



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:40 pm BST

PDB ID : 4OH3  
Title : Crystal structure of a nitrate transporter  
Authors : Sun, J.; Bankston, J.R.; Payandeh, J.; Hinds, T.R.; Zagotta, W.N.; Zheng, N.  
Deposited on : 2014-01-16  
Resolution : 3.25 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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 : 2.11  
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) : 2.11

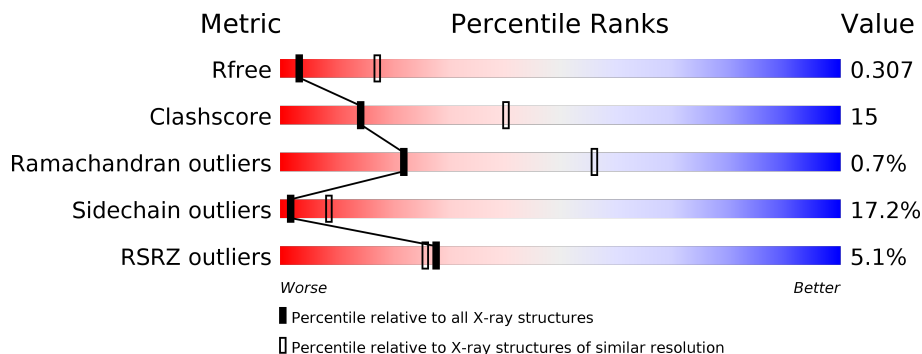
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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  $\geq 3$ , 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	599	
1	B	599	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8048 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.

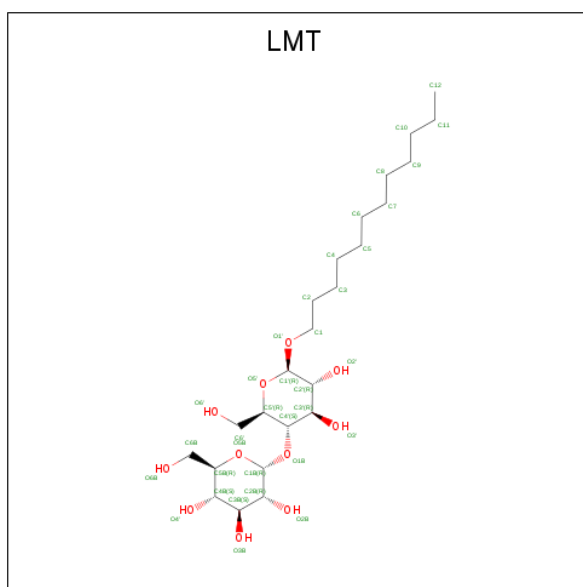
- Molecule 1 is a protein called Nitrate transporter 1.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	512	3930	2576	647	687	20	0	0	0
1	B	537	4062	2657	672	713	20	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

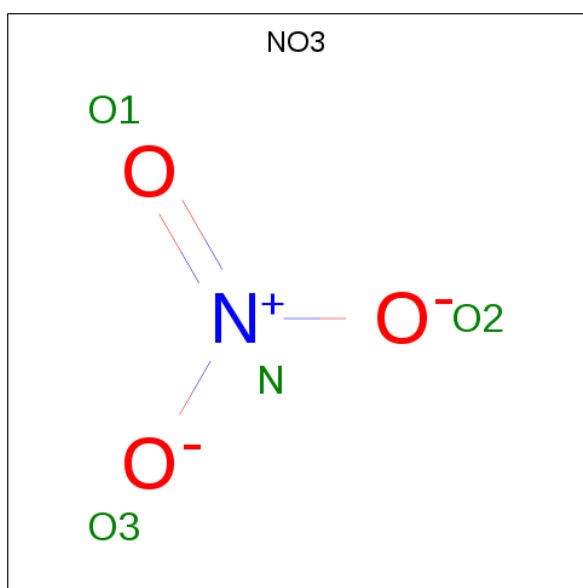
Chain	Residue	Modelled	Actual	Comment	Reference
A	591	ALA	-	EXPRESSION TAG	UNP Q05085
A	592	ALA	-	EXPRESSION TAG	UNP Q05085
A	593	ALA	-	EXPRESSION TAG	UNP Q05085
A	594	GLY	-	EXPRESSION TAG	UNP Q05085
A	595	SER	-	EXPRESSION TAG	UNP Q05085
A	596	LEU	-	EXPRESSION TAG	UNP Q05085
A	597	VAL	-	EXPRESSION TAG	UNP Q05085
A	598	PRO	-	EXPRESSION TAG	UNP Q05085
A	599	ARG	-	EXPRESSION TAG	UNP Q05085
B	591	ALA	-	EXPRESSION TAG	UNP Q05085
B	592	ALA	-	EXPRESSION TAG	UNP Q05085
B	593	ALA	-	EXPRESSION TAG	UNP Q05085
B	594	GLY	-	EXPRESSION TAG	UNP Q05085
B	595	SER	-	EXPRESSION TAG	UNP Q05085
B	596	LEU	-	EXPRESSION TAG	UNP Q05085
B	597	VAL	-	EXPRESSION TAG	UNP Q05085
B	598	PRO	-	EXPRESSION TAG	UNP Q05085
B	599	ARG	-	EXPRESSION TAG	UNP Q05085

- Molecule 2 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



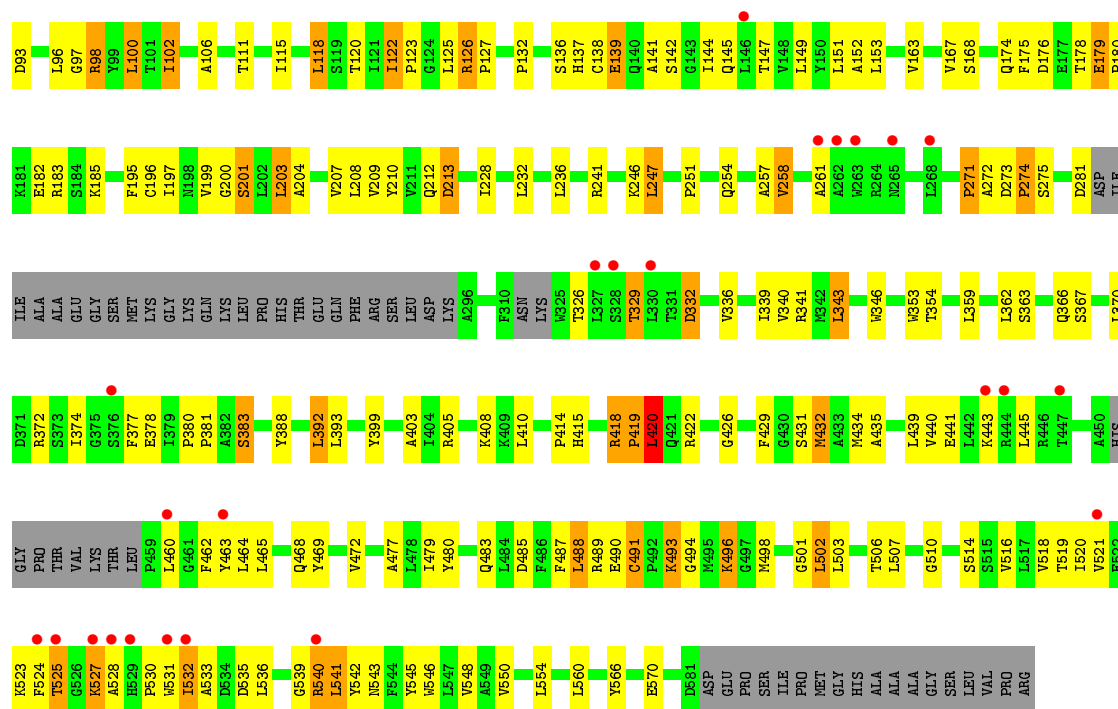
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			24	13	11		
2	B	1	Total	C	O	0	0
			24	13	11		

