Full wwPDB X-ray Structure Validation Report (i)

Nov 19, 2023 – 07:21 PM JST

PDB ID	:	6M0Z
Title	:	X-ray structure of Drosophila dopamine transporter with NET-like mutations (D121G/S426M/F471L) in L-norepinephrine bound form
Authors	:	Shabareesh, P.; Mallela, A.K.; Joseph, D.; Penmatsa, A.
Deposited on	:	2020-02-24
Resolution	:	2.88 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

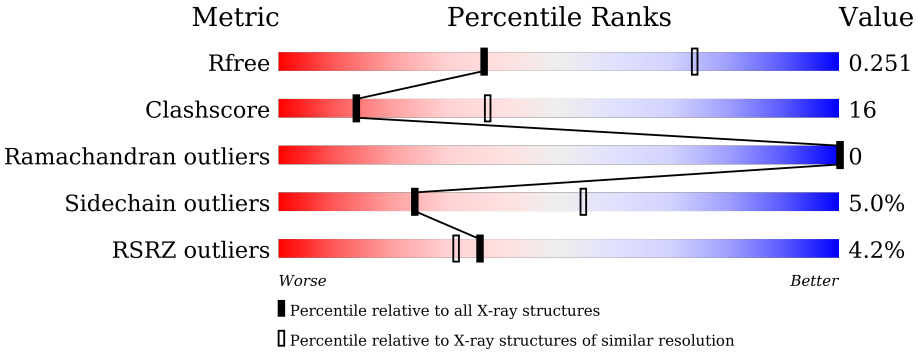
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.88 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	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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	536	2%, 65%, 33%, •
2	L	214	7%, 74%, 23%, •
3	H	219	7%, 69%, 29%, •

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 7665 atoms, of which 11 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Sodium-dependent dopamine transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	536	4244	2844	662	718	20	0	1	0

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	ALA	VAL	engineered mutation	UNP Q7K4Y6
A	121	GLY	ASP	engineered mutation	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	GLN	deletion	UNP Q7K4Y6
A	?	-	ASN	deletion	UNP Q7K4Y6
A	?	-	ALA	deletion	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	ARG	deletion	UNP Q7K4Y6
A	?	-	VAL	deletion	UNP Q7K4Y6
A	?	-	PRO	deletion	UNP Q7K4Y6
A	?	-	VAL	deletion	UNP Q7K4Y6
A	?	-	ILE	deletion	UNP Q7K4Y6
A	?	-	GLY	deletion	UNP Q7K4Y6
A	?	-	ASN	deletion	UNP Q7K4Y6
A	?	-	TYR	deletion	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	ASP	deletion	UNP Q7K4Y6
A	?	-	LEU	deletion	UNP Q7K4Y6
A	?	-	TYR	deletion	UNP Q7K4Y6
A	?	-	ALA	deletion	UNP Q7K4Y6
A	?	-	MET	deletion	UNP Q7K4Y6
A	?	-	GLY	deletion	UNP Q7K4Y6
A	?	-	ASN	deletion	UNP Q7K4Y6
A	?	-	GLN	deletion	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	LEU	deletion	UNP Q7K4Y6
A	?	-	LEU	deletion	UNP Q7K4Y6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	TYR	deletion	UNP Q7K4Y6
A	?	-	ASN	deletion	UNP Q7K4Y6
A	?	-	GLU	deletion	UNP Q7K4Y6
A	?	-	THR	deletion	UNP Q7K4Y6
A	?	-	TYR	deletion	UNP Q7K4Y6
A	?	-	MET	deletion	UNP Q7K4Y6
A	?	-	ASN	deletion	UNP Q7K4Y6
A	?	-	GLY	deletion	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	LEU	deletion	UNP Q7K4Y6
A	?	-	ASP	deletion	UNP Q7K4Y6
A	?	-	THR	deletion	UNP Q7K4Y6
A	?	-	SER	deletion	UNP Q7K4Y6
A	?	-	ALA	deletion	UNP Q7K4Y6
A	?	-	VAL	deletion	UNP Q7K4Y6
A	415	ALA	LEU	engineered mutation	UNP Q7K4Y6
A	426	MET	SER	engineered mutation	UNP Q7K4Y6
A	471	LEU	PHE	engineered mutation	UNP Q7K4Y6

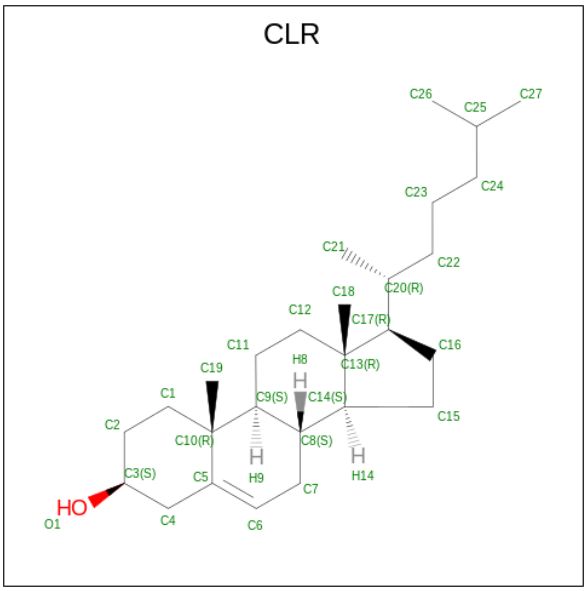
- Molecule 2 is a protein called Antibody fragment (Fab) 9D5 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	214	1620	1008	268	336	8	0	0	0

- Molecule 3 is a protein called Antibody fragment (Fab) 9D5 heavy chain.

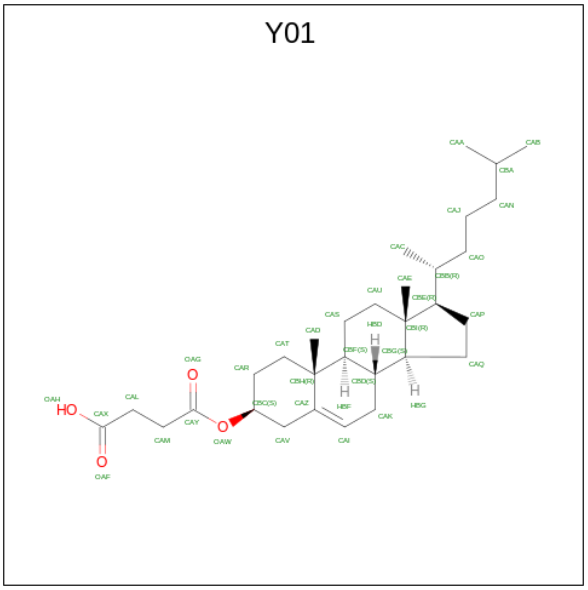
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	219	1643	1034	278	323	8	0	0	0

- Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



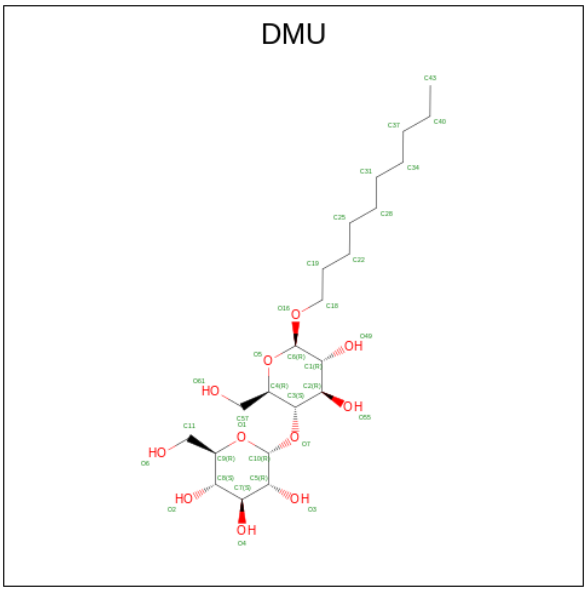
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	28	27	1	0	0

