W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Nov 5, 2023 – 02:59 PM EST

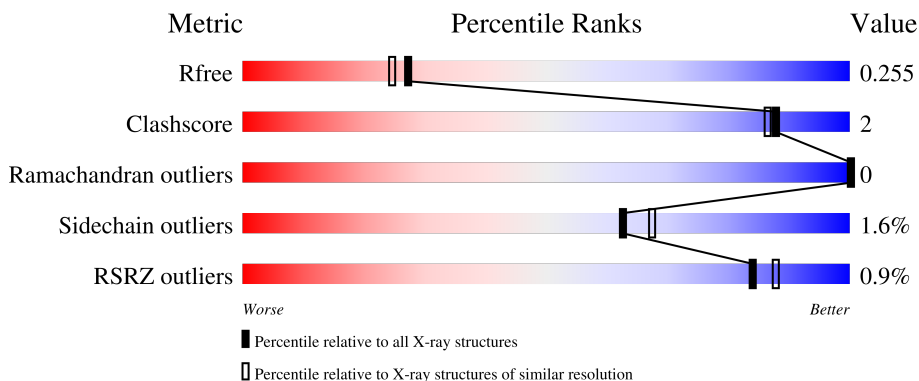|		
PDB ID	:	4WKM
Title	:	AmpR effector binding domain from Citrobacter freundii bound to UDP-Mur NAc-pentapeptide
Authors	:	Vadlamani, G.; Reeve, T.M.; Mark, B.L.
Deposited on	:	2014-10-02
Resolution	:	2.15 Å(reported)

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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 2.15 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	Percentile Ranks	Value
Rfree		0.255
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		1.6%
RSRZ outliers		0.9%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
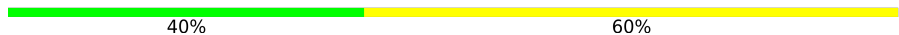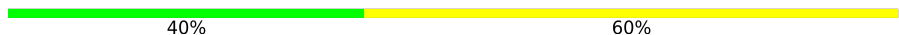
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	219	86% · 10%
1	B	219	2% 83% 7% 11%
1	C	219	83% 6% 11%
1	D	219	3% 84% 6% 11%
1	E	219	% 83% 7% 11%

