WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 06:31 PM JST

PDB ID	:	6JZ2
Title	:	b-glucuronidase from Ruminococcus gnavus in complex with uronic isofagomine at 1.3 Angstroms resolution
Authors	:	Dashnyam, P.; Lin, H.Y.
Deposited on	:	2019-04-30
Resolution	:	1.29 Å(reported)

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	:	2.36
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 1.29 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.
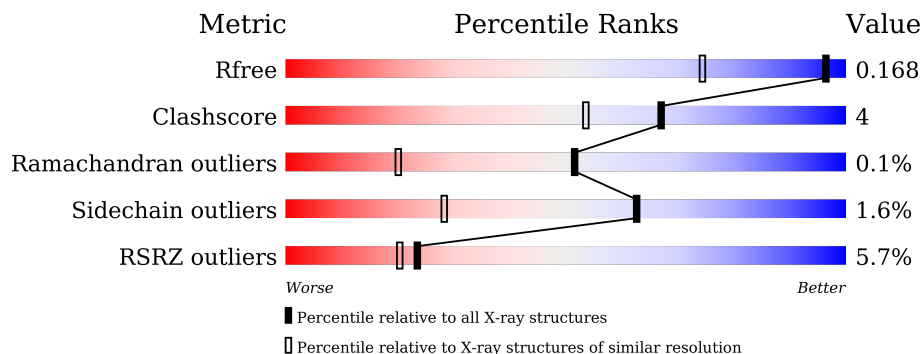
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	627	5% / 86% / 7% · 6%
1	B	627	6% / 88% / 7% 5%

2　Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 10909 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 Beta-glucuronidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	589	Total 4845	C 3125	N 791	O 905	S 24	0	1	0
1	B	596	Total 4891	C 3152	N 799	O 916	S 24	0	1	0

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

- Molecule 2 is (3S,4R,5R)-4,5-dihydroxypiperidine-3-carboxylic acid (three-letter code: SJ5) (formula: $C_6H_{11}NO_4$) (labeled as "Ligand of Interest" by depositor).
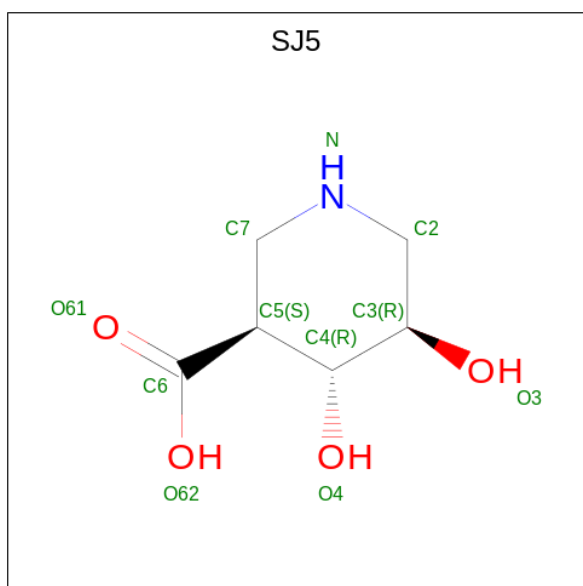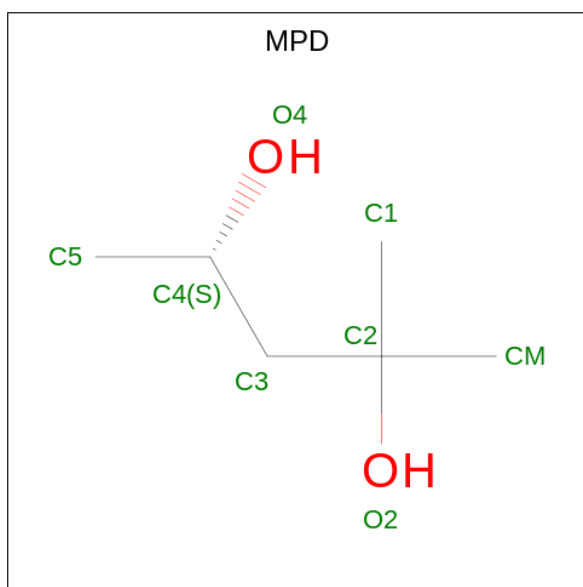
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 11	C 6	N 1	O 4	0	0
2	B	1	Total 11	C 6	N 1	O 4	0	0