- Molecule 5 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	35	31	4	0	0

- Molecule 6 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	33	22	11	0	0

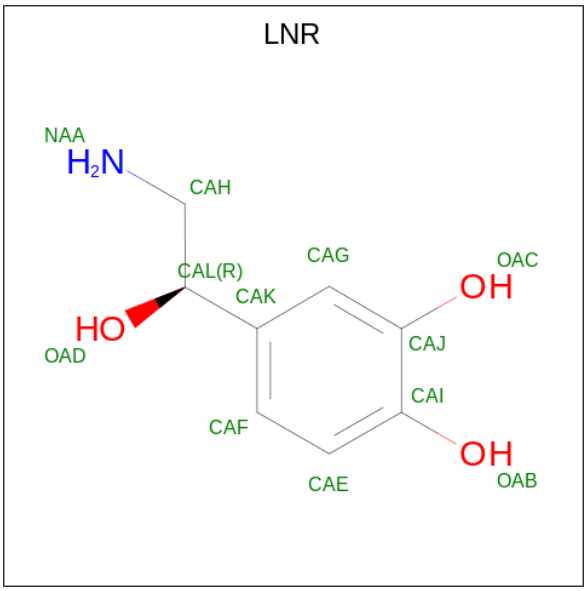
- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
7	A	2	2	2	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
8	A	1	1	1	0	0

- Molecule 9 is L-NOREPINEPHRINE (three-letter code: LNR) (formula: $C_8H_{11}NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
9	A	1	23	8	11	1	3	0	0

- Molecule 10 is water.

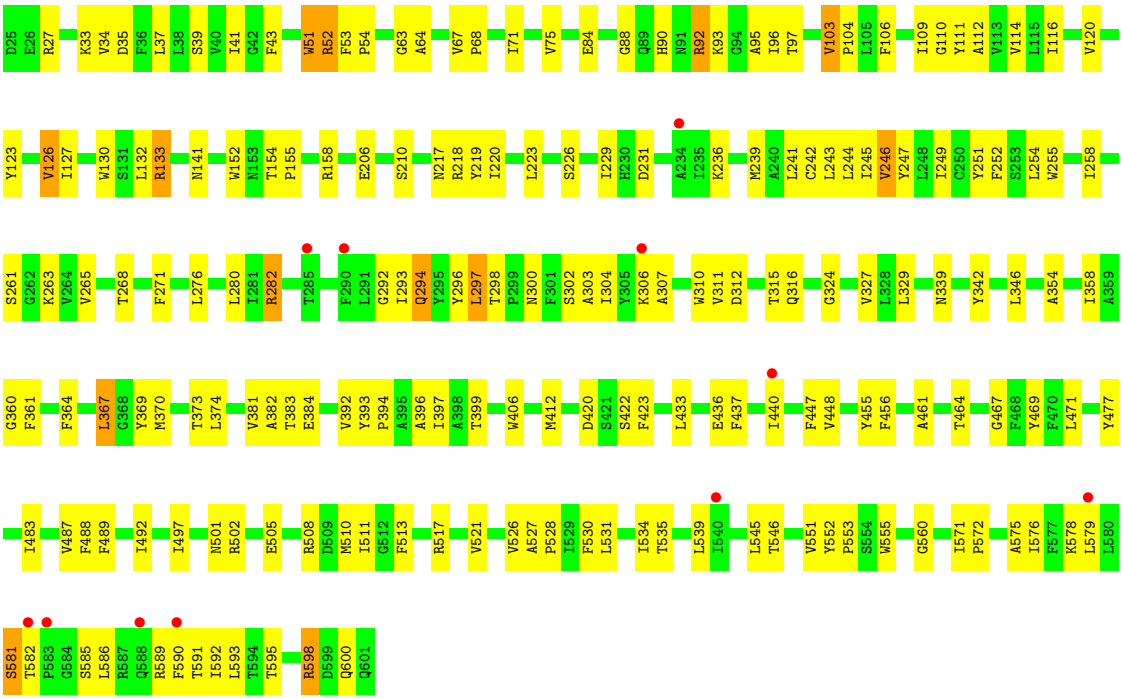
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	6	6	6	0	0
			Total	O		
10	L	11	11	11	0	0
			Total	O		
10	H	19	19	19	0	0

3 Residue-property plots (i)

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

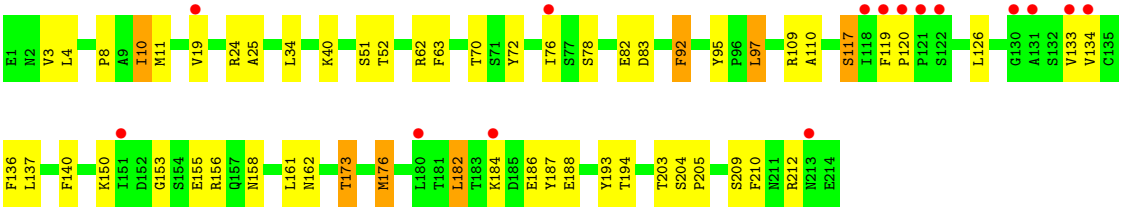
• Molecule 1: Sodium-dependent dopamine transporter

Chain A:



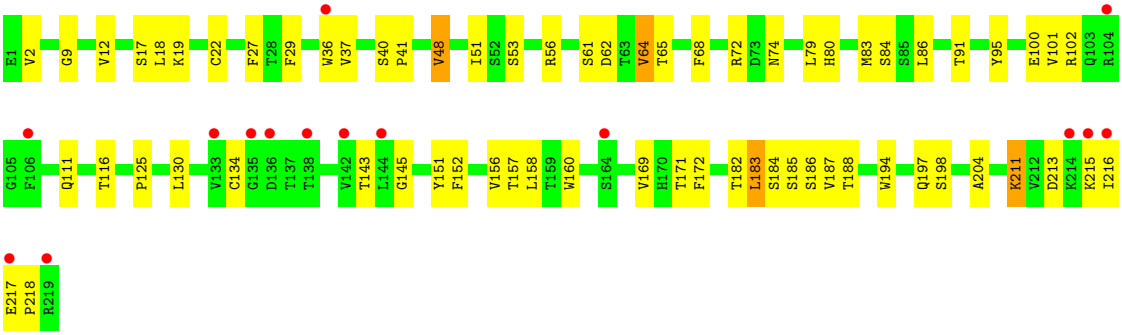
• Molecule 2: Antibody fragment (Fab) 9D5 Light chain

Chain L:



• Molecule 3: Antibody fragment (Fab) 9D5 heavy chain

Chain H:


E1
V2
G9
V12
S17
L18
K19
C22
F27
T28
F29
W36
V37
S40
P41
V48
I51
S52
S53
R56
S61
D62
T63
V64
T65
F68
R72
D73
N74
L79
H80
M83
S84
S85
L86
T91
Y95
E100
V101
R102
Q103
R104
G105
F106
Q111
T116
P125
L130
V133
C134
G135
D136
T137
T138
V142
T143
L144
G145
Y151
F152
V156
T157
L158
T159
W160
S164
V169
H170
T171
F172
T182
L183
S184
S185
S186
V187
T188
W194
Q197
S198
A204
K211
V212
D213
K214
K215
I216
E217
P218
R219

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	97.29Å 142.80Å 168.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.61 – 2.88 48.61 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.61-2.88) 99.9 (48.61-2.88)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.213 , 0.243 0.216 , 0.251	Depositor DCC
R_{free} test set	2687 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	93.6	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 63.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7665	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: DMU, CL, LNR, CLR, Y01, NA

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	0.25	0/4388	0.40	0/5991
2	L	0.25	0/1658	0.46	0/2255
3	H	0.25	0/1682	0.46	0/2292
All	All	0.25	0/7728	0.43	0/10538

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	4244	0	4186	145	0
2	L	1620	0	1525	39	0
3	H	1643	0	1590	57	0
4	A	28	0	46	3	0
5	A	35	0	49	0	0
6	A	33	0	42	4	0
7	A	2	0	0	0	0
8	A	1	0	0	0	0
9	A	12	11	11	0	0
10	A	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	H	19	0	0	3	0
10	L	11	0	0	0	0
All	All	7654	11	7449	238	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 16.

