



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 01:20 PM UTC

PDB ID : 6JTU / pdb_00006jtu
Title : Crystal structure of MHETase from Ideonella sakaiensis
Authors : Sagong, H.-Y.; Seo, H.; Kim, K.-J.
Deposited on : 2019-04-12
Resolution : 2.10 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

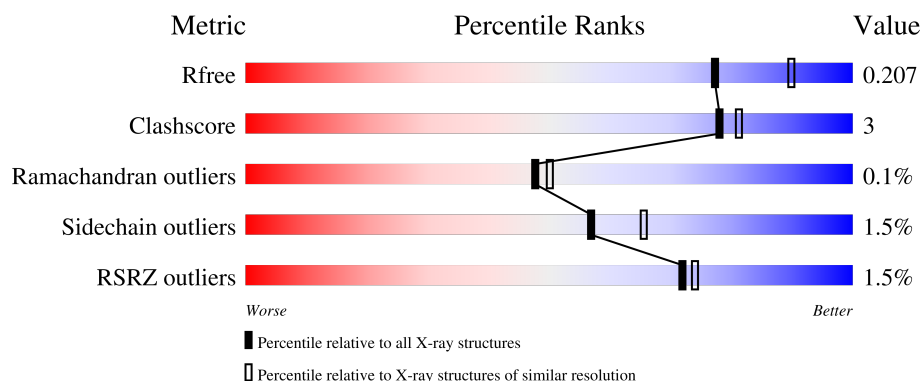
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	613	
1	B	613	
1	C	613	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13224 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 Mono(2-hydroxyethyl) terephthalate hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	561	Total	C	N	O	S	0	0	0
			4140	2592	728	792	28			
1	B	561	Total	C	N	O	S	0	0	0
			4140	2592	728	792	28			
1	C	561	Total	C	N	O	S	0	0	0
			4140	2592	728	792	28			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP A0A0K8P8E7
A	-8	MET	-	expression tag	UNP A0A0K8P8E7
A	-7	ILE	-	expression tag	UNP A0A0K8P8E7
A	-6	THR	-	expression tag	UNP A0A0K8P8E7
A	-5	LEU	-	expression tag	UNP A0A0K8P8E7
A	-4	ARG	-	expression tag	UNP A0A0K8P8E7
A	-3	LYS	-	expression tag	UNP A0A0K8P8E7
A	-2	LEU	-	expression tag	UNP A0A0K8P8E7
A	-1	PRO	-	expression tag	UNP A0A0K8P8E7
A	0	LEU	-	expression tag	UNP A0A0K8P8E7
A	1	ALA	-	expression tag	UNP A0A0K8P8E7
A	2	VAL	-	expression tag	UNP A0A0K8P8E7
A	3	ALA	-	expression tag	UNP A0A0K8P8E7
A	4	VAL	-	expression tag	UNP A0A0K8P8E7
A	5	ALA	-	expression tag	UNP A0A0K8P8E7
A	6	ALA	-	expression tag	UNP A0A0K8P8E7
A	7	GLY	-	expression tag	UNP A0A0K8P8E7
A	8	VAL	-	expression tag	UNP A0A0K8P8E7
A	9	MET	-	expression tag	UNP A0A0K8P8E7
A	10	SER	-	expression tag	UNP A0A0K8P8E7
A	11	ALA	-	expression tag	UNP A0A0K8P8E7
A	12	GLN	-	expression tag	UNP A0A0K8P8E7
A	13	ALA	-	expression tag	UNP A0A0K8P8E7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	14	MET	-	expression tag	UNP A0A0K8P8E7
A	15	ALA	-	expression tag	UNP A0A0K8P8E7
A	16	MET	-	expression tag	UNP A0A0K8P8E7
B	-9	MET	-	initiating methionine	UNP A0A0K8P8E7
B	-8	MET	-	expression tag	UNP A0A0K8P8E7
B	-7	ILE	-	expression tag	UNP A0A0K8P8E7
B	-6	THR	-	expression tag	UNP A0A0K8P8E7
B	-5	LEU	-	expression tag	UNP A0A0K8P8E7
B	-4	ARG	-	expression tag	UNP A0A0K8P8E7
B	-3	LYS	-	expression tag	UNP A0A0K8P8E7
B	-2	LEU	-	expression tag	UNP A0A0K8P8E7
B	-1	PRO	-	expression tag	UNP A0A0K8P8E7
B	0	LEU	-	expression tag	UNP A0A0K8P8E7
B	1	ALA	-	expression tag	UNP A0A0K8P8E7
B	2	VAL	-	expression tag	UNP A0A0K8P8E7
B	3	ALA	-	expression tag	UNP A0A0K8P8E7
B	4	VAL	-	expression tag	UNP A0A0K8P8E7
B	5	ALA	-	expression tag	UNP A0A0K8P8E7
B	6	ALA	-	expression tag	UNP A0A0K8P8E7
B	7	GLY	-	expression tag	UNP A0A0K8P8E7
B	8	VAL	-	expression tag	UNP A0A0K8P8E7
B	9	MET	-	expression tag	UNP A0A0K8P8E7
B	10	SER	-	expression tag	UNP A0A0K8P8E7
B	11	ALA	-	expression tag	UNP A0A0K8P8E7
B	12	GLN	-	expression tag	UNP A0A0K8P8E7
B	13	ALA	-	expression tag	UNP A0A0K8P8E7
B	14	MET	-	expression tag	UNP A0A0K8P8E7
B	15	ALA	-	expression tag	UNP A0A0K8P8E7
B	16	MET	-	expression tag	UNP A0A0K8P8E7
C	-9	MET	-	initiating methionine	UNP A0A0K8P8E7
C	-8	MET	-	expression tag	UNP A0A0K8P8E7
C	-7	ILE	-	expression tag	UNP A0A0K8P8E7
C	-6	THR	-	expression tag	UNP A0A0K8P8E7
C	-5	LEU	-	expression tag	UNP A0A0K8P8E7
C	-4	ARG	-	expression tag	UNP A0A0K8P8E7
C	-3	LYS	-	expression tag	UNP A0A0K8P8E7
C	-2	LEU	-	expression tag	UNP A0A0K8P8E7
C	-1	PRO	-	expression tag	UNP A0A0K8P8E7
C	0	LEU	-	expression tag	UNP A0A0K8P8E7
C	1	ALA	-	expression tag	UNP A0A0K8P8E7
C	2	VAL	-	expression tag	UNP A0A0K8P8E7
C	3	ALA	-	expression tag	UNP A0A0K8P8E7

