAL:O	2:D:100:MET:HE1	2.10	0.52
2:D:38:VAL:HB	2:D:67[B]:TYR:CZ	2.45	0.52
1:C:51:LYS:HG3	1:C:53:TRP:CZ2	2.45	0.51
1:C:86:LYS:HG3	5:C:610:HOH:O	2.10	0.50
1:C:103[A]:GLU:HB3	1:C:111[A]:ASN:OD1	2.12	0.49
1:C:149:ASN:HA	1:C:155[A]:ARG:HD2	1.94	0.48
1:A:122:ASP:HB3	1:A:134[A]:THR:HG21	1.97	0.46
1:A:75[B]:SER:HB3	1:A:79:ARG:HH12	1.81	0.45
2:D:50:VAL:CG1	2:D:67[A]:TYR:HD2	2.30	0.45
1:A:53:TRP:HB2	1:A:176[A]:SER:OG	2.17	0.45
1:C:252:VAL:HG12	5:C:556:HOH:O	2.17	0.44
1:A:71[A]:ARG:HD3	1:C:71[A]:ARG:HD3	1.99	0.44
1:C:189:ALA:HA	1:C:207:HIS:O	2.17	0.44
1:A:209:SER:CB	5:A:406:HOH:O	2.66	0.42
1:A:189:ALA:HA	1:A:207:HIS:O	2.19	0.42
1:A:129:THR:HG22	1:A:155[B]:ARG:HH11	1.85	0.42
1:C:127:GLN:NE2	5:C:409:HOH:O	2.49	0.41
2:D:92:LYS:NZ	5:D:213:HOH:O	2.53	0.41
2:B:65:LEU:N	2:B:65:LEU:HD23	2.35	0.41
1:C:152:LYS:HG3	1:C:155[B]:ARG:HH21	1.85	0.41
1:A:29:LEU:HD23	1:A:29:LEU:N	2.36	0.40
1:C:153:TRP:HZ3	3:C:301:AGH:HAB2	1.85	0.40
2:B:7:LYS:O	2:B:28:VAL:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	292/296 (99%)	285 (98%)	7 (2%)	0	100	100
1	C	297/296 (100%)	291 (98%)	6 (2%)	0	100	100
2	B	104/100 (104%)	103 (99%)	1 (1%)	0	100	100
2	D	103/100 (103%)	101 (98%)	2 (2%)	0	100	100
All	All	796/792 (100%)	780 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	257/256 (100%)	252 (98%)	5 (2%)	50	31
1	C	263/256 (103%)	260 (99%)	3 (1%)	65	52
2	B	101/95 (106%)	98 (97%)	3 (3%)	36	16
2	D	100/95 (105%)	98 (98%)	2 (2%)	48	29
All	All	721/702 (103%)	708 (98%)	13 (2%)	48	33

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	129	THR
1	A	145	ILE
1	A	146	GLN
1	A	209	SER
2	B	71	PHE
2	B	76	LYS
2	B	100	MET

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Mol	Chain	Res	Type
1	C	29	LEU
1	C	178	LYS
1	C	252	VAL
2	D	2	ILE
2	D	100	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	115	HIS
1	C	115	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	1PE	C	302	-	15,15,15	0.38	0	14,14,14	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AGH	C	301	-	60,60,60	0.79	1 (1%)	65,69,69	0.78	3 (4%)
3	AGH	A	301	-	60,60,60	0.67	1 (1%)	65,69,69	0.62	0
4	1PE	A	302	-	15,15,15	0.55	0	14,14,14	0.44	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
4	1PE	C	302	-	-	1/13/13/13	-
3	AGH	C	301	-	-	6/58/78/78	0/1/1/1
3	AGH	A	301	-	-	0/58/78/78	0/1/1/1
4	1PE	A	302	-	-	1/13/13/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	AGH	CAC-CAB	-3.79	1.38	1.52
3	A	301	AGH	O3-C3	2.22	1.48	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	301	AGH	C1-C2-N2	2.20	112.85	109.61
3	C	301	AGH	CAF-CAE-CAD	-2.12	103.67	114.42
3	C	301	AGH	C2-N2-CAA	-2.03	120.05	123.48

There are no chirality outliers.

