Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 02:14 AM BST

PDB ID	:	3M7O
Title	:	Crystal structure of mouse MD-1 in complex with phosphatidylcholine
Authors	:	Harada, H.; Ohto, U.; Satow, Y.
Deposited on	:	2010-03-17
Resolution	:	1.65 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 following versions of software and data (see references ⓘ) were used in the production of this report:

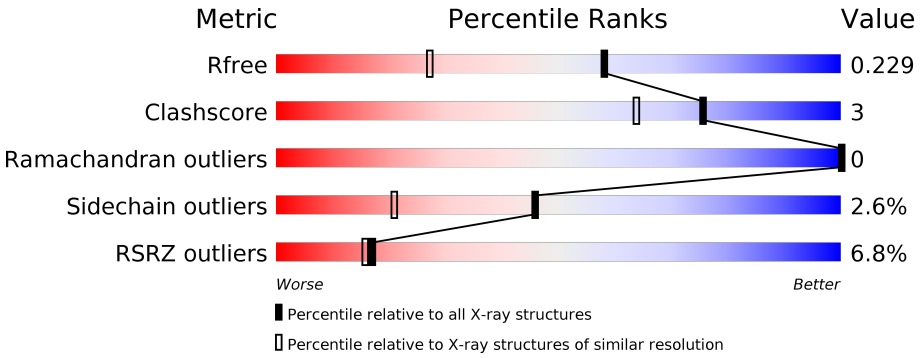
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 1.65 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	162	4% 75% 10% 15%
1	B	162	10% 75% 5% 19%
1	C	162	6% 77% 19%
1	D	162	2% 70% 9% 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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	201	X	-	-	X

2 Entry composition

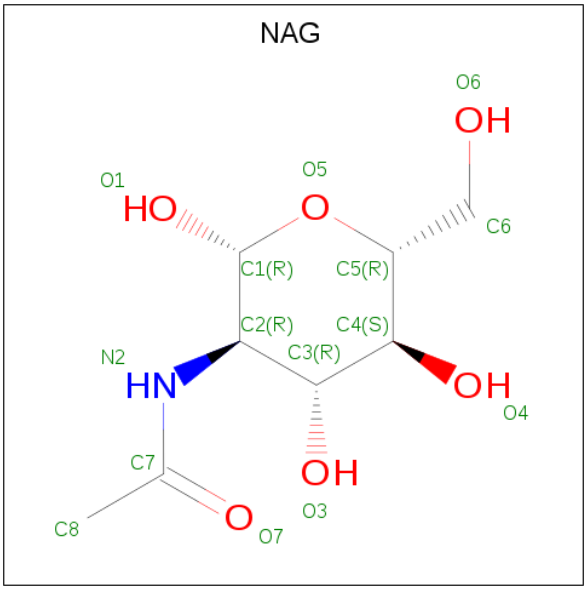
There are 5 unique types of molecules in this entry. The entry contains 4955 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lymphocyte antigen 86.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	137	Total	C	N	O	S	0	1	0
			1075	676	183	209	7			
1	B	131	Total	C	N	O	S	0	1	0
			1024	646	175	196	7			
1	C	131	Total	C	N	O	S	0	1	0
			1024	646	175	196	7			
1	D	131	Total	C	N	O	S	0	1	0
			1024	646	175	196	7			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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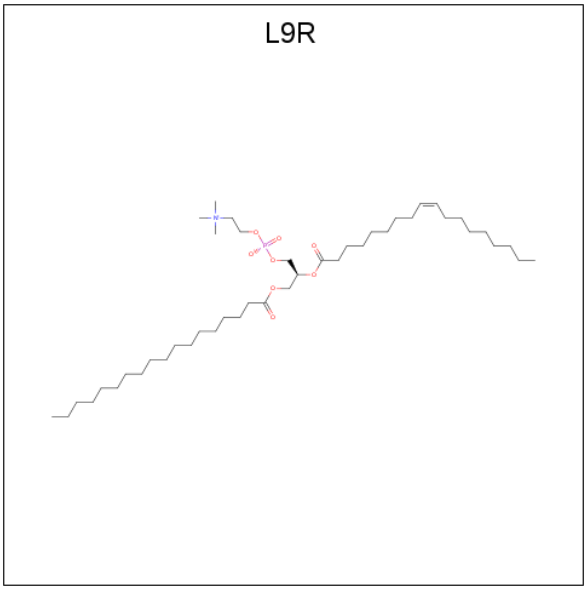
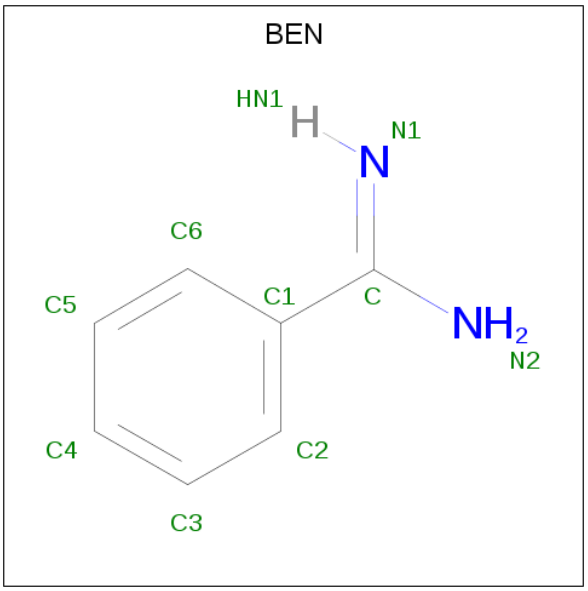
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	C	1	Total C N O 14 8 1 5	0	0
2	C	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0