- Molecule 3 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).
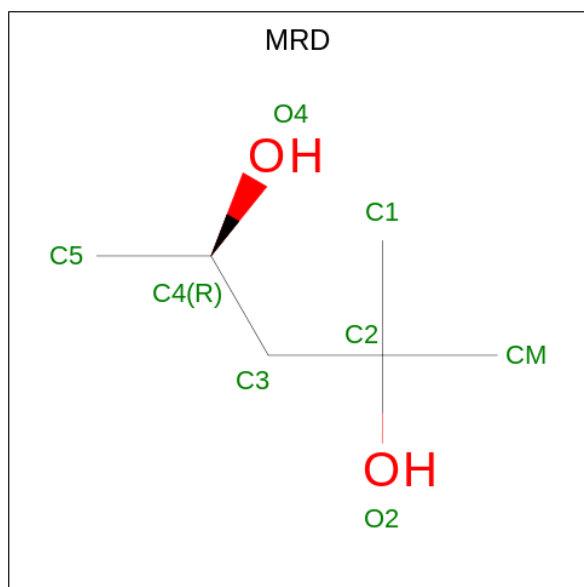
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 8	C 6	O 2	0	0
3	B	1	Total 8	C 6	O 2	0	0
3	B	1	Total 8	C 6	O 2	0	0

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 8	C 6	O 2	0	0
4	B	1	Total 8	C 6	O 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	544	Total 544	O 544	0	0
5	B	567	Total 567	O 567	0	0

3 Residue-property plots ⓘ

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
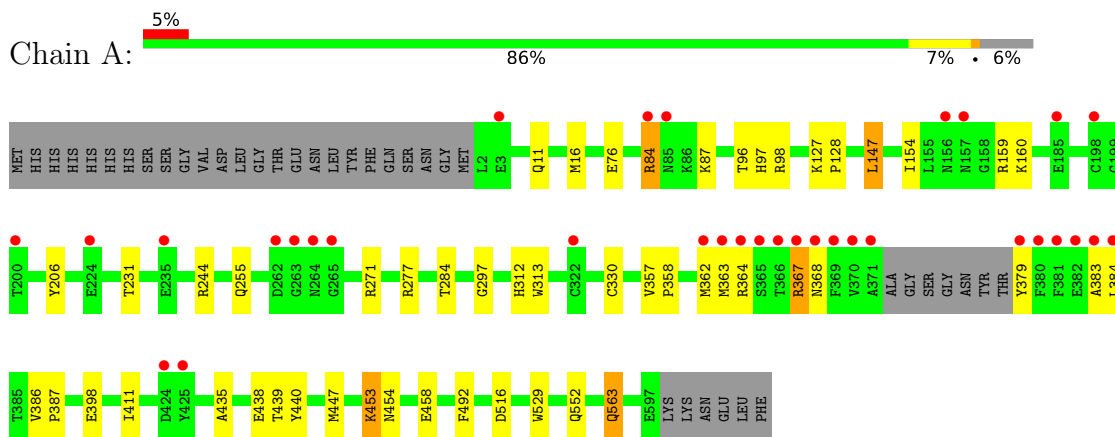
• Molecule 1: Beta-glucuronidase
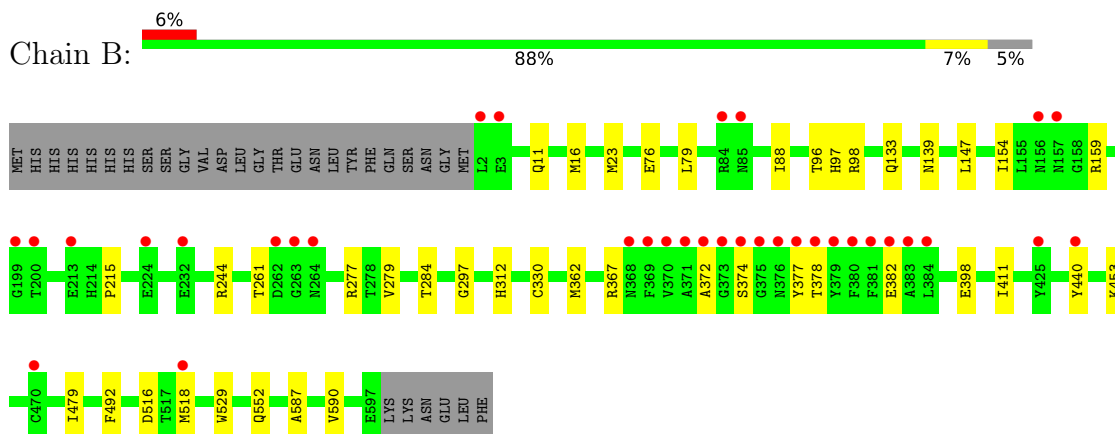
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	163.24Å 102.73Å 112.71Å 90.00° 130.94° 90.00°	Depositor
Resolution (Å)	27.09 – 1.29 28.15 – 1.29	Depositor EDS
% Data completeness (in resolution range)	93.5 (27.09-1.29) 93.5 (28.15-1.29)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 1.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.156 , 0.170 0.162 , 0.168	Depositor DCC
R_{free} test set	1998 reflections (0.60%)	wwPDB-VP
Wilson B-factor (Å^2)	14.1	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 56.7	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.012 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	10909	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, MRD, SJ5