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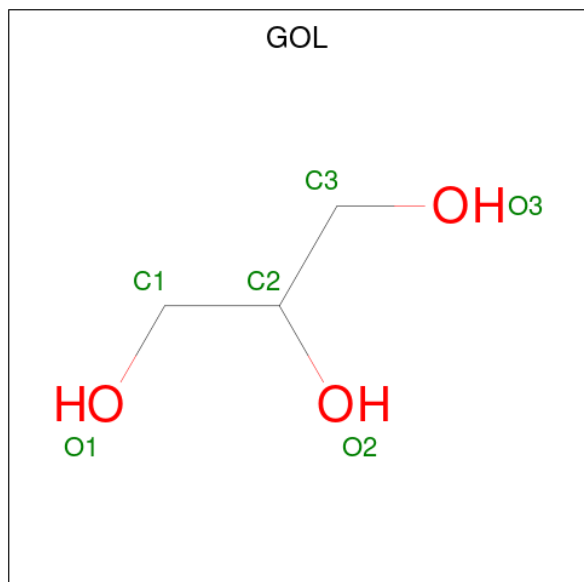
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Chain	Residue	Modelled	Actual	Comment	Reference
C	4	VAL	-	expression tag	UNP A0A0K8P8E7
C	5	ALA	-	expression tag	UNP A0A0K8P8E7
C	6	ALA	-	expression tag	UNP A0A0K8P8E7
C	7	GLY	-	expression tag	UNP A0A0K8P8E7
C	8	VAL	-	expression tag	UNP A0A0K8P8E7
C	9	MET	-	expression tag	UNP A0A0K8P8E7
C	10	SER	-	expression tag	UNP A0A0K8P8E7
C	11	ALA	-	expression tag	UNP A0A0K8P8E7
C	12	GLN	-	expression tag	UNP A0A0K8P8E7
C	13	ALA	-	expression tag	UNP A0A0K8P8E7
C	14	MET	-	expression tag	UNP A0A0K8P8E7
C	15	ALA	-	expression tag	UNP A0A0K8P8E7
C	16	MET	-	expression tag	UNP A0A0K8P8E7

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

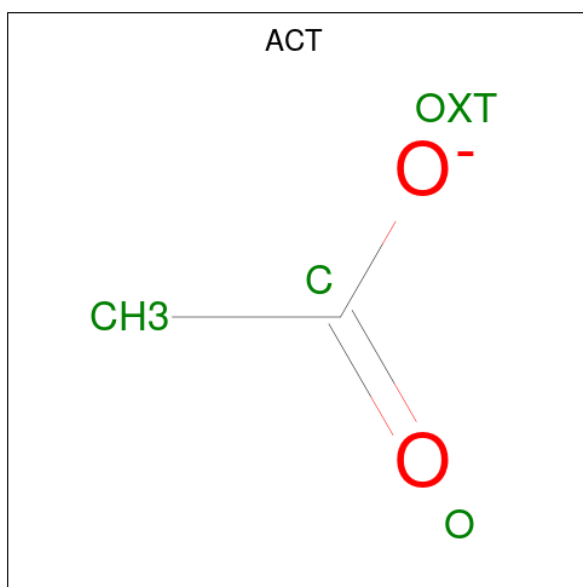
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



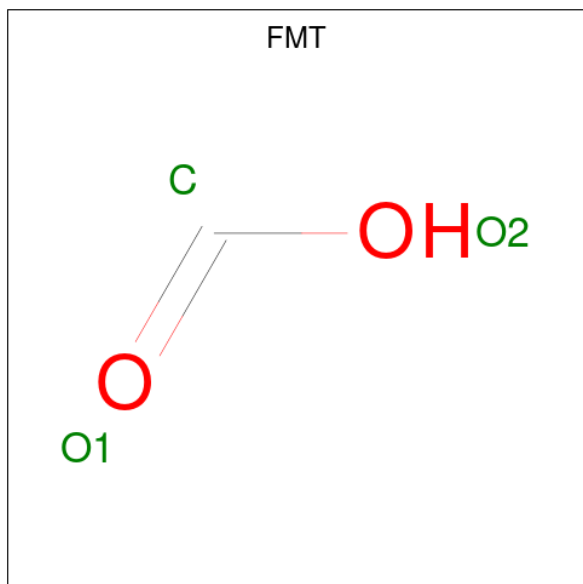
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

