



# Full wwPDB X-ray Structure Validation Report

May 16, 2020 – 03:14 pm BST

PDB ID : 6NTW  
Title : Crystal structure of E. coli YcbB  
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Deposited on : 2019-01-30  
Resolution : 2.76 Å(reported)

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

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

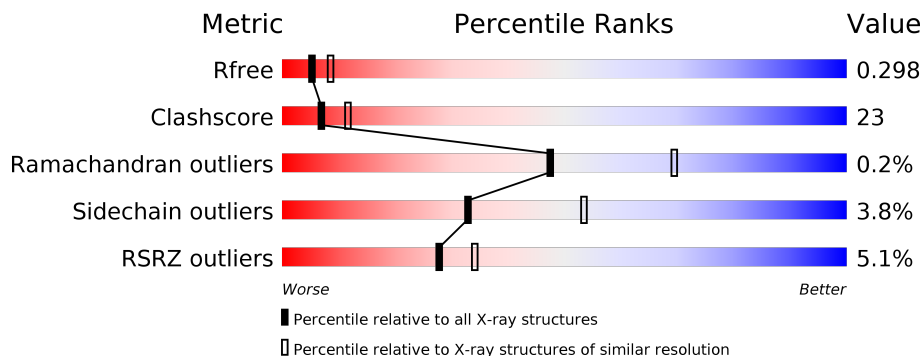
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.76 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	585	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MXR	A	701	-	-	X	-
3	SO4	A	703	-	-	X	-

## 2 Entry composition [i](#)

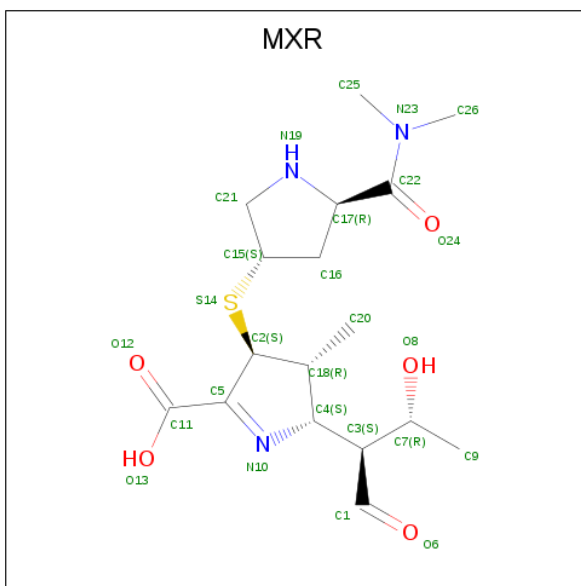
There are 4 unique types of molecules in this entry. The entry contains 4066 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Probable L,D-transpeptidase YcbB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	505	3994	2538	710	731	15	0	2	0

- Molecule 2 is (2S,3R,4S)-4-[[[(3S,5R)-5-(dimethylcarbamoyl)pyrrolidin-3-yl]sulfonyl]-2-[(2S,3R)-3-hydroxy-1-oxobutan-2-yl]-3-methyl-3,4-dihydro-2H-pyrrole-5-carboxylic acid (three-letter code: MXR) (formula: C<sub>17</sub>H<sub>27</sub>N<sub>3</sub>O<sub>5</sub>S).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