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	0.44	0/4983	0.60	0/6755
1	B	0.39	0/5031	0.58	0/6822
All	All	0.42	0/10014	0.59	0/13577

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	4845	0	4627	49	0
1	B	4891	0	4666	27	0
2	A	11	0	0	0	0
2	B	11	0	0	0	0
3	A	8	0	14	1	0
3	B	16	0	28	0	0
4	B	16	0	28	4	0
5	A	544	0	0	8	0
5	B	567	0	0	4	0
All	All	10909	0	9363	74	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 4.

All (74) 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:364:ARG:HG3	1:A:379:TYR:N	1.42	1.28
1:A:363:MET:O	1:A:367:ARG:HB3	1.61	1.00
1:A:76:GLU:HG3	5:A:811:HOH:O	1.73	0.86
1:A:84:ARG:HG2	1:A:128:PRO:HG2	1.58	0.85
1:A:76:GLU:CG	5:A:811:HOH:O	2.32	0.76
1:A:364:ARG:CG	1:A:379:TYR:N	2.38	0.75
1:A:98:ARG:HG3	3:A:702:MRD:O2	1.87	0.74
1:A:362:MET:HB2	5:A:1081:HOH:O	1.87	0.74
1:A:147:LEU:HD22	1:A:147:LEU:N	2.04	0.73
1:B:398:GLU:HG3	1:B:440:TYR:CE2	2.27	0.69
1:B:453:LYS:NZ	5:B:801:HOH:O	2.27	0.68
1:A:84:ARG:HG2	1:A:128:PRO:CG	2.24	0.67
1:B:453:LYS:HD2	1:B:479:ILE:CD1	2.25	0.65
1:B:453:LYS:HD2	1:B:479:ILE:HD11	1.79	0.65
1:A:312:HIS:HD2	1:B:312:HIS:HD2	1.44	0.63
1:A:563:GLN:NE2	5:A:802:HOH:O	2.31	0.62
1:A:154:ILE:HD13	1:A:160:LYS:HG2	1.82	0.60
1:A:255:GLN:NE2	1:A:271:ARG:HD3	2.16	0.60
1:A:364:ARG:HD3	1:A:368:ASN:ND2	2.16	0.60
1:A:87:LYS:NZ	5:A:803:HOH:O	2.34	0.59
1:B:367:ARG:NH1	1:B:382:GLU:OE2	2.35	0.59
1:A:312:HIS:HD2	1:B:312:HIS:CD2	2.21	0.58
1:A:84:ARG:HG2	1:A:128:PRO:CB	2.33	0.58
1:A:206:TYR:HE2	1:A:231:THR:HG21	1.68	0.58
1:B:398:GLU:HG3	1:B:440:TYR:CD2	2.39	0.57
1:A:312:HIS:CD2	1:B:312:HIS:HD2	2.23	0.57
1:A:438:GLU:HA	1:A:447:MET:HE1	1.89	0.54
1:B:284:THR:O	1:B:552:GLN:HG3	2.08	0.54
1:B:372:ALA:HB1	1:B:377:TYR:CE1	2.43	0.53
1:B:453:LYS:CD	1:B:479:ILE:HD11	2.37	0.53
1:A:284:THR:O	1:A:552:GLN:HG3	2.09	0.53
1:A:398:GLU:HB2	1:A:440:TYR:CE2	2.44	0.53
1:B:279:VAL:HG21	1:B:411:ILE:HG22	1.91	0.53
1:A:84:ARG:HH11	1:A:84:ARG:HG3	1.74	0.52
1:B:518:MET:HG3	5:B:1056:HOH:O	2.10	0.52
1:A:147:LEU:N	1:A:147:LEU:CD2	2.73	0.51
1:B:147:LEU:HD21	1:B:362:MET:CE	2.40	0.51
1:B:98:ARG:HG3	4:B:703:MPD:H4	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ILE:HD12	1:B:154:ILE:N	2.27	0.50
1:A:84:ARG:HG3	1:A:84:ARG:NH1	2.27	0.50
4:B:705:MPD:H31	5:B:919:HOH:O	2.12	0.49
1:A:383:ALA:O	1:A:386:VAL:HG23	2.13	0.49
1:A:435:ALA:O	1:A:439:THR:HG23	2.13	0.48
1:B:587:ALA:O	1:B:590:VAL:HG12	2.13	0.48
1:A:127:LYS:NZ	5:A:809:HOH:O	2.46	0.48
1:B:76:GLU:OE2	1:B:133:GLN:HG3	2.14	0.47
1:A:398:GLU:HA	1:A:440:TYR:CD2	2.49	0.47
1:A:147:LEU:HD11	1:A:362:MET:CE	2.45	0.47
1:A:363:MET:CE	1:A:364:ARG:H	2.28	0.46
1:B:79:LEU:HD21	1:B:88:ILE:HD13	1.97	0.46
4:B:703:MPD:C1	4:B:703:MPD:H52	2.46	0.46
1:A:147:LEU:HB3	1:A:358:PRO:O	2.17	0.45
1:A:458:GLU:HG3	5:A:814:HOH:O	2.16	0.45
1:A:159:ARG:HD2	5:A:970:HOH:O	2.18	0.43
1:A:206:TYR:CE2	1:A:231:THR:HG21	2.52	0.43
1:A:147:LEU:HD11	1:A:362:MET:HE2	2.00	0.43
1:B:159:ARG:HD2	5:B:908:HOH:O	2.18	0.43
1:B:297:GLY:HA3	1:B:330:CYS:O	2.19	0.43
1:A:386:VAL:N	1:A:387:PRO:CD	2.82	0.43
1:B:215:PRO:HD2	1:B:261:THR:O	2.19	0.43
1:A:87:LYS:HB3	1:A:87:LYS:HE2	1.77	0.42
1:B:96:THR:HA	1:B:97:HIS:HA	1.83	0.42
1:A:313:TRP:CD2	1:B:23:MET:HG2	2.55	0.42
1:A:206:TYR:OH	1:A:231:THR:HG23	2.19	0.42
1:A:297:GLY:HA3	1:A:330:CYS:O	2.20	0.42
1:A:364:ARG:HD3	1:A:368:ASN:HD21	1.84	0.41
1:A:96:THR:HA	1:A:97:HIS:HA	1.84	0.41
1:A:516:ASP:HB3	1:A:529:TRP:CZ3	2.56	0.41
1:A:453:LYS:HD2	1:A:454:ASN:N	2.35	0.41
1:B:516:ASP:HB3	1:B:529:TRP:CZ3	2.56	0.41
1:A:357:VAL:HG22	1:A:358:PRO:CD	2.51	0.41
1:B:139:ASN:CB	4:B:703:MPD:H51	2.51	0.40
1:A:411:ILE:C	1:A:411:ILE:HD12	2.41	0.40
1:A:398:GLU:HB2	1:A:440:TYR:CZ	2.57	0.40

