



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 10:28 AM EDT

PDB ID : 6JZ4
Title : b-glucuronidase from Ruminococcus gnavus in complex with D-glucaro-d-lactam
Authors : Dashnyam, P.; Lin, H.Y.
Deposited on : 2019-04-30
Resolution : 1.71 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

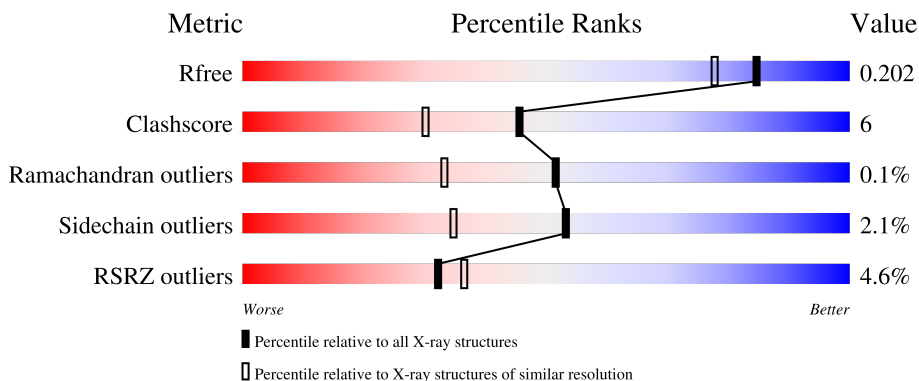
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

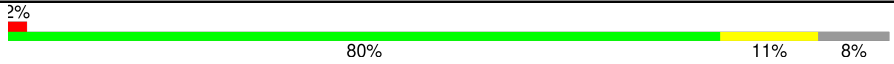

The reported resolution of this entry is 1.71 Å.

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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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 $\leq 5\%$. 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	627	
1	B	627	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10256 atoms, of which 30 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 Beta-glucuronidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	576	Total	C	N	O	S	0	0	0
			4717	3042	767	885	23			
1	B	577	Total	C	N	O	S	0	0	0
			4725	3047	768	886	24			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	initiating methionine	UNP Q6W7J7
A	-22	HIS	-	expression tag	UNP Q6W7J7
A	-21	HIS	-	expression tag	UNP Q6W7J7
A	-20	HIS	-	expression tag	UNP Q6W7J7
A	-19	HIS	-	expression tag	UNP Q6W7J7
A	-18	HIS	-	expression tag	UNP Q6W7J7
A	-17	HIS	-	expression tag	UNP Q6W7J7
A	-16	SER	-	expression tag	UNP Q6W7J7
A	-15	SER	-	expression tag	UNP Q6W7J7
A	-14	GLY	-	expression tag	UNP Q6W7J7
A	-13	VAL	-	expression tag	UNP Q6W7J7
A	-12	ASP	-	expression tag	UNP Q6W7J7
A	-11	LEU	-	expression tag	UNP Q6W7J7
A	-10	GLY	-	expression tag	UNP Q6W7J7
A	-9	THR	-	expression tag	UNP Q6W7J7
A	-8	GLU	-	expression tag	UNP Q6W7J7
A	-7	ASN	-	expression tag	UNP Q6W7J7
A	-6	LEU	-	expression tag	UNP Q6W7J7
A	-5	TYR	-	expression tag	UNP Q6W7J7
A	-4	PHE	-	expression tag	UNP Q6W7J7
A	-3	GLN	-	expression tag	UNP Q6W7J7
A	-2	SER	-	expression tag	UNP Q6W7J7
A	-1	ASN	-	expression tag	UNP Q6W7J7
A	0	GLY	-	expression tag	UNP Q6W7J7
B	-23	MET	-	initiating methionine	UNP Q6W7J7

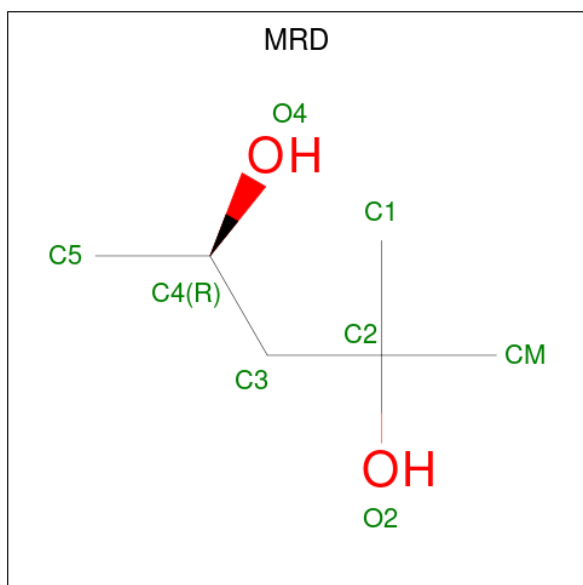
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	HIS	-	expression tag	UNP Q6W7J7
B	-21	HIS	-	expression tag	UNP Q6W7J7
B	-20	HIS	-	expression tag	UNP Q6W7J7
B	-19	HIS	-	expression tag	UNP Q6W7J7
B	-18	HIS	-	expression tag	UNP Q6W7J7
B	-17	HIS	-	expression tag	UNP Q6W7J7
B	-16	SER	-	expression tag	UNP Q6W7J7
B	-15	SER	-	expression tag	UNP Q6W7J7
B	-14	GLY	-	expression tag	UNP Q6W7J7
B	-13	VAL	-	expression tag	UNP Q6W7J7
B	-12	ASP	-	expression tag	UNP Q6W7J7
B	-11	LEU	-	expression tag	UNP Q6W7J7
B	-10	GLY	-	expression tag	UNP Q6W7J7
B	-9	THR	-	expression tag	UNP Q6W7J7
B	-8	GLU	-	expression tag	UNP Q6W7J7
B	-7	ASN	-	expression tag	UNP Q6W7J7
B	-6	LEU	-	expression tag	UNP Q6W7J7
B	-5	TYR	-	expression tag	UNP Q6W7J7
B	-4	PHE	-	expression tag	UNP Q6W7J7
B	-3	GLN	-	expression tag	UNP Q6W7J7
B	-2	SER	-	expression tag	UNP Q6W7J7
B	-1	ASN	-	expression tag	UNP Q6W7J7
B	0	GLY	-	expression tag	UNP Q6W7J7