All (8) torsion outliers are listed below:

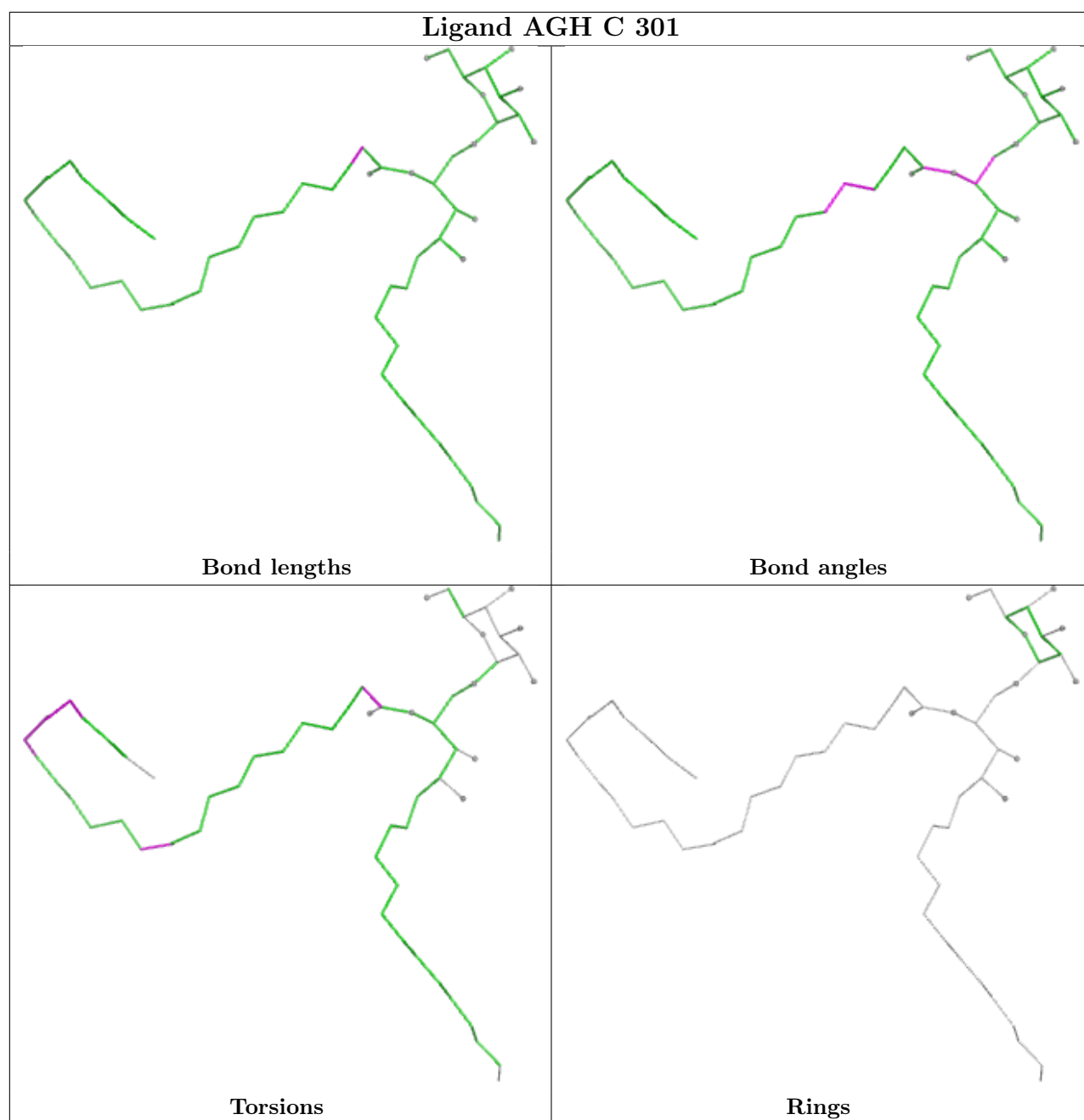
Mol	Chain	Res	Type	Atoms
4	A	302	1PE	OH4-C13-C23-OH3
3	C	301	AGH	CAR-CAS-CAT-CAU
3	C	301	AGH	CAT-CAU-CAV-CAW
4	C	302	1PE	C24-C14-OH5-C25
3	C	301	AGH	CAK-CAL-CAM-CAN
3	C	301	AGH	CAU-CAV-CAW-CAX
3	C	301	AGH	OAA-CAA-CAB-CAC
3	C	301	AGH	CAQ-CAR-CAS-CAT