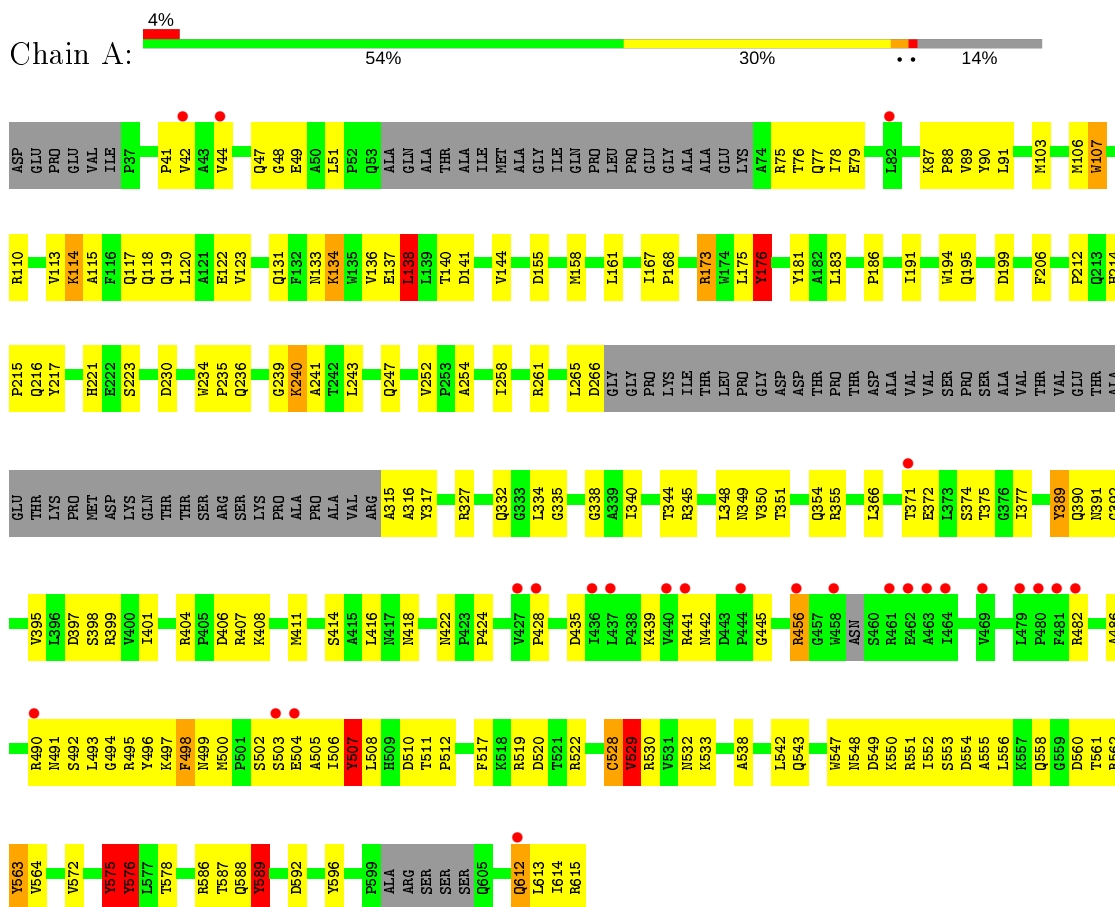
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total	O	0	0
			21	21		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Probable L,D-transpeptidase YcbB



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.50 Å 126.50 Å 88.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.45 – 2.76 89.45 – 2.76	Depositor EDS
% Data completeness (in resolution range)	99.3 (89.45-2.76) 99.3 (89.45-2.76)	Depositor EDS
$R_{merge}$	0.41	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 2.77 Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.256 , 0.298 0.256 , 0.298	Depositor DCC
$R_{free}$ test set	953 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.6	Xtrriage
Anisotropy	0.380	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 53.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4066	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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: MXR, SO4

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	0.67	0/4098	1.02	24/5587 (0.4%)

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	5

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	576	TYR	CB-CG-CD2	-14.19	112.49	121.00
1	A	445	GLY	C-N-CA	10.93	149.02	121.70
1	A	173	ARG	NE-CZ-NH1	10.72	125.66	120.30
1	A	507	TYR	CB-CG-CD2	-10.08	114.95	121.00
1	A	173	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	A	575	TYR	CB-CG-CD2	-8.05	116.17	121.00
1	A	576	TYR	CA-CB-CG	7.77	128.17	113.40
1	A	482	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	A	138	LEU	CA-CB-CG	7.00	131.41	115.30
1	A	576	TYR	CB-CG-CD1	6.96	125.17	121.00
1	A	589	TYR	CB-CG-CD2	-6.30	117.22	121.00
1	A	120	LEU	CB-CG-CD2	-6.17	100.52	111.00
1	A	114	LYS	CD-CE-NZ	-5.94	98.05	111.70
1	A	134	LYS	CB-CG-CD	-5.63	96.95	111.60
1	A	592	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	528	CYS	N-CA-CB	5.60	120.68	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	TRP	CA-CB-CG	-5.56	103.14	113.70
1	A	519	ARG	NE-CZ-NH1	-5.47	117.56	120.30
1	A	612	GLN	CA-CB-CG	5.46	125.42	113.40
1	A	366	LEU	CA-CB-CG	5.16	127.17	115.30
1	A	529	VAL	CG1-CB-CG2	5.15	119.14	110.90
1	A	173	ARG	CG-CD-NE	5.07	122.44	111.80
1	A	482	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	327	ARG	NE-CZ-NH1	-5.03	117.78	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	176	TYR	Sidechain
1	A	507	TYR	Sidechain
1	A	575	TYR	Sidechain
1	A	576	TYR	Sidechain
1	A	589	TYR	Sidechain

## 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	3994	0	3964	171	9
2	A	26	0	26	20	0
3	A	25	0	0	5	0
4	A	21	0	0	3	0
All	All	4066	0	3990	185	9

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 23.