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- The chemical structure of EVA (Ethyl Vinyl Acetate) is shown, highlighting the stereochemistry of the chiral centers. The structure is a six-membered ring with a nitrogen atom (N) at the top. The ring is substituted with various groups, including a carboxylic acid group (HO-C=O) and a hydroxyl group (OH). The stereochemistry is indicated by wedges and dashes. The labels CA(S), CB(R), CD1(R), and CG(S) are used to denote the stereochemistry of the chiral centers. The labels OXT, OAK, OAJ, and OD2 are used to denote the stereochemistry of the oxygen atoms. The labels C, N, and O are used to denote the atoms. The labels HO, OH, and O are used to denote the functional groups. The labels CA, CB, CD1, and CG are used to denote the chiral centers. The labels S, R, and R are used to denote the stereochemistry of the chiral centers. The labels S, R, and R are used to denote the stereochemistry of the chiral centers.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			21	6	8	1	6		
2	B	1	Total	C	H	N	O	0	0
			21	6	8	1	6		

- Molecule 3 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			22	6	14	2		

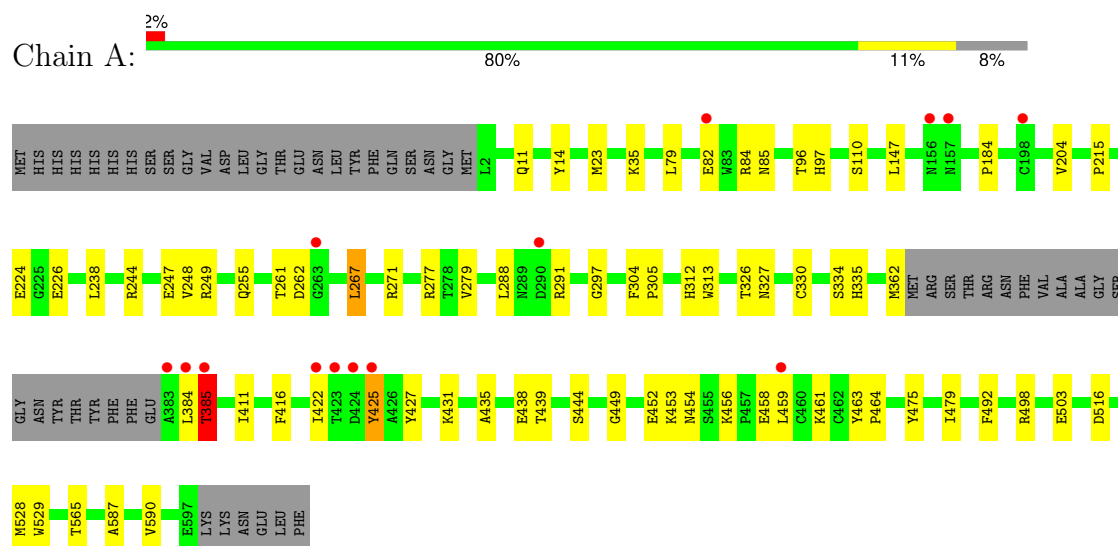
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	403	Total	O	0	0
			403	403		
4	B	347	Total	O	0	0
			347	347		