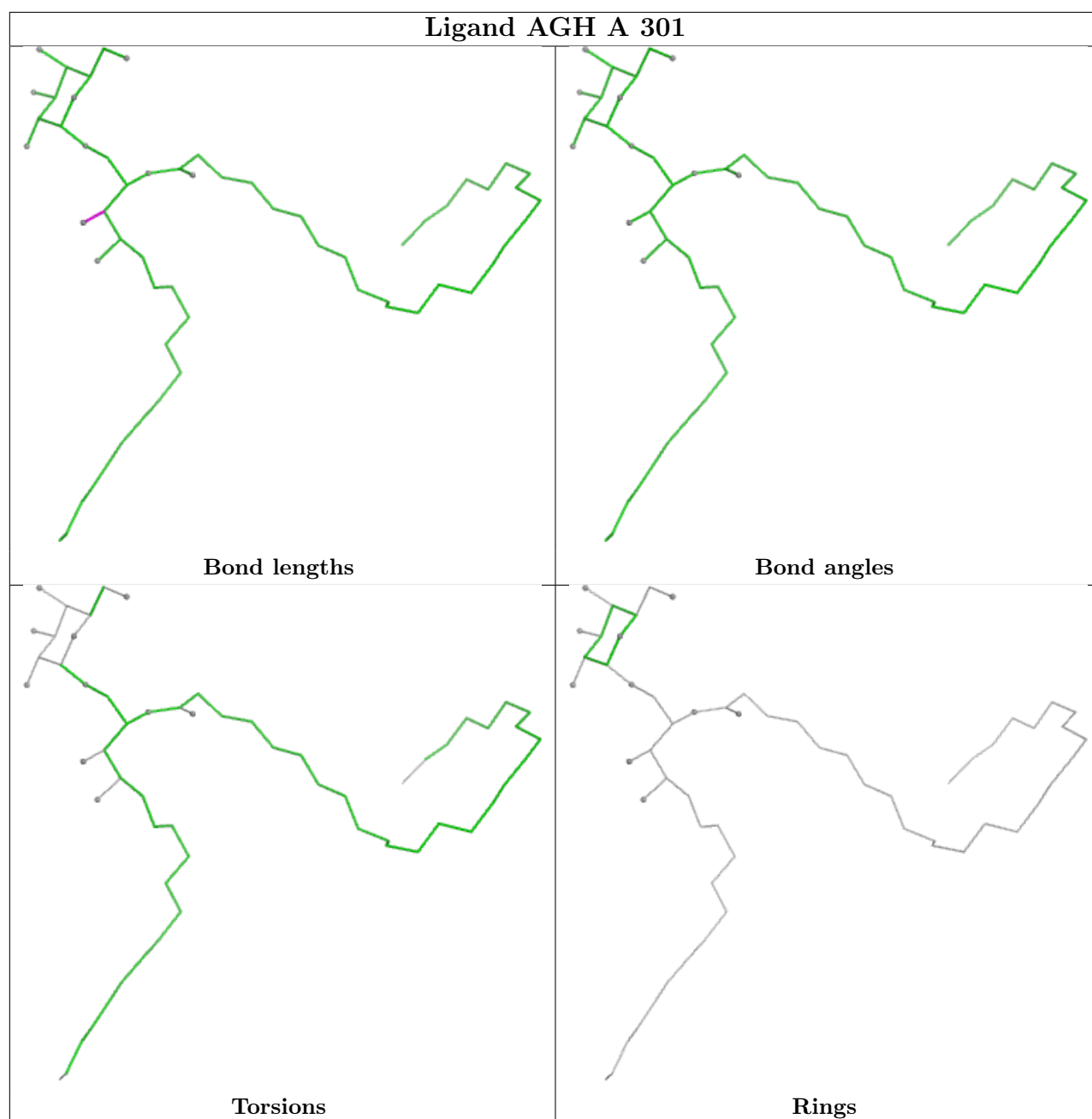
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	AGH	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	273/296 (92%)	0.51	19 (6%)	22 26	10, 31, 55, 86	17 (6%)
1	C	273/296 (92%)	0.80	33 (12%)	8 10	10, 34, 67, 119	19 (6%)
2	B	99/100 (99%)	0.38	9 (9%)	15 18	11, 29, 65, 83	4 (4%)
2	D	99/100 (99%)	0.48	3 (3%)	52 59	11, 30, 59, 87	5 (5%)
All	All	744/792 (93%)	0.59	64 (8%)	16 19	10, 32, 62, 119	45 (6%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	147	VAL	5.6
2	D	2	ILE	5.1
1	A	279	PRO	5.0
1	C	199	PRO	4.7
1	A	7	LEU	4.4
1	C	274	VAL	4.3
1	C	7	LEU	4.1
2	B	100	MET	4.1
1	C	107	GLY	3.8
1	C	106	PRO	3.7
1	C	246[A]	ARG	3.7
1	C	197	PRO	3.6
1	C	160	TRP	3.5
1	A	246[A]	ARG	3.5
1	C	104	VAL	3.3
1	C	200	GLY	3.2
1	A	109	ALA	3.2
1	A	150[A]	GLN	3.1
1	A	107	GLY	3.1
1	C	278	GLY	3.0
1	C	143	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	256	ALA	3.0
1	C	108	ASN	2.9
1	A	270	GLY	2.9
2	B	74	THR	2.9
1	A	148	LEU	2.9
2	D	100	MET	2.8
1	C	259	LEU	2.8
1	C	111[A]	ASN	2.8
1	C	61	GLN	2.8
1	C	279	PRO	2.7
1	A	143	LEU	2.7
1	A	61	GLN	2.7
1	C	181	LEU	2.7
2	B	2	ILE	2.6
1	A	106	PRO	2.6
1	C	112[A]	ASN	2.6
1	A	276	TYR	2.5
1	A	104	VAL	2.5
2	D	72	THR	2.5
1	C	147	VAL	2.5
1	C	252	VAL	2.5
1	C	84	PHE	2.5
1	C	144	ALA	2.5
2	B	93	ILE	2.5
1	C	196	SER	2.4
2	B	99	ASP	2.4
1	C	8	PHE	2.4
1	C	221	MET	2.4
1	C	129	THR	2.3
1	C	176	SER	2.3
1	C	174	LEU	2.3
1	A	274	VAL	2.3
1	A	48[A]	ARG	2.2
1	C	198	GLY	2.1
1	C	195	PRO	2.1
2	B	72	THR	2.1
2	B	75	GLU	2.1
2	B	19	GLY	2.1
1	C	148	LEU	2.1
1	A	108	ASN	2.0
2	B	20	LYS	2.0
1	A	84	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	244	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