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Mol	Chain	Length	Quality of chain
1	F	219	83% 7% 11%
1	G	219	85% • 11%
1	H	219	86% • 11%
2	I	5	60% 40%
2	J	5	60% 40%
2	K	5	60% 40%
2	L	5	60% 40%
2	M	5	60% 40%
2	N	5	60% 40%
2	O	5	40% 60%
2	P	5	40% 60%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 26109 atoms, of which 12401 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 LysR family transcriptional regulator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	197	Total	C	H	N	O	S	0	0	0
			3055	987	1513	264	281	10			
1	B	196	Total	C	H	N	O	S	0	0	0
			2987	975	1473	250	279	10			
1	C	196	Total	C	H	N	O	S	0	0	0
			3019	979	1494	257	279	10			
1	D	196	Total	C	H	N	O	S	0	0	0
			3018	980	1494	256	278	10			
1	E	196	Total	C	H	N	O	S	0	0	0
			3028	980	1501	260	277	10			
1	F	196	Total	C	H	N	O	S	0	0	0
			3057	987	1520	261	279	10			
1	G	196	Total	C	H	N	O	S	0	0	0
			3040	984	1509	258	279	10			
1	H	196	Total	C	H	N	O	S	0	0	0
			3036	982	1505	260	279	10			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	292	THR	-	expression tag	UNP K8QNC4
A	293	SER	-	expression tag	UNP K8QNC4
A	294	GLY	-	expression tag	UNP K8QNC4
A	295	SER	-	expression tag	UNP K8QNC4
A	296	HIS	-	expression tag	UNP K8QNC4
A	297	HIS	-	expression tag	UNP K8QNC4
A	298	HIS	-	expression tag	UNP K8QNC4
A	299	HIS	-	expression tag	UNP K8QNC4
A	300	HIS	-	expression tag	UNP K8QNC4
A	301	HIS	-	expression tag	UNP K8QNC4
B	292	THR	-	expression tag	UNP K8QNC4
B	293	SER	-	expression tag	UNP K8QNC4
B	294	GLY	-	expression tag	UNP K8QNC4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	295	SER	-	expression tag	UNP K8QNC4
B	296	HIS	-	expression tag	UNP K8QNC4
B	297	HIS	-	expression tag	UNP K8QNC4
B	298	HIS	-	expression tag	UNP K8QNC4
B	299	HIS	-	expression tag	UNP K8QNC4
B	300	HIS	-	expression tag	UNP K8QNC4
B	301	HIS	-	expression tag	UNP K8QNC4
C	292	THR	-	expression tag	UNP K8QNC4
C	293	SER	-	expression tag	UNP K8QNC4
C	294	GLY	-	expression tag	UNP K8QNC4
C	295	SER	-	expression tag	UNP K8QNC4
C	296	HIS	-	expression tag	UNP K8QNC4
C	297	HIS	-	expression tag	UNP K8QNC4
C	298	HIS	-	expression tag	UNP K8QNC4
C	299	HIS	-	expression tag	UNP K8QNC4
C	300	HIS	-	expression tag	UNP K8QNC4
C	301	HIS	-	expression tag	UNP K8QNC4
D	292	THR	-	expression tag	UNP K8QNC4
D	293	SER	-	expression tag	UNP K8QNC4
D	294	GLY	-	expression tag	UNP K8QNC4
D	295	SER	-	expression tag	UNP K8QNC4
D	296	HIS	-	expression tag	UNP K8QNC4
D	297	HIS	-	expression tag	UNP K8QNC4
D	298	HIS	-	expression tag	UNP K8QNC4
D	299	HIS	-	expression tag	UNP K8QNC4
D	300	HIS	-	expression tag	UNP K8QNC4
D	301	HIS	-	expression tag	UNP K8QNC4
E	292	THR	-	expression tag	UNP K8QNC4
E	293	SER	-	expression tag	UNP K8QNC4
E	294	GLY	-	expression tag	UNP K8QNC4
E	295	SER	-	expression tag	UNP K8QNC4
E	296	HIS	-	expression tag	UNP K8QNC4
E	297	HIS	-	expression tag	UNP K8QNC4
E	298	HIS	-	expression tag	UNP K8QNC4
E	299	HIS	-	expression tag	UNP K8QNC4
E	300	HIS	-	expression tag	UNP K8QNC4
E	301	HIS	-	expression tag	UNP K8QNC4
F	292	THR	-	expression tag	UNP K8QNC4
F	293	SER	-	expression tag	UNP K8QNC4
F	294	GLY	-	expression tag	UNP K8QNC4
F	295	SER	-	expression tag	UNP K8QNC4
F	296	HIS	-	expression tag	UNP K8QNC4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	297	HIS	-	expression tag	UNP K8QNC4
F	298	HIS	-	expression tag	UNP K8QNC4
F	299	HIS	-	expression tag	UNP K8QNC4
F	300	HIS	-	expression tag	UNP K8QNC4
F	301	HIS	-	expression tag	UNP K8QNC4
G	292	THR	-	expression tag	UNP K8QNC4
G	293	SER	-	expression tag	UNP K8QNC4
G	294	GLY	-	expression tag	UNP K8QNC4
G	295	SER	-	expression tag	UNP K8QNC4
G	296	HIS	-	expression tag	UNP K8QNC4
G	297	HIS	-	expression tag	UNP K8QNC4
G	298	HIS	-	expression tag	UNP K8QNC4
G	299	HIS	-	expression tag	UNP K8QNC4
G	300	HIS	-	expression tag	UNP K8QNC4
G	301	HIS	-	expression tag	UNP K8QNC4
H	292	THR	-	expression tag	UNP K8QNC4
H	293	SER	-	expression tag	UNP K8QNC4
H	294	GLY	-	expression tag	UNP K8QNC4
H	295	SER	-	expression tag	UNP K8QNC4
H	296	HIS	-	expression tag	UNP K8QNC4
H	297	HIS	-	expression tag	UNP K8QNC4
H	298	HIS	-	expression tag	UNP K8QNC4
H	299	HIS	-	expression tag	UNP K8QNC4
H	300	HIS	-	expression tag	UNP K8QNC4
H	301	HIS	-	expression tag	UNP K8QNC4