- Molecule 3 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O	0	0
			4	1	3		
3	B	1	Total	N	O	0	0
			4	1	3		





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.80Å 188.47Å 262.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.91 – 3.25 45.91 – 3.20	Depositor EDS
% Data completeness (in resolution range)	89.5 (45.91-3.25) 86.6 (45.91-3.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.78 (at 3.19Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.235 , 0.307 0.237 , 0.307	Depositor DCC
$R_{free}$ test set	1484 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	86.3	Xtrriage
Anisotropy	0.011	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 67.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	8048	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, NO3

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	0.54	0/4017	0.72	4/5459 (0.1%)
1	B	0.44	0/4149	0.68	6/5643 (0.1%)
All	All	0.49	0/8166	0.70	10/11102 (0.1%)

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	1
1	B	0	3
All	All	0	4

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	271	PRO	N-CA-CB	6.43	111.02	103.30
1	B	274	PRO	N-CA-CB	5.84	110.31	103.30
1	A	29	GLY	N-CA-C	-5.60	99.10	113.10
1	A	178	THR	N-CA-C	-5.52	96.09	111.00
1	B	420	LEU	CA-CB-CG	5.47	127.89	115.30
1	B	12	LEU	CA-CB-CG	5.29	127.48	115.30
1	B	247	LEU	CA-CB-CG	5.29	127.46	115.30
1	A	177	GLU	N-CA-C	-5.19	96.99	111.00
1	B	30	GLY	N-CA-C	5.19	126.08	113.10
1	A	30	GLY	N-CA-C	5.11	125.86	113.10

There are no chirality outliers.



All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	262	ALA	Peptide
1	B	175	PHE	Peptide
1	B	272	ALA	Peptide
1	B	418	ARG	Peptide

## 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	3930	0	4004	129	0
1	B	4062	0	4079	122	0
2	A	24	0	20	1	0
2	B	24	0	20	4	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
All	All	8048	0	8123	250	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 15.