All (238) 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)
3:H:9:GLY:HA2	3:H:18:LEU:HD21	1.21	1.13
3:H:169:VAL:HG12	3:H:187:VAL:HG12	1.35	1.04
1:A:75:VAL:CG1	1:A:526:VAL:HG11	2.00	0.91
3:H:9:GLY:HA2	3:H:18:LEU:CD2	2.07	0.84
1:A:396:ALA:O	1:A:399:THR:HG22	1.81	0.81
1:A:27:ARG:NH1	1:A:92:ARG:O	2.14	0.81
1:A:369:TYR:O	1:A:373:THR:HG22	1.82	0.80
1:A:589:ARG:HA	1:A:592:ILE:HG22	1.65	0.79
2:L:34:LEU:HD22	2:L:72:TYR:CG	2.19	0.77
1:A:75:VAL:HG12	1:A:526:VAL:HG11	1.65	0.77
1:A:303:ALA:HA	1:A:306:LYS:HE3	1.65	0.76
1:A:369:TYR:CE1	1:A:373:THR:HG21	2.23	0.74
1:A:282:ARG:O	1:A:282:ARG:HD3	1.88	0.74
1:A:27:ARG:HH12	1:A:93:LYS:HA	1.53	0.73
1:A:477:TYR:CD2	1:A:560:GLY:HA3	2.23	0.73
1:A:397:ILE:HG23	1:A:406:TRP:HB2	1.71	0.72
1:A:123:TYR:HB2	1:A:471:LEU:HD13	1.72	0.71
3:H:83:MET:HB3	3:H:86:LEU:HD21	1.73	0.70
1:A:294:GLN:O	1:A:298:THR:HG23	1.91	0.70
1:A:437:PHE:HB2	1:A:440:ILE:HD13	1.74	0.69
6:A:703:DMU:O55	6:A:703:DMU:O3	2.10	0.69
1:A:68:PRO:HD3	1:A:304:ILE:HD12	1.74	0.69
1:A:364:PHE:HA	1:A:367:LEU:HB2	1.74	0.69
1:A:258:ILE:HA	1:A:261:SER:HB3	1.75	0.69
3:H:183:LEU:HD12	3:H:184:SER:N	2.08	0.68
1:A:251:TYR:CE1	1:A:448:VAL:HG23	2.30	0.67
1:A:152:TRP:O	1:A:218:ARG:HD3	1.94	0.67
1:A:219:TYR:HD2	1:A:220:ILE:HD12	1.59	0.67
1:A:535:THR:O	1:A:539:LEU:HD13	1.95	0.67
1:A:591:THR:O	1:A:595:THR:HG23	1.95	0.67
2:L:194:THR:HG23	2:L:209:SER:OG	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:ALA:O	1:A:579:LEU:HB2	1.95	0.67
1:A:33:LYS:HE3	1:A:339:ASN:HD21	1.59	0.66
3:H:29:PHE:O	3:H:72:ARG:NH2	2.30	0.65
1:A:546:THR:HG22	1:A:551:VAL:HA	1.78	0.65
3:H:197:GLN:NE2	10:H:302:HOH:O	2.29	0.65
1:A:220:ILE:O	1:A:236:LYS:HE2	1.97	0.65
1:A:303:ALA:HA	1:A:306:LYS:CE	2.27	0.64
3:H:171:THR:HG22	3:H:185:SER:OG	1.96	0.64
1:A:133:ARG:NH2	6:A:703:DMU:H30	2.12	0.64
1:A:578:LYS:HA	1:A:581:SER:HB2	1.80	0.63
1:A:219:TYR:CD2	1:A:220:ILE:HD12	2.33	0.63
3:H:17:SER:HB3	3:H:84:SER:HA	1.80	0.63
1:A:369:TYR:OH	1:A:399:THR:HG23	1.99	0.62
3:H:169:VAL:CG1	3:H:187:VAL:HG12	2.21	0.62
3:H:125:PRO:HB3	3:H:151:TYR:HB3	1.82	0.62
3:H:91:THR:HG23	3:H:116:THR:HA	1.81	0.62
1:A:123:TYR:HB2	1:A:471:LEU:CD1	2.31	0.61
2:L:34:LEU:HD22	2:L:72:TYR:CD2	2.35	0.61
3:H:172:PHE:O	3:H:183:LEU:HD13	2.00	0.61
2:L:120:PRO:HB3	2:L:210:PHE:CE1	2.38	0.59
3:H:2:VAL:HG13	3:H:27:PHE:CD1	2.37	0.59
2:L:126:LEU:O	2:L:184:LYS:HD2	2.01	0.59
1:A:52:ARG:HG2	1:A:316:GLN:OE1	2.01	0.59
1:A:84:GLU:OE1	1:A:324:GLY:N	2.32	0.59
3:H:64:VAL:HG13	3:H:68:PHE:HB2	1.83	0.59
1:A:300:ASN:OD1	1:A:302:SER:HB3	2.03	0.58
2:L:134:VAL:HG21	3:H:130:LEU:HD13	1.85	0.58
3:H:36:TRP:O	3:H:48:VAL:HG13	2.03	0.58
1:A:93:LYS:HD2	1:A:97:THR:HG21	1.85	0.58
1:A:461:ALA:O	1:A:464:THR:HG22	2.04	0.58
1:A:508:ARG:HD2	1:A:508:ARG:O	2.04	0.57
1:A:123:TYR:O	1:A:126:VAL:HG13	2.04	0.57
1:A:370:MET:HE1	1:A:381:VAL:HB	1.86	0.57
1:A:53:PHE:HB3	1:A:54:PRO:HD3	1.86	0.57
1:A:545:LEU:HG	1:A:552:TYR:CD1	2.40	0.57
1:A:585:SER:O	1:A:589:ARG:HG3	2.04	0.56
1:A:282:ARG:HD3	1:A:282:ARG:C	2.23	0.56
2:L:136:PHE:C	2:L:137:LEU:HD12	2.25	0.56
1:A:97:THR:OG1	1:A:436:GLU:HG2	2.06	0.56
1:A:64:ALA:O	1:A:304:ILE:HD11	2.06	0.56
1:A:245:ILE:O	1:A:249:ILE:HG13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ILE:HD11	1:A:489:PHE:HB3	1.89	0.55
1:A:226:SER:OG	1:A:231:ASP:O	2.17	0.55
1:A:43:PHE:CD1	1:A:327:VAL:HG21	2.41	0.55
2:L:156:ARG:NH1	2:L:158:ASN:HB3	2.22	0.55
1:A:307:ALA:O	1:A:311:VAL:HG12	2.07	0.55
3:H:143:THR:HG22	3:H:188:THR:CG2	2.37	0.55
4:A:701:CLR:H121	4:A:701:CLR:H212	1.88	0.54
1:A:393:TYR:CE2	1:A:397:ILE:HD11	2.41	0.54
1:A:303:ALA:O	1:A:306:LYS:HG3	2.08	0.54
1:A:582:THR:OG1	1:A:589:ARG:HD2	2.07	0.54
1:A:370:MET:HE1	1:A:392:VAL:HG13	1.88	0.54
2:L:62:ARG:NH1	2:L:83:ASP:OD2	2.41	0.54
1:A:106:PHE:HE2	1:A:497:ILE:CD1	2.20	0.54
3:H:143:THR:HG22	3:H:188:THR:HB	1.90	0.54
2:L:140:PHE:O	2:L:173:THR:HG22	2.07	0.54
1:A:242:CYS:O	1:A:246:VAL:HG13	2.08	0.53
1:A:292:GLY:HA3	1:A:364:PHE:O	2.09	0.53
1:A:37:LEU:O	1:A:41:ILE:HG12	2.08	0.53
2:L:156:ARG:HH12	2:L:158:ASN:HB3	1.73	0.53
1:A:508:ARG:NE	3:H:100:GLU:O	2.32	0.53
1:A:95:ALA:HA	1:A:329:LEU:HD23	1.90	0.52
1:A:116:ILE:O	1:A:120:VAL:HG13	2.09	0.52
3:H:151:TYR:CE2	3:H:156:VAL:HG13	2.45	0.52
1:A:75:VAL:HG13	1:A:526:VAL:HG11	1.87	0.52
1:A:103:VAL:HG22	1:A:106:PHE:HB2	1.91	0.52
2:L:184:LYS:HE2	2:L:188:GLU:OE2	2.09	0.52
3:H:188:THR:HG23	10:H:307:HOH:O	2.09	0.52
1:A:110:GLY:O	1:A:114:VAL:HG23	2.10	0.52
1:A:303:ALA:CA	1:A:306:LYS:HE3	2.38	0.52
2:L:63:PHE:CE1	2:L:76:ILE:HG12	2.45	0.51
1:A:571:ILE:HB	1:A:572:PRO:CD	2.40	0.51
1:A:501:ASN:OD1	1:A:502:ARG:N	2.43	0.51
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.92	0.51
2:L:161:LEU:CD1	3:H:182:THR:HB	2.41	0.51
1:A:244:LEU:HB2	1:A:456:PHE:CE2	2.45	0.51
1:A:487:VAL:HG12	1:A:531:LEU:HD11	1.93	0.51
1:A:464:THR:HG23	1:A:467:GLY:N	2.26	0.51
1:A:513:PHE:HB3	3:H:101:VAL:HG13	1.92	0.51
1:A:35:ASP:OD2	1:A:263:LYS:HE3	2.10	0.51
1:A:95:ALA:HA	1:A:329:LEU:CD2	2.41	0.51
3:H:12:VAL:HG11	3:H:86:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:188:THR:O	10:H:301:HOH:O	2.19	0.50
1:A:223:LEU:HD11	1:A:469:TYR:CE2	2.46	0.50
1:A:96:ILE:HD13	1:A:111:TYR:CE1	2.46	0.50
1:A:276:LEU:O	1:A:280:LEU:HB2	2.11	0.50
1:A:354:ALA:O	1:A:358:ILE:HG12	2.12	0.50
1:A:39:SER:HA	1:A:265:VAL:HG11	1.94	0.50
1:A:271:PHE:CE2	1:A:412:MET:HG3	2.46	0.50
1:A:367:LEU:HD21	1:A:382:ALA:HA	1.93	0.50
1:A:219:TYR:HD2	1:A:220:ILE:CD1	2.25	0.50
1:A:63:GLY:N	1:A:297:LEU:O	2.30	0.50
1:A:433:LEU:HD12	1:A:447:PHE:CZ	2.47	0.50
1:A:104:PRO:HD2	1:A:593:LEU:O	2.11	0.50
1:A:293:ILE:HD12	1:A:361:PHE:HD1	1.77	0.50
1:A:154:THR:HB	1:A:155:PRO:HD2	1.94	0.49
1:A:511:ILE:HD12	1:A:513:PHE:CZ	2.47	0.49
2:L:95:TYR:OH	3:H:102:ARG:NH2	2.44	0.49
3:H:19:LYS:HE2	3:H:80:HIS:ND1	2.26	0.49
1:A:296:TYR:CD1	1:A:297:LEU:HD13	2.48	0.49
1:A:572:PRO:O	1:A:576:ILE:HG12	2.11	0.49
3:H:9:GLY:CA	3:H:18:LEU:HD21	2.15	0.49
2:L:120:PRO:HB3	2:L:210:PHE:CZ	2.47	0.49
2:L:187:TYR:O	2:L:193:TYR:OH	2.30	0.49
1:A:293:ILE:HD12	1:A:361:PHE:CD1	2.48	0.49
2:L:119:PHE:HB2	2:L:134:VAL:HG22	1.94	0.49
3:H:143:THR:HG22	3:H:188:THR:HG22	1.95	0.49
1:A:252:PHE:HA	1:A:255:TRP:HB2	1.94	0.49
3:H:211:LYS:NZ	3:H:213:ASP:OD1	2.46	0.48
1:A:296:TYR:CG	1:A:297:LEU:HD13	2.48	0.48
1:A:571:ILE:HB	1:A:572:PRO:HD3	1.95	0.48
3:H:40:SER:HB2	3:H:41:PRO:HD2	1.93	0.48
1:A:103:VAL:CG2	1:A:106:PHE:HB2	2.44	0.48
1:A:96:ILE:CG2	1:A:436:GLU:HG3	2.44	0.48
2:L:137:LEU:HD12	2:L:137:LEU:N	2.28	0.48
2:L:162:ASN:HB3	2:L:176:MET:HE2	1.96	0.48
1:A:251:TYR:O	1:A:255:TRP:HB2	2.14	0.47
1:A:370:MET:HE1	1:A:381:VAL:CG1	2.44	0.47
2:L:187:TYR:CZ	2:L:212:ARG:HD3	2.48	0.47
3:H:130:LEU:HB2	3:H:145:GLY:CA	2.44	0.47
1:A:27:ARG:NH1	1:A:93:LYS:HA	2.25	0.47
1:A:505:GLU:OE1	3:H:56:ARG:HD3	2.15	0.47
4:A:701:CLR:H212	4:A:701:CLR:H183	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:CD1	1:A:246:VAL:HG12	2.45	0.46
1:A:370:MET:O	1:A:374:LEU:HB2	2.14	0.46
2:L:4:LEU:HD22	2:L:25:ALA:HB2	1.98	0.46
1:A:383:THR:OG1	1:A:384:GLU:N	2.48	0.46
2:L:109:ARG:HG3	2:L:110:ALA:O	2.15	0.46
1:A:502:ARG:HG3	3:H:56:ARG:NH1	2.31	0.46
2:L:182:LEU:HB3	2:L:186:GLU:HG2	1.97	0.46
1:A:67:VAL:HB	1:A:68:PRO:HD3	1.98	0.46
3:H:18:LEU:HD12	3:H:19:LYS:H	1.80	0.45
1:A:545:LEU:HG	1:A:552:TYR:CE1	2.51	0.45
3:H:215:LYS:HE2	3:H:217:GLU:CD	2.37	0.45
1:A:254:LEU:HD21	1:A:423:PHE:CD1	2.51	0.45
2:L:92:PHE:CE1	2:L:97:LEU:HD21	2.52	0.45
2:L:117:SER:HB2	2:L:119:PHE:HE1	1.82	0.45
3:H:72:ARG:NE	3:H:74:ASN:OD1	2.42	0.45
3:H:143:THR:HG22	3:H:188:THR:CB	2.47	0.45
1:A:90:HIS:HB2	1:A:510:MET:SD	2.56	0.45
6:A:703:DMU:H38	6:A:703:DMU:H28	1.55	0.45
2:L:188:GLU:O	2:L:212:ARG:NH2	2.50	0.45
3:H:143:THR:HA	3:H:187:VAL:O	2.16	0.45
1:A:370:MET:CE	1:A:381:VAL:HB	2.47	0.45
2:L:11:MET:CE	2:L:19:VAL:HG13	2.47	0.44
1:A:530:PHE:O	1:A:534:ILE:HG13	2.16	0.44
1:A:132:LEU:HD12	1:A:246:VAL:HG12	1.99	0.44
1:A:488:PHE:O	1:A:492:ILE:HG12	2.17	0.44
3:H:37:VAL:O	3:H:95:TYR:HB2	2.17	0.44
1:A:67:VAL:HB	1:A:68:PRO:CD	2.48	0.44
1:A:103:VAL:CG2	1:A:103:VAL:O	2.65	0.44
1:A:133:ARG:HD2	1:A:133:ARG:HA	1.49	0.44
1:A:342:TYR:CZ	1:A:346:LEU:HD11	2.53	0.44
1:A:120:VAL:HA	1:A:123:TYR:CE2	2.53	0.44
2:L:162:ASN:HB3	2:L:176:MET:CE	2.47	0.44
1:A:517:ARG:O	1:A:521:VAL:HG23	2.18	0.43
2:L:161:LEU:HD13	3:H:182:THR:HB	2.00	0.43
1:A:158:ARG:O	1:A:210:SER:HA	2.18	0.43
1:A:296:TYR:CZ	1:A:360:GLY:HA3	2.52	0.43
1:A:553:PRO:HB2	1:A:555:TRP:CD1	2.53	0.43
2:L:150:LYS:HG2	2:L:155:GLU:HA	1.99	0.43
1:A:370:MET:HE1	1:A:381:VAL:CB	2.48	0.43
2:L:40:LYS:NZ	2:L:82:GLU:O	2.42	0.43
3:H:27:PHE:CE2	3:H:29:PHE:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:ARG:C	1:A:600:GLN:H	2.22	0.43
3:H:143:THR:CG2	3:H:188:THR:HG22	2.48	0.43
1:A:130:TRP:HD1	1:A:239:MET:HE1	1.84	0.43
2:L:150:LYS:HD2	2:L:153:GLY:O	2.19	0.43
3:H:156:VAL:CG2	3:H:183:LEU:HD23	2.49	0.43
1:A:241:LEU:CD2	6:A:703:DMU:H12	2.49	0.42
3:H:151:TYR:O	3:H:152:PHE:HB2	2.19	0.42
3:H:157:THR:OG1	3:H:204:ALA:HB3	2.19	0.42
3:H:62:ASP:O	3:H:65:THR:HG22	2.19	0.42
1:A:440:ILE:N	1:A:440:ILE:HD12	2.34	0.42
3:H:158:LEU:C	3:H:158:LEU:HD23	2.40	0.42
1:A:268:THR:OG1	1:A:420:ASP:OD1	2.14	0.42
1:A:247:TYR:CZ	1:A:455:TYR:HB3	2.55	0.42
1:A:312:ASP:O	1:A:315:THR:HG22	2.19	0.42
1:A:393:TYR:HB3	1:A:394:PRO:HD3	2.02	0.42
2:L:10:ILE:N	2:L:10:ILE:HD12	2.35	0.42
3:H:194:TRP:CH2	3:H:218:PRO:HG3	2.54	0.42
1:A:88:GLY:CA	1:A:329:LEU:HD12	2.50	0.41
3:H:22:CYS:HB3	3:H:79:LEU:HB3	2.02	0.41
3:H:169:VAL:HA	3:H:186:SER:O	2.20	0.41
1:A:243:LEU:O	1:A:246:VAL:HG22	2.19	0.41
1:A:71:ILE:HD12	1:A:310:TRP:HH2	1.85	0.41
3:H:51:ILE:HD13	3:H:72:ARG:HB2	2.01	0.41
1:A:112:ALA:O	1:A:116:ILE:HG13	2.20	0.41
2:L:161:LEU:C	2:L:161:LEU:HD23	2.40	0.41
1:A:315:THR:HA	1:A:534:ILE:HD13	2.01	0.41
4:A:701:CLR:H121	4:A:701:CLR:C21	2.51	0.41
3:H:216:ILE:N	3:H:216:ILE:HD12	2.35	0.41
2:L:24:ARG:NH2	2:L:70:THR:OG1	2.53	0.41
1:A:370:MET:SD	1:A:396:ALA:HB2	2.60	0.41
1:A:236:LYS:HB3	1:A:236:LYS:HE3	1.84	0.41
2:L:8:PRO:HG2	2:L:11:MET:HB3	2.02	0.41
1:A:127:ILE:HD13	1:A:130:TRP:CZ3	2.56	0.41
1:A:43:PHE:CE1	1:A:327:VAL:HG21	2.56	0.40
1:A:483:ILE:HD12	1:A:483:ILE:HA	1.90	0.40
3:H:160:TRP:CE2	3:H:187:VAL:HG13	2.55	0.40
1:A:585:SER:OG	1:A:586:LEU:N	2.54	0.40
2:L:204:SER:HB2	2:L:205:PRO:HD2	2.02	0.40
3:H:64:VAL:CG1	3:H:68:PHE:HB2	2.48	0.40
1:A:51:TRP:CD1	1:A:51:TRP:C	2.95	0.40
1:A:280:LEU:HD23	1:A:280:LEU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:51:SER:O	2:L:52:THR:HB	2.20	0.40
3:H:130:LEU:HB2	3:H:145:GLY:HA3	2.04	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	535/536 (100%)	512 (96%)	23 (4%)	0	100	100
2	L	212/214 (99%)	198 (93%)	14 (7%)	0	100	100
3	H	217/219 (99%)	202 (93%)	15 (7%)	0	100	100
All	All	964/969 (100%)	912 (95%)	52 (5%)	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	436/440 (99%)	416 (95%)	20 (5%)	27	58
2	L	182/187 (97%)	171 (94%)	11 (6%)	19	46
3	H	181/187 (97%)	172 (95%)	9 (5%)	24	54
All	All	799/814 (98%)	759 (95%)	40 (5%)	24	54