- Molecule 2 is a protein (with D amino acids) called ALA-FGA-API-DAL-DAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	5	Total	C	H	N	O	0	0	0
			69	21	32	6	10			
2	J	5	Total	C	H	N	O	0	0	0
			69	21	32	6	10			
2	K	5	Total	C	H	N	O	0	0	0
			69	21	32	6	10			
2	L	5	Total	C	H	N	O	0	0	0
			69	21	32	6	10			
2	M	5	Total	C	H	N	O	0	0	0
			69	21	32	6	10			
2	N	5	Total	C	H	N	O	0	0	0
			69	21	32	6	10			
2	O	5	Total	C	H	N	O	0	0	0
			69	21	32	6	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	5	Total	C	H	N	O	0	0	0
			69	21	32	6	10			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	C	1	Total	C	H	O	0	0
			14	3	8	3		
3	D	1	Total	C	H	O	0	0
			14	3	8	3		
3	E	1	Total	C	H	O	0	0
			14	3	8	3		
3	F	1	Total	C	H	O	0	0
			14	3	8	3		
3	G	1	Total	C	H	O	0	0
			14	3	8	3		
3	H	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 4 is N-acetyl-alpha-muramic acid (three-letter code: MUB) (formula: $C_{11}H_{19}NO_8$).

MUB
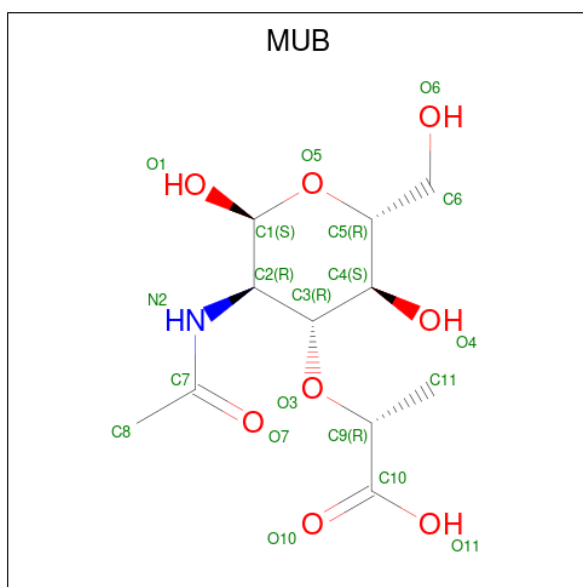
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	I	1	Total 37	C 11	H 18	N 1	O 7	0	0
4	J	1	Total 9	C 3	H 4	O 2		0	0
4	K	1	Total 37	C 11	H 18	N 1	O 7	0	0
4	L	1	Total 5	C 3	O 2			0	0
4	M	1	Total 5	C 3	O 2			0	0
4	N	1	Total 37	C 11	H 18	N 1	O 7	0	0
4	O	1	Total 9	C 3	H 4	O 2		0	0
4	P	1	Total 37	C 11	H 18	N 1	O 7	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	111	Total 111	O 111	0	0
5	B	89	Total 89	O 89	0	0
5	C	116	Total 116	O 116	0	0
5	D	113	Total 113	O 113	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	131	Total 131	O 131	0	0
5	F	144	Total 144	O 144	0	0
5	G	127	Total 127	O 127	0	0
5	H	157	Total 157	O 157	0	0
5	I	4	Total 4	O 4	0	0
5	J	6	Total 6	O 6	0	0
5	K	9	Total 9	O 9	0	0
5	L	5	Total 5	O 5	0	0
5	M	7	Total 7	O 7	0	0
5	N	10	Total 10	O 10	0	0
5	O	10	Total 10	O 10	0	0
5	P	4	Total 4	O 4	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: LysR family transcriptional regulator