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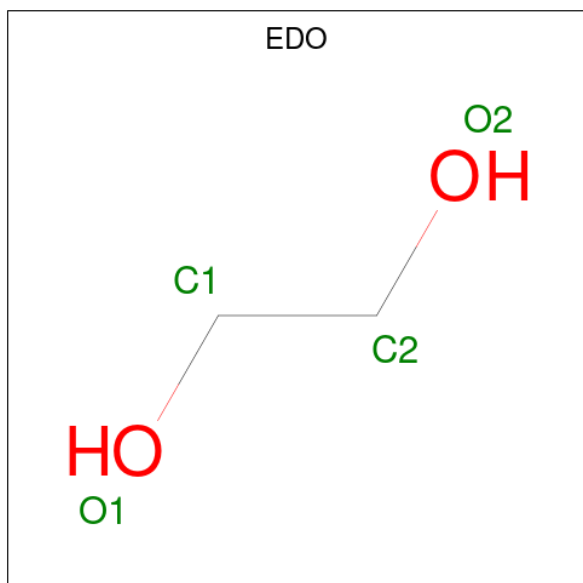
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	1	2		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).

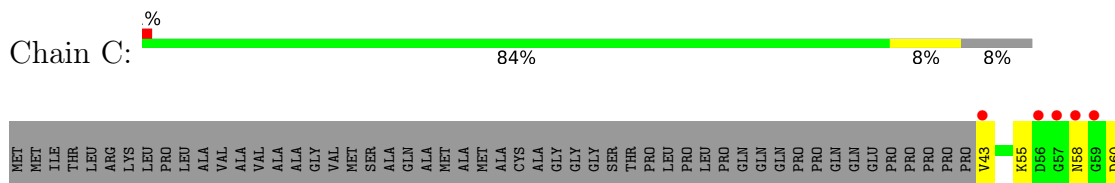


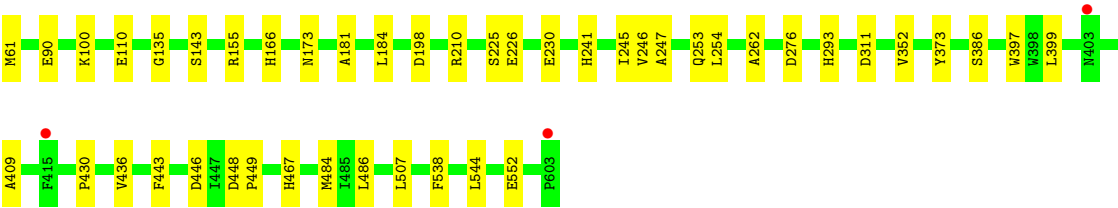
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	205	Total 205	O 205	0	0
7	B	260	Total 260	O 260	0	0
7	C	253	Total 253	O 253	0	0

- Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	214.93Å 173.16Å 107.22Å 90.00° 119.86° 90.00°	Depositor
Resolution (Å)	33.21 – 2.10 33.21 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.6 (33.21-2.10) 97.6 (33.21-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.79 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.171 , 0.198 0.182 , 0.207	Depositor DCC
R_{free} test set	9652 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 32.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13224	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: EDO, FMT, CA, GOL, ACT

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	1.17	4/4248 (0.1%)	1.37	14/5785 (0.2%)
1	B	1.16	4/4248 (0.1%)	1.34	5/5785 (0.1%)
1	C	1.17	4/4248 (0.1%)	1.34	7/5785 (0.1%)
All	All	1.16	12/12744 (0.1%)	1.35	26/17355 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	130	GLY	C-O	7.41	1.30	1.24
1	C	538	PHE	C-O	6.13	1.31	1.23
1	B	582	ILE	C-O	5.72	1.29	1.23
1	B	575	PRO	C-O	-5.64	1.17	1.23
1	C	397	TRP	C-O	5.45	1.30	1.24
1	A	294	LEU	C-O	5.25	1.30	1.24
1	B	236	GLN	C-O	-5.21	1.17	1.23
1	A	581	GLN	C-O	5.18	1.30	1.23
1	C	446	ASP	C-O	-5.17	1.17	1.24
1	B	566	TYR	C-O	-5.05	1.17	1.24
1	C	430	PRO	C-O	-5.01	1.18	1.23
1	A	64	PRO	C-O	-5.00	1.17	1.24