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	VAL
1	A	51	TRP
1	A	52	ARG
1	A	92	ARG
1	A	103	VAL
1	A	126	VAL
1	A	133	ARG
1	A	141	ASN
1	A	206	GLU
1	A	217	ASN
1	A	229	ILE
1	A	246	VAL
1	A	282	ARG
1	A	294	GLN
1	A	297	LEU
1	A	367	LEU
1	A	422	SER
1	A	581	SER
1	A	590	PHE
1	A	598	ARG
2	L	3	VAL
2	L	10	ILE
2	L	78	SER
2	L	92	PHE
2	L	97	LEU
2	L	117	SER
2	L	133	VAL
2	L	173	THR
2	L	176	MET
2	L	182	LEU
2	L	203	THR
3	H	48	VAL
3	H	53	SER
3	H	61	SER
3	H	64	VAL
3	H	111	GLN
3	H	134	CYS
3	H	183	LEU
3	H	198	SER
3	H	211	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	DMU	A	703	-	34,34,34	0.57	1 (2%)	45,45,45	0.67	0
9	LNR	A	707	-	12,12,12	2.62	7 (58%)	15,16,16	0.60	0
5	Y01	A	702	-	38,38,38	0.71	1 (2%)	57,57,57	1.58	9 (15%)
4	CLR	A	701	-	31,31,31	0.63	0	48,48,48	1.65	10 (20%)