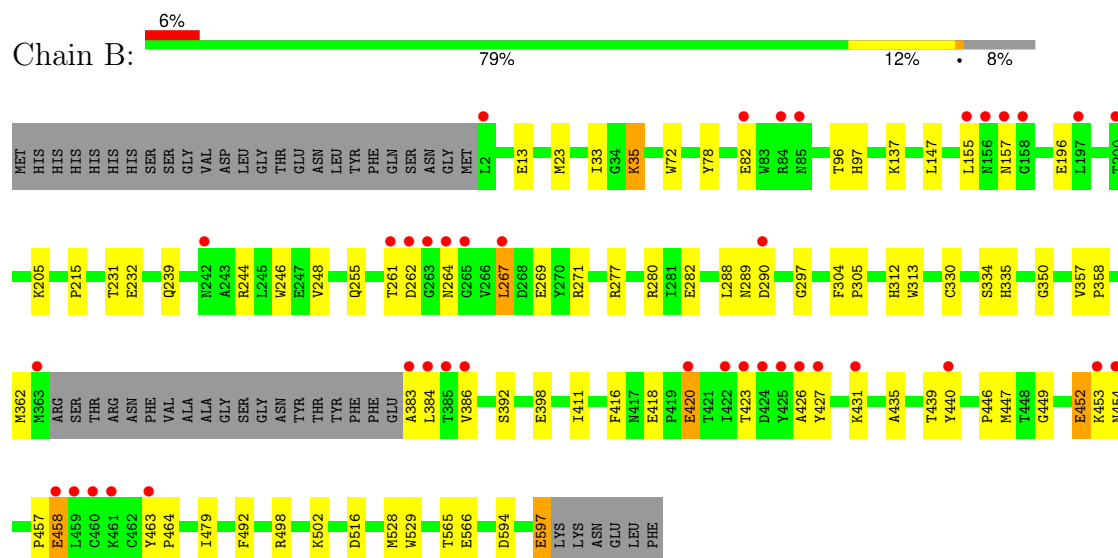
3 Residue-property plots [i](#)

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: Beta-glucuronidase



• Molecule 1: Beta-glucuronidase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	161.21Å 101.90Å 111.30Å 90.00° 130.90° 90.00°	Depositor
Resolution (Å)	28.50 – 1.71 28.50 – 1.71	Depositor EDS
% Data completeness (in resolution range)	62.0 (28.50-1.71) 88.8 (28.50-1.71)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 1.72Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.168 , 0.203 0.180 , 0.202	Depositor DCC
R_{free} test set	2019 reflections (1.48%)	wwPDB-VP
Wilson B-factor (Å ²)	12.2	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10256	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MRD, EVA

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	0.52	0/4851	0.58	1/6579 (0.0%)
1	B	0.47	1/4859 (0.0%)	0.57	0/6589
All	All	0.49	1/9710 (0.0%)	0.57	1/13168 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	566	GLU	CD-OE2	-5.33	1.19	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	385	THR	N-CA-CB	5.01	119.81	110.30

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	4717	0	4506	56	0
1	B	4725	0	4515	70	0
2	A	13	8	8	0	0
2	B	13	8	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	8	14	14	1	0
4	A	403	0	0	2	0
4	B	347	0	0	2	0
All	All	10226	30	9051	119	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 6.