All (250) 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:A:179:GLU:HG2	1:A:181:LYS:H	1.37	0.90
1:B:392:LEU:HD12	1:B:477:ALA:HB2	1.60	0.84
1:A:98:ARG:HG2	1:A:170:PHE:HB2	1.59	0.82
1:A:24:ASP:OD1	1:A:27:LYS:N	2.12	0.81
1:B:45:ARG:HH21	1:B:197:ILE:HG21	1.46	0.80
1:B:102:ILE:HD12	1:B:167:VAL:HG23	1.63	0.80
1:B:142:SER:H	1:B:145:GLN:HE21	1.28	0.79
1:A:57:THR:HG22	1:A:217:ARG:HH12	1.48	0.79
1:A:303:ASP:O	1:A:341:ARG:NH2	2.17	0.78
1:B:408:LYS:HB2	1:B:414:PRO:HB3	1.64	0.78
1:B:340:VAL:HA	1:B:343:LEU:HD22	1.66	0.77
1:B:93:ASP:OD1	1:B:98:ARG:NH1	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:THR:O	1:B:126:ARG:NH2	2.23	0.71
1:B:399:TYR:OH	1:B:422:ARG:NH1	2.25	0.70
1:B:374:ILE:HB	1:B:377:PHE:HB3	1.75	0.69
1:A:434:MET:HG3	1:A:548:VAL:HG12	1.75	0.68
1:B:329:THR:HG23	1:B:332:ASP:HB2	1.75	0.68
1:B:429:PHE:HA	1:B:432:MET:HB2	1.75	0.68
1:B:12:LEU:HD12	1:B:14:ASP:HB3	1.76	0.66
1:B:462:PHE:CG	1:B:463:TYR:N	2.64	0.66
1:A:251:PRO:HB3	1:A:495:MET:HB3	1.78	0.65
1:A:54:ASN:OD1	1:A:57:THR:HB	1.97	0.65
1:A:197:ILE:O	1:A:201:SER:N	2.30	0.64
1:B:106:ALA:HB3	1:B:232:LEU:HD12	1.80	0.64
1:A:98:ARG:O	1:A:102:ILE:HG22	1.98	0.64
1:B:127:PRO:HG3	1:B:141:ALA:HA	1.79	0.63
1:B:195:PHE:HD1	2:B:601:LMT:H6E	1.64	0.63
1:B:142:SER:H	1:B:145:GLN:NE2	1.98	0.62
1:B:480:TYR:CE2	1:B:503:LEU:HD21	2.35	0.62
1:A:179:GLU:O	1:A:183:ARG:HB3	2.00	0.62
1:B:353:TRP:HB2	1:B:510:GLY:HA3	1.82	0.61
1:A:421:GLN:O	1:A:425:LEU:HB2	2.01	0.61
1:A:543:ASN:HA	1:A:546:TRP:HB2	1.83	0.61
1:B:540:ARG:HB2	1:B:542:TYR:CE2	2.35	0.60
1:A:141:ALA:HB3	1:A:146:LEU:HD13	1.84	0.60
1:A:45:ARG:HH21	1:A:197:ILE:HG21	1.67	0.60
1:B:31:TRP:HE1	1:B:185:LYS:HG2	1.67	0.60
1:B:393:LEU:HD22	2:B:601:LMT:H2'	1.84	0.59
1:A:563:SER:O	1:A:567:VAL:HG22	2.04	0.58
1:B:366:GLN:HG3	1:B:465:LEU:HD11	1.85	0.58
1:A:479:ILE:O	1:A:483:GLN:HB2	2.04	0.58
1:A:99:TYR:HB2	1:A:170:PHE:CE1	2.38	0.57
1:A:463:TYR:HA	1:A:466:ILE:HG13	1.86	0.57
1:B:408:LYS:CB	1:B:414:PRO:HB3	2.35	0.57
1:B:354:THR:HG23	1:B:514:SER:HB2	1.86	0.57
1:A:198:ASN:N	1:A:198:ASN:OD1	2.35	0.57
1:B:420:LEU:H	1:B:420:LEU:HD12	1.69	0.57
1:A:37:ILE:HG21	1:A:170:PHE:HD2	1.68	0.56
1:A:179:GLU:HG2	1:A:181:LYS:N	2.15	0.56
1:B:490:GLU:OE1	1:B:566:TYR:OH	2.10	0.56
1:B:246:LYS:O	1:B:247:LEU:HB2	2.05	0.56
1:A:540:ARG:NE	1:A:542:TYR:OH	2.22	0.56
1:B:54:ASN:HB3	1:B:212:GLN:NE2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:VAL:O	1:A:340:VAL:HG23	2.06	0.55
1:B:494:GLY:H	1:B:496:LYS:HE3	1.71	0.55
1:A:37:ILE:HD13	1:A:170:PHE:CD2	2.42	0.55
1:B:115:ILE:HG22	1:B:152:ALA:HB2	1.87	0.55
1:A:334:GLU:HA	1:A:337:LYS:HB2	1.89	0.55
1:A:413:TYR:HD1	1:A:416:GLY:O	1.90	0.55
1:B:370:LEU:HD11	1:B:465:LEU:HG	1.88	0.55
1:B:50:GLY:HA3	1:B:208:LEU:HD12	1.87	0.54
1:B:399:TYR:HD1	1:B:403:ALA:HB3	1.72	0.54
1:B:431:SER:O	1:B:435:ALA:N	2.35	0.54
1:B:527:LYS:HD3	1:B:528:ALA:H	1.71	0.54
1:A:351:LEU:HD12	1:A:555:ASN:HB2	1.88	0.54
1:B:275:SER:O	1:B:281:ASP:HA	2.08	0.54
1:B:179:GLU:HG2	1:B:180:PRO:HD2	1.87	0.54
1:B:257:ALA:O	1:B:261:ALA:HB3	2.08	0.54
1:A:493:LYS:HA	1:A:493:LYS:NZ	2.22	0.54
1:A:530:PRO:HG2	1:A:533:ALA:HB2	1.90	0.54
1:B:533:ALA:HB3	1:B:536:LEU:HD23	1.89	0.54
1:A:122:ILE:HG23	1:A:123:PRO:HD2	1.90	0.53
1:A:40:ILE:HG22	1:A:231:ALA:HB1	1.90	0.53
1:A:334:GLU:OE1	1:A:338:GLN:NE2	2.41	0.53
1:A:344:PRO:HG2	1:A:345:ILE:HD12	1.90	0.53
1:B:254:GLN:NE2	1:B:332:ASP:OD2	2.42	0.53
1:A:37:ILE:HD13	1:A:170:PHE:CE2	2.44	0.53
1:A:470:LEU:HG	1:A:474:ILE:HD11	1.90	0.53
1:B:362:LEU:HD13	1:B:541:LEU:HD21	1.90	0.53
1:A:55:LEU:HD23	1:A:74:VAL:HG22	1.90	0.52
1:B:207:VAL:O	1:B:210:TYR:HB3	2.10	0.52
1:A:361:THR:OG1	1:A:362:LEU:N	2.43	0.52
1:B:531:TRP:CG	1:B:543:ASN:HB3	2.45	0.52
1:A:258:VAL:HG22	1:A:333:VAL:HG12	1.92	0.52
1:A:209:VAL:HG11	1:A:383:SER:HB3	1.92	0.52
1:B:196:CYS:O	1:B:200:GLY:N	2.33	0.51
1:A:105:PHE:HE2	1:A:158:LEU:HD11	1.75	0.51
1:A:250:SER:HB3	1:A:253:THR:HG23	1.93	0.51
1:A:163:VAL:HG13	1:A:167:VAL:HG21	1.93	0.51
1:A:258:VAL:HG21	1:A:333:VAL:HA	1.93	0.50
1:B:516:VAL:O	1:B:520:ILE:HG13	2.11	0.50
1:A:102:ILE:HD12	1:A:167:VAL:HG22	1.92	0.50
1:A:345:ILE:H	1:A:345:ILE:HD12	1.76	0.50
1:A:404:ILE:HD12	1:A:408:LYS:HZ1	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:THR:HG21	1:A:531:TRP:CD1	2.47	0.49
1:B:251:PRO:HB2	1:B:498:MET:HG2	1.94	0.49
1:A:353:TRP:HB2	1:A:510:GLY:HA3	1.93	0.49
1:A:397:ALA:HB2	2:A:701:LMT:H6E	1.95	0.49
1:B:195:PHE:CD1	2:B:601:LMT:H6E	2.45	0.49
1:B:380:PRO:HB2	1:B:383:SER:HB2	1.94	0.49
1:A:370:LEU:HD11	1:A:465:LEU:HG	1.94	0.49
1:B:142:SER:HB3	1:B:144:ILE:HG22	1.95	0.48
1:A:122:ILE:O	1:A:126:ARG:NH2	2.46	0.48
1:A:335:GLU:HG2	1:A:492:PRO:HB3	1.94	0.48
1:B:487:PHE:O	1:B:491:CYS:HB2	2.13	0.48
1:A:104:ILE:HG12	1:B:236:LEU:HB3	1.94	0.48
1:A:198:ASN:HA	1:A:201:SER:HB2	1.95	0.48
1:B:441:GLU:HG2	1:B:541:LEU:HB3	1.95	0.48
1:B:59:LEU:HB3	1:B:65:LEU:HD12	1.96	0.48
1:B:59:LEU:HA	1:B:63:MET:HB2	1.95	0.48
1:A:330:LEU:HA	1:A:333:VAL:HG22	1.96	0.48
1:B:254:GLN:O	1:B:258:VAL:HG13	2.14	0.47
1:A:32:ALA:O	1:A:35:ALA:HB3	2.14	0.47
1:B:343:LEU:O	1:B:346:TRP:HB3	2.14	0.47
1:A:420:LEU:H	1:A:420:LEU:HD12	1.80	0.47
1:A:359:LEU:HA	1:A:359:LEU:HD12	1.69	0.47
1:A:484:LEU:O	1:A:488:LEU:HB2	2.14	0.47
1:B:367:SER:O	1:B:372:ARG:NE	2.48	0.47
1:A:352:PHE:HE2	1:A:476:GLU:HG3	1.79	0.47
1:A:17:ASP:HB2	1:A:21:ARG:O	2.13	0.47
1:A:480:TYR:CE1	1:A:503:LEU:HD21	2.50	0.47
1:B:213:ASP:OD2	1:B:381:PRO:HD2	2.15	0.47
1:A:31:TRP:CG	1:A:32:ALA:N	2.83	0.47
1:A:255:VAL:HG22	1:A:336:VAL:HG22	1.97	0.47
1:A:535:ASP:OD2	1:A:538:LYS:NZ	2.40	0.47
1:B:118:LEU:HA	1:B:118:LEU:HD13	1.74	0.47