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
6	DMU	A	703	-	-	7/19/59/59	0/2/2/2
9	LNR	A	707	-	-	1/6/6/6	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	Y01	A	702	-	-	11/19/77/77	0/4/4/4
4	CLR	A	701	-	-	2/10/68/68	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	707	LNR	CAG-CAJ	4.70	1.45	1.38
9	A	707	LNR	OAC-CAJ	4.34	1.45	1.36
9	A	707	LNR	CAH-CAL	3.45	1.62	1.51
9	A	707	LNR	OAB-CAI	2.75	1.42	1.36
9	A	707	LNR	CAI-CAJ	-2.74	1.35	1.40
9	A	707	LNR	CAF-CAE	2.68	1.43	1.38
5	A	702	Y01	CBH-CBF	-2.33	1.52	1.56
9	A	707	LNR	OAD-CAL	-2.27	1.37	1.42
6	A	703	DMU	O16-C6	2.12	1.43	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	702	Y01	CBI-CBE-CBB	-4.52	112.40	119.49
5	A	702	Y01	OAW-CAY-CAM	4.04	120.21	111.50
4	A	701	CLR	C19-C10-C9	-4.00	106.91	111.68
4	A	701	CLR	C13-C17-C20	-3.41	114.15	119.49
4	A	701	CLR	C4-C5-C10	3.35	120.87	116.42
4	A	701	CLR	C15-C14-C13	-2.87	100.38	103.84
5	A	702	Y01	CAS-CAU-CBI	-2.84	107.92	112.78
4	A	701	CLR	C13-C14-C8	-2.68	110.42	114.38
5	A	702	Y01	CBI-CBG-CBD	-2.66	110.44	114.38
5	A	702	Y01	CAQ-CBG-CBI	-2.66	100.64	103.84
5	A	702	Y01	CAD-CBH-CBF	-2.65	108.52	111.68
5	A	702	Y01	CAK-CBD-CBG	-2.63	107.09	110.91
4	A	701	CLR	C2-C3-C4	-2.60	106.75	110.31
4	A	701	CLR	C4-C5-C6	-2.54	116.95	120.61
4	A	701	CLR	C7-C8-C14	-2.34	107.52	110.91
5	A	702	Y01	CAC-CBB-CBE	-2.21	109.53	112.92
4	A	701	CLR	C15-C14-C8	-2.18	115.49	119.08
5	A	702	Y01	CAQ-CBG-CBD	-2.12	115.58	119.08
4	A	701	CLR	C18-C13-C14	-2.03	107.92	111.71