All (119) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:LYS:HE3	1:B:35:LYS:H	1.37	0.89
1:A:255:GLN:NE2	1:A:271:ARG:HD3	1.88	0.88
1:A:427:TYR:CE2	1:A:431:LYS:HE2	2.19	0.78
1:B:35:LYS:H	1:B:35:LYS:CE	1.96	0.78
1:A:255:GLN:HE21	1:A:271:ARG:HD3	1.47	0.78
1:B:35:LYS:H	1:B:35:LYS:CD	1.98	0.77
1:A:255:GLN:NE2	1:A:271:ARG:HH11	1.84	0.75
1:A:452:GLU:OE1	1:A:454:ASN:ND2	2.21	0.74
1:A:384:LEU:O	1:A:385:THR:HG23	1.88	0.73
1:B:423:THR:HG23	1:B:426:ALA:H	1.55	0.72
1:B:35:LYS:HE3	1:B:35:LYS:N	2.07	0.70
1:B:248:VAL:HG23	1:B:288:LEU:HD22	1.75	0.68
1:B:453:LYS:HD3	1:B:479:ILE:HD11	1.75	0.68
1:A:23:MET:HG2	1:B:313:TRP:CD2	2.29	0.67
1:B:280:ARG:NH2	1:B:290:ASP:OD1	2.29	0.66
1:A:587:ALA:O	1:A:590:VAL:HG12	1.96	0.66
1:A:313:TRP:CD2	1:B:23:MET:HG2	2.31	0.65
1:A:312:HIS:HD2	1:B:312:HIS:HD2	1.43	0.64
1:B:594:ASP:O	1:B:597:GLU:CG	2.46	0.64
1:A:565:THR:HG23	4:A:903:HOH:O	1.97	0.64
1:B:458:GLU:HG3	1:B:458:GLU:O	1.98	0.63
1:B:248:VAL:CG2	1:B:288:LEU:HD22	2.29	0.62
1:A:147:LEU:HD21	1:A:362:MET:CE	2.30	0.62
1:B:416:PHE:CE1	1:B:449:GLY:HA3	2.35	0.62
1:A:248:VAL:HG23	1:A:288:LEU:CD2	2.31	0.60
1:B:594:ASP:O	1:B:597:GLU:HG3	2.01	0.60
1:B:35:LYS:H	1:B:35:LYS:HD2	1.67	0.59
1:A:247:GLU:OE2	1:A:291:ARG:NH2	2.37	0.58
1:A:248:VAL:CG2	1:A:288:LEU:HD22	2.34	0.58
1:A:453:LYS:HE3	1:A:475:TYR:OH	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:GLU:OE2	1:A:226:GLU:OE2	2.22	0.57
1:A:279:VAL:HG22	1:A:288:LEU:HD12	1.87	0.56
1:B:280:ARG:NH1	1:B:282:GLU:OE1	2.39	0.56
1:A:248:VAL:HG23	1:A:288:LEU:HD23	1.89	0.55
1:A:312:HIS:CD2	1:B:312:HIS:HD2	2.24	0.55
1:A:255:GLN:HE22	1:A:271:ARG:HH11	1.54	0.54
1:B:463:TYR:OH	1:B:502:LYS:NZ	2.40	0.54
1:A:458:GLU:OE2	1:A:498:ARG:HD2	2.09	0.53
1:A:312:HIS:HD2	1:B:312:HIS:CD2	2.24	0.53
1:B:13:GLU:H	1:B:13:GLU:CD	2.12	0.53
1:B:262:ASP:HB2	1:B:267:LEU:HD13	1.91	0.53
1:A:453:LYS:HD2	1:A:479:ILE:CD1	2.40	0.52
1:B:255:GLN:OE1	1:B:271:ARG:NH1	2.37	0.52
1:B:147:LEU:HD21	1:B:362:MET:CE	2.40	0.52
1:A:11:GLN:HG2	1:B:78:TYR:HB3	1.91	0.52
1:A:422:ILE:O	1:A:461:LYS:HE2	2.10	0.52
1:A:147:LEU:HD21	1:A:362:MET:HE2	1.93	0.51
1:A:435:ALA:O	1:A:439:THR:HG23	2.10	0.51
1:B:418:GLU:HG2	1:B:452:GLU:HB3	1.91	0.51
1:B:196:GLU:OE2	1:B:205:LYS:NZ	2.31	0.50
1:B:155:LEU:HB2	1:B:157:ASN:OD1	2.11	0.50
1:B:35:LYS:HE3	1:B:72:TRP:HZ2	1.77	0.49
1:B:357:VAL:HG22	1:B:358:PRO:HD2	1.94	0.49
1:B:528:MET:O	1:B:529:TRP:HB2	2.12	0.49
1:B:416:PHE:CZ	1:B:449:GLY:HA3	2.47	0.49
1:B:289:ASN:O	1:B:290:ASP:HB2	2.13	0.49
1:A:248:VAL:CG2	1:A:288:LEU:CD2	2.90	0.49
1:B:435:ALA:O	1:B:439:THR:HG23	2.13	0.48
1:A:590:VAL:CG1	4:A:838:HOH:O	2.61	0.48
1:A:463:TYR:N	1:A:464:PRO:CD	2.76	0.48
1:A:297:GLY:HA3	1:A:330:CYS:O	2.14	0.48
1:B:463:TYR:CG	1:B:464:PRO:HD3	2.49	0.48
1:B:453:LYS:CD	1:B:479:ILE:HD11	2.42	0.48
1:A:528:MET:O	1:A:529:TRP:HB2	2.14	0.47
1:B:458:GLU:HB3	1:B:498:ARG:HH22	1.79	0.47
1:B:427:TYR:CE2	1:B:431:LYS:HE3	2.49	0.47
1:A:82:GLU:HB2	1:B:82:GLU:OE1	2.13	0.47
1:B:248:VAL:HG23	1:B:288:LEU:CD2	2.44	0.47
1:B:357:VAL:HG22	1:B:358:PRO:CD	2.45	0.46
1:A:279:VAL:HG21	1:A:411:ILE:HG22	1.97	0.46
1:A:248:VAL:HG22	1:A:288:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:GLU:CG	1:B:452:GLU:HB3	2.45	0.46
1:B:304:PHE:CG	1:B:305:PRO:HD2	2.51	0.46
1:A:84:ARG:O	1:A:85:ASN:HB2	2.16	0.45
1:B:516:ASP:O	1:B:529:TRP:HA	2.16	0.45
1:B:231:THR:HG22	1:B:232:GLU:N	2.32	0.45
1:B:463:TYR:N	1:B:464:PRO:CD	2.80	0.45
1:B:383:ALA:O	1:B:386:VAL:HG23	2.16	0.45
1:A:14:TYR:O	1:A:184:PRO:HD3	2.17	0.45
1:B:96:THR:HA	1:B:97:HIS:HA	1.80	0.45
1:A:82:GLU:HG2	1:A:82:GLU:O	2.17	0.45
1:A:96:THR:HA	1:A:97:HIS:HA	1.80	0.45
1:B:398:GLU:HG3	1:B:440:TYR:CE1	2.52	0.45
1:B:147:LEU:HD21	1:B:362:MET:HE2	1.99	0.45
1:B:196:GLU:HG3	1:B:205:LYS:NZ	2.32	0.45
1:B:297:GLY:HA3	1:B:330:CYS:O	2.17	0.45
1:B:334:SER:HA	1:B:335:HIS:HA	1.77	0.45
1:A:425:TYR:HD1	1:A:425:TYR:O	2.00	0.44
1:B:147:LEU:CD2	1:B:362:MET:HE2	2.47	0.44
1:A:147:LEU:HD21	1:A:362:MET:HE3	2.00	0.44
1:B:262:ASP:HB2	1:B:267:LEU:CD1	2.48	0.43
1:B:431:LYS:HE3	1:B:431:LYS:HB2	1.83	0.43
1:A:438:GLU:OE2	1:A:444:SER:OG	2.26	0.43
1:B:35:LYS:HZ3	1:B:137:LYS:HE3	1.82	0.43
1:A:35:LYS:HD2	1:A:35:LYS:HA	1.68	0.43
1:B:516:ASP:HB3	1:B:529:TRP:CZ3	2.54	0.43
1:A:215:PRO:HD2	1:A:261:THR:O	2.19	0.43
1:A:262:ASP:HB3	1:A:267:LEU:HD21	2.01	0.43
1:B:411:ILE:O	1:B:446:PRO:HD2	2.19	0.42
1:B:565:THR:HG23	4:B:907:HOH:O	2.19	0.42
1:A:334:SER:HA	1:A:335:HIS:HA	1.80	0.42
1:B:452:GLU:OE2	1:B:454:ASN:ND2	2.49	0.42
1:A:456:LYS:HD2	1:A:459:LEU:HD12	2.02	0.42
1:A:247:GLU:CD	1:A:291:ARG:HH22	2.23	0.42
1:B:33:ILE:C	1:B:33:ILE:HD12	2.39	0.42
1:B:269:GLU:OE2	1:B:271:ARG:NE	2.30	0.42
1:B:457:PRO:O	1:B:502:LYS:NZ	2.53	0.42
1:B:420:GLU:H	1:B:420:GLU:HG2	1.69	0.42
1:A:255:GLN:HE22	1:A:271:ARG:HD3	1.79	0.42
1:B:594:ASP:O	1:B:597:GLU:HG2	2.19	0.42
1:B:215:PRO:HB2	1:B:261:THR:CG2	2.50	0.41
1:A:416:PHE:CZ	1:A:449:GLY:HA3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:TRP:CZ2	1:B:350:GLY:HA2	2.56	0.41
1:B:447:MET:HG3	4:B:896:HOH:O	2.21	0.40
1:A:204:VAL:HB	1:A:238:LEU:HB2	2.03	0.40
1:A:110:SER:HB3	3:A:702:MRD:H1C1	2.03	0.40
1:A:304:PHE:CG	1:A:305:PRO:HD2	2.57	0.40
1:A:326:THR:O	1:A:327:ASN:HB2	2.21	0.40
1:A:516:ASP:HB3	1:A:529:TRP:CZ3	2.57	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	572/627 (91%)	555 (97%)	16 (3%)	1 (0%)	47	30
1	B	573/627 (91%)	556 (97%)	17 (3%)	0	100	100
All	All	1145/1254 (91%)	1111 (97%)	33 (3%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	385	THR