There are no symmetry-related clashes.

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	586/627 (94%)	566 (97%)	20 (3%)	0	100	100
1	B	595/627 (95%)	575 (97%)	19 (3%)	1 (0%)	47	19
All	All	1181/1254 (94%)	1141 (97%)	39 (3%)	1 (0%)	51	20

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	374	SER

5.3.2 Protein sidechains ⓘ

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	515/546 (94%)	504 (98%)	11 (2%)	53	16
1	B	519/546 (95%)	513 (99%)	6 (1%)	71	40
All	All	1034/1092 (95%)	1017 (98%)	17 (2%)	62	28

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	16	MET
1	A	84	ARG
1	A	147	LEU
1	A	244	ARG

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Mol	Chain	Res	Type
1	A	277	ARG
1	A	367	ARG
1	A	384	LEU
1	A	453	LYS
1	A	492	PHE
1	A	563	GLN
1	B	11	GLN
1	B	16	MET
1	B	244	ARG
1	B	277	ARG
1	B	378	THR
1	B	492	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	255	GLN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

7 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	MRD	A	702	-	7,7,7	0.75	0	9,10,10	0.52	0
2	SJ5	B	701	-	11,11,11	0.58	0	11,15,15	1.68	1 (9%)
3	MRD	B	702	-	7,7,7	0.62	0	9,10,10	0.50	0
3	MRD	B	704	-	7,7,7	0.64	0	9,10,10	0.71	0
4	MPD	B	703	-	7,7,7	0.58	0	9,10,10	0.71	0
4	MPD	B	705	-	7,7,7	0.59	0	9,10,10	0.85	0
2	SJ5	A	701	-	11,11,11	0.52	0	11,15,15	1.74	1 (9%)