1:A:491:CYS:HB3	1:A:495:MET:O	2.15	0.47
1:B:419:PRO:HD2	1:B:420:LEU:HD12	1.96	0.47
1:A:471:ILE:HA	1:A:474:ILE:HD12	1.97	0.46
1:A:518:VAL:HG22	1:A:532:ILE:CD1	2.46	0.46
1:A:25:ARG:HH21	1:A:179:GLU:CD	2.18	0.46
1:A:84:LEU:HD23	1:A:84:LEU:HA	1.70	0.46
1:A:98:ARG:HG3	1:A:166:SER:HB3	1.97	0.46
1:B:195:PHE:HA	2:B:601:LMT:H6E	1.97	0.46
1:B:87:LEU:O	1:B:91:ILE:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:LEU:HD23	1:B:501:GLY:HA2	1.98	0.46
1:A:441:GLU:HG2	1:A:541:LEU:HB3	1.97	0.46
1:B:434:MET:HE3	1:B:545:TYR:HA	1.97	0.46
1:A:536:LEU:HD23	1:A:536:LEU:HA	1.81	0.46
1:B:57:THR:O	1:B:61:GLY:N	2.48	0.46
1:A:154:TYR:HA	1:A:154:TYR:HD1	1.51	0.46
1:A:551:LEU:HA	1:A:551:LEU:HD23	1.61	0.46
1:B:258:VAL:HG21	1:B:336:VAL:HG21	1.98	0.45
1:B:422:ARG:NH2	1:B:485:ASP:OD1	2.50	0.45
1:A:459:PRO:HB2	1:A:460:LEU:H	1.51	0.45
1:B:483:GLN:NE2	1:B:506:THR:OG1	2.49	0.45
1:B:98:ARG:O	1:B:102:ILE:HG23	2.16	0.45
1:B:199:VAL:O	1:B:203:LEU:HD22	2.16	0.45
1:A:131:ASN:ND2	1:A:133:THR:HB	2.31	0.45
1:B:533:ALA:HB2	1:B:539:GLY:HA3	1.98	0.45
1:A:371:ASP:HB3	1:A:461:GLY:HA2	1.98	0.45
1:A:59:LEU:HD21	1:A:149:LEU:HD11	1.99	0.45
1:B:531:TRP:HB3	1:B:543:ASN:HB3	1.99	0.45
1:B:49:LEU:HD12	1:B:53:VAL:HG23	1.99	0.45
1:A:24:ASP:OD1	1:A:26:SER:N	2.50	0.45
1:A:127:PRO:HG3	1:A:141:ALA:HA	1.97	0.45
1:B:399:TYR:CD1	1:B:403:ALA:HB3	2.50	0.44
1:A:49:LEU:HD23	1:A:49:LEU:HA	1.74	0.44
1:A:60:THR:O	1:A:64:HIS:HA	2.17	0.44
1:A:59:LEU:HA	1:A:59:LEU:HD23	1.64	0.44
1:B:86:LEU:CD2	1:B:501:GLY:HA2	2.48	0.44
1:B:46:LEU:HG	1:B:204:ALA:HB2	1.99	0.44
1:B:29:GLY:O	1:B:33:SER:HB3	2.18	0.44
1:A:96:LEU:HD22	1:A:100:LEU:HB3	2.00	0.44
1:B:414:PRO:HD2	1:B:415:HIS:NE2	2.32	0.44
1:A:155:LEU:HD23	1:A:155:LEU:HA	1.74	0.44
1:A:419:PRO:HB2	1:A:486:PHE:HB2	2.00	0.44
1:B:106:ALA:HB1	1:B:228:ILE:HD11	1.98	0.44
1:A:535:ASP:HB3	1:A:538:LYS:HB2	2.00	0.43
1:B:525:THR:O	1:B:530:PRO:HB3	2.19	0.43
1:A:351:LEU:HA	1:A:351:LEU:HD23	1.65	0.43
1:B:142:SER:HB2	1:B:145:GLN:HG2	2.00	0.43
1:B:370:LEU:HD13	1:B:462:PHE:HD1	1.82	0.43
1:B:363:SER:HA	1:B:366:GLN:HG2	2.01	0.43
1:B:550:VAL:O	1:B:554:LEU:HG	2.19	0.43
1:A:145:GLN:HG2	1:A:145:GLN:H	1.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LEU:HG	1:A:204:ALA:HB2	1.99	0.43
1:B:209:VAL:O	1:B:213:ASP:HB2	2.19	0.43
1:B:16:TRP:CZ2	1:B:246:LYS:HE3	2.53	0.43
1:B:531:TRP:CB	1:B:543:ASN:HB3	2.49	0.43
1:A:517:LEU:HA	1:A:517:LEU:HD12	1.71	0.43
1:B:336:VAL:O	1:B:339:ILE:HB	2.19	0.43
1:B:362:LEU:HB3	1:B:541:LEU:HD11	2.01	0.43
1:A:425:LEU:HA	1:A:425:LEU:HD23	1.86	0.43
1:A:99:TYR:HD2	1:A:100:LEU:HD22	1.83	0.43
1:B:122:ILE:HA	1:B:123:PRO:HD3	1.83	0.43
1:B:380:PRO:HA	1:B:381:PRO:HD3	1.77	0.43
1:B:434:MET:HG3	1:B:548:VAL:CG1	2.49	0.43
1:B:533:ALA:HB1	1:B:535:ASP:O	2.19	0.43
1:A:14:ASP:HA	1:A:16:TRP:CH2	2.54	0.42
1:A:16:TRP:HZ3	1:A:246:LYS:HB2	1.83	0.42
1:A:370:LEU:HD21	1:A:444:ARG:HD2	2.01	0.42
1:A:25:ARG:NH1	1:A:177:GLU:OE2	2.51	0.42
1:B:176:ASP:OD1	1:B:183:ARG:HG2	2.19	0.42
1:B:502:LEU:O	1:B:506:THR:HG23	2.19	0.42
1:B:100:LEU:HD23	1:B:100:LEU:H	1.83	0.42
1:B:127:PRO:HB3	1:B:139:GLU:HB3	2.00	0.42
1:A:194:PHE:HD1	1:A:194:PHE:HA	1.78	0.42
1:A:467:PRO:O	1:A:471:ILE:HG12	2.20	0.42
1:B:122:ILE:HG12	1:B:125:LEU:HD22	2.00	0.42
1:B:392:LEU:HD12	1:B:392:LEU:HA	1.84	0.42
1:B:47:THR:HG23	1:B:51:ILE:HD12	2.00	0.42
1:A:146:LEU:O	1:A:150:TYR:HD1	2.01	0.42
1:A:423:ILE:HD11	1:A:483:GLN:HA	2.01	0.42
1:A:197:ILE:HD13	1:A:197:ILE:HA	1.78	0.42
1:B:132:PRO:HA	1:B:136:SER:O	2.20	0.42
1:B:254:GLN:HA	1:B:257:ALA:HB3	2.02	0.42
1:B:527:LYS:HE2	1:B:527:LYS:HA	2.02	0.42
1:A:404:ILE:HG23	1:A:408:LYS:HZ2	1.85	0.42
1:B:197:ILE:O	1:B:201:SER:N	2.46	0.41
1:B:426:GLY:HA3	1:B:479:ILE:HB	2.02	0.41
1:A:439:LEU:HG	1:A:546:TRP:CZ2	2.55	0.41
1:B:136:SER:OG	1:B:137:HIS:N	2.53	0.41
1:B:153:LEU:HD23	1:B:153:LEU:HA	1.88	0.41
1:A:330:LEU:HA	1:A:330:LEU:HD22	1.85	0.41
1:A:343:LEU:HD23	1:A:343:LEU:HA	1.76	0.41
1:B:258:VAL:CG2	1:B:336:VAL:HG21	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:VAL:O	1:B:521:VAL:HG22	2.20	0.41
1:A:173:ASP:HA	1:A:176:ASP:OD1	2.21	0.41
1:A:346:TRP:HE1	1:A:505:SER:HB3	1.86	0.41
1:B:203:LEU:HA	1:B:203:LEU:HD12	1.98	0.41
1:A:146:LEU:HG	1:A:150:TYR:HE1	1.85	0.41
1:B:440:VAL:CG2	1:B:464:LEU:HB3	2.51	0.41
1:A:226:PHE:CE2	1:A:230:LEU:HD22	2.56	0.41
1:B:468:GLN:O	1:B:472:VAL:HG23	2.21	0.41
1:B:493:LYS:HD3	1:B:493:LYS:HA	1.66	0.41
1:A:379:ILE:HA	1:A:380:PRO:HD3	1.90	0.41
1:A:404:ILE:HA	1:A:408:LYS:HE3	2.02	0.41
1:A:426:GLY:HA3	1:A:479:ILE:HB	2.02	0.41
1:B:465:LEU:O	1:B:469:TYR:HD1	2.02	0.41
1:A:116:LEU:O	1:A:119:SER:HB3	2.21	0.41
1:B:434:MET:HG3	1:B:548:VAL:HG12	2.03	0.41
1:A:366:GLN:NE2	1:A:441:GLU:HB2	2.36	0.41
1:A:493:LYS:HZ3	1:A:493:LYS:HA	1.86	0.41
1:B:533:ALA:HB3	1:B:536:LEU:HA	2.02	0.41
1:A:118:LEU:HA	1:A:118:LEU:HD12	1.76	0.40
1:A:219:TRP:O	1:A:223:ILE:HG12	2.21	0.40
1:A:404:ILE:HG23	1:A:408:LYS:HE3	2.02	0.40
1:A:470:LEU:HD12	1:A:470:LEU:HA	1.73	0.40
1:A:372:ARG:HA	1:A:462:PHE:CD2	2.56	0.40
1:A:117:THR:O	1:A:121:ILE:HG22	2.21	0.40
1:A:99:TYR:CD2	1:A:100:LEU:HD22	2.56	0.40
1:B:353:TRP:CD2	1:B:507:LEU:HD13	2.56	0.40
1:A:445:LEU:HD12	1:A:445:LEU:HA	1.91	0.40
1:B:359:LEU:HA	1:B:359:LEU:HD12	1.80	0.40
1:A:99:TYR:O	1:A:102:ILE:HG23	2.22	0.40
1:A:119:SER:HA	1:A:125:LEU:HD23	2.03	0.40
1:A:566:TYR:O	1:A:570:GLU:HB2	2.21	0.40
1:B:488:LEU:HA	1:B:488:LEU:HD12	1.79	0.40
1:B:97:GLY:H	1:B:100:LEU:HD21	1.87	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	504/599 (84%)	470 (93%)	32 (6%)	2 (0%)	34	67
1	B	529/599 (88%)	474 (90%)	50 (10%)	5 (1%)	17	50
All	All	1033/1198 (86%)	944 (91%)	82 (8%)	7 (1%)	22	56