- Molecule 3 is (2S)-3-(octadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: L9R) (formula: $C_{44}H_{86}NO_8P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 54 44 1 8 1	0	0
3	D	1	Total C N O P 54 44 1 8 1	0	0

- Molecule 4 is BENZAMIDINE (three-letter code: BEN) (formula: $C_7H_8N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 9 7 2	0	0
4	A	1	Total C N 9 7 2	0	0
4	A	1	Total C N 9 7 2	0	0
4	A	1	Total C N 9 7 2	0	0
4	A	1	Total C N 9 7 2	0	0
4	B	1	Total C N 9 7 2	0	0
4	B	1	Total C N 9 7 2	0	0
4	B	1	Total C N 9 7 2	0	0
4	C	1	Total C N 9 7 2	0	0
4	C	1	Total C N 9 7 2	0	0
4	C	1	Total C N 9 7 2	0	0
4	D	1	Total C N 9 7 2	0	0
4	D	1	Total C N 9 7 2	0	0
4	D	1	Total C N 9 7 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C N 9 7 2	0	0
4	D	1	Total C N 9 7 2	0	0

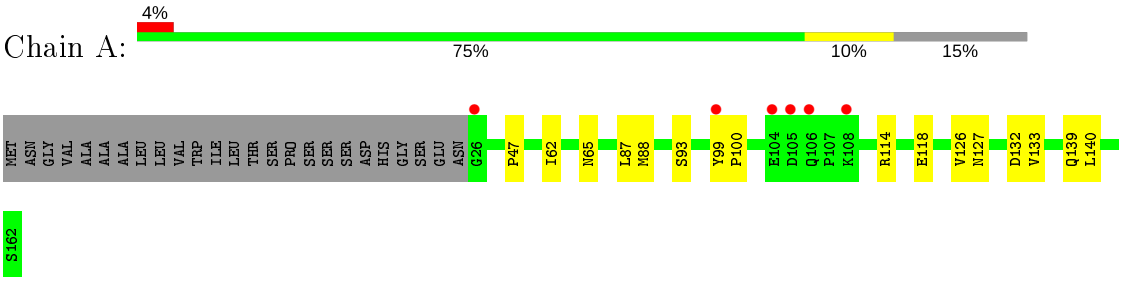
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	128	Total O 128 128	0	0
5	B	97	Total O 97 97	0	0
5	C	104	Total O 104 104	0	0
5	D	115	Total O 115 115	0	0

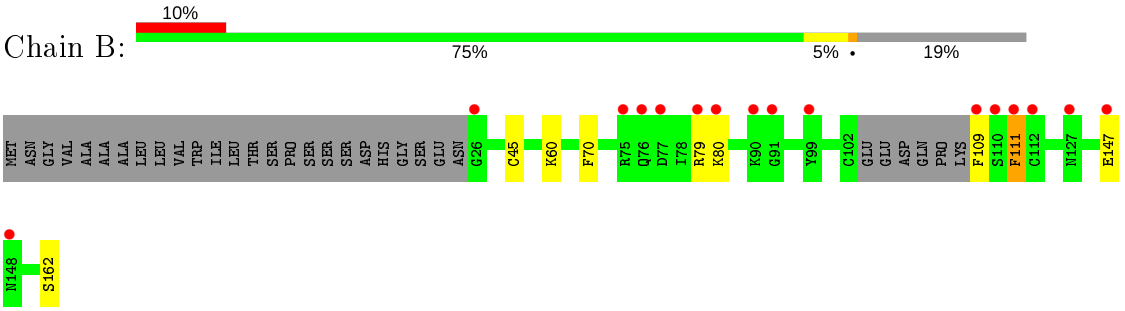
3 Residue-property plots

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.