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
3	MRD	A	702	-	-	0/5/5/5	-
2	SJ5	B	701	-	-	2/4/18/18	0/1/1/1
3	MRD	B	702	-	-	2/5/5/5	-
3	MRD	B	704	-	-	1/5/5/5	-
4	MPD	B	703	-	-	1/5/5/5	-
4	MPD	B	705	-	-	5/5/5/5	-
2	SJ5	A	701	-	-	3/4/18/18	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	SJ5	C7-N-C2	5.28	117.50	111.70
2	B	701	SJ5	C7-N-C2	5.00	117.19	111.70

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	703	MPD	C2-C3-C4-O4
4	B	705	MPD	C1-C2-C3-C4
4	B	705	MPD	O2-C2-C3-C4
3	B	704	MRD	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	B	702	MRD	CM-C2-C3-C4
4	B	705	MPD	CM-C2-C3-C4
2	A	701	SJ5	C4-C5-C6-O61
3	B	702	MRD	O2-C2-C3-C4
2	A	701	SJ5	C4-C5-C6-O62
2	B	701	SJ5	C4-C5-C6-O62
2	B	701	SJ5	C4-C5-C6-O61
4	B	705	MPD	C2-C3-C4-C5
2	A	701	SJ5	C7-C5-C6-O62
4	B	705	MPD	C2-C3-C4-O4

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	MRD	1	0
4	B	703	MPD	3	0
4	B	705	MPD	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand SJ5 B 701