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	ASP	CA-CB-CG	7.41	120.01	112.60
1	A	593	THR	CA-CB-OG1	-6.59	99.72	109.60
1	B	465	ASP	CA-CB-CG	6.48	119.08	112.60
1	A	388	THR	CA-CB-OG1	-6.23	100.25	109.60
1	A	389	THR	CA-CB-OG1	-6.15	100.38	109.60
1	A	465	ASP	CA-CB-CG	6.05	118.65	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	388	THR	CA-CB-CG2	5.67	120.15	110.50
1	B	455	THR	CA-CB-OG1	-5.67	101.09	109.60
1	C	276	ASP	CA-CB-CG	5.57	118.17	112.60
1	B	593	THR	CA-CB-OG1	-5.54	101.28	109.60
1	A	535	THR	CA-C-O	-5.51	116.04	122.37
1	C	443	PHE	CA-CB-CG	5.50	119.30	113.80
1	A	589	GLY	CA-C-O	-5.44	118.53	122.45
1	A	500	THR	N-CA-C	-5.42	105.45	111.36
1	A	455	THR	CA-CB-OG1	-5.17	101.84	109.60
1	C	436	VAL	CA-C-O	-5.11	115.76	121.17
1	C	262	ALA	N-CA-C	-5.10	105.72	111.28
1	A	414	GLY	CA-C-N	5.09	127.10	120.28
1	A	414	GLY	C-N-CA	5.09	127.10	120.28
1	B	359	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	B	167	ASP	CB-CA-C	5.07	118.24	110.14
1	C	90	GLU	CA-C-O	-5.05	115.59	121.15
1	C	507	LEU	CA-C-N	5.04	125.57	119.98
1	C	507	LEU	C-N-CA	5.04	125.57	119.98
1	A	121	TRP	CA-C-O	-5.02	115.39	120.71
1	A	272	ALA	CA-C-O	-5.01	116.10	121.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4140	0	3931	23	0
1	B	4140	0	3929	19	0
1	C	4140	0	3929	23	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	6	0	8	0	0
3	B	36	0	48	2	0
3	C	18	0	24	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	4	0	3	0	0
4	B	4	0	3	0	0
4	C	4	0	3	0	0
5	A	3	0	1	1	0
6	A	8	0	12	0	0
7	A	205	0	0	0	0
7	B	260	0	0	2	0
7	C	253	0	0	5	0
All	All	13224	0	11891	64	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 3.

All (64) 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:C:253:GLN:HE22	3:C:704:GOL:H2	1.50	0.77
1:B:321:GLN:HE22	1:B:378:TRP:H	1.33	0.76
1:A:51:CYS:HG	1:A:92:CYS:HG	0.81	0.73
1:C:373:TYR:O	3:C:704:GOL:H11	1.90	0.71
1:A:60:ASP:HB2	1:A:210:ARG:HH12	1.55	0.70
1:C:166:HIS:HE1	7:C:863:HOH:O	1.81	0.63
1:A:56:ASP:HB2	1:A:59:GLY:H	1.64	0.63
1:C:60:ASP:OD1	1:C:210:ARG:NH2	2.32	0.62
1:B:166:HIS:HD2	7:B:925:HOH:O	1.85	0.58
1:A:246:VAL:HG23	1:A:544:LEU:HD22	1.87	0.57
1:C:247:ALA:HB3	1:C:486:LEU:HD23	1.88	0.55
1:A:60:ASP:HB3	1:A:210:ARG:HH22	1.71	0.55
1:B:166:HIS:HE1	7:B:851:HOH:O	1.88	0.55
1:A:198:ASP:OD1	1:A:241:HIS:HE1	1.90	0.54
1:C:135:GLY:HA2	1:C:166:HIS:O	2.07	0.54
1:C:155:ARG:NH2	7:C:801:HOH:O	2.35	0.54
1:B:84:SER:O	1:B:149:ILE:HG13	2.08	0.54
1:C:246:VAL:HG23	1:C:544:LEU:HD22	1.90	0.53
1:A:108:PRO:HG2	1:A:170:VAL:HG11	1.90	0.53
1:B:246:VAL:HG23	1:B:544:LEU:HD22	1.90	0.52
1:B:254:LEU:HD13	1:B:495:PHE:CE1	2.44	0.52
1:A:294:LEU:HD11	1:A:331:ASN:ND2	2.25	0.51
1:A:331:ASN:C	1:A:331:ASN:OD1	2.53	0.51
1:A:60:ASP:CB	1:A:210:ARG:HH12	2.22	0.51
1:A:411:ARG:HH21	5:A:704:FMT:H	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:VAL:HG23	7:C:1007:HOH:O	2.10	0.50
1:B:198:ASP:OD1	1:B:241:HIS:HE1	1.95	0.50
1:A:484:MET:HE3	1:A:486:LEU:HD11	1.95	0.49
1:C:166:HIS:HD2	7:C:945:HOH:O	1.94	0.49
1:C:253:GLN:NE2	3:C:704:GOL:H2	2.24	0.48
1:C:143:SER:HA	3:C:702:GOL:H2	1.94	0.47
1:B:143:SER:HA	3:B:703:GOL:H2	1.97	0.47
1:C:226:GLU:OE2	1:C:230:GLU:OE1	2.32	0.47
1:A:528:HIS:O	1:A:529:CYS:HB2	2.15	0.46
1:C:293:HIS:HD2	7:C:1029:HOH:O	1.98	0.46
1:B:64:PRO:HA	3:B:705:GOL:H11	1.96	0.46
1:A:299:ILE:O	1:A:303:CYS:HB2	2.16	0.45
1:C:173:ASN:HB3	1:C:181:ALA:CB	2.46	0.45
1:B:254:LEU:HD13	1:B:495:PHE:HE1	1.80	0.45
1:A:173:ASN:HB3	1:A:181:ALA:CB	2.47	0.45
1:C:245:ILE:O	1:C:484:MET:HA	2.17	0.45
1:B:341:VAL:HG12	1:C:311:ASP:HA	2.00	0.44
1:B:418:ARG:HD3	1:B:433:MET:CE	2.48	0.44
1:A:108:PRO:HG2	1:A:170:VAL:CG1	2.48	0.44
1:B:366:ASN:HB2	1:B:446:ASP:OD1	2.18	0.44
1:B:253:GLN:HE22	1:B:256:LYS:NZ	2.15	0.44
1:A:399:LEU:C	1:A:409:ALA:HB2	2.43	0.43
1:B:60:ASP:OD1	1:B:210:ARG:NH2	2.49	0.43
1:A:263:TRP:CD2	1:A:364:PRO:HA	2.53	0.43
1:A:263:TRP:HB2	1:A:364:PRO:HB3	2.01	0.43
1:C:61:MET:HA	1:C:210:ARG:NH1	2.33	0.43
1:A:448:ASP:N	1:A:449:PRO:CD	2.82	0.43
1:C:100:LYS:HD2	1:C:110:GLU:OE1	2.19	0.42
1:A:535:THR:HG21	1:A:574:ARG:HB2	2.01	0.42
1:B:177:LEU:HA	1:B:433:MET:HE3	2.02	0.41
1:B:251:GLY:O	1:B:254:LEU:HB2	2.21	0.41
1:A:484:MET:O	1:A:518:ALA:HA	2.20	0.41
1:B:487:TYR:HA	1:B:521:PHE:O	2.20	0.41
1:C:198:ASP:OD1	1:C:241:HIS:HE1	2.03	0.41
1:C:448:ASP:N	1:C:449:PRO:CD	2.83	0.41
1:A:339:GLN:HE21	1:A:354:VAL:HB	1.86	0.41
1:C:399:LEU:C	1:C:409:ALA:HB2	2.46	0.41
1:C:55:LYS:O	1:C:58:ASN:HB2	2.21	0.41
1:B:198:ASP:OD1	1:B:241:HIS:CE1	2.74	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	559/613 (91%)	540 (97%)	18 (3%)	1 (0%)	43	44
1	B	559/613 (91%)	540 (97%)	19 (3%)	0	100	100
1	C	559/613 (91%)	540 (97%)	18 (3%)	1 (0%)	43	44
All	All	1677/1839 (91%)	1620 (97%)	55 (3%)	2 (0%)	48	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	225	SER
1	A	225	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	407/446 (91%)	402 (99%)	5 (1%)	63	72
1	B	407/446 (91%)	400 (98%)	7 (2%)	53	62
1	C	407/446 (91%)	401 (98%)	6 (2%)	57	65
All	All	1221/1338 (91%)	1203 (98%)	18 (2%)	57	65