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	273	ASP
1	B	532	ILE
1	B	274	PRO
1	A	493	LYS
1	A	492	PRO
1	B	271	PRO
1	B	419	PRO

### 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	409/494 (83%)	337 (82%)	72 (18%)	2	8
1	B	412/494 (83%)	343 (83%)	69 (17%)	2	9
All	All	821/988 (83%)	680 (83%)	141 (17%)	2	9

All (141) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	10	ASP
1	A	14	ASP
1	A	17	ASP
1	A	25	ARG
1	A	27	LYS
1	A	40	ILE
1	A	45	ARG
1	A	57	THR
1	A	75	THR
1	A	78	LEU
1	A	83	MET
1	A	95	PHE
1	A	100	LEU
1	A	102	ILE
1	A	108	ILE
1	A	109	GLN
1	A	111	THR
1	A	118	LEU
1	A	121	ILE
1	A	126	ARG
1	A	140	GLN
1	A	144	ILE
1	A	145	GLN
1	A	146	LEU
1	A	149	LEU
1	A	160	THR
1	A	178	THR
1	A	183	ARG
1	A	187	THR
1	A	188	TYR
1	A	194	PHE
1	A	198	ASN
1	A	201	SER
1	A	202	LEU
1	A	203	LEU
1	A	208	LEU
1	A	217	ARG
1	A	228	ILE
1	A	232	LEU
1	A	241	ARG
1	A	252	MET
1	A	255	VAL
1	A	329	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	330	LEU
1	A	337	LYS
1	A	341	ARG
1	A	351	LEU
1	A	359	LEU
1	A	368	GLU
1	A	379	ILE
1	A	388	TYR
1	A	394	LEU
1	A	411	PHE
1	A	415	HIS
1	A	417	LEU
1	A	418	ARG
1	A	425	LEU
1	A	443	LYS
1	A	447	THR
1	A	468	GLN
1	A	488	LEU
1	A	495	MET
1	A	502	LEU
1	A	509	LEU
1	A	515	SER
1	A	517	LEU
1	A	525	THR
1	A	541	LEU
1	A	551	LEU
1	A	560	LEU
1	A	570	GLU
1	A	573	LEU
1	B	12	LEU
1	B	13	LEU
1	B	27	LYS
1	B	31	TRP
1	B	46	LEU
1	B	48	THR
1	B	62	THR
1	B	63	MET
1	B	80	THR
1	B	87	LEU
1	B	96	LEU
1	B	98	ARG
1	B	100	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	102	ILE
1	B	111	THR
1	B	118	LEU
1	B	122	ILE
1	B	126	ARG
1	B	138	CYS
1	B	139	GLU
1	B	147	THR
1	B	149	LEU
1	B	151	LEU
1	B	163	VAL
1	B	168	SER
1	B	174	GLN
1	B	178	THR
1	B	179	GLU
1	B	182	GLU
1	B	201	SER
1	B	203	LEU
1	B	213	ASP
1	B	241	ARG
1	B	258	VAL
1	B	326	THR
1	B	329	THR
1	B	332	ASP
1	B	341	ARG
1	B	343	LEU
1	B	378	GLU
1	B	383	SER
1	B	388	TYR
1	B	392	LEU
1	B	405	ARG
1	B	410	LEU
1	B	418	ARG
1	B	420	LEU
1	B	432	MET
1	B	439	LEU
1	B	443	LYS
1	B	445	LEU
1	B	460	LEU
1	B	488	LEU
1	B	489	ARG
1	B	491	CYS