Chain A:

- Molecule 1: LysR family transcriptional regulator

Chain B:

- Molecule 1: LysR family transcriptional regulator

Chain C:

- Molecule 1: LysR family transcriptional regulator

Chain D:

- Molecule 1: LysR family transcriptional regulator

Chain E:

• Molecule 1: LysR family transcriptional regulator

Chain F:

83% 7% 11%

MET LEU ASP ARG PHE ALA THR LYS GLN THR GLN **E94** K97 I98 **F110** P111 L112 L113 **D124** L125 **H126** I127 **E139** D154 **S210** V217 Q270 **P273** R283 **L289** HIS LYS THR SER GLY SER HIS HIS HIS HIS HIS HIS

• Molecule 1: LysR family transcriptional regulator

Chain G:

85% · 11%

MET LEU ASP ARG PHE ALA THR LYS GLN THR GLN **E94** K95 L113 **D124** I127 **C161** L199 R240 L261 **A277** S282 **L289** HIS LYS THR SER GLY SER HIS HIS HIS HIS HIS HIS

• Molecule 1: LysR family transcriptional regulator

Chain H:

86% · 11%

MET LEU ASP ARG PHE ALA THR LYS GLN THR GLN **E94** **F110** P111 P136 L141 L199 R279 R283 **L289** HIS LYS THR SER GLY SER HIS HIS HIS HIS HIS HIS

• Molecule 2: ALA-FGA-API-DAL-DAL

Chain I:

60% 40%

A1 E2 K3 A4 A5

• Molecule 2: ALA-FGA-API-DAL-DAL

Chain J:

60% 40%

A1 E2 K3 A4 A5

• Molecule 2: ALA-FGA-API-DAL-DAL

Chain K:

60% 40%

A1 E2 K3 A4 A5

• Molecule 2: ALA-FGA-API-DAL-DAL

Chain L:

60% 40%

A1 E2 K3 A4 A5

• Molecule 2: ALA-FGA-API-DAL-DAL

Chain M:

60% 40%

A1 E2 K3 A4 A5

• Molecule 2: ALA-FGA-API-DAL-DAL

Chain N:

60%   40%

A1 E2 K3 A4 A5

• Molecule 2: ALA-FGA-API-DAL-DAL

Chain O:

40%   60%

A1 E2 K3 A4 A5

• Molecule 2: ALA-FGA-API-DAL-DAL

Chain P:

40%   60%

A1 E2 K3 A4 A5

4　Data and refinement statistics　ⓘ

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	62.70Å　　183.60Å　　197.81Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	52.96　–　2.15 52.96　–　2.15	Depositor EDS
% Data completeness (in resolution range)	96.7 (52.96-2.15) 96.7 (52.96-2.15)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.75 (at 2.16Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9pre_1669)	Depositor
R, R_{free}	0.201　,　0.254 0.208　,　0.255	Depositor DCC
R_{free} test set	2724 reflections (2.25%)	wwPDB-VP
Wilson B-factor (Å^2)	31.4	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 47.9	EDS
L-test for twinning [2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	26109	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.50 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.8214e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DAL, GOL, FGA, MUB, API

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	0.58	0/1585	0.63	1/2164 (0.0%)
1	B	0.59	0/1557	0.66	0/2129
1	C	0.63	0/1568	0.67	0/2142
1	D	0.65	0/1567	0.69	0/2140
1	E	0.60	0/1570	0.64	0/2144
1	F	0.63	0/1580	0.69	0/2155
1	G	0.63	0/1574	0.67	0/2148
1	H	0.65	0/1574	0.70	0/2149
2	I	0.71	0/4	1.27	0/4
2	J	0.51	0/4	1.71	0/4
2	K	0.55	0/4	2.29	0/4
2	L	0.46	0/4	2.03	0/4
2	M	0.70	0/4	1.71	0/4
2	N	0.52	0/4	0.93	0/4
2	O	0.38	0/4	2.84	1/4 (25.0%)
2	P	0.45	0/4	1.30	0/4
All	All	0.62	0/12607	0.67	2/17203 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	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})
1	A	260	ASP	CB-CG-OD1	5.33	123.10	118.30
2	O	1	ALA	CB-CA-C	-5.31	102.14	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	194	ARG	Peptide