All (185) 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:173:ARG:NH1	3:A:703:SO4:S	2.16	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ARG:NH1	3:A:703:SO4:O3	1.89	1.04
1:A:117:GLN:HB3	1:A:612:GLN:HE22	1.22	1.02
2:A:701:MXR:H26	2:A:701:MXR:H32	1.42	0.98
2:A:701:MXR:H27	2:A:701:MXR:C11	1.95	0.95
1:A:247:GLN:O	1:A:316:ALA:O	1.85	0.94
1:A:252:VAL:HB	1:A:315:ALA:HB3	1.53	0.88
1:A:422:ASN:O	1:A:561:THR:OG1	1.92	0.87
1:A:374:SER:OG	1:A:392:GLY:N	2.10	0.84
1:A:345:ARG:O	1:A:349:ASN:ND2	2.13	0.81
2:A:701:MXR:H32	2:A:701:MXR:C21	2.10	0.81
1:A:113:VAL:HG12	1:A:117:GLN:HE21	1.46	0.80
2:A:701:MXR:H23	2:A:701:MXR:O8	1.81	0.80
1:A:508:LEU:HD23	1:A:529:VAL:HG22	1.66	0.77
2:A:701:MXR:C26	2:A:701:MXR:H26	2.16	0.75
1:A:252:VAL:CB	1:A:315:ALA:HB3	2.18	0.73
2:A:701:MXR:H32	2:A:701:MXR:H18	1.70	0.73
1:A:551:ARG:NH2	1:A:562[B]:ARG:HH12	1.87	0.73
1:A:131:GLN:HG2	1:A:183:LEU:HD11	1.71	0.73
1:A:41:PRO:O	1:A:44:VAL:HG22	1.89	0.72
1:A:317:TYR:OH	1:A:338:GLY:O	2.05	0.72
1:A:173:ARG:NH1	3:A:703:SO4:O2	2.13	0.71
1:A:214:HIS:O	4:A:801:HOH:O	2.09	0.71
1:A:507:TYR:CE1	1:A:528:CYS:SG	2.84	0.70
1:A:117:GLN:CB	1:A:612:GLN:HE22	2.03	0.70
1:A:492:SER:HA	1:A:512:PRO:HG3	1.74	0.69
1:A:441:ARG:NH1	3:A:706:SO4:O4	2.26	0.68
2:A:701:MXR:H27	2:A:701:MXR:C5	2.23	0.68
1:A:41:PRO:HD2	1:A:199:ASP:OD2	1.95	0.67
2:A:701:MXR:H23	2:A:701:MXR:C7	2.23	0.67
2:A:701:MXR:H32	2:A:701:MXR:C16	2.25	0.67
1:A:122:GLU:OE2	1:A:221:HIS:ND1	2.28	0.66
1:A:75:ARG:NE	1:A:75:ARG:HA	2.09	0.66
1:A:486:ALA:O	1:A:491:ASN:ND2	2.24	0.66
1:A:75:ARG:HD3	1:A:77:GLN:H	1.59	0.66
2:A:701:MXR:C26	2:A:701:MXR:H18	2.23	0.65
1:A:497:LYS:HE3	1:A:507:TYR:CD2	2.32	0.65
1:A:334:LEU:HD13	1:A:344:THR:HG22	1.79	0.64
1:A:428:PRO:HG2	2:A:701:MXR:H3	1.78	0.64
1:A:134:LYS:HE3	1:A:138:LEU:CD2	2.28	0.63
1:A:167:ILE:HG22	1:A:168:PRO:HD3	1.81	0.63
1:A:175:LEU:C	1:A:176:TYR:HD1	2.01	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:TYR:N	1:A:176:TYR:HD1	1.96	0.63
1:A:235:PRO:HG2	1:A:258:ILE:HG13	1.79	0.63
1:A:497:LYS:NZ	4:A:802:HOH:O	2.32	0.63
1:A:236:GLN:HE22	1:A:349:ASN:HB3	1.64	0.63
1:A:547:TRP:CH2	1:A:562[A]:ARG:HG2	2.35	0.62
1:A:375:THR:HA	1:A:389:TYR:O	2.00	0.62
1:A:176:TYR:N	1:A:176:TYR:CD1	2.68	0.61
1:A:528:CYS:HB2	2:A:701:MXR:H11	1.81	0.61
1:A:106:MET:CE	1:A:195:GLN:HE22	2.13	0.61
1:A:106:MET:HE2	1:A:195:GLN:HE22	1.66	0.60
1:A:223:SER:OG	1:A:586:ARG:NH1	2.35	0.60
1:A:110:ARG:NH2	1:A:114:LYS:HZ1	1.99	0.60
1:A:558:GLN:HG3	1:A:558:GLN:O	2.01	0.59
1:A:42:VAL:HG21	1:A:195:GLN:OE1	2.02	0.59
1:A:500:MET:SD	1:A:572:VAL:HG21	2.43	0.59
1:A:498:PHE:N	1:A:498:PHE:CD1	2.70	0.59
1:A:134:LYS:HE3	1:A:138:LEU:HD21	1.85	0.59
1:A:240:LYS:N	1:A:345:ARG:HH12	2.00	0.57
1:A:186:PRO:HG2	1:A:191:ILE:HD11	1.86	0.57
1:A:141:ASP:O	1:A:144:VAL:HG22	2.05	0.57
1:A:498:PHE:HD1	1:A:498:PHE:N	2.03	0.56
1:A:492:SER:HA	1:A:512:PRO:HD3	1.86	0.56
