



Full wwPDB X-ray Structure Validation Report i

Nov 7, 2023 – 06:46 PM JST

PDB ID : 8HX8
Title : Crystal structure of 4-amino-4-deoxychorismate synthase from Streptomyces venezuelae co-crystallized with chorismate
Authors : Nakamichi, Y.; Watanabe, M.
Deposited on : 2023-01-04
Resolution : 2.55 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

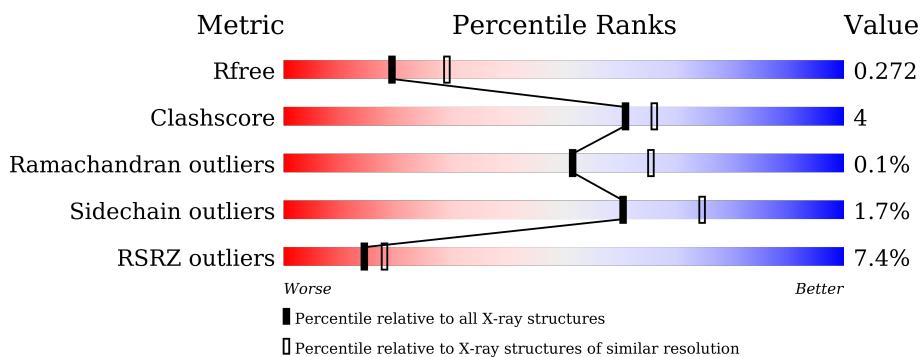
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

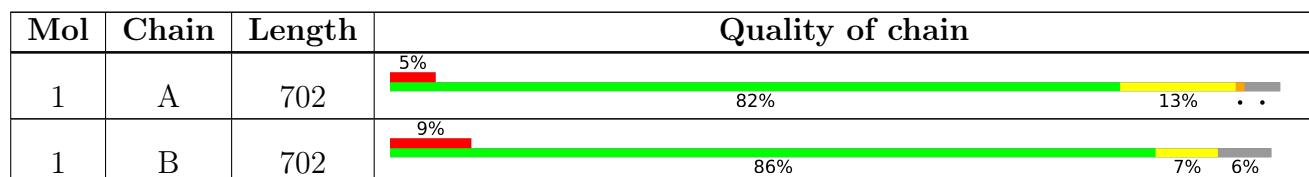
The reported resolution of this entry is 2.55 Å.

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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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.



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10317 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 4-amino-4-deoxychorismate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	673	Total	C	N	O	S	0	0	0
			5174	3243	930	983	18			
1	B	661	Total	C	N	O	S	0	0	0
			5101	3196	921	967	17			

There are 32 discrepancies between the modelled and reference sequences:

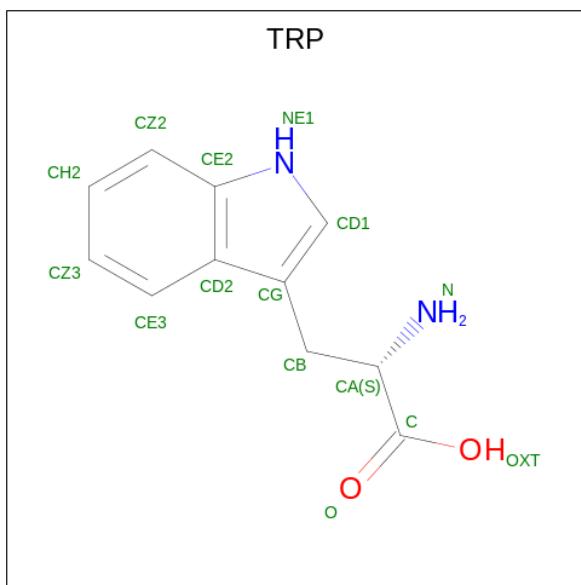
Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP Q6L8Q5
A	-14	ASN	-	expression tag	UNP Q6L8Q5
A	-13	HIS	-	expression tag	UNP Q6L8Q5
A	-12	LYS	-	expression tag	UNP Q6L8Q5
A	-11	VAL	-	expression tag	UNP Q6L8Q5
A	-10	HIS	-	expression tag	UNP Q6L8Q5
A	-9	HIS	-	expression tag	UNP Q6L8Q5
A	-8	HIS	-	expression tag	UNP Q6L8Q5
A	-7	HIS	-	expression tag	UNP Q6L8Q5
A	-6	HIS	-	expression tag	UNP Q6L8Q5
A	-5	HIS	-	expression tag	UNP Q6L8Q5
A	-4	ILE	-	expression tag	UNP Q6L8Q5
A	-3	GLU	-	expression tag	UNP Q6L8Q5
A	-2	GLY	-	expression tag	UNP Q6L8Q5
A	-1	ARG	-	expression tag	UNP Q6L8Q5
A	0	HIS	-	expression tag	UNP Q6L8Q5
B	-15	MET	-	initiating methionine	UNP Q6L8Q5
B	-14	ASN	-	expression tag	UNP Q6L8Q5
B	-13	HIS	-	expression tag	UNP Q6L8Q5
B	-12	LYS	-	expression tag	UNP Q6L8Q5
B	-11	VAL	-	expression tag	UNP Q6L8Q5
B	-10	HIS	-	expression tag	UNP Q6L8Q5
B	-9	HIS	-	expression tag	UNP Q6L8Q5
B	-8	HIS	-	expression tag	UNP Q6L8Q5
B	-7	HIS	-	expression tag	UNP Q6L8Q5