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	502/546 (92%)	494 (98%)	8 (2%)	62	47
1	B	503/546 (92%)	490 (97%)	13 (3%)	46	26
All	All	1005/1092 (92%)	984 (98%)	21 (2%)	53	35

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LEU
1	A	244	ARG
1	A	249	ARG
1	A	267	LEU
1	A	277	ARG
1	A	425	TYR
1	A	492	PHE
1	A	503	GLU
1	B	35	LYS
1	B	239	GLN
1	B	244	ARG
1	B	264	ASN
1	B	267	LEU
1	B	277	ARG
1	B	384	LEU
1	B	392	SER
1	B	420	GLU
1	B	452	GLU
1	B	458	GLU
1	B	492	PHE
1	B	597	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	A	255	GLN
1	A	454	ASN
1	A	505	ASN
1	B	41	ASN

5.3.3 RNA ⓘ

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](#)

3 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$
2	EVA	A	701	-	13,13,13	1.57	2 (15%)	13,19,19	1.70	1 (7%)
3	MRD	A	702	-	7,7,7	1.33	1 (14%)	9,10,10	1.17	1 (11%)
2	EVA	B	701	-	13,13,13	1.61	2 (15%)	13,19,19	1.65	1 (7%)

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	EVA	A	701	-	-	1/3/24/24	0/1/1/1
3	MRD	A	702	-	-	3/5/5/5	-
2	EVA	B	701	-	-	0/3/24/24	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	EVA	CG-CD1	-4.08	1.47	1.53
2	B	701	EVA	CG-CD1	-3.88	1.47	1.53
3	A	702	MRD	O2-C2	-2.99	1.37	1.44
2	B	701	EVA	CG-CB	2.47	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	EVA	CG-CB	2.17	1.58	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	EVA	OAK-CAE-N	-4.93	116.15	122.67
2	B	701	EVA	OAK-CAE-N	-4.61	116.57	122.67
3	A	702	MRD	CM-C2-C1	-2.89	104.16	110.63

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	EVA	O-C-CA-N
3	A	702	MRD	C1-C2-C3-C4
3	A	702	MRD	C2-C3-C4-O4
3	A	702	MRD	CM-C2-C3-C4