1:A:230:ASP:OD1	1:A:261:ARG:NH2	2.32	0.56
1:A:377:ILE:HB	1:A:572:VAL:HG12	1.86	0.56
1:A:335:GLY:HA3	1:A:520:ASP:OD2	2.05	0.55
1:A:558:GLN:HG3	1:A:560:ASP:H	1.71	0.55
1:A:113:VAL:CG1	1:A:117:GLN:HE21	2.16	0.55
1:A:265:LEU:O	1:A:266:ASP:HB2	2.07	0.55
1:A:214:HIS:CE1	1:A:216:GLN:HG3	2.42	0.55
1:A:507:TYR:CD1	1:A:528:CYS:SG	3.00	0.55
1:A:588:GLN:C	1:A:589:TYR:HD1	2.09	0.55
1:A:88:PRO:HG2	1:A:91:LEU:HB2	1.89	0.54
1:A:503:SER:O	1:A:504:GLU:HG2	2.06	0.54
1:A:507:TYR:CD1	1:A:507:TYR:N	2.76	0.54
1:A:89:VAL:HG22	1:A:90:TYR:CD2	2.42	0.54
1:A:397:ASP:O	1:A:533:LYS:HD2	2.08	0.54
1:A:551:ARG:NH2	1:A:562[B]:ARG:NH1	2.55	0.54
1:A:243:LEU:HD23	1:A:340:ILE:HD12	1.88	0.54
1:A:492:SER:HA	1:A:512:PRO:CG	2.38	0.53
1:A:240:LYS:H	1:A:345:ARG:NH1	2.06	0.53
1:A:49:GLU:N	1:A:49:GLU:OE1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:ALA:O	1:A:506:ILE:HG13	2.09	0.53
1:A:547:TRP:HH2	1:A:562[A]:ARG:HG2	1.72	0.53
1:A:492:SER:HA	1:A:512:PRO:CD	2.39	0.52
1:A:497:LYS:HE3	1:A:507:TYR:CE2	2.44	0.52
2:A:701:MXR:C21	2:A:701:MXR:C5	2.84	0.52
1:A:252:VAL:HB	1:A:315:ALA:CB	2.34	0.52
1:A:507:TYR:HD1	1:A:507:TYR:N	2.08	0.52
1:A:553:SER:HA	1:A:556:LEU:HD12	1.92	0.52
1:A:240:LYS:H	1:A:345:ARG:HH12	1.57	0.51
1:A:543:GLN:NE2	1:A:549:ASP:HB3	2.25	0.51
1:A:117:GLN:HB3	1:A:612:GLN:NE2	2.07	0.51
1:A:78:ILE:HD13	1:A:103:MET:HG3	1.93	0.51
1:A:351:THR:OG1	1:A:354:GLN:HG3	2.10	0.51
1:A:528:CYS:SG	2:A:701:MXR:H11	2.51	0.51
1:A:494:GLY:HA3	1:A:510:ASP:OD2	2.11	0.50
1:A:176:TYR:CE2	1:A:411:MET:SD	3.04	0.50
1:A:614:ILE:O	1:A:614:ILE:HG13	2.11	0.50
1:A:375:THR:HG1	1:A:391:ASN:H	1.59	0.50
1:A:575:TYR:H	1:A:575:TYR:HD1	1.59	0.50
1:A:214:HIS:CG	1:A:215:PRO:HD2	2.47	0.50
1:A:371:THR:HG22	1:A:372:GLU:HG3	1.92	0.49
1:A:554:ASP:OD1	1:A:555:ALA:N	2.45	0.49
1:A:507:TYR:O	1:A:528:CYS:HB3	2.12	0.49
1:A:548:ASN:ND2	1:A:550:LYS:HD2	2.27	0.49
1:A:133:ASN:HA	1:A:136:VAL:HG22	1.94	0.48
1:A:398:SER:HB2	1:A:533:LYS:HB2	1.96	0.48
1:A:435:ASP:OD1	1:A:439:LYS:NZ	2.46	0.48
1:A:508:LEU:HD23	1:A:529:VAL:CG2	2.40	0.48
2:A:701:MXR:C26	2:A:701:MXR:C21	2.86	0.48
1:A:119:GLN:O	1:A:123:VAL:HG23	2.14	0.48
1:A:418:ASN:OD1	1:A:499:ASN:HB2	2.14	0.48
1:A:555:ALA:O	1:A:558:GLN:HB3	2.14	0.48
1:A:547:TRP:CE3	1:A:551:ARG:HG3	2.49	0.48
1:A:252:VAL:CG1	1:A:315:ALA:CB	2.92	0.48
1:A:137:GLU:O	1:A:140:THR:HG22	2.13	0.47
1:A:42:VAL:CG2	1:A:195:GLN:HB3	2.43	0.47
1:A:332:GLN:HE22	1:A:355:ARG:HH22	1.61	0.47
1:A:495:ARG:NH2	1:A:556:LEU:O	2.48	0.47
1:A:76:THR:HA	1:A:79:GLU:HB2	1.97	0.47
1:A:414:SER:HB2	1:A:502:SER:HB2	1.97	0.47
1:A:542:LEU:HD23	1:A:552:ILE:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:GLY:HA3	1:A:510:ASP:HB3	1.97	0.46
1:A:408:LYS:NZ	1:A:596:TYR:OH	2.43	0.46
1:A:252:VAL:HG11	1:A:315:ALA:CB	2.46	0.46
1:A:418:ASN:HB2	1:A:564:VAL:O	2.15	0.46
1:A:576:TYR:CE1	1:A:578:THR:HG23	2.51	0.46
1:A:110:ARG:CZ	1:A:114:LYS:HZ1	2.29	0.46