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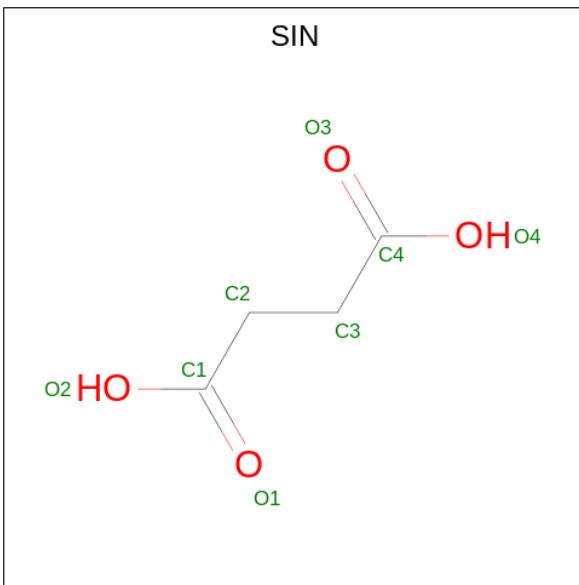
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP Q6L8Q5
B	-5	HIS	-	expression tag	UNP Q6L8Q5
B	-4	ILE	-	expression tag	UNP Q6L8Q5
B	-3	GLU	-	expression tag	UNP Q6L8Q5
B	-2	GLY	-	expression tag	UNP Q6L8Q5
B	-1	ARG	-	expression tag	UNP Q6L8Q5
B	0	HIS	-	expression tag	UNP Q6L8Q5

- Molecule 2 is TRYPTOPHAN (three-letter code: TRP) (formula: C₁₁H₁₂N₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 15 11 2 2	0	0
2	B	1	Total C N O 15 11 2 2	0	0

- Molecule 3 is SUCCINIC ACID (three-letter code: SIN) (formula: C₄H₆O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 8 4 4	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mg 2 2	0	0

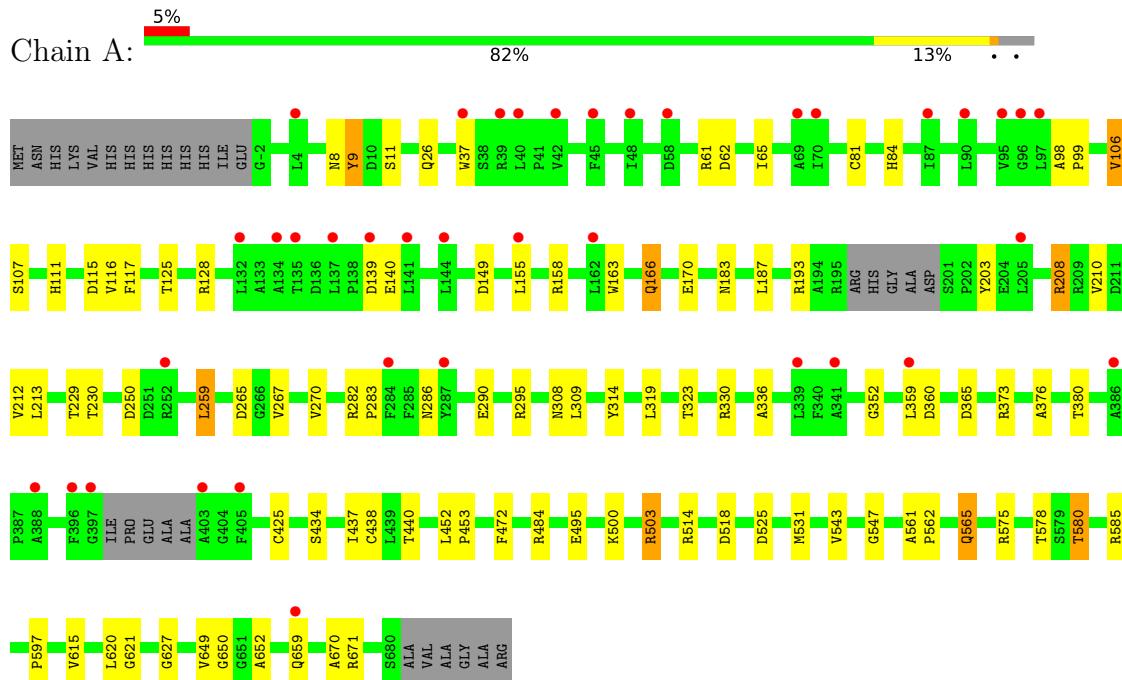
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total O 2 2	0	0