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Mol	Chain	Res	Type
1	B	493	LYS
1	B	496	LYS
1	B	502	LEU
1	B	519	THR
1	B	523	LYS
1	B	524	PHE
1	B	525	THR
1	B	527	LYS
1	B	532	ILE
1	B	540	ARG
1	B	541	LEU
1	B	546	TRP
1	B	560	LEU
1	B	570	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	145	GLN
1	B	254	GLN
1	B	366	GLN
1	B	468	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates 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
3	NO3	A	702	-	1,3,3	0.06	0	0,3,3	0.00	-
2	LMT	A	701	-	25,25,36	1.61	4 (16%)	36,36,47	2.20	11 (30%)
2	LMT	B	601	-	25,25,36	1.59	3 (12%)	36,36,47	1.59	6 (16%)
3	NO3	B	602	-	1,3,3	0.09	0	0,3,3	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMT	A	701	-	-	5/10/50/61	0/2/2/2
2	LMT	B	601	-	-	5/10/50/61	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	LMT	C3'-C4'	-3.99	1.41	1.52
2	B	601	LMT	O5B-C1B	3.89	1.51	1.41
2	A	701	LMT	O5B-C1B	3.52	1.50	1.41
2	B	601	LMT	C3'-C4'	-3.51	1.42	1.52
2	A	701	LMT	O3'-C3'	2.57	1.49	1.43
2	B	601	LMT	O3'-C3'	2.34	1.48	1.43
2	A	701	LMT	O5'-C5'	2.07	1.49	1.44

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	LMT	C1-O1'-C1'	8.64	126.61	113.27
2	B	601	LMT	C1-O1'-C1'	4.09	119.58	113.27
2	A	701	LMT	C4B-C3B-C2B	3.56	117.03	110.82
2	B	601	LMT	C1B-O5B-C5B	3.51	120.58	113.69
2	A	701	LMT	C1B-C2B-C3B	3.47	117.22	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	LMT	O5B-C5B-C4B	3.17	115.45	109.69
2	A	701	LMT	O5B-C5B-C6B	3.11	114.17	106.44
2	B	601	LMT	C2'-C3'-C4'	2.85	116.19	109.68
2	A	701	LMT	C1'-C2'-C3'	2.67	115.57	110.00
2	A	701	LMT	O6'-C6'-C5'	2.53	119.96	111.29
2	B	601	LMT	O1'-C1'-C2'	2.43	111.00	108.15
2	A	701	LMT	O1'-C1'-C2'	2.35	110.91	108.15
2	A	701	LMT	C2'-C3'-C4'	2.30	114.92	109.68
2	A	701	LMT	O6B-C6B-C5B	2.29	119.14	111.29
2	A	701	LMT	O2'-C2'-C1'	-2.23	104.62	110.05
2	B	601	LMT	C1'-C2'-C3'	2.16	114.50	110.00
2	A	701	LMT	O5B-C1B-C2B	2.04	114.67	110.35

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	LMT	C2'-C1'-O1'-C1
2	A	701	LMT	O5'-C1'-O1'-C1
2	B	601	LMT	O5'-C1'-O1'-C1
2	B	601	LMT	C2'-C1'-O1'-C1
2	B	601	LMT	C4B-C5B-C6B-O6B
2	B	601	LMT	O5B-C5B-C6B-O6B
2	A	701	LMT	O5'-C5'-C6'-O6'
2	A	701	LMT	O5B-C5B-C6B-O6B
2	A	701	LMT	O5B-C1B-O1B-C4'
2	B	601	LMT	O5'-C5'-C6'-O6'

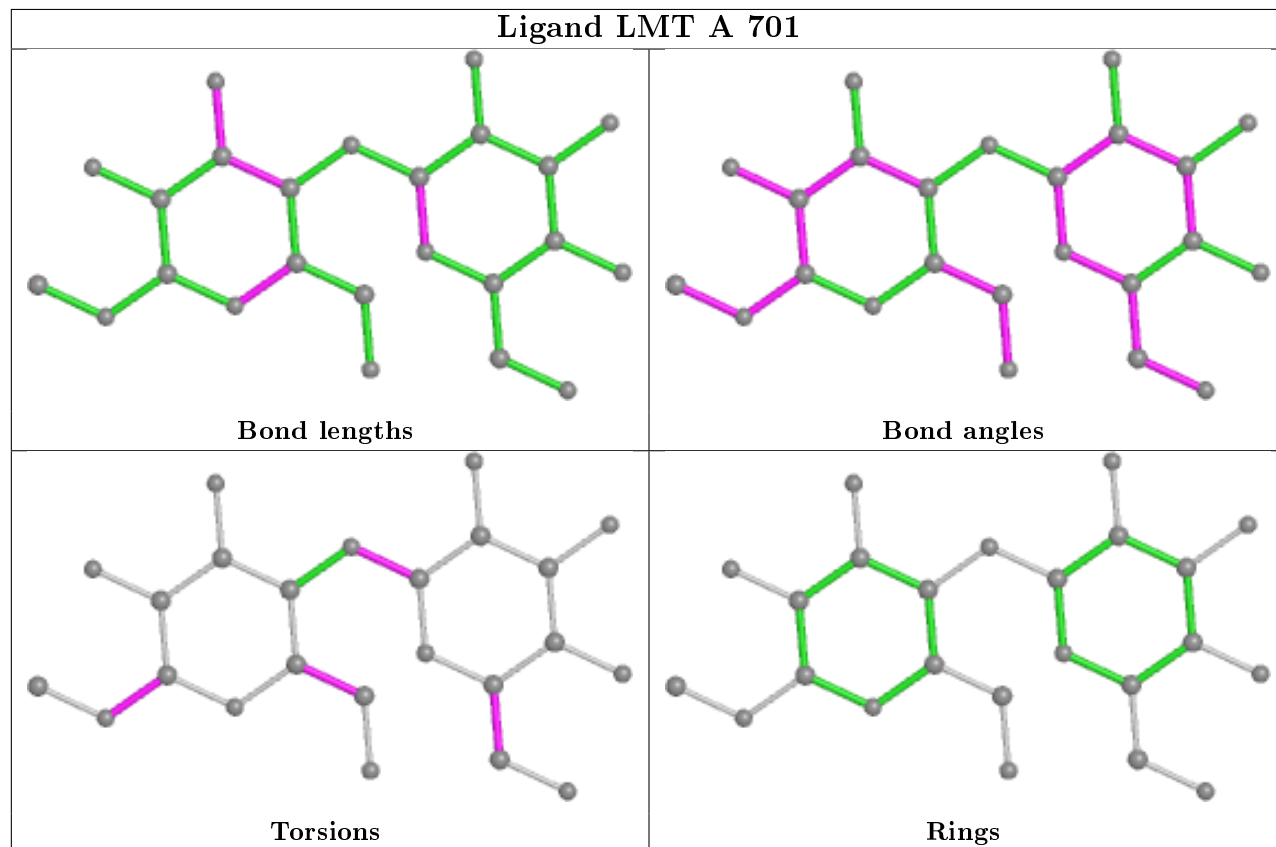
There are no ring outliers.