1:A:131:GLN:HG2	1:A:183:LEU:CD1	2.43	0.46
1:A:401:ILE:HB	1:A:530:ARG:HB2	1.97	0.46
1:A:390:GLN:HB3	1:A:395:VAL:HG21	1.98	0.46
1:A:404:ARG:HH21	1:A:407:ARG:CZ	2.29	0.45
1:A:588:GLN:C	1:A:589:TYR:CD1	2.90	0.45
1:A:212:PRO:HD2	1:A:217:TYR:CE1	2.50	0.45
1:A:517:PHE:CD1	1:A:532:ASN:HB2	2.52	0.45
1:A:194:TRP:HB2	1:A:206:PHE:CE2	2.51	0.45
1:A:214:HIS:HE1	1:A:216:GLN:HG3	1.81	0.45
1:A:252:VAL:HG11	1:A:315:ALA:HB1	1.98	0.45
1:A:133:ASN:O	1:A:137:GLU:HG2	2.17	0.44
1:A:155:ASP:O	1:A:158:MET:HB2	2.17	0.44
1:A:47:GLN:HG2	1:A:48:GLY:H	1.82	0.44
1:A:586:ARG:HD2	1:A:587:THR:H	1.83	0.44
1:A:345:ARG:HA	1:A:348:LEU:HD12	2.00	0.44
1:A:589:TYR:N	1:A:589:TYR:HD1	2.16	0.44
1:A:254:ALA:CB	4:A:809:HOH:O	2.66	0.44
1:A:110:ARG:CZ	1:A:114:LYS:NZ	2.81	0.43
1:A:134:LYS:HD2	1:A:134:LYS:HA	1.68	0.43
1:A:134:LYS:HD2	1:A:134:LYS:O	2.19	0.43
1:A:428:PRO:HG2	2:A:701:MXR:H24	1.99	0.43
1:A:563:TYR:CD1	1:A:563:TYR:N	2.87	0.43
1:A:589:TYR:N	1:A:589:TYR:CD1	2.86	0.43
2:A:701:MXR:N10	2:A:701:MXR:H16	2.33	0.43
1:A:87:LYS:HE3	1:A:91:LEU:HD22	2.01	0.43
1:A:161:LEU:HD23	1:A:161:LEU:HA	1.84	0.43
2:A:701:MXR:N10	2:A:701:MXR:C15	2.81	0.43
1:A:374:SER:HB2	1:A:392:GLY:HA2	2.00	0.43
1:A:528:CYS:CB	2:A:701:MXR:H11	2.47	0.43
1:A:252:VAL:CG1	1:A:315:ALA:HB3	2.49	0.43
1:A:115:ALA:O	1:A:118:GLN:HB3	2.19	0.42
1:A:401:ILE:O	1:A:529:VAL:HA	2.19	0.42
1:A:496:TYR:CD1	1:A:538:ALA:CB	3.02	0.42
1:A:344:THR:HG23	3:A:705:SO4:O1	2.19	0.42
1:A:350:VAL:HA	1:A:354:GLN:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:TRP:HB2	1:A:206:PHE:CZ	2.55	0.42
1:A:243:LEU:HB3	1:A:340:ILE:HB	2.01	0.42
1:A:87:LYS:HE3	1:A:91:LEU:CD2	2.50	0.42
1:A:181:TYR:CE1	1:A:183:LEU:HD23	2.55	0.42
1:A:234:TRP:CZ2	1:A:258:ILE:HG23	2.54	0.42
1:A:47:GLN:HB3	1:A:49:GLU:OE1	2.20	0.42
1:A:240:LYS:N	1:A:345:ARG:NH1	2.66	0.41
1:A:511:THR:HG21	1:A:517:PHE:HE2	1.85	0.41
1:A:118:GLN:OE1	1:A:613:LEU:HD22	2.20	0.41
1:A:528:CYS:SG	2:A:701:MXR:C9	2.95	0.41
1:A:399:ARG:HB3	1:A:522:ARG:NH2	2.36	0.41
1:A:497:LYS:HG3	1:A:507:TYR:HD2	1.86	0.41
1:A:191:ILE:HG23	1:A:191:ILE:HD12	1.83	0.41
1:A:406:ASP:OD1	1:A:406:ASP:N	2.52	0.41
1:A:561:THR:HG22	1:A:563:TYR:HE1	1.86	0.41
1:A:107:TRP:HE3	1:A:113:VAL:HG22	1.86	0.40
1:A:110:ARG:NH2	1:A:615:ARG:CZ	2.85	0.40
1:A:110:ARG:HH21	1:A:615:ARG:HD2	1.87	0.40
1:A:239:GLY:C	1:A:241:ALA:H	2.24	0.40
1:A:416:LEU:HD12	1:A:499:ASN:O	2.21	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:ARG:CZ	1:A:456:ARG:CZ[8_556]	0.64	1.56
1:A:456:ARG:CZ	1:A:456:ARG:NH1[8_556]	0.69	1.51
1:A:456:ARG:NE	1:A:456:ARG:NH1[8_556]	0.96	1.24
1:A:456:ARG:NH1	1:A:456:ARG:NH2[8_556]	1.34	0.86
1:A:456:ARG:CD	1:A:456:ARG:CD[8_556]	1.58	0.62
1:A:456:ARG:CZ	1:A:456:ARG:NH2[8_556]	1.68	0.52
1:A:456:ARG:NH2	1:A:456:ARG:NH2[8_556]	1.72	0.48
1:A:456:ARG:NE	1:A:456:ARG:CZ[8_556]	1.79	0.41
1:A:456:ARG:NH1	1:A:456:ARG:NH1[8_556]	1.99	0.21