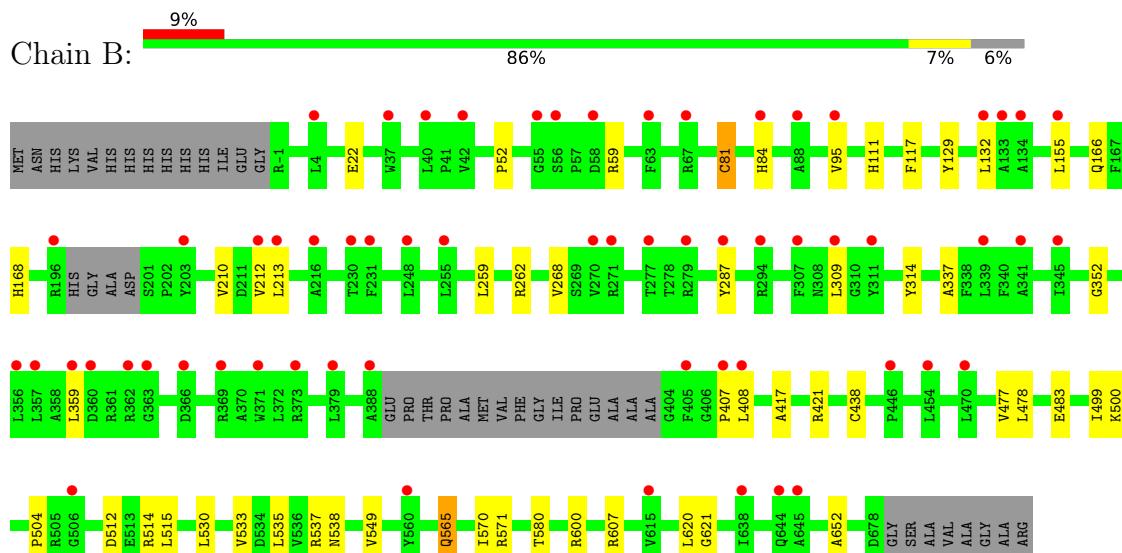
3 Residue-property plots [\(i\)](#)

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: 4-amino-4-deoxychorismate synthase



- Molecule 1: 4-amino-4-deoxychorismate synthase



4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	98.33Å 172.85Å 161.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.50 – 2.55 47.50 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.50-2.55) 99.9 (47.50-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	1.48 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R , R_{free}	0.206 , 0.268 0.211 , 0.272	Depositor DCC
R_{free} test set	2260 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	70.2	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 62.7	EDS
L-test for twinning ²	$< L > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.001 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.013 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10317	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: OCS, SIN, MG

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	0.29	0/5281	0.51	0/7172
1	B	0.28	0/5205	0.50	0/7067
All	All	0.28	0/10486	0.51	0/14239

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	5174	0	5059	62	1
1	B	5101	0	4993	34	0
2	A	15	0	9	0	0
2	B	15	0	9	0	0
3	A	8	0	4	0	0
4	A	2	0	0	0	0
5	A	2	0	0	0	0
All	All	10317	0	10074	91	1