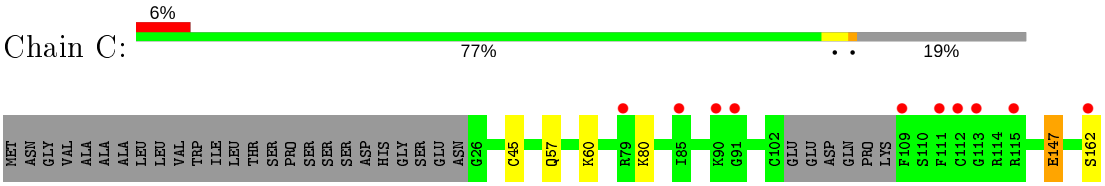
- Molecule 1: Lymphocyte antigen 86



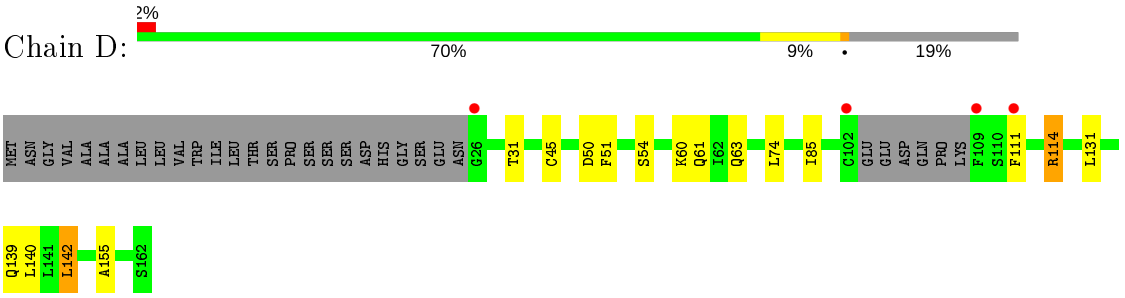
- Molecule 1: Lymphocyte antigen 86



- Molecule 1: Lymphocyte antigen 86



- Molecule 1: Lymphocyte antigen 86



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	90.30Å 90.30Å 86.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 1.65 29.96 – 1.65	Depositor EDS
% Data completeness (in resolution range)	98.1 (29.96-1.65) 84.6 (29.96-1.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.94 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.195 , 0.227 0.196 , 0.229	Depositor DCC
R_{free} test set	3551 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	27.0	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 53.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.017 for -h,-l,-k 0.001 for -h,l,k 0.001 for l,-k,h 0.018 for -l,-k,-h 0.033 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4955	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BEN, NAG, L9R

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	0.53	0/1099	0.69	1/1487 (0.1%)
1	B	0.49	0/1046	0.65	0/1414
1	C	0.52	0/1046	0.65	0/1414
1	D	0.59	0/1046	0.72	2/1414 (0.1%)
All	All	0.53	0/4237	0.68	3/5729 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	50	ASP	CB-CG-OD2	6.07	123.76	118.30
1	D	140	LEU	CA-CB-CG	5.87	128.79	115.30
1	A	140	LEU	CA-CB-CG	5.77	128.58	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1075	0	1045	10	0
1	B	1024	0	1000	6	0
1	C	1024	0	1000	2	0
1	D	1024	0	1000	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	28	0	26	0	0
2	B	28	0	26	0	0
2	C	28	0	26	0	0
2	D	28	0	26	0	0
3	A	54	0	86	2	0
3	D	54	0	86	1	0
4	A	45	0	35	0	0
4	B	27	0	21	0	0
4	C	27	0	21	1	0
4	D	45	0	35	3	0
5	A	128	0	0	1	0
5	B	97	0	0	0	0
5	C	104	0	0	0	0
5	D	115	0	0	1	0
All	All	4955	0	4433	28	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 3.

All (28) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:LYS:HB2	1:B:147:GLU:HG3	1.56	0.88
1:B:60:LYS:HD2	1:B:162:SER:O	1.80	0.80
1:D:31:THR:HB	4:D:164:BEN:H5	1.69	0.74
1:D:139:GLN:NE2	5:D:318:HOH:O	2.22	0.72
1:C:60:LYS:HD2	1:C:162:SER:O	1.90	0.71
1:D:61:GLN:HE21	1:D:63:GLN:HE22	1.46	0.64
1:A:139:GLN:NE2	5:A:212:HOH:O	2.31	0.63
1:A:114:ARG:HD3	1:A:118:GLU:OE1	2.00	0.60
1:A:127:ASN:H	3:A:301:L9R:H12A	1.71	0.56
1:D:74:LEU:CD1	1:D:114:ARG:HB3	2.35	0.56
1:A:87:LEU:HD21	3:A:301:L9R:H44	1.88	0.56
1:A:65:ASN:HA	1:A:126:VAL:O	2.06	0.56
1:D:31:THR:CB	4:D:164:BEN:H5	2.35	0.55
1:B:70:PHE:CE2	1:B:111:PHE:CZ	2.96	0.53
1:A:65:ASN:HD22	1:A:127:ASN:HA	1.73	0.53
1:B:70:PHE:HE2	1:B:111:PHE:CZ	2.27	0.52
1:D:74:LEU:HD11	1:D:114:ARG:HB3	1.93	0.50
1:D:131:LEU:HD21	3:D:301:L9R:H43	1.94	0.49
1:B:109:PHE:HD2	1:B:111:PHE:HB2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:PHE:CD2	1:B:111:PHE:HB2	2.49	0.48
1:C:80:LYS:HB2	1:C:147:GLU:HG3	1.96	0.48
1:A:47:PRO:O	4:C:163:BEN:H5	2.16	0.45
1:A:88:MET:HG2	1:A:93:SER:HA	1.98	0.45
1:A:99:TYR:HA	1:A:100:PRO:HD3	1.90	0.45
1:D:51:PHE:HZ	1:D:155:ALA:HB2	1.83	0.44
1:D:54:SER:HB2	4:D:167:BEN:H3	2.02	0.42
1:A:62:ILE:HD12	1:A:133:VAL:CG2	2.51	0.41
1:D:85:ILE:HG12	1:D:142:LEU:HD23	2.02	0.40

There are no symmetry-related clashes.

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	136/162 (84%)	132 (97%)	4 (3%)	0	100	100
1	B	128/162 (79%)	126 (98%)	2 (2%)	0	100	100
1	C	128/162 (79%)	125 (98%)	3 (2%)	0	100	100
1	D	128/162 (79%)	125 (98%)	3 (2%)	0	100	100
All	All	520/648 (80%)	508 (98%)	12 (2%)	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	120/139 (86%)	119 (99%)	1 (1%)	81 70
1	B	114/139 (82%)	111 (97%)	3 (3%)	46 21
1	C	114/139 (82%)	111 (97%)	3 (3%)	46 21
1	D	114/139 (82%)	109 (96%)	5 (4%)	28 7
All	All	462/556 (83%)	450 (97%)	12 (3%)	46 21