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	1542	1513	1513	4	0
1	B	1514	1473	1471	9	0
1	C	1525	1494	1494	8	0
1	D	1524	1494	1494	8	0
1	E	1527	1501	1501	6	0
1	F	1537	1520	1520	10	0
1	G	1531	1509	1509	4	0
1	H	1531	1505	1505	3	0
2	I	37	32	27	0	0
2	J	37	32	27	0	0
2	K	37	32	27	0	0
2	L	37	32	27	0	0
2	M	37	32	26	0	0
2	N	37	32	27	0	0
2	O	37	32	26	0	0
2	P	37	32	27	1	0
3	A	6	8	8	0	0
3	C	6	8	8	0	0
3	D	6	8	8	0	0
3	E	6	8	8	0	0
3	F	6	8	8	0	0
3	G	6	8	8	0	0
3	H	6	8	8	0	0
4	I	19	18	18	0	0
4	J	5	4	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	19	18	18	0	0
4	L	5	0	4	0	0
4	M	5	0	4	0	0
4	N	19	18	18	0	0
4	O	5	4	4	0	0
4	P	19	18	18	1	0
5	A	111	0	0	2	1
5	B	89	0	0	2	0
5	C	116	0	0	1	1
5	D	113	0	0	1	0
5	E	131	0	0	1	0
5	F	144	0	0	1	1
5	G	127	0	0	1	0
5	H	157	0	0	0	0
5	I	4	0	0	0	0
5	J	6	0	0	0	0
5	K	9	0	0	0	0
5	L	5	0	0	0	0
5	M	7	0	0	0	0
5	N	10	0	0	0	0
5	O	10	0	0	0	0
5	P	4	0	0	0	0
All	All	13708	12401	12365	49	2

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 2.

The worst 5 of 49 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:H:279:ARG:O	1:H:283:ARG:HG3	1.95	0.65
1:B:202:GLN:OE1	1:D:202:GLN:NE2	2.30	0.65
1:B:284:TRP:O	1:B:288:VAL:HG13	2.02	0.60
1:D:207:ALA:O	5:D:594:HOH:O	2.17	0.58
1:B:190:ARG:HD3	1:B:215:VAL:HG11	1.89	0.55

All (2) 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)
5:C:501:HOH:O	5:C:501:HOH:O[2_775]	2.09	0.11
5:A:509:HOH:O	5:F:514:HOH:O[4_577]	2.16	0.04

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	195/219 (89%)	188 (96%)	7 (4%)	0	100	100
1	B	194/219 (89%)	184 (95%)	10 (5%)	0	100	100
1	C	194/219 (89%)	187 (96%)	7 (4%)	0	100	100
1	D	194/219 (89%)	188 (97%)	6 (3%)	0	100	100
1	E	194/219 (89%)	188 (97%)	6 (3%)	0	100	100
1	F	194/219 (89%)	191 (98%)	3 (2%)	0	100	100
1	G	194/219 (89%)	189 (97%)	5 (3%)	0	100	100
1	H	194/219 (89%)	190 (98%)	4 (2%)	0	100	100
All	All	1553/1752 (89%)	1505 (97%)	48 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	167/189 (88%)	165 (99%)	2 (1%)	71	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	162/189 (86%)	159 (98%)	3 (2%)	57	61
1	C	165/189 (87%)	164 (99%)	1 (1%)	86	90
1	D	164/189 (87%)	163 (99%)	1 (1%)	86	90
1	E	165/189 (87%)	160 (97%)	5 (3%)	41	40
1	F	167/189 (88%)	163 (98%)	4 (2%)	49	51
1	G	166/189 (88%)	163 (98%)	3 (2%)	59	63
1	H	166/189 (88%)	164 (99%)	2 (1%)	71	76
All	All	1322/1512 (87%)	1301 (98%)	21 (2%)	62	67