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

All (91) 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:503:ARG:NH1	1:A:518:ASP:OD2	2.21	0.72
1:A:565:GLN:HE21	1:A:565:GLN:HA	1.56	0.71
1:B:438:CYS:SG	1:B:500:LYS:NZ	2.68	0.64
1:B:259:LEU:HD21	1:B:268:VAL:HG13	1.83	0.59
1:A:170:GLU:O	1:B:537:ARG:NH1	2.30	0.59
1:A:330:ARG:CB	1:A:330:ARG:HH11	2.15	0.58
1:A:314:TYR:CD1	1:A:615:VAL:HG13	2.37	0.58
1:A:84:HIS:CE1	1:A:166:GLN:HG2	2.39	0.58
1:A:98:ALA:HB1	1:A:99:PRO:HD2	1.85	0.58
1:A:11:SER:HB3	1:B:535:LEU:HD13	1.86	0.57
1:A:37:TRP:HB2	1:A:65:ILE:HD11	1.86	0.57
1:A:62:ASP:OD1	1:B:600:ARG:NH2	2.38	0.57
1:A:323:THR:HG22	1:A:585:ARG:HG3	1.85	0.57
1:A:440:THR:HG22	1:A:650:GLY:HA3	1.86	0.57
1:A:514:ARG:HH11	1:A:514:ARG:HG2	1.71	0.56
1:A:500:LYS:HE3	1:A:652:ALA:HB2	1.89	0.55
1:A:565:GLN:HA	1:A:565:GLN:NE2	2.22	0.53
1:A:438:CYS:SG	1:A:500:LYS:NZ	2.75	0.51
1:B:95:VAL:HG12	1:B:132:LEU:HD23	1.93	0.51
1:A:434:SER:HA	1:A:597:PRO:HD2	1.92	0.51
1:B:213:LEU:HD22	1:B:352:GLY:HA2	1.91	0.51
1:B:314:TYR:CE2	1:B:337:ALA:HB3	2.45	0.51
1:A:580:THR:HG21	1:A:627:GLY:O	2.11	0.50
1:B:500:LYS:HE3	1:B:652:ALA:HB2	1.93	0.50
1:B:210:VAL:HG12	1:B:212:VAL:HG22	1.92	0.50
1:A:193:ARG:NH1	1:A:575:ARG:O	2.44	0.50
1:B:84:HIS:CE1	1:B:166:GLN:HB2	2.47	0.50
1:A:309:LEU:HD13	1:A:359:LEU:HG	1.93	0.50
1:A:155:LEU:HD12	1:A:155:LEU:C	2.32	0.50
1:B:111:HIS:ND1	1:B:117:PHE:HB3	2.27	0.49
1:A:330:ARG:HB2	1:A:330:ARG:NH1	2.27	0.49
1:B:620:LEU:HD23	1:B:621:GLY:N	2.28	0.49
1:B:565:GLN:HE21	1:B:565:GLN:HA	1.78	0.48
1:A:265:ASP:HB2	1:A:267:VAL:HG22	1.95	0.48
1:A:503:ARG:NH2	1:A:525:ASP:OD2	2.46	0.48
1:A:360:ASP:CG	1:A:365:ASP:O	2.52	0.48
1:B:483:GLU:HB2	1:B:499:ILE:HD12	1.95	0.48
1:A:330:ARG:HH11	1:A:330:ARG:HB2	1.79	0.48
1:A:376:ALA:O	1:A:380:THR:HG23	2.14	0.47
1:A:360:ASP:OD1	1:A:365:ASP:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:LEU:HD22	1:A:352:GLY:HA2	1.95	0.47
1:A:106:VAL:HG13	1:A:125:THR:HG23	1.97	0.47
1:A:230:THR:HG22	1:A:250:ASP:HB3	1.97	0.47
1:A:61:ARG:O	1:A:62:ASP:HB2	2.15	0.47
1:B:155:LEU:C	1:B:155:LEU:HD12	2.36	0.46
1:B:549:VAL:HA	1:B:571:ARG:O	2.15	0.46
1:A:140:GLU:O	1:A:158:ARG:HG3	2.16	0.46
1:B:52:PRO:HB3	1:B:81:OCS:HB2	1.97	0.46
1:B:259:LEU:HD11	1:B:287:TYR:HE1	1.79	0.46
1:A:8:ASN:O	1:A:9:TYR:C	2.54	0.46
1:B:407:PRO:HB2	1:B:408:LEU:HD22	1.96	0.46
1:A:203:TYR:OH	1:A:295:ARG:NH1	2.50	0.45
1:B:514:ARG:HH11	1:B:514:ARG:HG2	1.80	0.45
1:A:319:LEU:HD11	1:A:336:ALA:HB2	1.98	0.45
1:A:259:LEU:N	1:A:259:LEU:HD23	2.32	0.45
1:B:477:VAL:C	1:B:478:LEU:HD12	2.37	0.45
1:A:283:PRO:HG2	1:A:286:ASN:HB2	1.98	0.44
1:A:308:ASN:O	1:A:309:LEU:HB2	2.18	0.44
1:A:547:GLY:HA2	1:B:22:GLU:OE2	2.18	0.44
1:A:208:ARG:HG3	1:A:208:ARG:HH11	1.83	0.44
1:B:417:ALA:O	1:B:421:ARG:HG2	2.17	0.44
1:A:128:ARG:HH12	1:A:149:ASP:CB	2.31	0.43
1:A:163:TRP:CE2	1:A:187:LEU:HD13	2.53	0.43
1:B:166:GLN:HG3	1:B:166:GLN:O	2.18	0.43
1:B:309:LEU:HD12	1:B:359:LEU:HG	2.00	0.43
1:A:425:CYS:HB3	1:A:437:ILE:HD12	2.00	0.43
1:A:649:VAL:HG11	1:A:670:ALA:HB2	2.00	0.43
1:A:452:LEU:HB3	1:A:453:PRO:HD3	2.00	0.43
1:A:561:ALA:HB3	1:A:562:PRO:HD3	1.99	0.43
1:B:52:PRO:HG3	1:B:168:HIS:CE1	2.54	0.42
1:A:531:MET:HG2	1:B:129:TYR:CE2	2.54	0.42
1:A:210:VAL:HG12	1:A:212:VAL:HG22	2.01	0.42
1:A:229:THR:HG23	1:A:472:PHE:HD1	1.84	0.42
1:B:620:LEU:HD23	1:B:620:LEU:C	2.40	0.42
1:A:514:ARG:HG2	1:A:514:ARG:NH1	2.35	0.42
1:A:26:GLN:HE21	1:A:26:GLN:HA	1.85	0.41
1:A:543:VAL:HB	1:A:578:THR:HG21	2.02	0.41
1:A:116:VAL:HA	1:A:183:ASN:HB3	2.02	0.41
1:A:309:LEU:CD1	1:A:359:LEU:HG	2.50	0.41
1:A:484:ARG:NH1	1:A:495:GLU:OE2	2.53	0.41
1:A:620:LEU:HD23	1:A:621:GLY:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:PRO:O	1:B:515:LEU:HD13	2.21	0.41
1:A:265:ASP:CB	1:A:267:VAL:HG22	2.51	0.41
1:A:111:HIS:ND1	1:A:117:PHE:HB3	2.36	0.40
1:A:115:ASP:HB3	1:A:187:LEU:HD11	2.03	0.40
1:B:533:VAL:HA	1:B:570:ILE:HD11	2.03	0.40
1:B:530:LEU:C	1:B:530:LEU:HD23	2.41	0.40
1:B:535:LEU:O	1:B:538:ASN:HB3	2.21	0.40
1:A:282:ARG:HH22	1:A:290:GLU:HG3	1.86	0.40
1:A:565:GLN:HE21	1:A:565:GLN:CA	2.24	0.40
1:B:262:ARG:HG2	1:B:262:ARG:HH11	1.86	0.40

All (1) 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:286:ASN:OD1	1:A:286:ASN:OD1[3_655]	1.97	0.23

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	666/702 (95%)	624 (94%)	41 (6%)	1 (0%)	47 60
1	B	654/702 (93%)	627 (96%)	27 (4%)	0	100 100
All	All	1320/1404 (94%)	1251 (95%)	68 (5%)	1 (0%)	51 65

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	TYR

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	539/560 (96%)	526 (98%)	13 (2%)	49 64
1	B	532/560 (95%)	527 (99%)	5 (1%)	78 86
All	All	1071/1120 (96%)	1053 (98%)	18 (2%)	60 75

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	VAL
1	A	107	SER
1	A	139	ASP
1	A	166	GLN
1	A	208	ARG
1	A	259	LEU
1	A	270	VAL
1	A	373	ARG
1	A	503	ARG
1	A	565	GLN
1	A	580	THR
1	A	659	GLN
1	A	671	ARG
1	B	59	ARG
1	B	512	ASP
1	B	565	GLN
1	B	580	THR
1	B	607	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	84	HIS
1	A	85	GLN
1	A	130	HIS