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	702	Y01	OAG-CAY-OAW-CBC
6	A	703	DMU	C19-C18-O16-C6
5	A	702	Y01	CAM-CAY-OAW-CBC
6	A	703	DMU	C3-C4-C57-O61
5	A	702	Y01	CAJ-CAO-CBB-CAC
6	A	703	DMU	O5-C4-C57-O61
4	A	701	CLR	C22-C23-C24-C25
6	A	703	DMU	C25-C28-C31-C34
6	A	703	DMU	C19-C22-C25-C28
6	A	703	DMU	C31-C34-C37-C40
5	A	702	Y01	CAJ-CAO-CBB-CBE
5	A	702	Y01	CAC-CBB-CBE-CBI
5	A	702	Y01	CAJ-CAN-CBA-CAB
6	A	703	DMU	O5-C6-O16-C18
5	A	702	Y01	CAO-CBB-CBE-CBI
5	A	702	Y01	CAJ-CAN-CBA-CAA
5	A	702	Y01	CAM-CAL-CAX-OAF
5	A	702	Y01	CAM-CAL-CAX-OAH
4	A	701	CLR	C16-C17-C20-C22
9	A	707	LNR	NAA-CAH-CAL-OAD
5	A	702	Y01	CAC-CBB-CBE-CAP

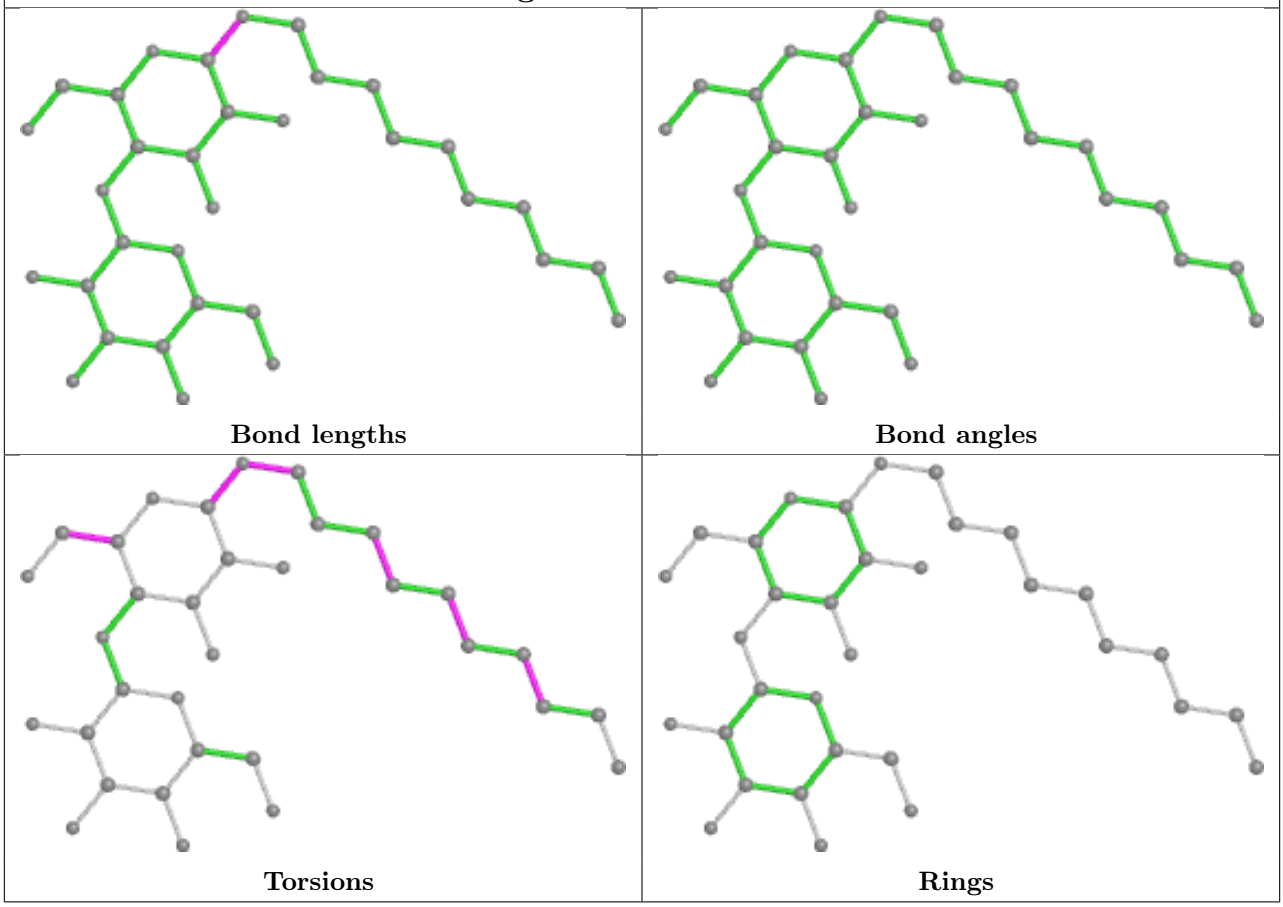
There are no ring outliers.

2 monomers are involved in 7 short contacts:

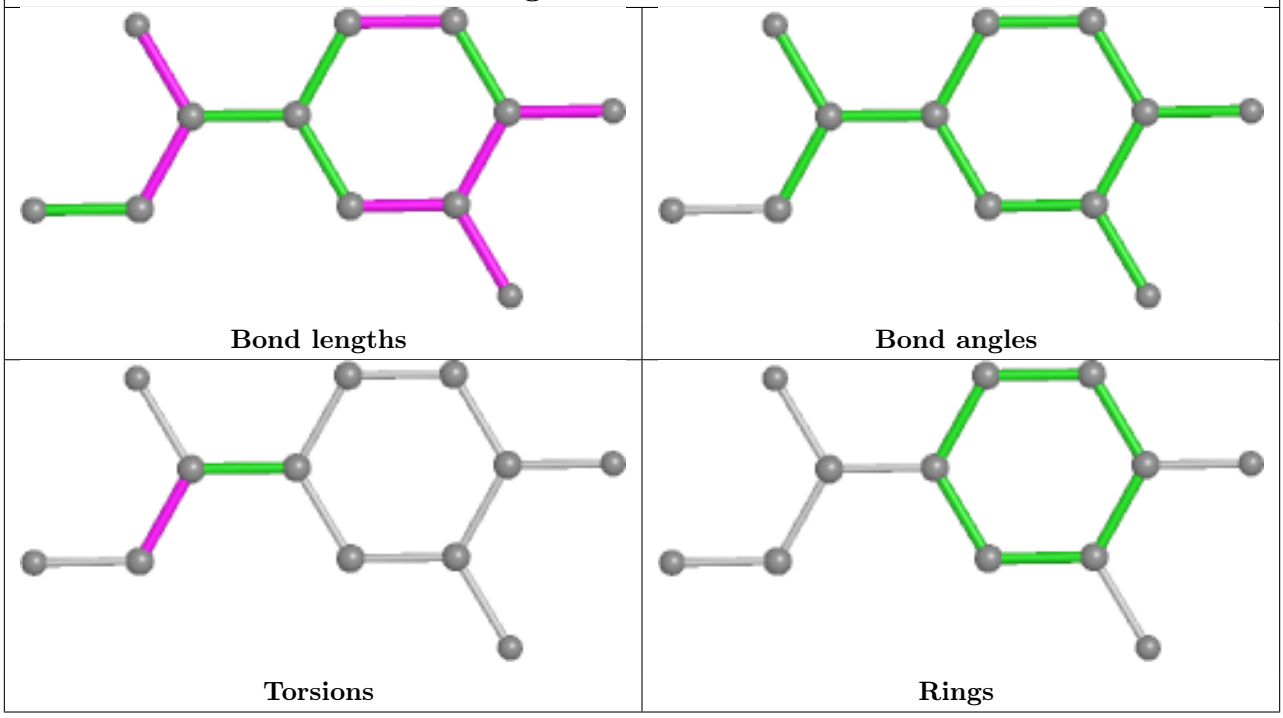
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	703	DMU	4	0
4	A	701	CLR	3	0

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.