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

Mol	Chain	Res	Type
1	A	58	ASN

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Mol	Chain	Res	Type
1	A	254	LEU
1	A	388	THR
1	A	433	MET
1	A	467	HIS
1	B	43	VAL
1	B	131	SER
1	B	254	LEU
1	B	336	GLN
1	B	401	SER
1	B	450	LEU
1	B	467	HIS
1	C	43	VAL
1	C	184	LEU
1	C	254	LEU
1	C	386	SER
1	C	467	HIS
1	C	552	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	202	GLN
1	A	241	HIS
1	A	278	GLN
1	A	339	GLN
1	A	435	GLN
1	B	156	ASN
1	B	166	HIS
1	B	241	HIS
1	B	253	GLN
1	B	297	GLN
1	B	321	GLN
1	B	461	GLN
1	C	156	ASN
1	C	166	HIS
1	C	241	HIS
1	C	293	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 3 are monoatomic - leaving 16 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	$\# Z > 2$
3	GOL	B	706	-	5,5,5	0.08	0	5,5,5	0.24	0
3	GOL	C	704	-	5,5,5	0.25	0	5,5,5	0.84	0
3	GOL	C	702	-	5,5,5	0.10	0	5,5,5	0.62	0
6	EDO	A	705	-	3,3,3	0.20	0	2,2,2	0.16	0
6	EDO	A	706	-	3,3,3	0.42	0	2,2,2	0.39	0
3	GOL	A	702	-	5,5,5	0.26	0	5,5,5	0.52	0
3	GOL	B	703	-	5,5,5	0.31	0	5,5,5	0.72	0
3	GOL	C	703	-	5,5,5	0.49	0	5,5,5	1.34	1 (20%)
3	GOL	B	704	-	5,5,5	0.28	0	5,5,5	0.53	0
4	ACT	A	703	-	3,3,3	1.37	1 (33%)	3,3,3	1.51	0
4	ACT	C	705	-	3,3,3	1.58	0	3,3,3	0.22	0
5	FMT	A	704	-	2,2,2	0.63	0	1,1,1	0.26	0
3	GOL	B	707	-	5,5,5	0.30	0	5,5,5	0.60	0
4	ACT	B	708	-	3,3,3	1.70	0	3,3,3	0.35	0
3	GOL	B	705	-	5,5,5	0.25	0	5,5,5	0.59	0
3	GOL	B	702	-	5,5,5	0.23	0	5,5,5	0.91	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
3	GOL	B	706	-	-	0/4/4/4	-
3	GOL	C	704	-	-	4/4/4/4	-
3	GOL	C	702	-	-	2/4/4/4	-
6	EDO	A	705	-	-	1/1/1/1	-
6	EDO	A	706	-	-	0/1/1/1	-
3	GOL	A	702	-	-	0/4/4/4	-
3	GOL	B	703	-	-	2/4/4/4	-
3	GOL	C	703	-	-	2/4/4/4	-
3	GOL	B	704	-	-	0/4/4/4	-
3	GOL	B	707	-	-	2/4/4/4	-
3	GOL	B	705	-	-	2/4/4/4	-
3	GOL	B	702	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	ACT	CH3-C	2.03	1.57	1.49