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	ASP
1	B	45	CYS
1	B	79	ARG
1	B	111	PHE
1	C	45	CYS
1	C	57	GLN
1	C	147	GLU
1	D	45	CYS
1	D	60	LYS
1	D	111	PHE
1	D	114	ARG
1	D	142	LEU

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

Mol	Chain	Res	Type
1	A	49	GLN
1	A	65	ASN
1	A	139	GLN
1	B	49	GLN
1	B	57	GLN
1	B	63	GLN
1	B	139	GLN
1	C	49	GLN
1	C	139	GLN
1	D	43	GLN
1	D	49	GLN
1	D	61	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	BEN	D	167	-	9,9,9	1.29	1 (11%)	7,11,11	1.01	1 (14%)
2	NAG	A	202	1	14,14,15	0.63	0	17,19,21	1.48	2 (11%)
4	BEN	D	163	-	9,9,9	1.31	1 (11%)	7,11,11	0.97	0
2	NAG	D	202	1	14,14,15	0.65	0	17,19,21	0.88	0
4	BEN	C	163	-	9,9,9	1.35	1 (11%)	7,11,11	0.74	0
2	NAG	A	201	1	14,14,15	0.59	0	17,19,21	1.07	1 (5%)
4	BEN	D	164	-	9,9,9	1.41	1 (11%)	7,11,11	1.07	1 (14%)
3	L9R	D	301	-	53,53,53	1.13	3 (5%)	59,61,61	0.90	2 (3%)
4	BEN	C	165	-	9,9,9	1.35	1 (11%)	7,11,11	1.09	1 (14%)
4	BEN	A	165	-	9,9,9	1.16	1 (11%)	7,11,11	1.57	1 (14%)
2	NAG	B	202	1	14,14,15	0.67	1 (7%)	17,19,21	0.95	0
2	NAG	D	201	1	14,14,15	0.59	0	17,19,21	1.19	1 (5%)
2	NAG	B	201	1	14,14,15	0.45	0	17,19,21	1.27	3 (17%)
4	BEN	B	164	-	9,9,9	1.20	1 (11%)	7,11,11	1.28	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	C	201	1	14,14,15	0.65	0	17,19,21	1.07	2 (11%)
4	BEN	A	163	-	9,9,9	1.12	1 (11%)	7,11,11	1.50	1 (14%)
4	BEN	C	164	-	9,9,9	1.28	1 (11%)	7,11,11	1.09	1 (14%)
4	BEN	B	165	-	9,9,9	1.31	1 (11%)	7,11,11	0.65	0
4	BEN	A	164	-	9,9,9	1.21	1 (11%)	7,11,11	0.97	0
4	BEN	D	165	-	9,9,9	1.32	1 (11%)	7,11,11	0.76	0
3	L9R	A	301	-	53,53,53	1.10	3 (5%)	59,61,61	0.91	2 (3%)
2	NAG	C	202	1	14,14,15	0.66	0	17,19,21	0.70	0
4	BEN	D	166	-	9,9,9	1.38	1 (11%)	7,11,11	0.74	0
4	BEN	B	163	-	9,9,9	1.40	1 (11%)	7,11,11	1.07	1 (14%)
4	BEN	A	166	-	9,9,9	1.31	1 (11%)	7,11,11	1.04	1 (14%)
4	BEN	A	167	-	9,9,9	1.47	1 (11%)	7,11,11	1.10	1 (14%)