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	210	SER
1	G	124	ASP
1	H	283	ARG
1	G	282	SER
1	G	95	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

32 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
2	FGA	N	2	2	7,8,9	1.01	0	7,9,11	1.82	3 (42%)
2	FGA	J	2	2	7,8,9	0.94	0	7,9,11	1.94	2 (28%)
2	FGA	O	2	2	7,8,9	1.11	1 (14%)	7,9,11	2.12	2 (28%)
2	API	N	3	2	9,11,12	1.18	0	7,13,15	1.16	1 (14%)
2	API	K	3	2	9,11,12	0.96	0	7,13,15	1.54	2 (28%)
2	API	L	3	2	9,11,12	1.24	1 (11%)	7,13,15	1.36	2 (28%)
2	FGA	M	2	2	7,8,9	1.12	1 (14%)	7,9,11	1.99	2 (28%)
2	FGA	K	2	2	7,8,9	1.07	1 (14%)	7,9,11	1.51	1 (14%)
2	FGA	I	2	2	7,8,9	1.12	0	7,9,11	1.64	1 (14%)
2	API	I	3	2	9,11,12	0.85	0	7,13,15	1.40	1 (14%)
2	API	J	3	2	9,11,12	1.19	1 (11%)	7,13,15	1.46	2 (28%)
2	API	O	3	2	9,11,12	1.34	1 (11%)	7,13,15	1.12	1 (14%)
2	API	M	3	2	9,11,12	1.20	0	7,13,15	1.79	2 (28%)
2	FGA	L	2	2	7,8,9	1.13	0	7,9,11	1.68	1 (14%)
2	API	P	3	2	9,11,12	1.24	1 (11%)	7,13,15	1.07	0
2	FGA	P	2	2	7,8,9	1.01	0	7,9,11	1.43	1 (14%)

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	FGA	N	2	2	-	0/7/8/9	-
2	FGA	J	2	2	-	1/7/8/9	-
2	FGA	O	2	2	-	0/7/8/9	-
2	API	N	3	2	-	0/11/12/14	-
2	API	K	3	2	-	1/11/12/14	-
2	API	L	3	2	-	0/11/12/14	-
2	FGA	M	2	2	-	0/7/8/9	-
2	FGA	K	2	2	-	0/7/8/9	-
2	FGA	I	2	2	-	0/7/8/9	-
2	API	I	3	2	-	0/11/12/14	-
2	API	J	3	2	-	1/11/12/14	-
2	API	O	3	2	-	0/11/12/14	-
2	API	M	3	2	-	0/11/12/14	-
2	FGA	L	2	2	-	0/7/8/9	-
2	API	P	3	2	-	0/11/12/14	-
2	FGA	P	2	2	-	0/7/8/9	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	3	API	C3-CA	-2.56	1.50	1.53
2	O	3	API	C3-CA	-2.46	1.50	1.53
2	J	3	API	C3-CA	-2.42	1.50	1.53
2	M	2	FGA	O-C	2.23	1.28	1.22
2	K	2	FGA	O-C	2.15	1.28	1.22

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	2	FGA	CB-CG-CD	-4.24	100.20	112.29
2	M	3	API	O4-C7-O3	-3.86	115.34	124.09
2	O	2	FGA	CB-CG-CD	-3.82	101.41	112.29
2	L	2	FGA	CB-CG-CD	-3.47	102.39	112.29
2	I	2	FGA	OXT-C-O	-3.19	116.84	124.09

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	2	FGA	CA-CB-CG-CD
2	J	3	API	N6-C6-C7-O4
2	K	3	API	N6-C6-C7-O4