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	703	GOL	C3-C2-C1	2.43	120.71	111.80

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	702	GOL	O1-C1-C2-C3
3	B	707	GOL	O1-C1-C2-C3
3	C	702	GOL	O1-C1-C2-C3
3	C	703	GOL	O1-C1-C2-C3
3	C	704	GOL	O1-C1-C2-C3
3	C	704	GOL	C1-C2-C3-O3
3	C	702	GOL	O1-C1-C2-O2
3	C	703	GOL	O1-C1-C2-O2
3	B	703	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	B	702	GOL	O1-C1-C2-O2
3	B	703	GOL	O2-C2-C3-O3
3	B	707	GOL	O1-C1-C2-O2
3	C	704	GOL	O2-C2-C3-O3
3	C	704	GOL	O1-C1-C2-O2
3	B	705	GOL	O1-C1-C2-C3
6	A	705	EDO	O1-C1-C2-O2
3	B	705	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	704	GOL	3	0
3	C	702	GOL	1	0
3	B	703	GOL	1	0
5	A	704	FMT	1	0
3	B	705	GOL	1	0

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	561/613 (91%)	-0.10	9 (1%) 70 73	22, 32, 47, 92	0
1	B	561/613 (91%)	-0.29	8 (1%) 73 75	22, 28, 43, 85	0
1	C	561/613 (91%)	-0.28	8 (1%) 73 75	23, 29, 42, 89	0
All	All	1683/1839 (91%)	-0.22	25 (1%) 72 74	22, 30, 46, 92	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	57	GLY	3.6
1	C	603	PRO	3.4
1	C	57	GLY	3.4
1	B	43	VAL	3.3
1	B	59	GLY	3.1
1	C	59	GLY	3.0
1	A	43	VAL	2.9
1	C	43	VAL	2.8
1	B	56	ASP	2.7
1	A	56	ASP	2.7
1	C	56	ASP	2.6
1	A	388	THR	2.6
1	B	603	PRO	2.5
1	C	58	ASN	2.5
1	A	415	PHE	2.5
1	A	442	LYS	2.4
1	A	57	GLY	2.4
1	B	60	ASP	2.4
1	A	58	ASN	2.3
1	A	59	GLY	2.3
1	C	403	ASN	2.3
1	A	603	PRO	2.3
1	B	58	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	149	ILE	2.1
1	C	415	PHE	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 oligosaccharides 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.