## 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	497/585 (85%)	478 (96%)	18 (4%)	1 (0%)	47 69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	240	LYS

### 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	426/488 (87%)	410 (96%)	16 (4%)	33 53

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	138	LEU
1	A	176	TYR
1	A	389	TYR
1	A	424	PRO
1	A	442	ASN
1	A	456	ARG
1	A	490	ARG
1	A	493	LEU
1	A	498	PHE

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Mol	Chain	Res	Type
1	A	507	TYR
1	A	529	VAL
1	A	563	TYR
1	A	575	TYR
1	A	576	TYR
1	A	589	TYR

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

Mol	Chain	Res	Type
1	A	195	GLN
1	A	236	GLN
1	A	543	GLN
1	A	612	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](#)

6 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	SO4	A	704	-	4,4,4	0.15	0	6,6,6	0.41	0
3	SO4	A	706	-	4,4,4	0.41	0	6,6,6	0.06	0
3	SO4	A	702	-	4,4,4	0.07	0	6,6,6	0.45	0
3	SO4	A	705	-	4,4,4	0.12	0	6,6,6	0.27	0
2	MXR	A	701	1	22,27,27	3.23	7 (31%)	13,39,39	2.18	4 (30%)
3	SO4	A	703	-	4,4,4	0.11	0	6,6,6	0.56	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MXR	A	701	1	-	12/18/51/51	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	MXR	C2-C18	-10.12	1.48	1.55
2	A	701	MXR	C5-N10	-5.35	1.24	1.28
2	A	701	MXR	C15-S14	-5.22	1.73	1.82
2	A	701	MXR	C2-S14	-4.67	1.73	1.84
2	A	701	MXR	C11-C5	-4.51	1.45	1.52
2	A	701	MXR	C22-N23	-2.79	1.30	1.34
2	A	701	MXR	C17-C22	-2.62	1.48	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	MXR	O6-C1-C3	-5.45	111.44	125.23
2	A	701	MXR	C17-C22-N23	-3.50	114.40	118.57
2	A	701	MXR	C20-C18-C2	-2.86	108.28	113.35
2	A	701	MXR	C22-C17-N19	-2.39	107.41	111.74

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	MXR	C1-C3-C7-O8
2	A	701	MXR	C1-C3-C7-C9
2	A	701	MXR	C4-C3-C7-O8