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Mol	Chain	Res	Type
1	A	166	GLN
1	A	350	GLN
1	A	659	GLN

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	OCS	B	81	1	7,8,9	1.64	1 (14%)	6,11,13	2.50	2 (33%)
1	OCS	A	81	1	7,8,9	1.00	1 (14%)	6,11,13	0.95	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
1	OCS	B	81	1	-	4/4/7/9	-
1	OCS	A	81	1	-	4/4/7/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	81	OCS	OD1-SG	4.02	1.56	1.45
1	A	81	OCS	OD2-SG	2.26	1.55	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	OCS	OD1-SG-CB	-4.92	101.09	106.94
1	B	81	OCS	OD2-SG-OD3	3.08	118.80	111.27

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	81	OCS	N-CA-CB-SG
1	A	81	OCS	CA-CB-SG-OD1
1	A	81	OCS	CA-CB-SG-OD2
1	A	81	OCS	CA-CB-SG-OD3
1	B	81	OCS	N-CA-CB-SG
1	B	81	OCS	CA-CB-SG-OD3
1	B	81	OCS	CA-CB-SG-OD1
1	B	81	OCS	CA-CB-SG-OD2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	81	OCS	1	0

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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
2	TRP	B	701	-	14,16,16	0.73	0	16,22,22	0.88	0
3	SIN	A	702	-	7,7,7	1.07	0	8,8,8	1.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TRP	A	701	-	14,16,16	0.77	0	16,22,22	0.90	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	TRP	B	701	-	-	1/7/8/8	0/2/2/2
3	SIN	A	702	-	-	3/5/5/5	-
2	TRP	A	701	-	-	0/7/8/8	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

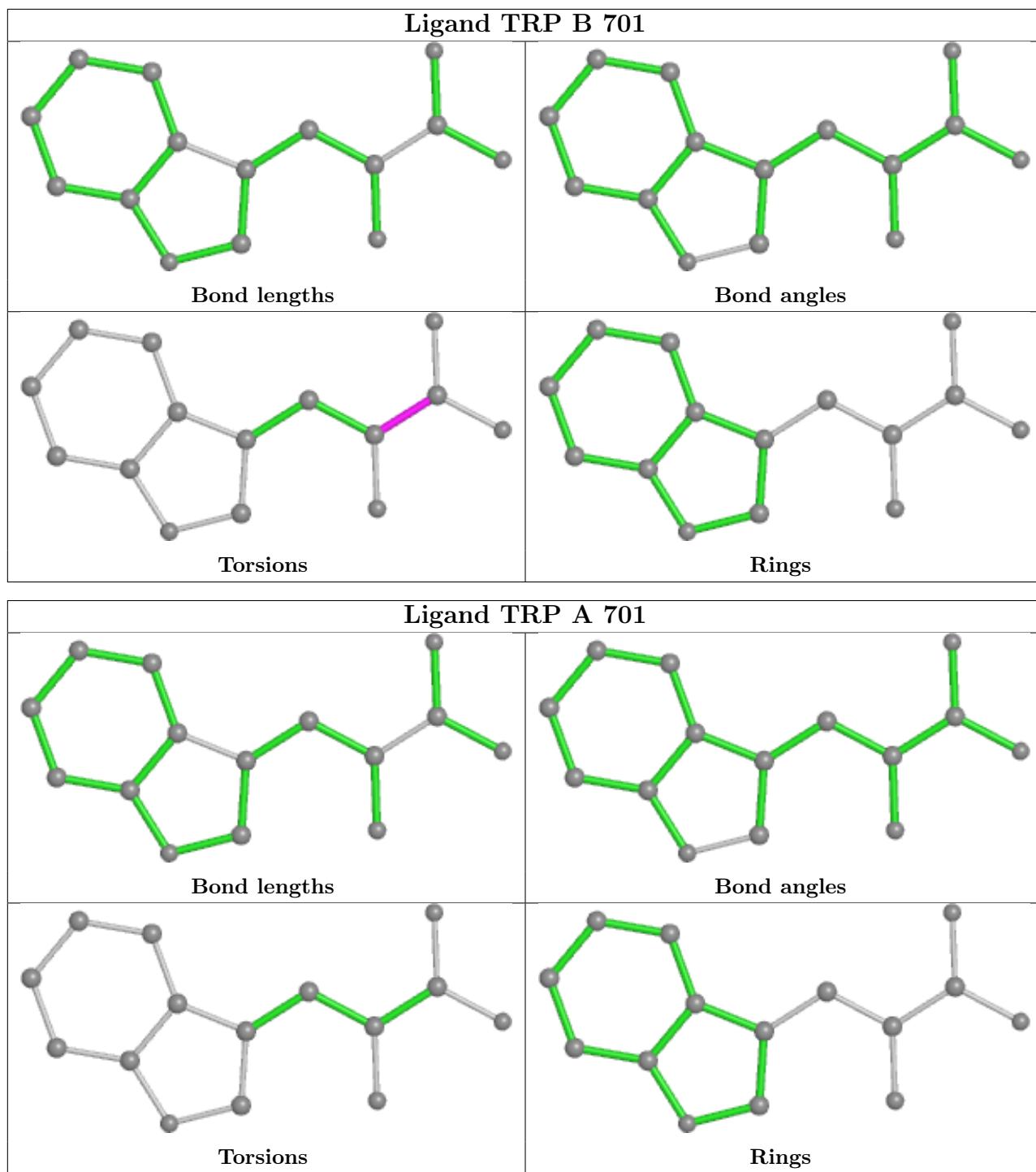
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	SIN	C1-C2-C3-C4
3	A	702	SIN	C2-C3-C4-O3
3	A	702	SIN	C2-C3-C4-O4
2	B	701	TRP	OXT-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