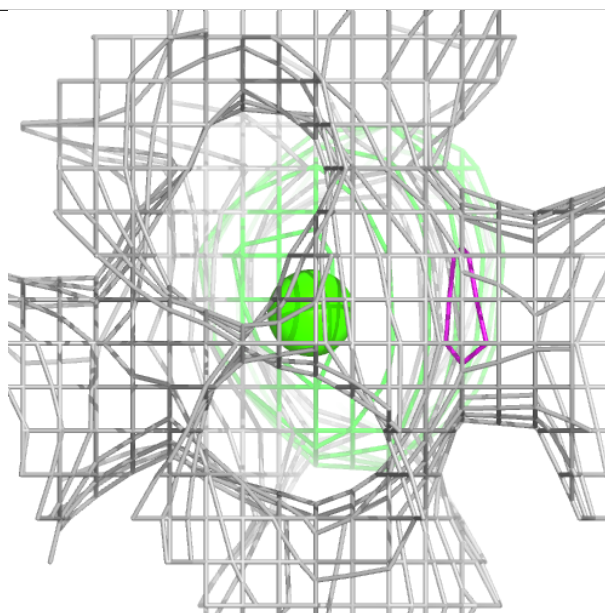
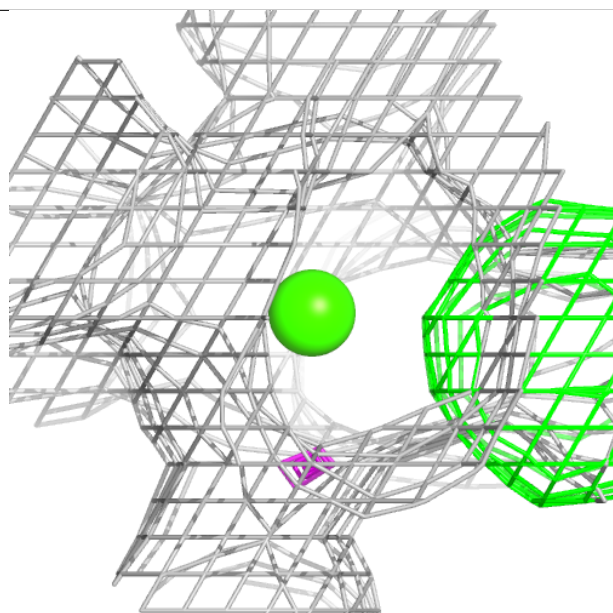
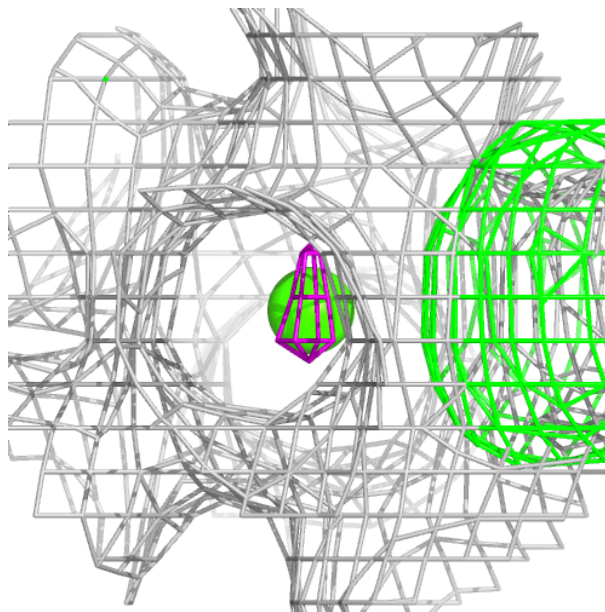
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	C	704	6/6	0.84	0.17	40,52,56,65	0
4	ACT	B	708	4/4	0.84	0.20	36,44,44,51	0
4	ACT	C	705	4/4	0.84	0.18	42,42,43,44	0
4	ACT	A	703	4/4	0.85	0.19	41,43,44,55	0
5	FMT	A	704	3/3	0.87	0.15	41,41,43,44	0
3	GOL	B	705	6/6	0.89	0.15	49,55,58,61	0
3	GOL	B	702	6/6	0.91	0.11	30,35,38,39	0
3	GOL	B	703	6/6	0.91	0.14	36,42,53,57	0
3	GOL	C	702	6/6	0.92	0.14	30,45,48,52	0
3	GOL	B	707	6/6	0.92	0.13	52,55,60,61	0
6	EDO	A	705	4/4	0.92	0.14	42,50,51,55	0
3	GOL	C	703	6/6	0.93	0.12	34,41,47,48	0
3	GOL	B	706	6/6	0.94	0.10	41,48,51,56	0
6	EDO	A	706	4/4	0.94	0.14	36,47,51,56	0
3	GOL	A	702	6/6	0.96	0.10	34,43,47,49	0
3	GOL	B	704	6/6	0.96	0.09	33,40,42,43	0
2	CA	C	701	1/1	0.98	0.03	26,26,26,26	0
2	CA	B	701	1/1	0.99	0.03	32,32,32,32	0
2	CA	A	701	1/1	0.99	0.03	36,36,36,36	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.

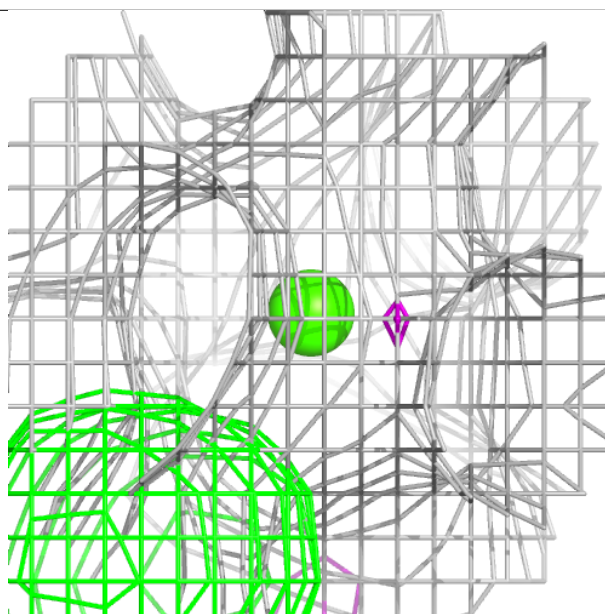
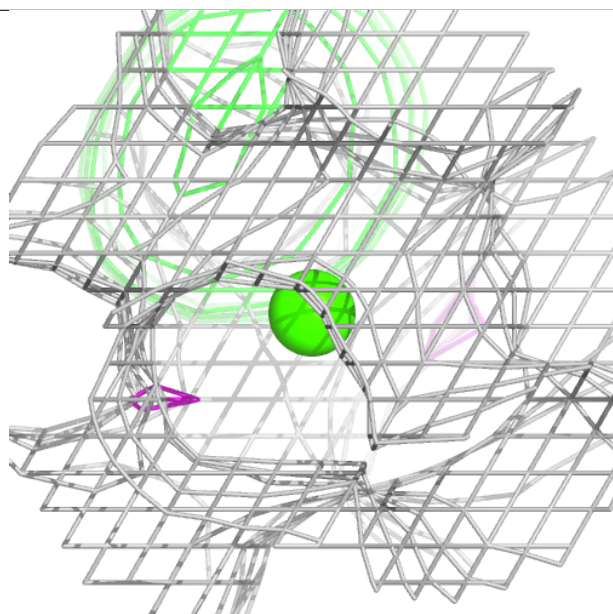
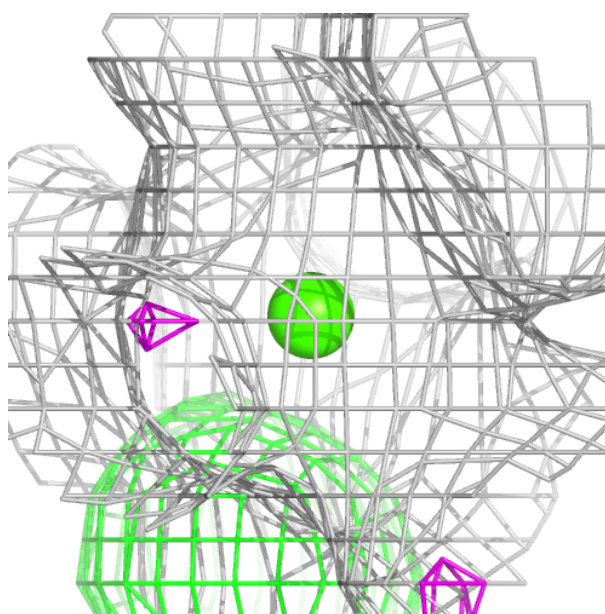
Electron density around CA C 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