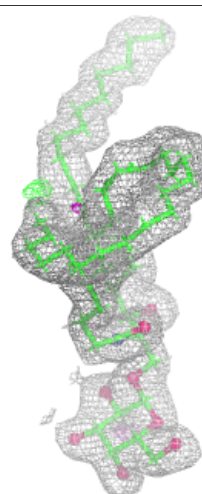
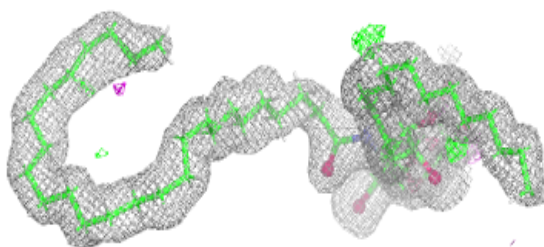
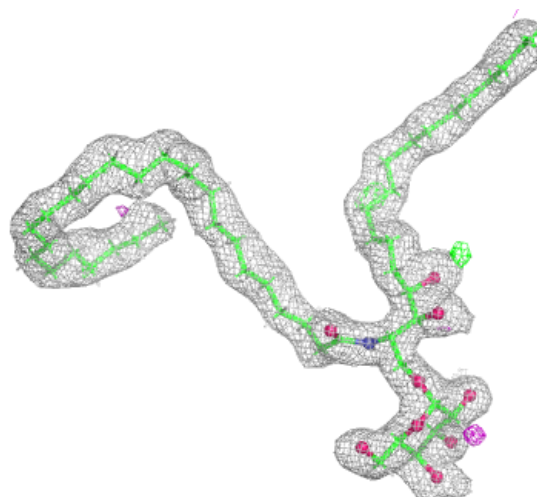
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	AGH	A	301	60/60	0.93	0.08	22,29,39,40	0
3	AGH	C	301	60/60	0.93	0.09	21,29,43,44	0
4	1PE	A	302	16/16	0.93	0.10	27,40,59,59	0
4	1PE	C	302	16/16	0.93	0.09	33,50,60,60	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.