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 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	672/702 (95%)	0.55	38 (5%) 23 28	54, 88, 130, 154	0
1	B	660/702 (94%)	0.61	61 (9%) 9 10	60, 95, 140, 154	0
All	All	1332/1404 (94%)	0.58	99 (7%) 14 18	54, 91, 135, 154	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	359	LEU	6.6
1	A	96	GLY	6.5
1	A	95	VAL	5.9
1	B	134	ALA	5.8
1	A	70	ILE	5.7
1	B	470	LEU	5.5
1	B	95	VAL	5.3
1	A	134	ALA	4.8
1	B	363	GLY	4.8
1	B	132	LEU	4.7
1	B	84	HIS	4.6
1	B	58	ASP	4.5
1	B	379	LEU	4.3
1	A	40	LEU	4.3
1	A	141	LEU	4.1
1	B	63	PHE	4.0
1	A	37	TRP	3.9
1	B	294	ARG	3.9
1	A	359	LEU	3.9
1	A	287	TYR	3.9
1	A	97	LEU	3.8
1	A	58	ASP	3.8
1	A	87	ILE	3.7
1	B	408	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	212	VAL	3.6
1	B	255	LEU	3.5
1	B	360	ASP	3.4
1	A	4	LEU	3.4
1	A	388	ALA	3.3
1	B	645	ALA	3.3
1	B	56	SER	3.3
1	A	137	LEU	3.3
1	B	42	VAL	3.3
1	B	270	VAL	3.2
1	A	139	ASP	3.1
1	B	88	ALA	3.1
1	B	357	LEU	3.1
1	B	37	TRP	3.0
1	B	362	ARG	3.0
1	B	560	TYR	3.0
1	B	277	THR	3.0
1	B	454	LEU	3.0
1	B	407	PRO	3.0
1	B	271	ARG	3.0
1	A	339	LEU	3.0
1	B	341	ALA	3.0
1	B	279	ARG	2.9
1	B	231	PHE	2.9
1	A	252	ARG	2.9
1	B	309	LEU	2.9
1	B	615	VAL	2.9
1	A	396	PHE	2.9
1	B	196	ARG	2.8
1	A	162	LEU	2.8
1	B	345	ILE	2.8
1	B	388	ALA	2.8
1	A	155	LEU	2.8
1	A	69	ALA	2.8
1	B	216	ALA	2.8
1	B	55	GLY	2.7
1	B	373	ARG	2.7
1	B	446	PRO	2.7
1	A	284	PHE	2.7
1	B	4	LEU	2.7
1	A	39	ARG	2.7
1	B	203	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	67	ARG	2.6
1	B	133	ALA	2.6
1	B	405	PHE	2.6
1	B	311	TYR	2.5
1	A	205	LEU	2.5
1	B	638	ILE	2.5
1	B	339	LEU	2.4
1	B	213	LEU	2.4
1	B	287	TYR	2.4
1	A	45	PHE	2.4
1	A	403	ALA	2.3
1	A	405	PHE	2.3
1	A	42	VAL	2.3
1	B	230	THR	2.3
1	B	40	LEU	2.3
1	A	386	ALA	2.3
1	A	132	LEU	2.3
1	A	659	GLN	2.3
1	A	90	LEU	2.3
1	B	307	PHE	2.2
1	B	356	LEU	2.2
1	A	48	ILE	2.2
1	A	341	ALA	2.2
1	A	397	GLY	2.2
1	B	369	ARG	2.1
1	A	144	LEU	2.1
1	B	371	TRP	2.1
1	A	135	THR	2.1
1	B	155	LEU	2.1
1	B	248	LEU	2.1
1	B	366	ASP	2.0
1	B	644	GLN	2.0
1	B	506	GLY	2.0

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

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
1	OCS	B	81	9/10	0.89	0.12	80,95,104,106	0
1	OCS	A	81	9/10	0.94	0.12	92,103,112,117	0