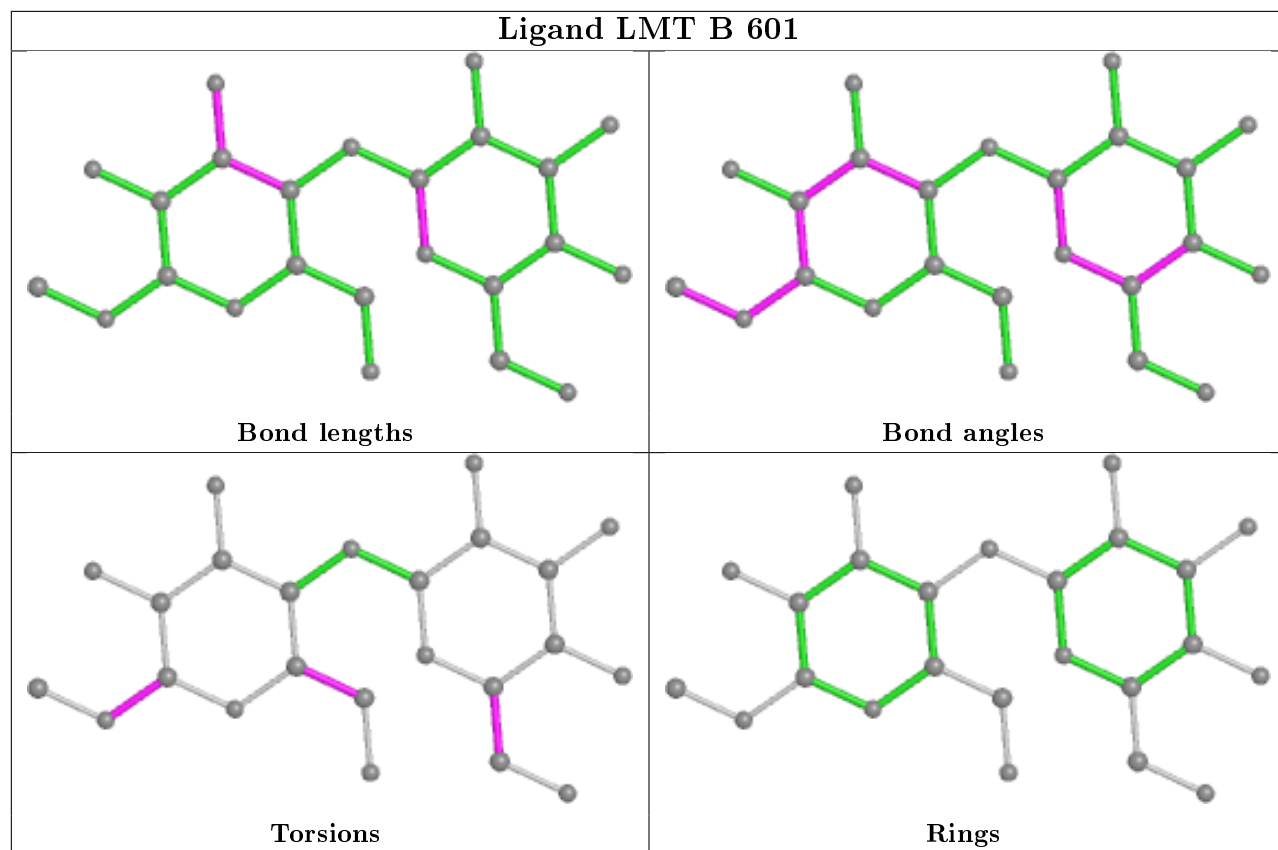
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	LMT	1	0
2	B	601	LMT	4	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	512/599 (85%)	-0.09	22 (4%) 35 33	36, 71, 159, 228	0
1	B	537/599 (89%)	0.08	31 (5%) 23 22	47, 93, 170, 237	0
All	All	1049/1198 (87%)	-0.00	53 (5%) 28 26	36, 84, 167, 237	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	529	HIS	6.1
1	A	527	LYS	5.2
1	A	572	ARG	5.1
1	B	524	PHE	4.8
1	A	263	TRP	4.6
1	B	447	THR	4.4
1	A	529	HIS	4.2
1	A	330	LEU	3.9
1	A	568	TYR	3.8
1	B	460	LEU	3.7
1	B	463	TYR	3.7
1	B	327	LEU	3.7
1	A	176	ASP	3.6
1	B	262	ALA	3.6
1	A	573	LEU	3.5
1	B	531	TRP	3.5
1	B	540	ARG	3.4
1	A	262	ALA	3.3
1	B	443	LYS	3.2
1	A	329	THR	3.2
1	B	330	LEU	3.2
1	A	14	ASP	3.2
1	B	10	ASP	3.1
1	B	527	LYS	3.0

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	B	25	ARG	3.0
1	B	263	TRP	3.0
1	B	528	ALA	3.0
1	A	261	ALA	2.8
1	A	328	SER	2.8
1	B	11	ILE	2.8
1	A	526	GLY	2.7
1	A	12	LEU	2.7
1	A	31	TRP	2.6
1	B	66	GLY	2.6
1	B	532	ILE	2.6
1	A	308	VAL	2.5
1	B	261	ALA	2.5
1	A	265	ASN	2.4
1	B	70	ALA	2.3
1	B	525	THR	2.3
1	B	444	ARG	2.3
1	B	146	LEU	2.3
1	B	328	SER	2.3
1	B	21	ARG	2.3
1	B	376	SER	2.3
1	A	576	VAL	2.2
1	A	570	GLU	2.2
1	A	188	TYR	2.1
1	B	265	ASN	2.1
1	B	268	LEU	2.0
1	B	12	LEU	2.0
1	A	414	PRO	2.0
1	B	521	VAL	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](#)