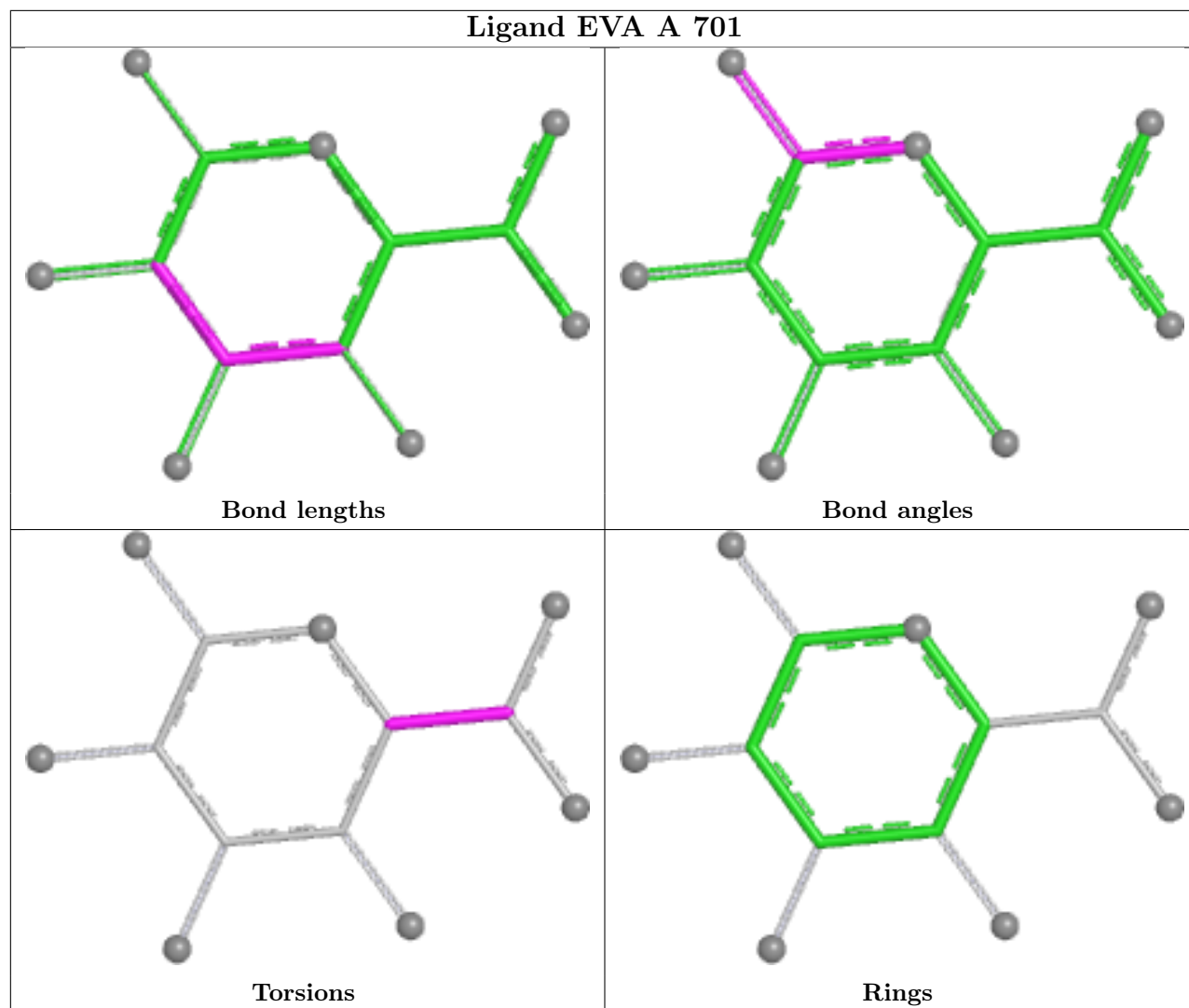
There are no ring outliers.

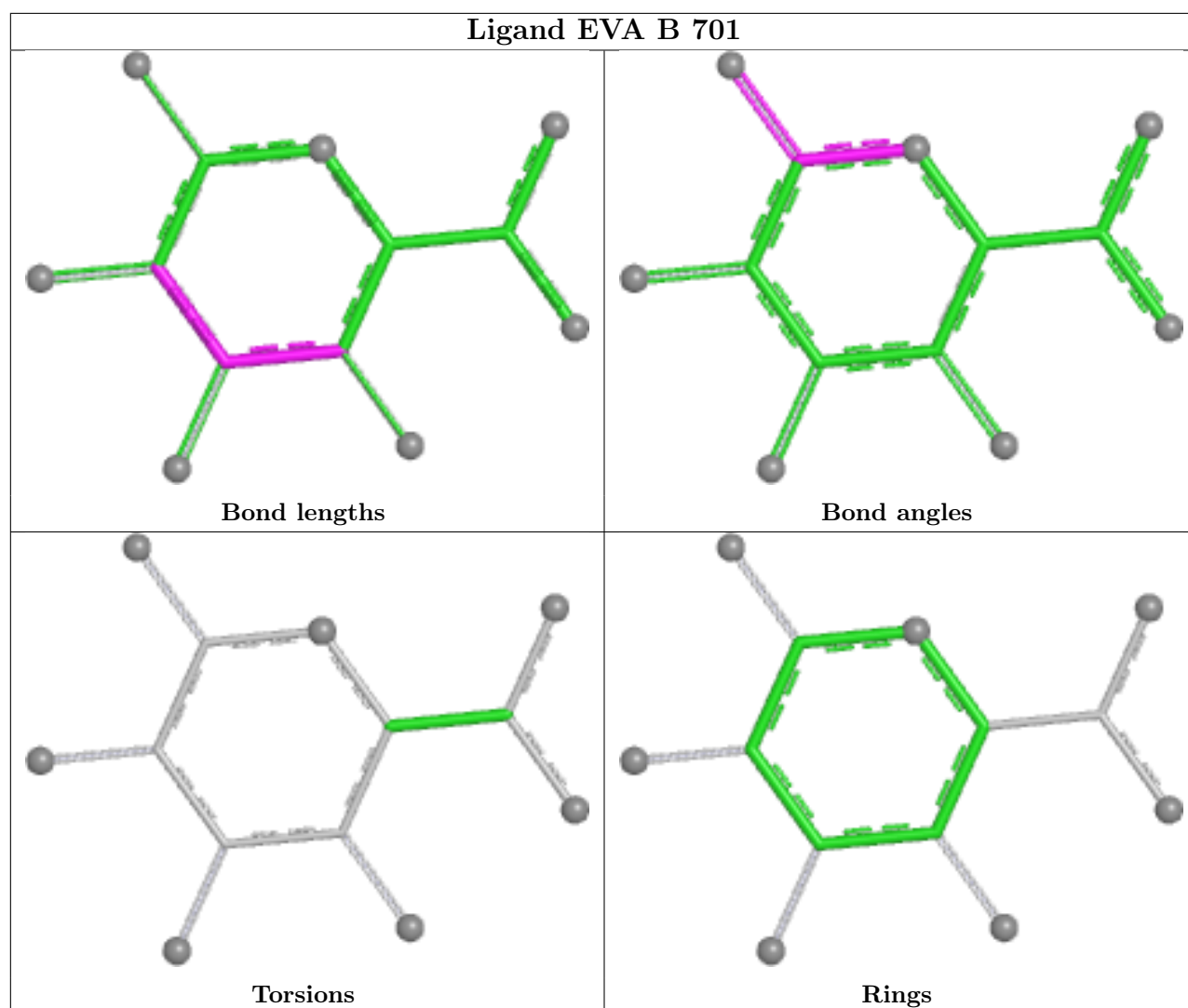
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	MRD	1	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.