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	BEN	D	167	-	-	1/4/4/4	0/1/1/1
2	NAG	A	202	1	-	0/6/23/26	0/1/1/1
4	BEN	D	163	-	-	0/4/4/4	0/1/1/1
2	NAG	D	202	1	-	0/6/23/26	0/1/1/1
4	BEN	C	163	-	-	1/4/4/4	0/1/1/1
2	NAG	A	201	1	-	2/6/23/26	0/1/1/1
4	BEN	D	164	-	-	0/4/4/4	0/1/1/1
3	L9R	D	301	-	-	29/57/57/57	-
4	BEN	C	165	-	-	0/4/4/4	0/1/1/1
4	BEN	A	165	-	-	0/4/4/4	0/1/1/1
2	NAG	B	202	1	-	0/6/23/26	0/1/1/1
2	NAG	D	201	1	-	0/6/23/26	0/1/1/1
2	NAG	B	201	1	1/1/5/7	4/6/23/26	0/1/1/1
4	BEN	B	164	-	-	0/4/4/4	0/1/1/1
2	NAG	C	201	1	-	2/6/23/26	0/1/1/1
4	BEN	A	163	-	-	0/4/4/4	0/1/1/1
4	BEN	C	164	-	-	0/4/4/4	0/1/1/1
4	BEN	B	165	-	-	0/4/4/4	0/1/1/1
4	BEN	A	164	-	-	0/4/4/4	0/1/1/1
4	BEN	D	165	-	-	0/4/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	L9R	A	301	-	-	26/57/57/57	-
2	NAG	C	202	1	-	0/6/23/26	0/1/1/1
4	BEN	D	166	-	-	4/4/4/4	0/1/1/1
4	BEN	B	163	-	-	2/4/4/4	0/1/1/1
4	BEN	A	166	-	-	0/4/4/4	0/1/1/1
4	BEN	A	167	-	-	0/4/4/4	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	301	L9R	O2-C31	4.59	1.47	1.34
3	D	301	L9R	O3-C11	4.56	1.46	1.33
3	A	301	L9R	O3-C11	4.43	1.46	1.33
3	A	301	L9R	O2-C31	4.39	1.46	1.34
4	A	167	BEN	C1-C	-4.07	1.40	1.47
4	D	164	BEN	C1-C	-3.88	1.40	1.47
3	A	301	L9R	C40-C39	3.71	1.53	1.31
4	C	163	BEN	C1-C	-3.65	1.40	1.47
4	B	163	BEN	C1-C	-3.62	1.40	1.47
3	D	301	L9R	C40-C39	3.61	1.52	1.31
4	D	166	BEN	C1-C	-3.50	1.41	1.47
4	A	166	BEN	C1-C	-3.43	1.41	1.47
4	C	165	BEN	C1-C	-3.41	1.41	1.47
4	D	165	BEN	C1-C	-3.40	1.41	1.47
4	D	167	BEN	C1-C	-3.37	1.41	1.47
4	C	164	BEN	C1-C	-3.24	1.41	1.47
4	B	165	BEN	C1-C	-3.18	1.41	1.47
4	D	163	BEN	C1-C	-3.18	1.41	1.47
4	A	164	BEN	C1-C	-3.06	1.41	1.47
4	B	164	BEN	C1-C	-2.88	1.42	1.47
4	A	165	BEN	C1-C	-2.87	1.42	1.47
4	A	163	BEN	C1-C	-2.50	1.42	1.47
2	B	202	NAG	C1-C2	2.18	1.55	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	165	BEN	C1-C-N2	3.92	123.96	118.05
3	D	301	L9R	O2-C31-C32	3.85	119.80	111.50
3	A	301	L9R	O2-C31-C32	3.82	119.74	111.50
2	D	201	NAG	C1-O5-C5	3.77	117.29	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	202	NAG	O7-C7-N2	3.69	128.73	121.95
4	B	164	BEN	C1-C-N2	3.29	123.00	118.05
2	B	201	NAG	C1-O5-C5	3.24	116.58	112.19
2	A	202	NAG	O5-C1-C2	-3.10	106.40	111.29
4	C	164	BEN	C1-C-N2	2.76	122.22	118.05
4	C	165	BEN	C1-C-N2	2.64	122.03	118.05
3	D	301	L9R	O3-C11-C12	2.63	120.16	111.91
2	C	201	NAG	C4-C3-C2	2.53	114.73	111.02
4	A	163	BEN	C1-C-N2	2.49	121.80	118.05
4	D	167	BEN	C1-C-N2	2.49	121.79	118.05
4	A	167	BEN	C1-C-N2	2.43	121.72	118.05
4	B	163	BEN	C1-C-N2	2.38	121.64	118.05
3	A	301	L9R	O3-C11-C12	2.33	119.22	111.91
4	D	164	BEN	C1-C-N2	2.24	121.42	118.05
2	B	201	NAG	C2-N2-C7	2.17	126.00	122.90
2	A	201	NAG	O5-C5-C6	2.14	110.55	107.20
4	A	166	BEN	C1-C-N2	2.06	121.16	118.05
2	B	201	NAG	C8-C7-N2	2.03	119.53	116.10
2	C	201	NAG	O5-C5-C6	2.01	110.36	107.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	201	NAG	C1

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	301	L9R	C1-O3P-P-O4P
3	D	301	L9R	C4-O4P-P-O1P
3	D	301	L9R	O4P-C4-C5-N
3	A	301	L9R	O4P-C4-C5-N
3	A	301	L9R	O11-C11-O3-C3
3	A	301	L9R	C12-C11-O3-C3
3	A	301	L9R	C14-C15-C16-C17
2	B	201	NAG	C4-C5-C6-O6
2	B	201	NAG	C8-C7-N2-C2
2	B	201	NAG	O7-C7-N2-C2
3	D	301	L9R	C31-C32-C33-C34
3	A	301	L9R	C11-C12-C13-C14
3	A	301	L9R	C31-C32-C33-C34
3	D	301	L9R	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
2	B	201	NAG	O5-C5-C6-O6
3	D	301	L9R	C12-C13-C14-C15
3	D	301	L9R	C33-C34-C35-C36
3	D	301	L9R	C42-C43-C44-C45
3	A	301	L9R	C13-C14-C15-C16
3	D	301	L9R	C35-C36-C37-C38
3	D	301	L9R	C16-C17-C18-C19
3	D	301	L9R	C17-C18-C19-C20
2	A	201	NAG	C4-C5-C6-O6
3	D	301	L9R	C19-C20-C21-C22
3	A	301	L9R	C18-C19-C20-C21
3	A	301	L9R	C32-C33-C34-C35
2	A	201	NAG	O5-C5-C6-O6
3	D	301	L9R	C1-C2-C3-O3
3	D	301	L9R	C40-C41-C42-C43
3	D	301	L9R	C18-C19-C20-C21
3	D	301	L9R	C20-C21-C22-C23
3	D	301	L9R	C12-C11-O3-C3
3	A	301	L9R	C32-C31-O2-C2
3	A	301	L9R	O31-C31-O2-C2
2	C	201	NAG	C4-C5-C6-O6
3	D	301	L9R	C4-O4P-P-O3P
3	A	301	L9R	C34-C35-C36-C37
3	A	301	L9R	C15-C16-C17-C18
3	D	301	L9R	O11-C11-O3-C3
3	A	301	L9R	C23-C24-C25-C26
3	D	301	L9R	C45-C46-C47-C48
3	D	301	L9R	C14-C15-C16-C17
3	A	301	L9R	O3P-C1-C2-C3
3	A	301	L9R	C16-C17-C18-C19
3	D	301	L9R	C11-C12-C13-C14
3	D	301	L9R	C43-C44-C45-C46
3	A	301	L9R	C19-C20-C21-C22
3	A	301	L9R	C41-C42-C43-C44
3	A	301	L9R	C33-C34-C35-C36
3	A	301	L9R	O3P-C1-C2-O2
2	C	201	NAG	O5-C5-C6-O6
3	D	301	L9R	O2-C2-C3-O3
3	A	301	L9R	C44-C45-C46-C47
4	D	167	BEN	N1-C-C1-C2
4	B	163	BEN	N1-C-C1-C6
3	D	301	L9R	C1-O3P-P-O1P