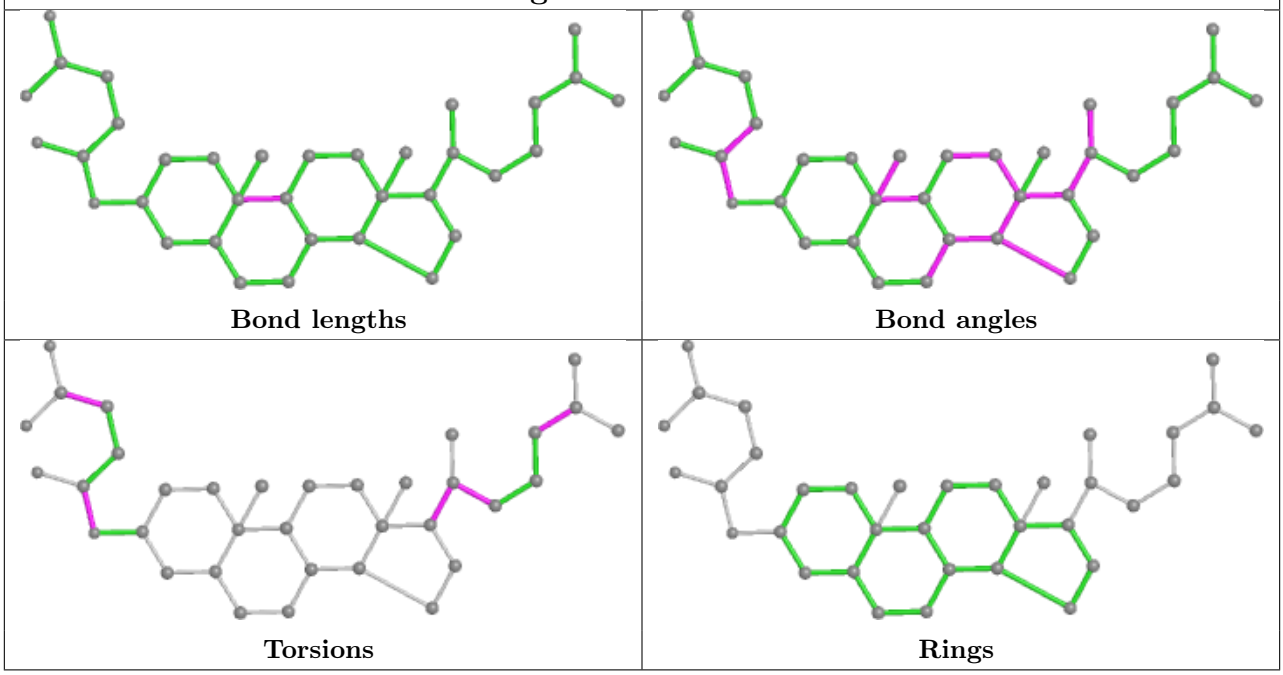
Ligand DMU A 703



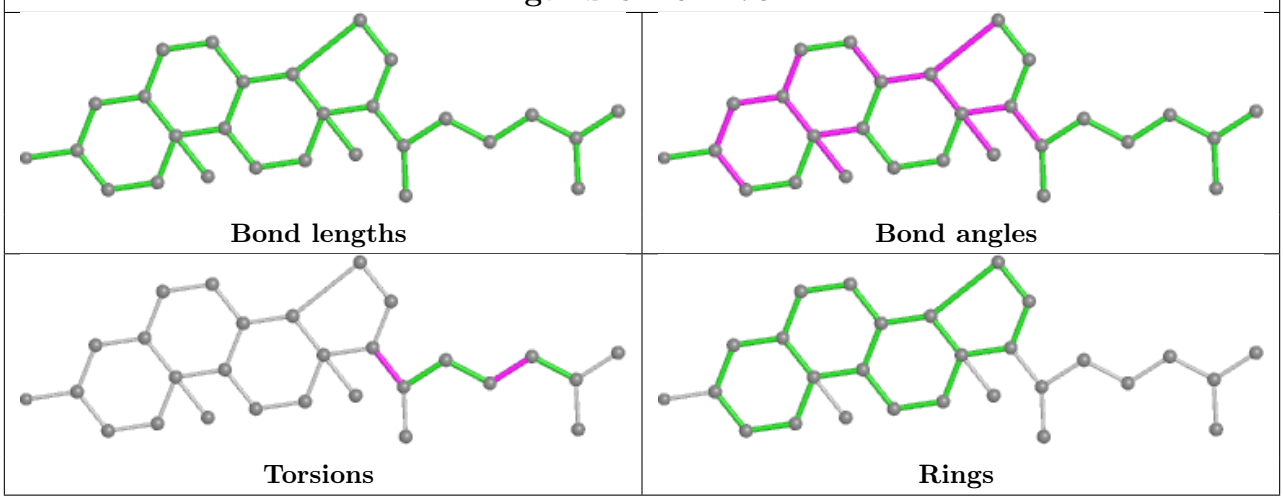
Ligand LNR A 707



Ligand Y01 A 702



Ligand CLR A 701



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, 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	536/536 (100%)	0.16	11 (2%)	63	62	71, 88, 111, 149	0
2	L	214/214 (100%)	0.26	15 (7%)	16	12	65, 84, 113, 148	0
3	H	219/219 (100%)	0.27	15 (6%)	17	13	71, 85, 119, 177	0
All	All	969/969 (100%)	0.21	41 (4%)	36	32	65, 86, 113, 177	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	133	VAL	4.9
3	H	138	THR	4.3
2	L	131	ALA	3.3
1	A	290	PHE	3.3
1	A	582	THR	3.3
1	A	234	ALA	3.3
2	L	119	PHE	3.2
2	L	121	PRO	3.2
2	L	213	ASN	3.0
2	L	180	LEU	3.0
3	H	136	ASP	2.9
2	L	133	VAL	2.9
1	A	590	PHE	2.8
2	L	151	ILE	2.7
3	H	215	LYS	2.7
3	H	216	ILE	2.7
1	A	588	GLN	2.6
3	H	164	SER	2.6
1	A	285	THR	2.6
2	L	122	SER	2.6
2	L	120	PRO	2.6
3	H	219	ARG	2.5
1	A	579	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	L	184	LYS	2.5
3	H	135	GLY	2.5
2	L	134	VAL	2.4
3	H	217	GLU	2.4
2	L	130	GLY	2.3
3	H	142	VAL	2.3
2	L	76	ILE	2.3
1	A	583	PRO	2.2
3	H	36	TRP	2.2
2	L	19	VAL	2.1
1	A	440	ILE	2.1
1	A	540	ILE	2.1
3	H	104	ARG	2.1
1	A	306	LYS	2.1
3	H	214	LYS	2.1
3	H	106	PHE	2.1
2	L	118	ILE	2.1
3	H	144	LEU	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, 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
9	LNR	A	707	12/12	0.82	0.30	95,114,126,148	0
6	DMU	A	703	33/33	0.88	0.23	105,126,135,137	0
7	NA	A	705	1/1	0.89	0.21	80,80,80,80	0
7	NA	A	704	1/1	0.89	0.30	88,88,88,88	0
5	Y01	A	702	35/35	0.93	0.22	93,104,127,130	0