Ligand EVA 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

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, 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	576/627 (91%)	0.01	14 (2%) 59 63	7, 15, 32, 50	0
1	B	577/627 (92%)	0.25	39 (6%) 17 19	7, 17, 38, 61	0
All	All	1153/1254 (91%)	0.13	53 (4%) 32 36	7, 15, 35, 61	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	384	LEU	13.2
1	B	384	LEU	11.5
1	B	425	TYR	10.2
1	A	425	TYR	8.3
1	B	422	ILE	6.8
1	B	363	MET	6.4
1	B	264	ASN	6.3
1	B	423	THR	5.6
1	B	156	ASN	4.9
1	B	263	GLY	4.9
1	B	458	GLU	4.9
1	B	385	THR	4.8
1	A	383	ALA	4.6
1	B	424	ASP	4.0
1	B	383	ALA	3.9
1	B	459	LEU	3.9
1	B	460	CYS	3.8
1	B	262	ASP	3.7
1	A	424	ASP	3.6
1	B	261	THR	3.6
1	A	385	THR	3.5
1	B	290	ASP	3.5
1	A	156	ASN	3.5
1	B	463	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	422	ILE	3.4
1	B	426	ALA	3.3
1	B	420	GLU	3.3
1	B	157	ASN	3.2
1	B	453	LYS	3.0
1	B	386	VAL	3.0
1	A	459	LEU	2.9
1	B	2	LEU	2.8
1	A	198	CYS	2.8
1	A	82	GLU	2.8
1	B	265	GLY	2.7
1	B	267	LEU	2.7
1	B	427	TYR	2.6
1	A	263	GLY	2.5
1	A	423	THR	2.5
1	B	158	GLY	2.4
1	B	461	LYS	2.4
1	B	155	LEU	2.4
1	B	200	THR	2.4
1	B	242	ASN	2.4
1	B	84	ARG	2.2
1	B	440	TYR	2.2
1	A	290	ASP	2.2
1	B	82	GLU	2.2
1	B	85	ASN	2.2
1	B	197	LEU	2.1
1	B	431	LYS	2.1
1	B	454	ASN	2.0
1	A	157	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands

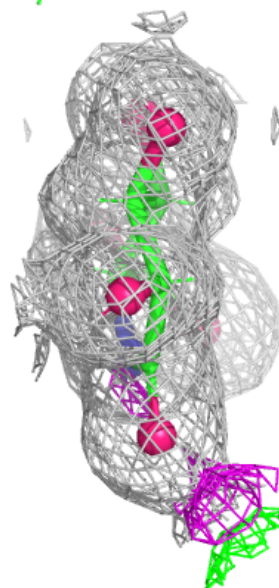
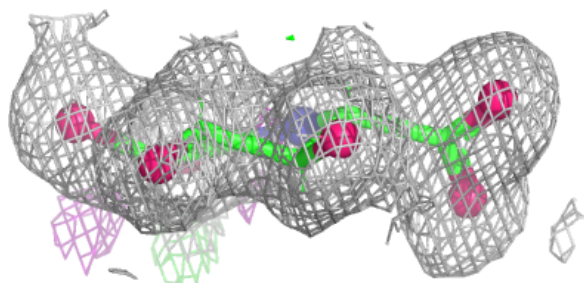
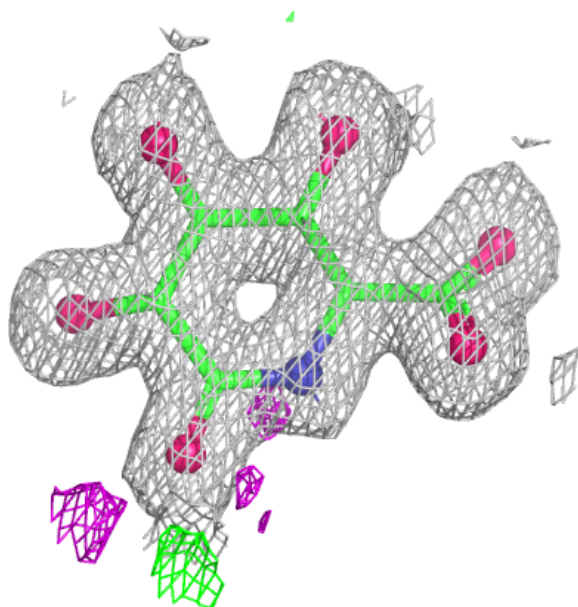
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