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

15 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	GOL	D	401	-	5,5,5	0.37	0	5,5,5	0.36	0
3	GOL	A	401	-	5,5,5	0.36	0	5,5,5	0.42	0
3	GOL	F	401	-	5,5,5	0.44	0	5,5,5	0.53	0
3	GOL	H	401	-	5,5,5	0.54	0	5,5,5	0.28	0
4	MUB	N	401	2	18,19,20	1.29	2 (11%)	21,26,28	1.09	1 (4%)
4	MUB	P	401	2	18,19,20	1.27	2 (11%)	21,26,28	0.97	1 (4%)
3	GOL	G	401	-	5,5,5	0.49	0	5,5,5	0.42	0
4	MUB	I	401	2	18,19,20	1.02	1 (5%)	21,26,28	0.97	1 (4%)
3	GOL	E	401	-	5,5,5	0.50	0	5,5,5	0.46	0
4	MUB	O	401	2	1,4,20	1.49	0	3,4,28	1.34	1 (33%)
4	MUB	M	401	2	1,4,20	1.63	0	3,4,28	1.17	0
4	MUB	J	101	2	1,4,20	2.18	1 (100%)	3,4,28	1.16	0
4	MUB	K	401	2	18,19,20	1.22	4 (22%)	21,26,28	1.02	1 (4%)
4	MUB	L	401	2	1,4,20	1.84	0	3,4,28	1.22	1 (33%)
3	GOL	C	401	-	5,5,5	0.24	0	5,5,5	0.44	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	D	401	-	-	4/4/4/4	-
3	GOL	A	401	-	-	2/4/4/4	-
3	GOL	F	401	-	-	2/4/4/4	-
3	GOL	H	401	-	-	2/4/4/4	-
4	MUB	N	401	2	-	3/10/32/34	0/1/1/1
4	MUB	P	401	2	-	4/10/32/34	0/1/1/1
3	GOL	G	401	-	-	0/4/4/4	-
4	MUB	I	401	2	-	3/10/32/34	0/1/1/1
3	GOL	E	401	-	-	2/4/4/4	-
4	MUB	O	401	2	-	0/0/2/34	-
4	MUB	M	401	2	-	0/0/2/34	-
4	MUB	J	101	2	-	0/0/2/34	-
4	MUB	K	401	2	-	3/10/32/34	0/1/1/1
4	MUB	L	401	2	-	0/0/2/34	-

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WORLDWIDE
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PROTEIN DATA BANK

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	401	-	-	0/4/4/4	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	401	MUB	C1-C2	3.25	1.56	1.52
4	P	401	MUB	C1-C2	3.22	1.56	1.52
4	P	401	MUB	C7-N2	2.93	1.44	1.34
4	K	401	MUB	C7-N2	2.63	1.43	1.34
4	K	401	MUB	C2-N2	-2.53	1.41	1.45

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	401	MUB	C8-C7-N2	2.46	120.27	116.10
4	I	401	MUB	C8-C7-N2	2.45	120.24	116.10
4	N	401	MUB	C8-C7-N2	2.33	120.05	116.10
4	K	401	MUB	C8-C7-N2	2.33	120.04	116.10
4	O	401	MUB	O10-C10-C9	-2.18	120.57	124.78

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	GOL	O1-C1-C2-C3
3	D	401	GOL	O1-C1-C2-C3
3	E	401	GOL	O1-C1-C2-C3
3	H	401	GOL	O1-C1-C2-C3
4	N	401	MUB	C10-C9-O3-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	P	401	MUB	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 MUB N 401