6.3 Carbohydrates [\(i\)](#)

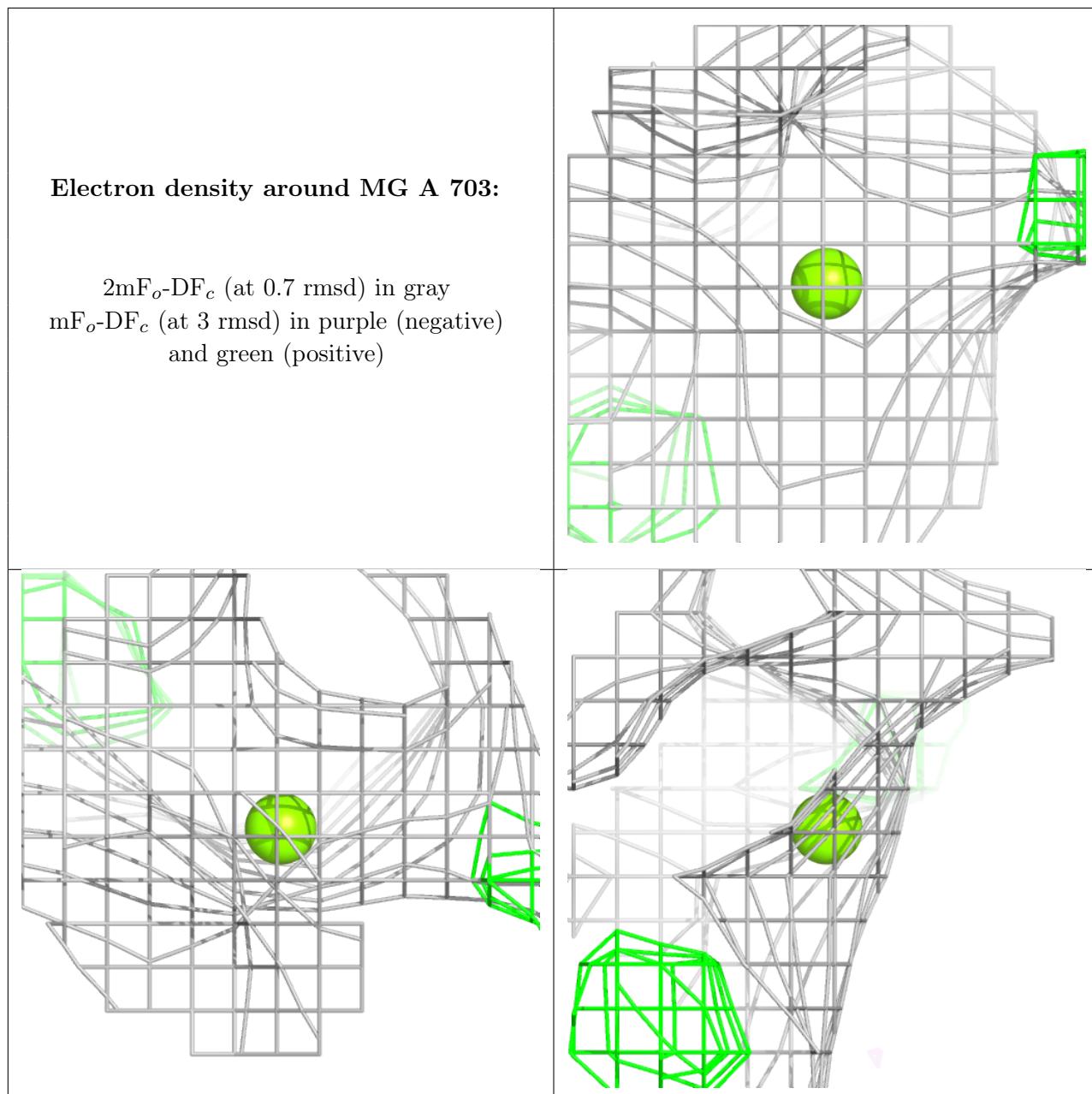
There are no monosaccharides in this entry.

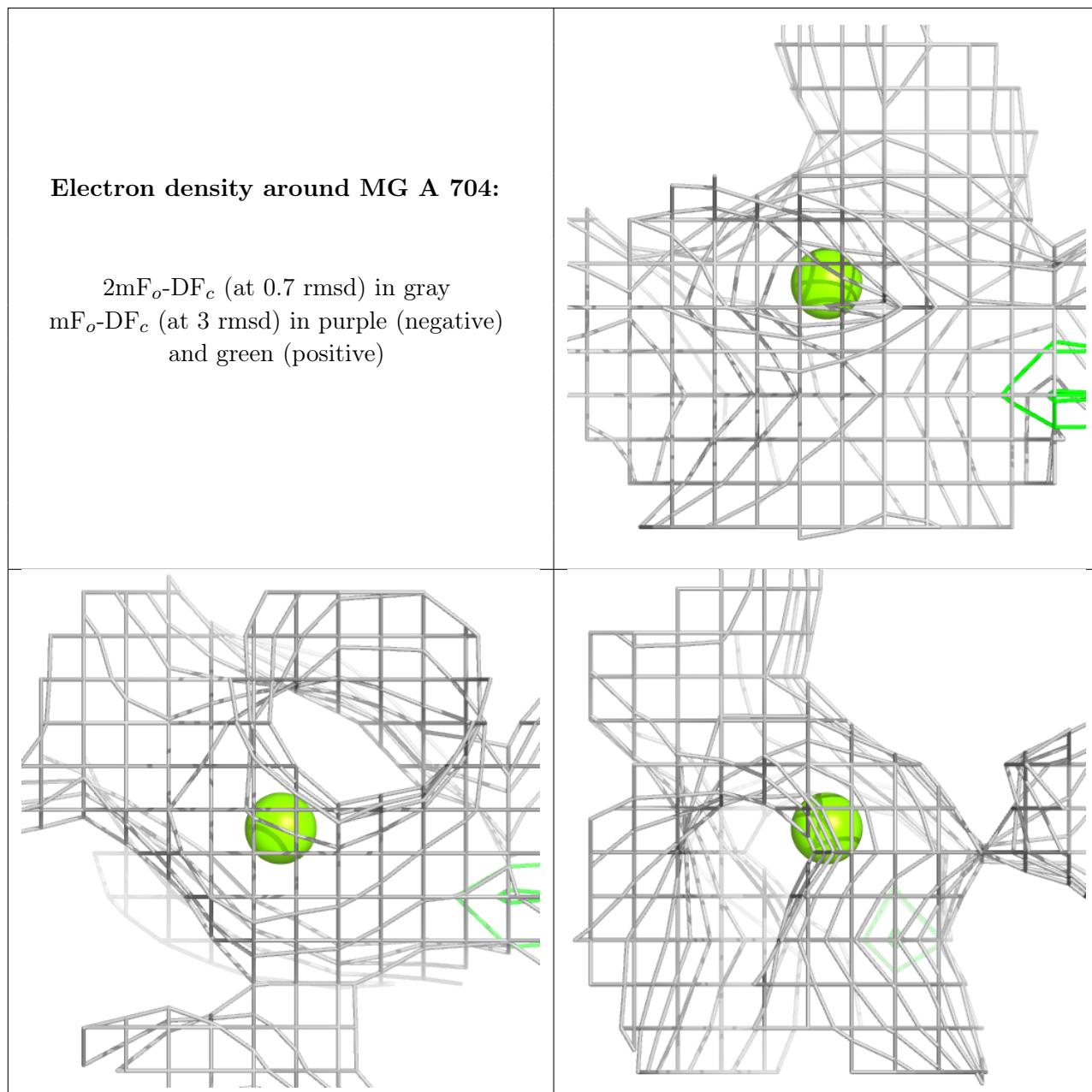
6.4 Ligands [\(i\)](#)