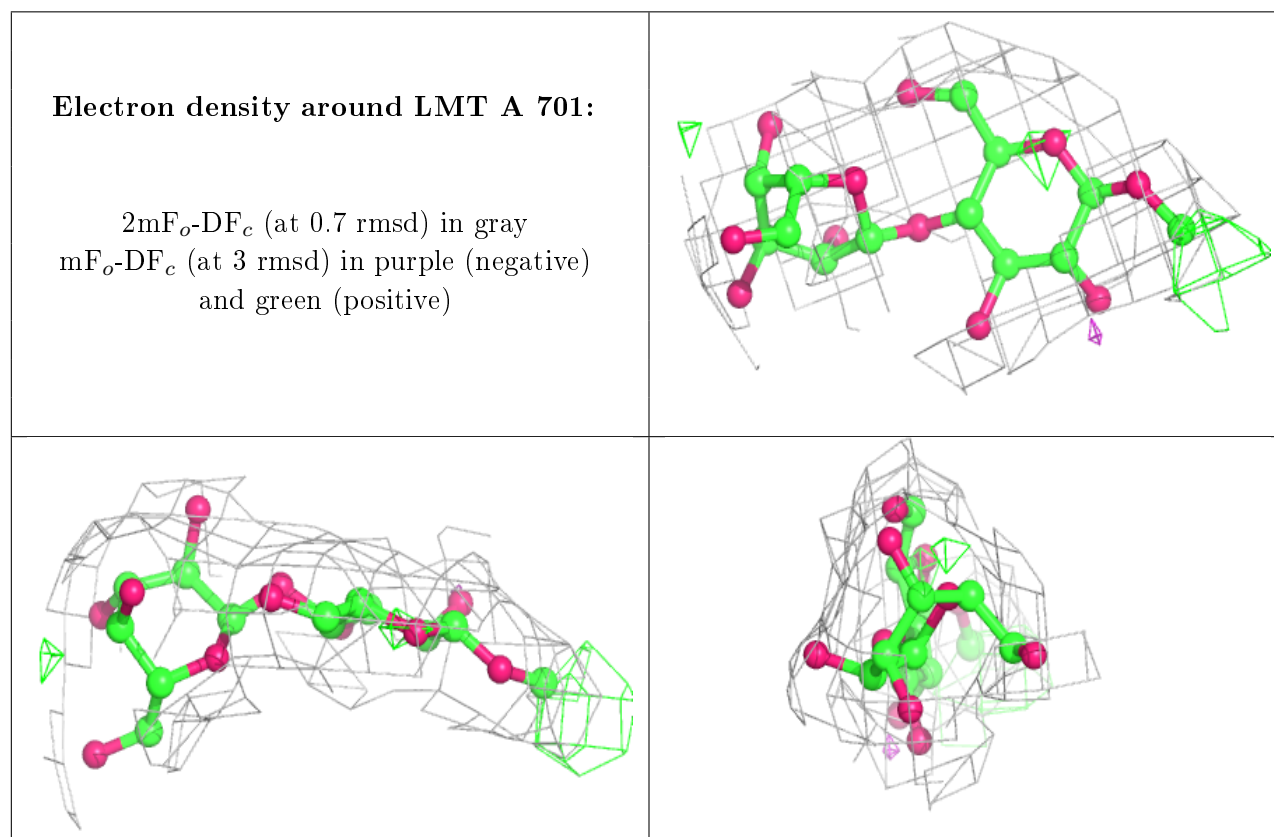
There are no carbohydrates in this entry.

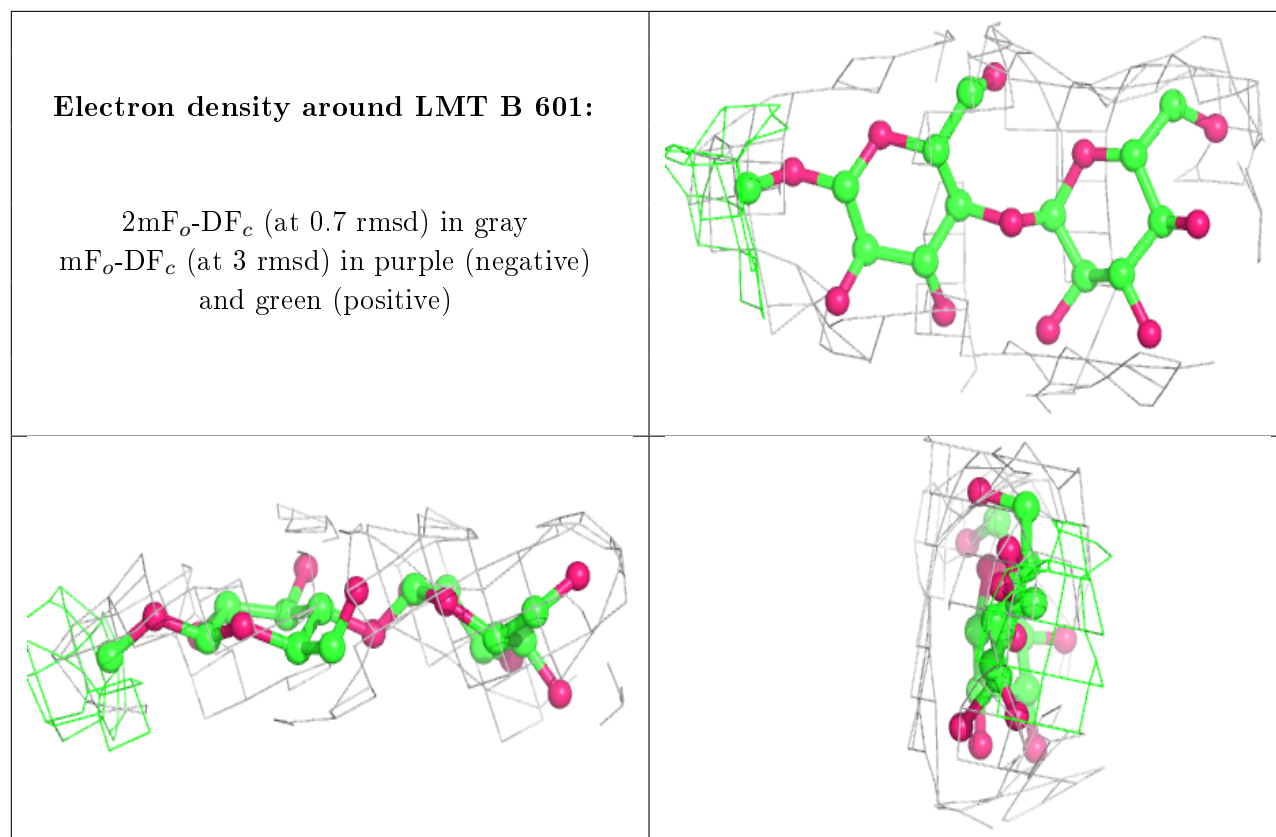
## 6.4 Ligands [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	NO3	A	702	4/4	0.90	0.26	78,78,78,78	0
2	LMT	A	701	24/35	0.90	0.14	80,83,85,86	0
2	LMT	B	601	24/35	0.92	0.11	96,96,97,97	0
3	NO3	B	602	4/4	0.93	0.37	109,109,109,109	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.