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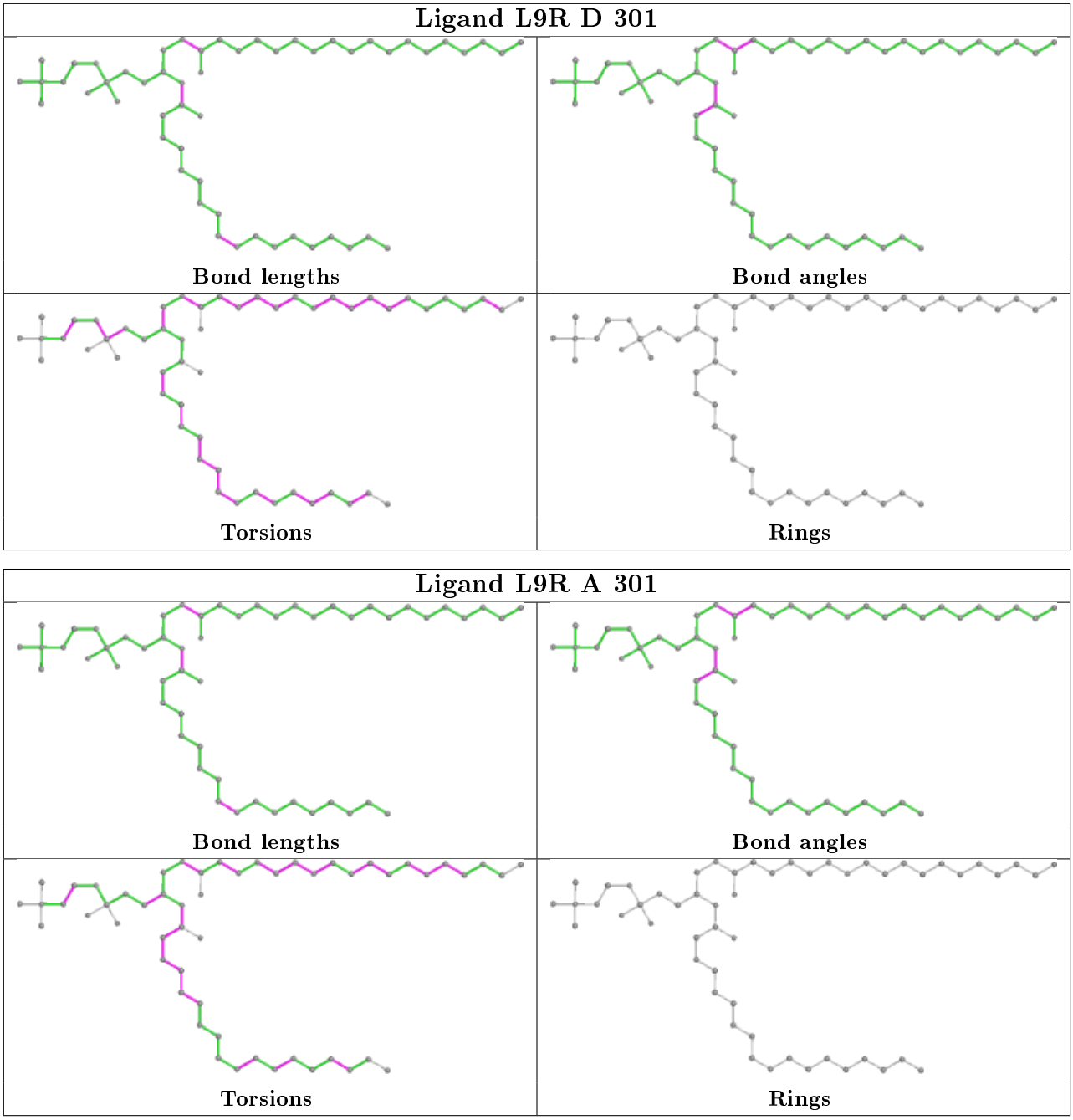
Mol	Chain	Res	Type	Atoms
3	D	301	L9R	C37-C38-C39-C40
3	A	301	L9R	C21-C22-C23-C24
3	D	301	L9R	C36-C37-C38-C39
4	D	166	BEN	N2-C-C1-C2
4	D	166	BEN	N2-C-C1-C6
3	D	301	L9R	C13-C14-C15-C16
3	D	301	L9R	C25-C26-C27-C28
3	A	301	L9R	C39-C40-C41-C42
3	A	301	L9R	C22-C23-C24-C25
4	C	163	BEN	N1-C-C1-C2
4	D	166	BEN	N1-C-C1-C2
4	D	166	BEN	N1-C-C1-C6
4	B	163	BEN	N1-C-C1-C2
3	A	301	L9R	O2-C31-C32-C33
3	A	301	L9R	O31-C31-C32-C33