Bond lengths

Bond angles

Torsions

Rings

Ligand SJ5 A 701
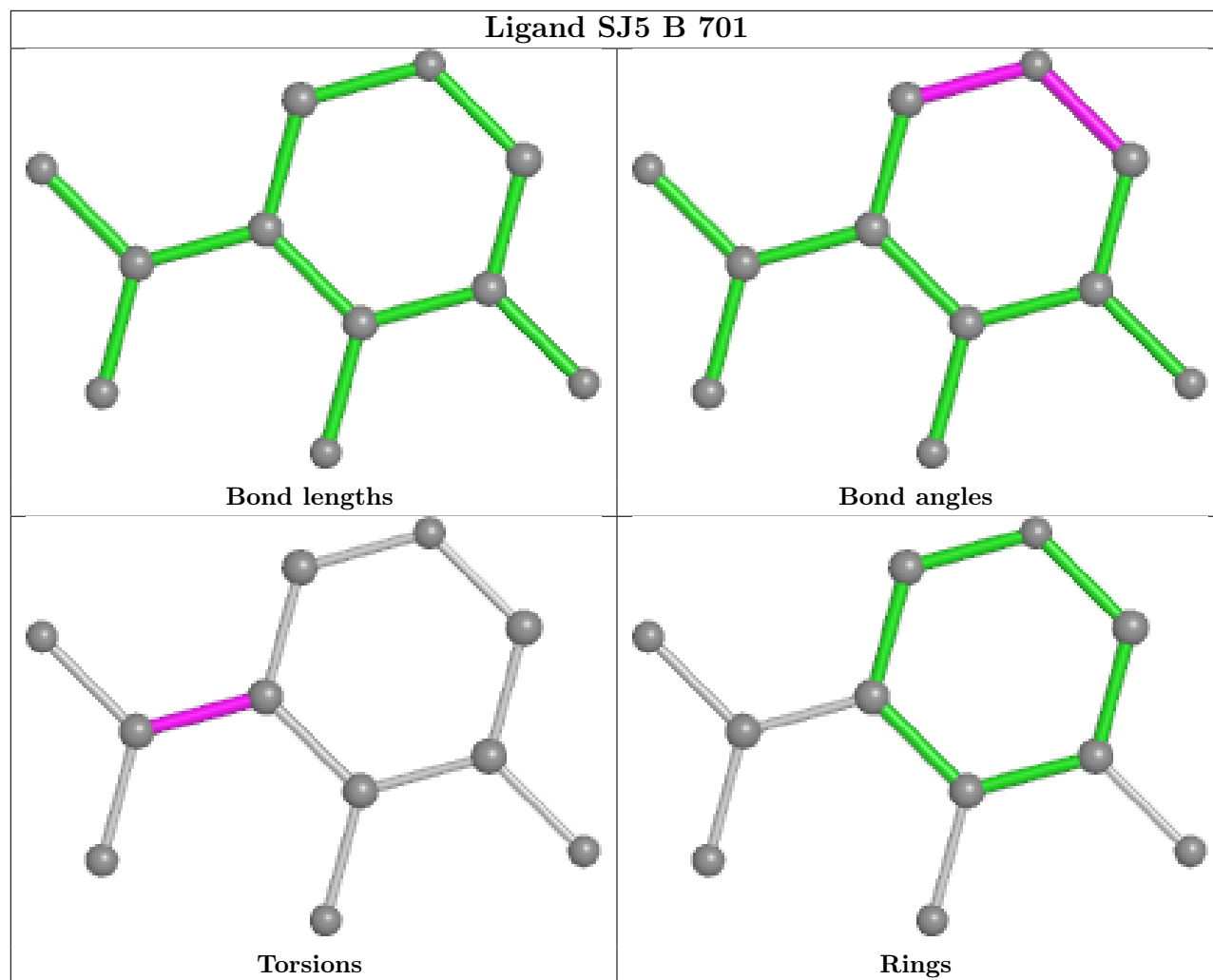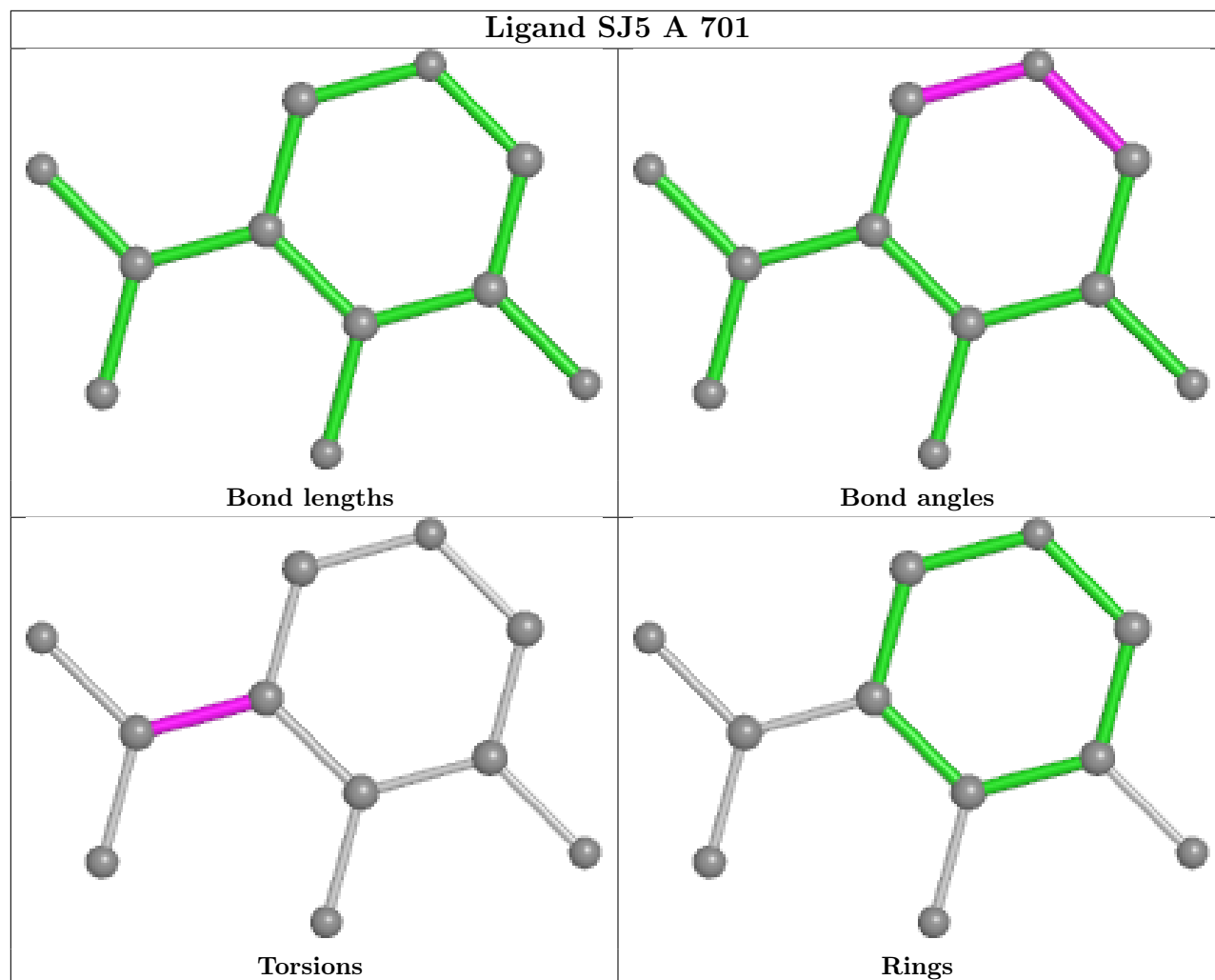
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	589/627 (93%)	0.14	33 (5%)	24	21	10, 17, 31, 68	0
1	B	596/627 (95%)	0.23	35 (5%)	22	19	11, 17, 33, 57	0
All	All	1185/1254 (94%)	0.18	68 (5%)	23	20	10, 17, 32, 68	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	374	SER	18.2
1	A	379	TYR	14.9
1	B	377	TYR	14.2
1	B	373	GLY	13.5
1	A	369	PHE	13.3
1	B	378	THR	11.6
1	B	381	PHE	11.5
1	B	379	TYR	11.4
1	B	380	PHE	11.3
1	B	372	ALA	11.2
1	B	375	GLY	11.1
1	A	264	ASN	8.6
1	A	370	VAL	8.0
1	A	425	TYR	7.8
1	A	263	GLY	7.7
1	A	368	ASN	7.6
1	A	366	THR	7.4
1	A	364	ARG	7.1
1	B	264	ASN	7.0
1	B	376	ASN	6.8
1	A	371	ALA	6.6
1	A	381	PHE	6.2
1	B	425	TYR	6.2