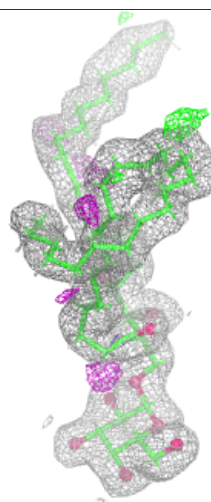
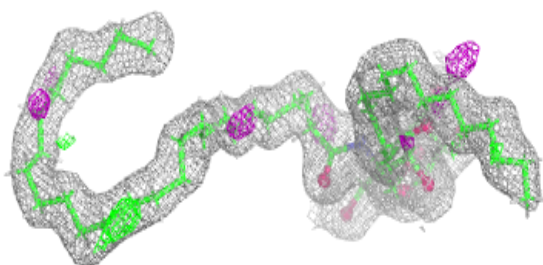
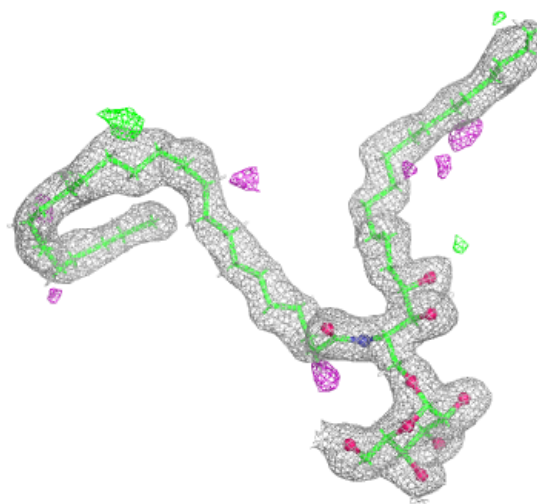
Electron density around AGH A 301:

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



Electron density around AGH C 301:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.