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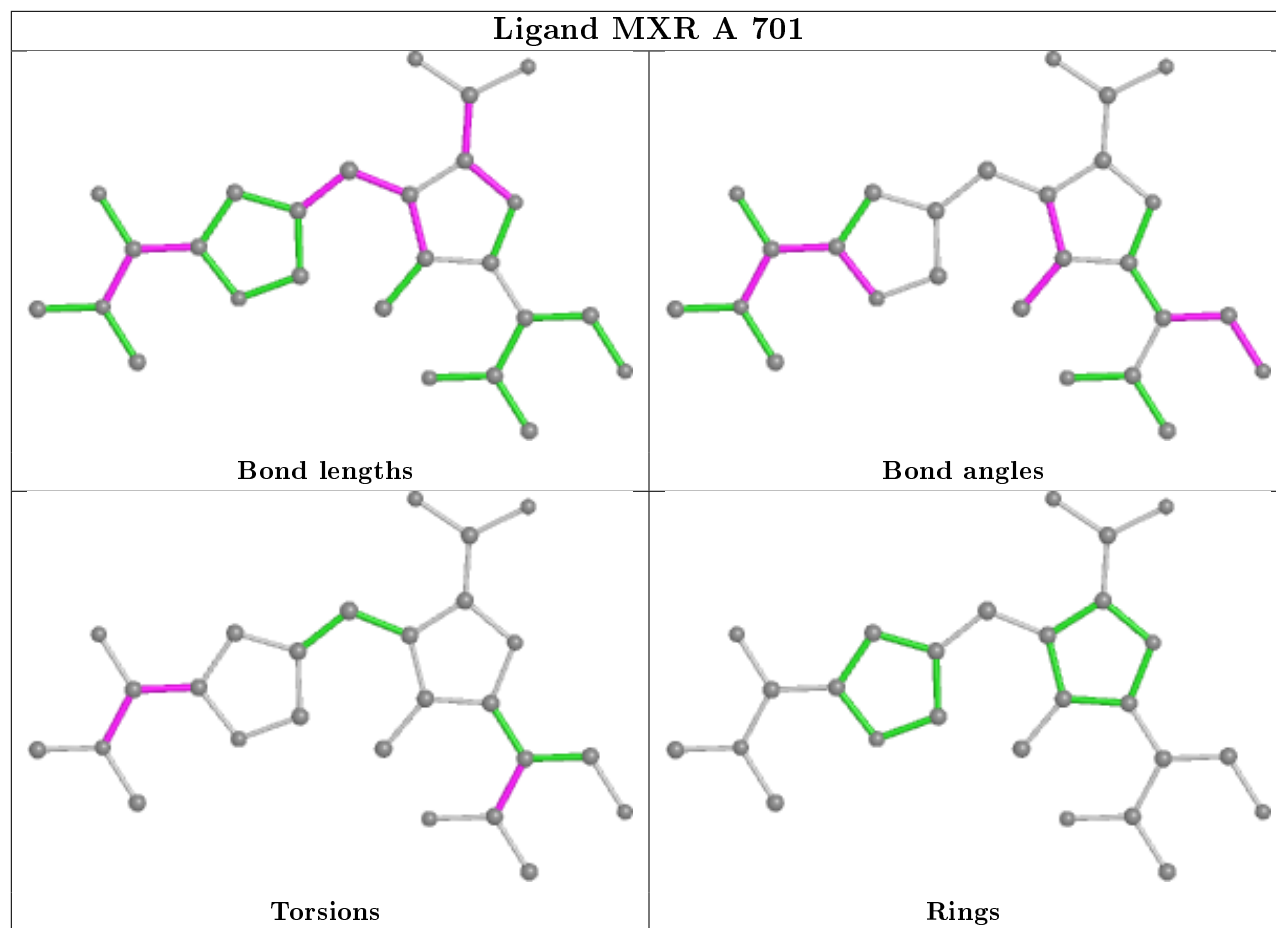
Mol	Chain	Res	Type	Atoms
2	A	701	MXR	C4-C3-C7-C9
2	A	701	MXR	C16-C17-C22-N23
2	A	701	MXR	C16-C17-C22-O24
2	A	701	MXR	C17-C22-N23-C25
2	A	701	MXR	C17-C22-N23-C26
2	A	701	MXR	O24-C22-N23-C25
2	A	701	MXR	O24-C22-N23-C26
2	A	701	MXR	N19-C17-C22-O24
2	A	701	MXR	N19-C17-C22-N23

There are no ring outliers.