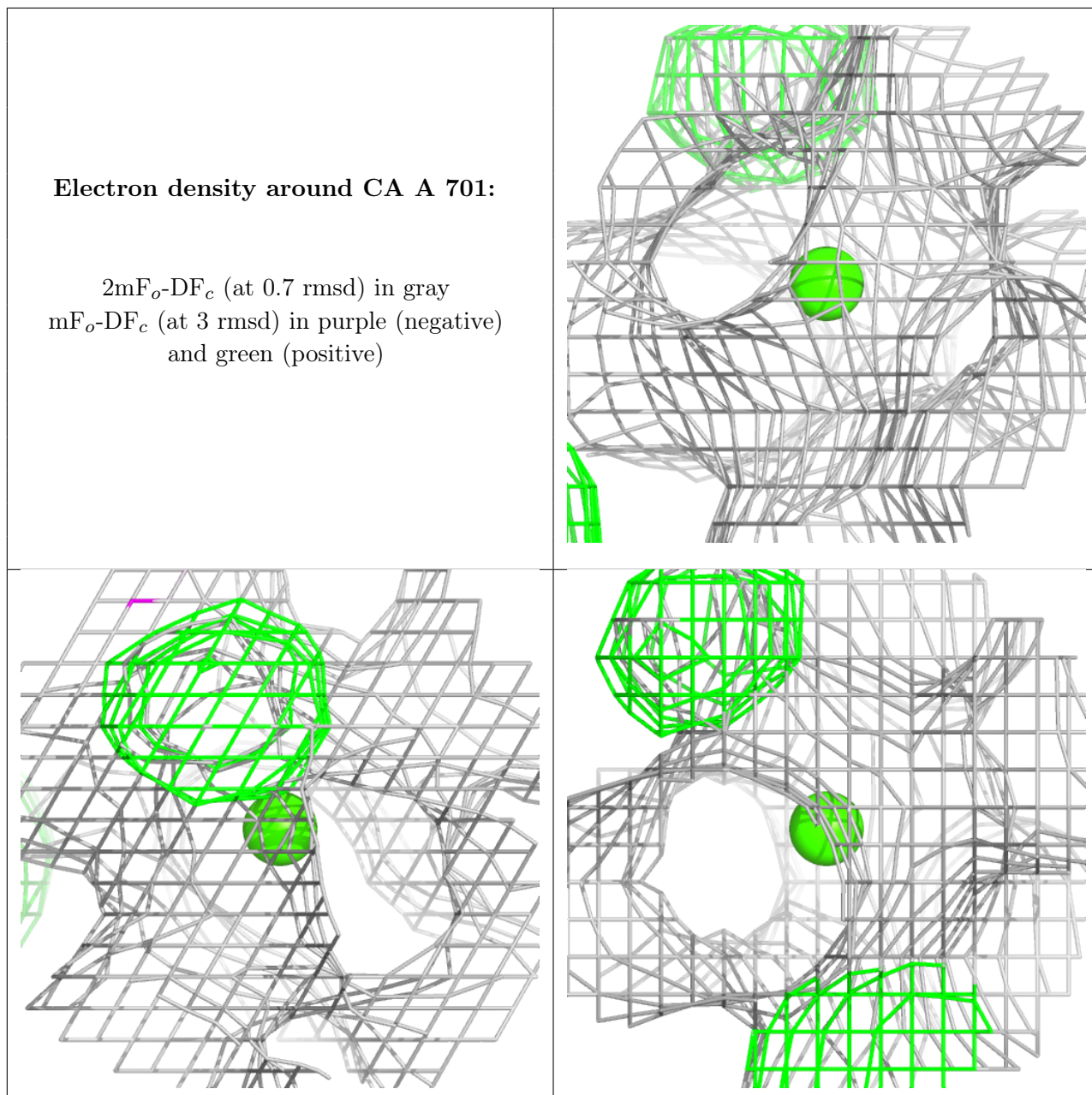
Electron density around CA B 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA 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** [i](#)

There are no such residues in this entry.