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	167	BEN	1	0
4	C	163	BEN	1	0
4	D	164	BEN	2	0
3	D	301	L9R	1	0
3	A	301	L9R	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 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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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>2	OWAB(Å^2)	Q<0.9
1	A	137/162 (84%)	0.23	6 (4%) 34 34	22, 32, 52, 68	0
1	B	131/162 (80%)	0.62	16 (12%) 4 3	25, 37, 60, 68	0
1	C	131/162 (80%)	0.30	10 (7%) 13 13	23, 33, 57, 62	0
1	D	131/162 (80%)	0.16	4 (3%) 49 49	22, 31, 49, 65	0
All	All	530/648 (81%)	0.33	36 (6%) 17 16	22, 33, 56, 68	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	26	GLY	6.6
1	B	91	GLY	4.9
1	C	79	ARG	4.8
1	A	105	ASP	4.7
1	D	26	GLY	4.5
1	B	109	PHE	4.4
1	B	79	ARG	4.1
1	C	113	GLY	4.1
1	B	112	CYS	4.1
1	B	110	SER	3.9
1	C	109	PHE	3.7
1	D	109	PHE	3.7
1	A	106	GLN	3.6
1	B	147	GLU	3.4
1	B	99	TYR	3.3
1	C	112	CYS	3.3
1	C	91	GLY	3.3
1	A	104	GLU	3.2
1	B	148	ASN	3.2
1	B	111	PHE	3.1
1	B	26	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	90	LYS	2.9
1	B	80	LYS	2.9
1	B	77	ASP	2.8
1	D	102	CYS	2.7
1	B	127	ASN	2.6
1	B	76	GLN	2.6
1	B	75	ARG	2.4
1	A	99	TYR	2.4
1	C	85	ILE	2.3
1	C	162	SER	2.3
1	B	90	LYS	2.3
1	C	115	ARG	2.2
1	A	108	LYS	2.1
1	C	111	PHE	2.0
1	D	111	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	B-factors(Å^2)	Q<0.9
2	NAG	C	201	14/15	0.53	0.29	68,78,80,81	0
4	BEN	D	164	9/9	0.55	0.22	63,66,69,69	0
3	L9R	A	301	54/54	0.61	0.27	51,74,104,106	0
4	BEN	D	167	9/9	0.62	0.25	48,55,58,60	0
4	BEN	A	167	9/9	0.62	0.30	53,63,66,68	0
4	BEN	D	166	9/9	0.65	0.20	60,65,67,68	0
4	BEN	B	165	9/9	0.66	0.21	48,53,54,55	0
3	L9R	D	301	54/54	0.70	0.21	46,73,94,96	0

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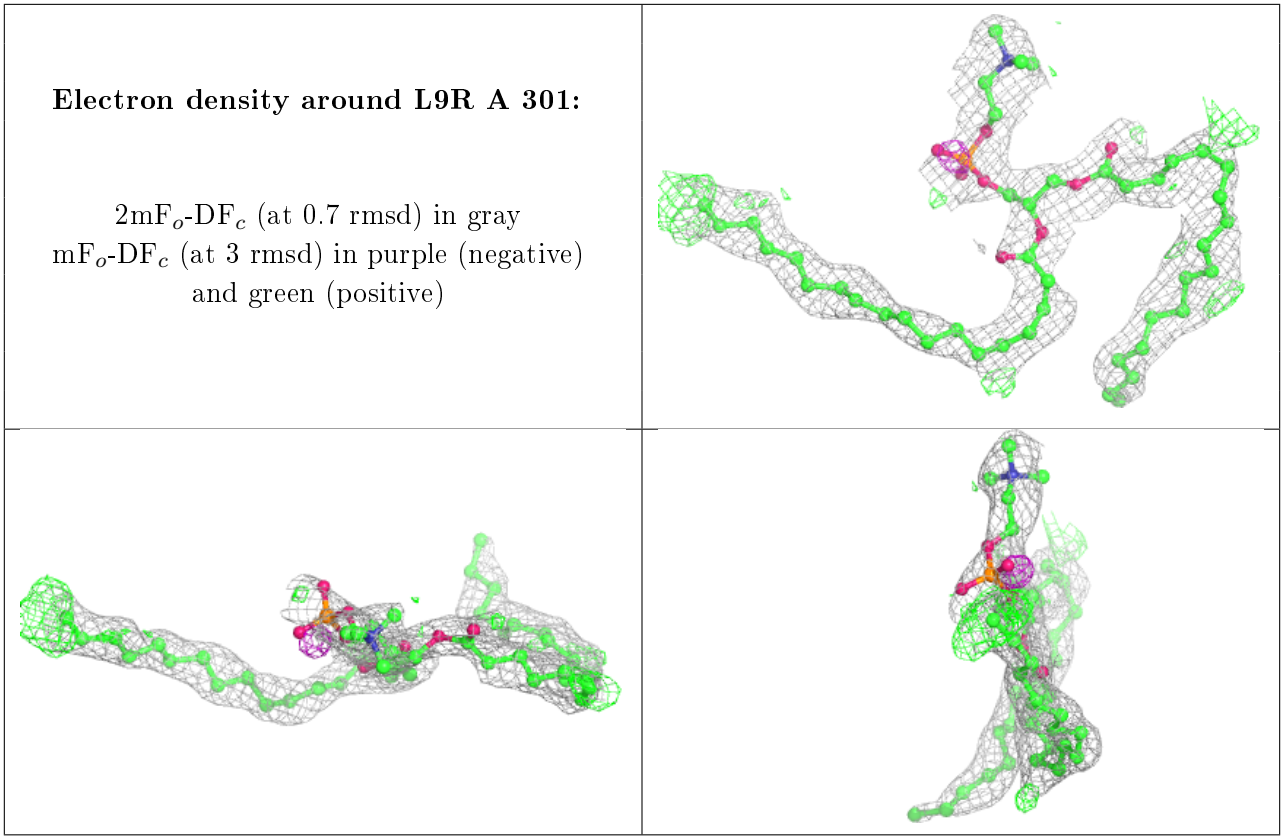
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BEN	B	164	9/9	0.76	0.16	44,46,51,56	0
2	NAG	B	201	14/15	0.76	0.41	76,83,89,90	0
2	NAG	D	201	14/15	0.77	0.21	43,56,64,69	0
2	NAG	A	201	14/15	0.77	0.23	45,56,63,65	0
4	BEN	A	166	9/9	0.79	0.18	37,44,50,51	0
4	BEN	D	165	9/9	0.81	0.22	52,56,57,58	0
4	BEN	B	163	9/9	0.85	0.19	40,45,47,47	0
4	BEN	C	165	9/9	0.86	0.12	36,37,42,42	0
4	BEN	C	164	9/9	0.87	0.14	48,52,53,55	0
4	BEN	A	165	9/9	0.93	0.12	23,23,27,29	0
4	BEN	C	163	9/9	0.94	0.17	35,36,39,39	0
4	BEN	A	164	9/9	0.94	0.15	23,26,27,27	0
4	BEN	A	163	9/9	0.95	0.14	23,24,25,27	0
2	NAG	D	202	14/15	0.97	0.09	19,22,27,27	0
2	NAG	B	202	14/15	0.97	0.08	20,23,26,26	0
4	BEN	D	163	9/9	0.98	0.16	21,23,25,26	0
2	NAG	C	202	14/15	0.98	0.09	21,23,24,26	0
2	NAG	A	202	14/15	0.98	0.09	22,23,27,28	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.