4 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	706	SO4	1	0
3	A	705	SO4	1	0
2	A	701	MXR	20	0
3	A	703	SO4	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 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	505/585 (86%)	0.43	26 (5%) <span style="border: 1px solid red; padding: 2px;">28</span> <span style="border: 1px solid red; padding: 2px;">34</span>	43, 69, 127, 176	1 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	479	LEU	5.2
1	A	503	SER	3.8
1	A	458	TRP	3.5
1	A	463	ALA	3.2
1	A	371	THR	2.8
1	A	462	GLU	2.6
1	A	456	ARG	2.6
1	A	461	ARG	2.6
1	A	482	ARG	2.6
1	A	42	VAL	2.5
1	A	427	VAL	2.5
1	A	490	ARG	2.5
1	A	612	GLN	2.4
1	A	436	ILE	2.4
1	A	44	VAL	2.3
1	A	464	ILE	2.3
1	A	437	LEU	2.3
1	A	480	PRO	2.3
1	A	440	VAL	2.3
1	A	481	PHE	2.2
1	A	469	VAL	2.2
1	A	504	GLU	2.1
1	A	82	LEU	2.1
1	A	441	ARG	2.0
1	A	428	PRO	2.0
1	A	444	PRO	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](#)

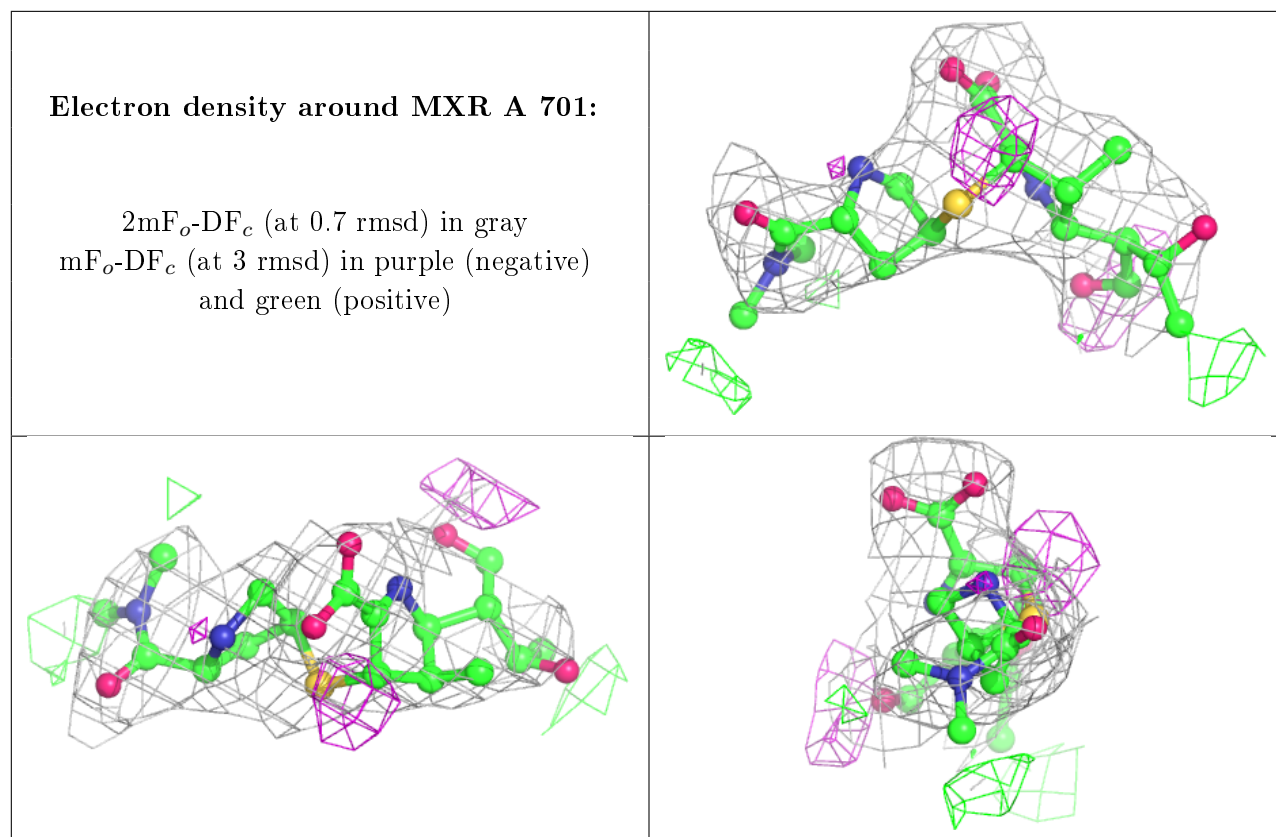
There are no carbohydrates in this entry.

## 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	SO4	A	706	5/5	0.60	0.23	130,134,141,141	5
3	SO4	A	705	5/5	0.86	0.20	64,64,71,75	5
2	MXR	A	701	26/26	0.88	0.23	74,83,94,98	0
3	SO4	A	703	5/5	0.92	0.17	68,71,86,86	0
3	SO4	A	702	5/5	0.95	0.14	55,55,59,60	5
3	SO4	A	704	5/5	0.97	0.09	77,80,88,91	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.