1	B	263	GLY	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	384	LEU	5.9
1	B	369	PHE	5.8
1	B	156	ASN	5.8
1	A	365	SER	5.6
1	B	85	ASN	5.6
1	B	383	ALA	5.3
1	A	322	CYS	5.2
1	A	380	PHE	5.2
1	A	262	ASP	5.0
1	B	371	ALA	4.6
1	B	84	ARG	4.6
1	A	363	MET	4.6
1	B	157	ASN	4.5
1	A	382	GLU	4.3
1	A	156	ASN	4.3
1	A	157	ASN	4.2
1	A	384	LEU	4.1
1	A	367	ARG	3.9
1	B	3	GLU	3.8
1	A	85	ASN	3.8
1	B	470	CYS	3.7
1	B	370	VAL	3.6
1	B	440	TYR	3.4
1	A	200	THR	3.3
1	A	3	GLU	3.2
1	A	198	CYS	3.1
1	B	382	GLU	2.8
1	B	224	GLU	2.7
1	B	200	THR	2.7
1	A	84	ARG	2.6
1	A	265	GLY	2.6
1	B	518	MET	2.5
1	A	424	ASP	2.5
1	A	383	ALA	2.4
1	B	213	GLU	2.3
1	B	232	GLU	2.3
1	A	362	MET	2.3
1	B	262	ASP	2.2
1	A	185	GLU	2.1
1	A	224	GLU	2.1
1	B	2	LEU	2.1
1	A	235	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	199	GLY	2.0
1	B	368	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.