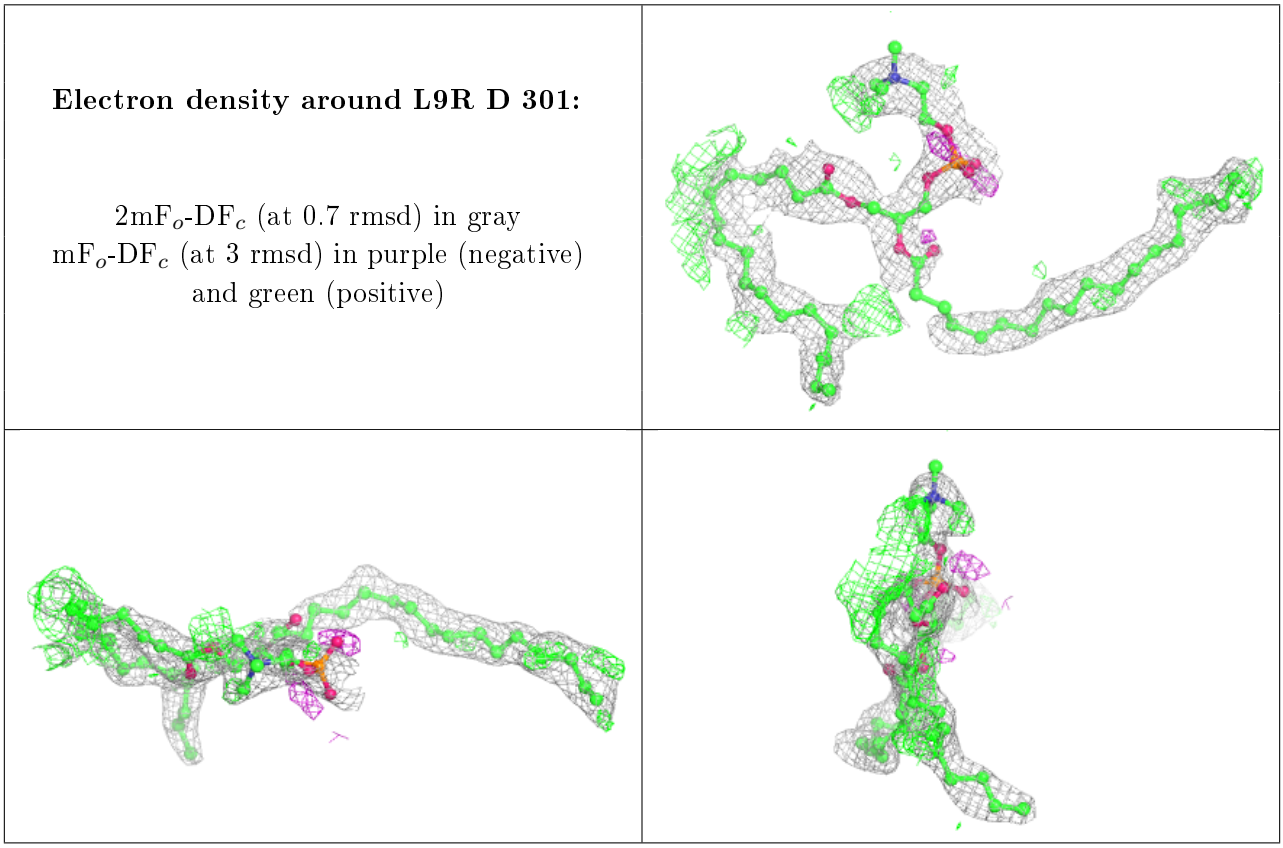
Electron density around L9R A 301:

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



Electron density around L9R D 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.