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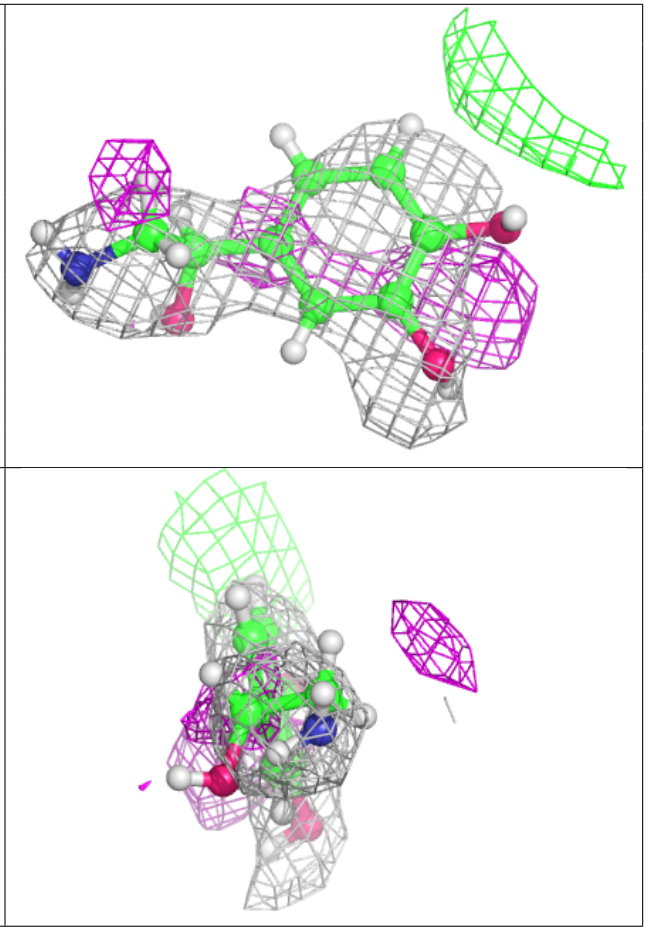
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CLR	A	701	28/28	0.95	0.30	82,92,99,103	0
8	CL	A	706	1/1	0.99	0.14	83,83,83,83	0

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.

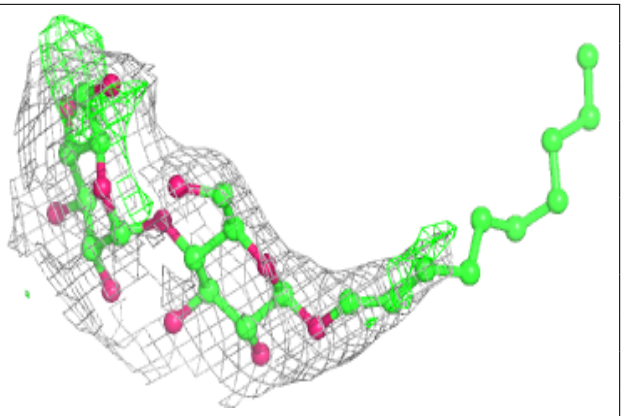
Electron density around LNR A 707:

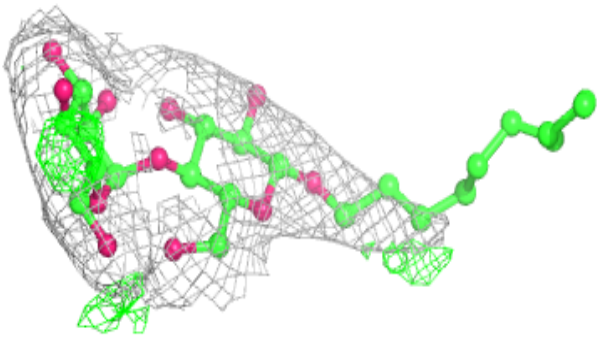
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

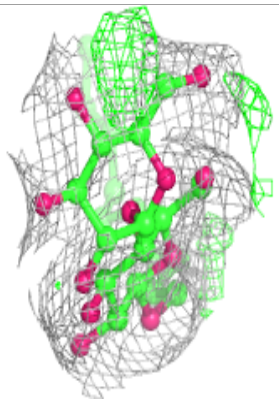


Electron density around DMU A 703:

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

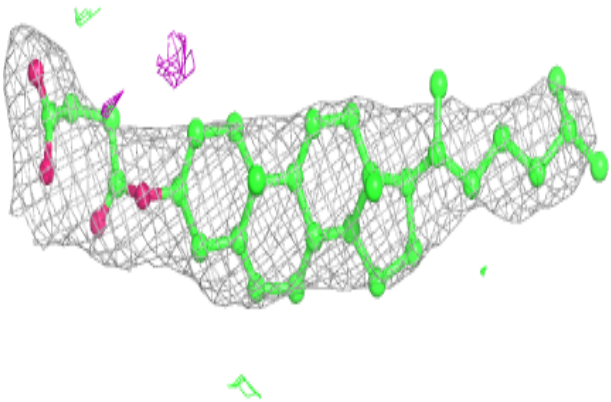


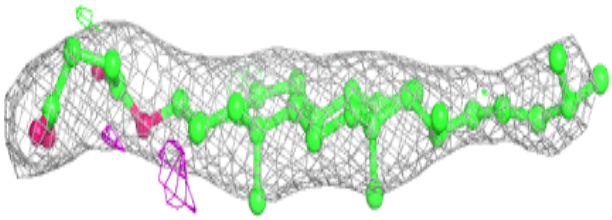


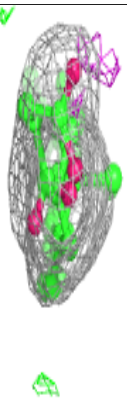


Electron density around Y01 A 702:

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

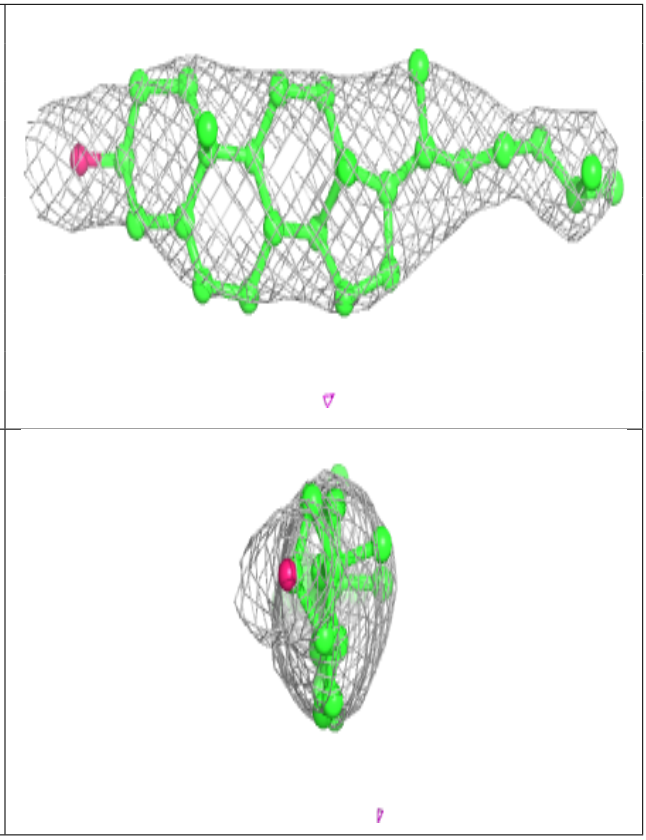






Electron density around CLR A 701:

$2mF_o$-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.