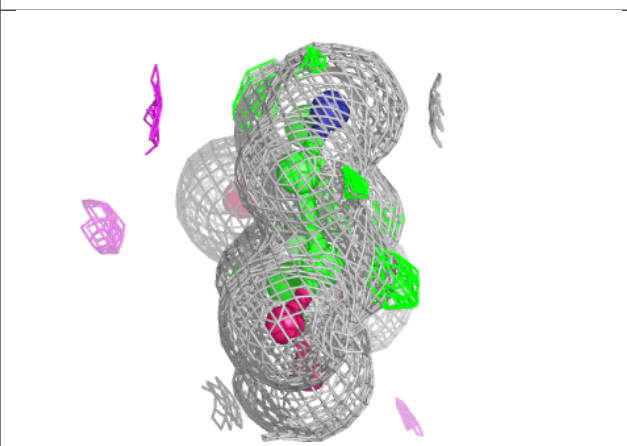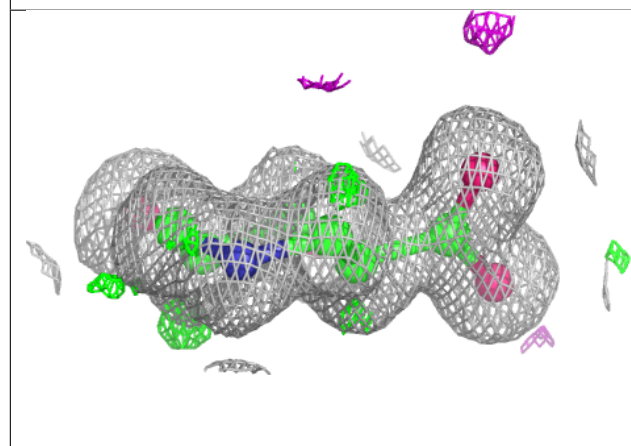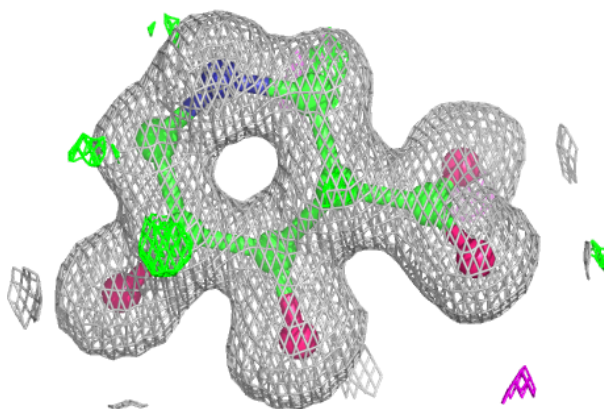| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MRD	A	702	8/8	0.68	0.26	31,35,41,54	0
4	MPD	B	705	8/8	0.74	0.24	28,37,45,46	0
3	MRD	B	702	8/8	0.79	0.14	25,32,35,40	0
4	MPD	B	703	8/8	0.81	0.15	23,31,37,40	0
3	MRD	B	704	8/8	0.86	0.11	24,28,40,43	0
2	SJ5	B	701	11/11	0.98	0.07	10,11,12,12	0
2	SJ5	A	701	11/11	0.98	0.07	11,12,13,13	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 SJ5 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)
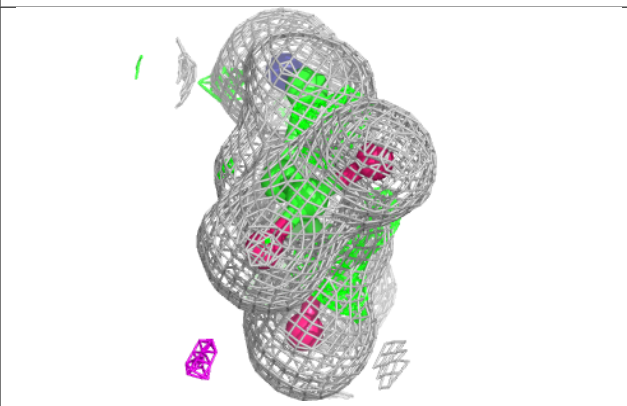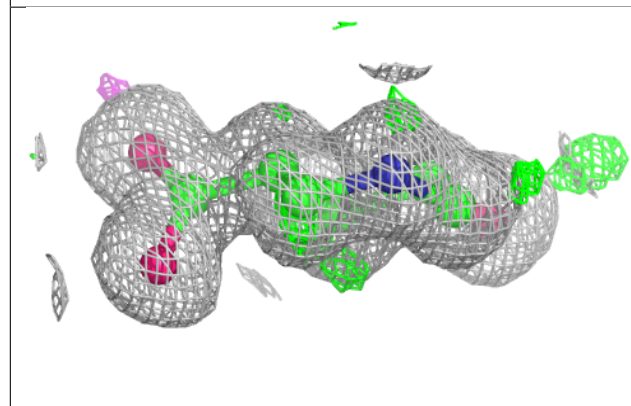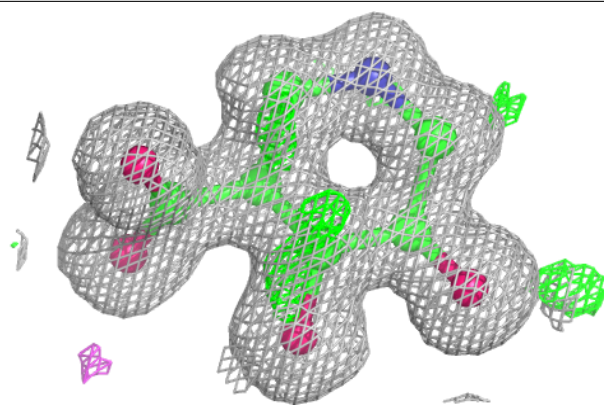
Electron density around SJ5 A 701:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.