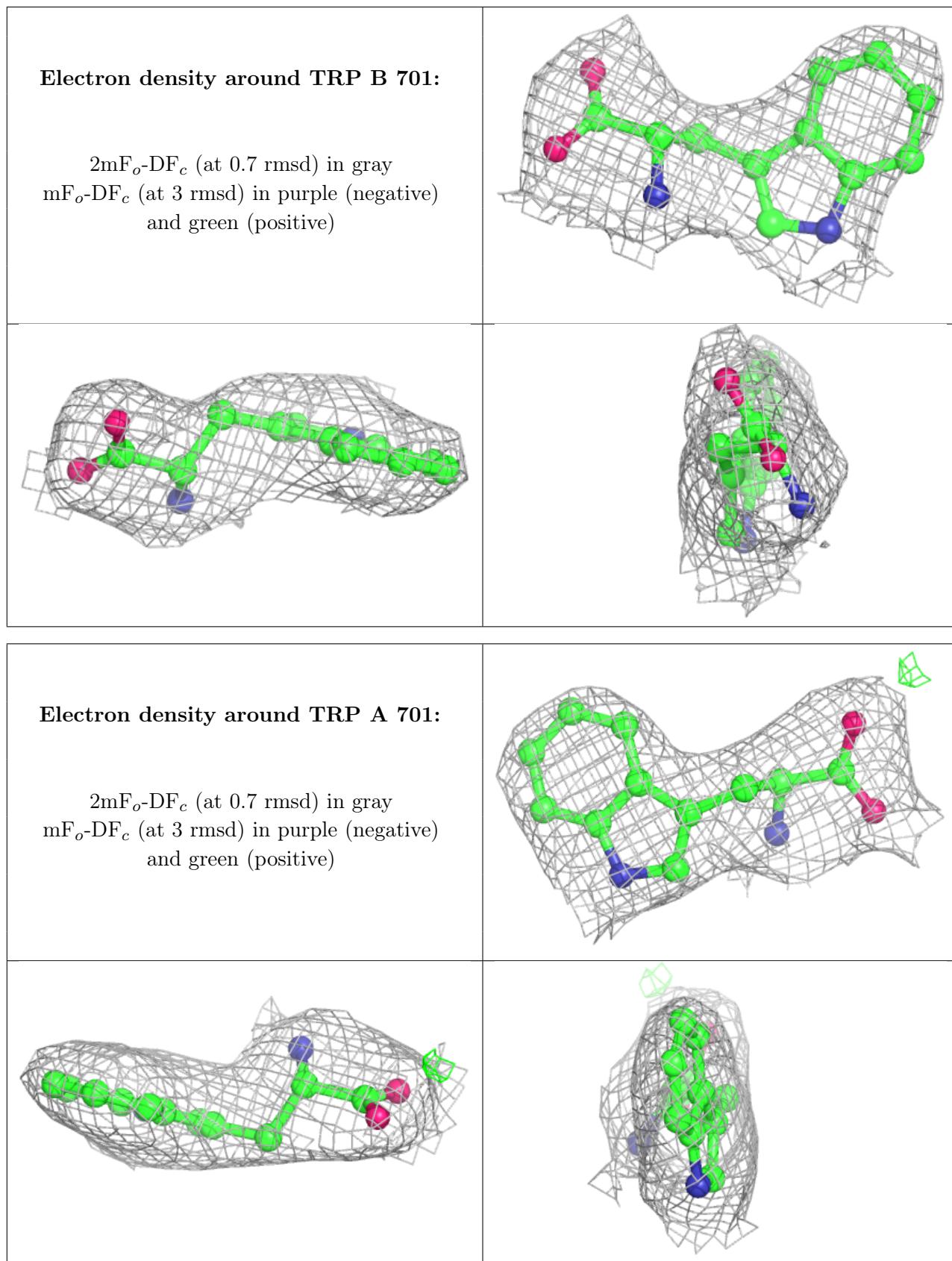
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	A	703	1/1	0.73	0.13	87,87,87,87	0
4	MG	A	704	1/1	0.82	0.14	89,89,89,89	0
2	TRP	B	701	15/15	0.94	0.13	80,86,89,90	0
2	TRP	A	701	15/15	0.95	0.17	62,63,65,69	0
3	SIN	A	702	8/8	0.96	0.19	78,87,88,92	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.