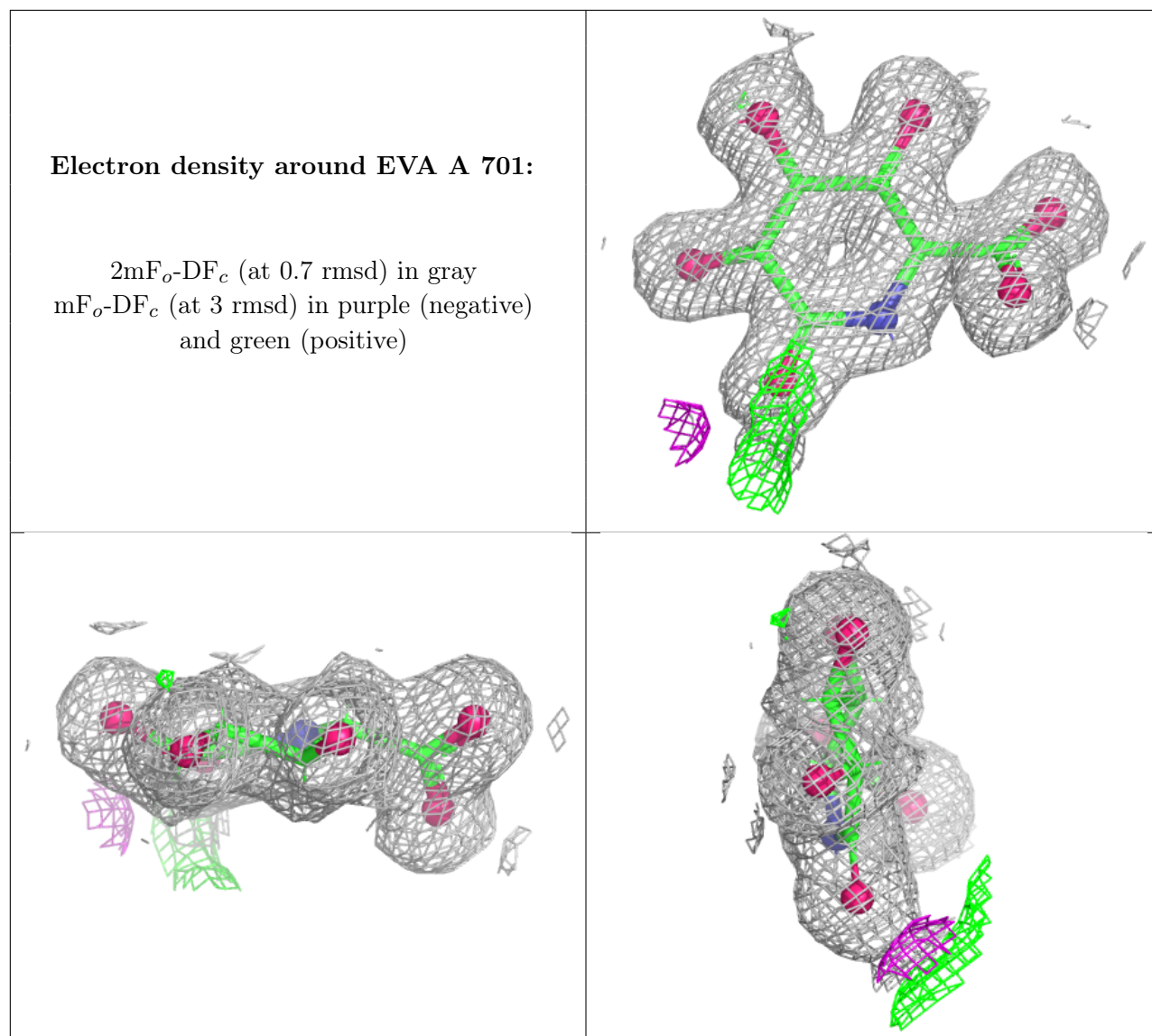
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MRD	A	702	8/8	0.90	0.27	20,20,20,20	0
2	EVA	B	701	13/13	0.97	0.07	9,12,14,15	0
2	EVA	A	701	13/13	0.98	0.07	8,10,12,13	0

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 EVA B 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 ⓘ

There are no such residues in this entry.