Bond lengths

Bond angles

Torsions

Rings

Ligand MUB P 401

Bond lengths

Bond angles

Torsions

Rings

Ligand MUB I 401

Bond lengths

Bond angles

Torsions

Rings

Ligand MUB O 401

Bond lengths

Bond angles

Torsions

Rings

Ligand MUB J 101

Bond lengths

Bond angles

Torsions

Rings

Ligand MUB K 401

Bond lengths

Bond angles

Torsions

Rings

Ligand MUB L 401

Bond lengths

Bond angles

Torsions

Rings
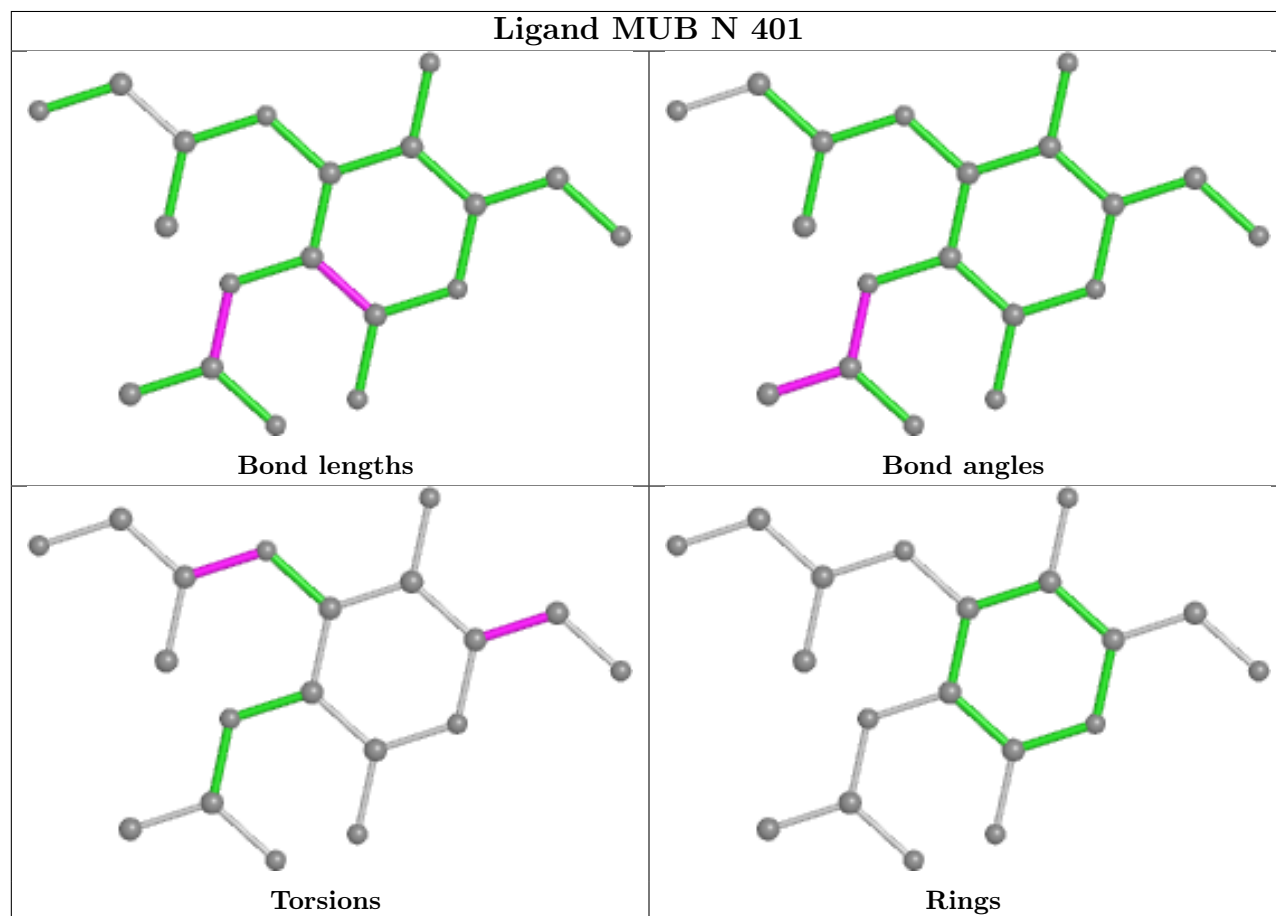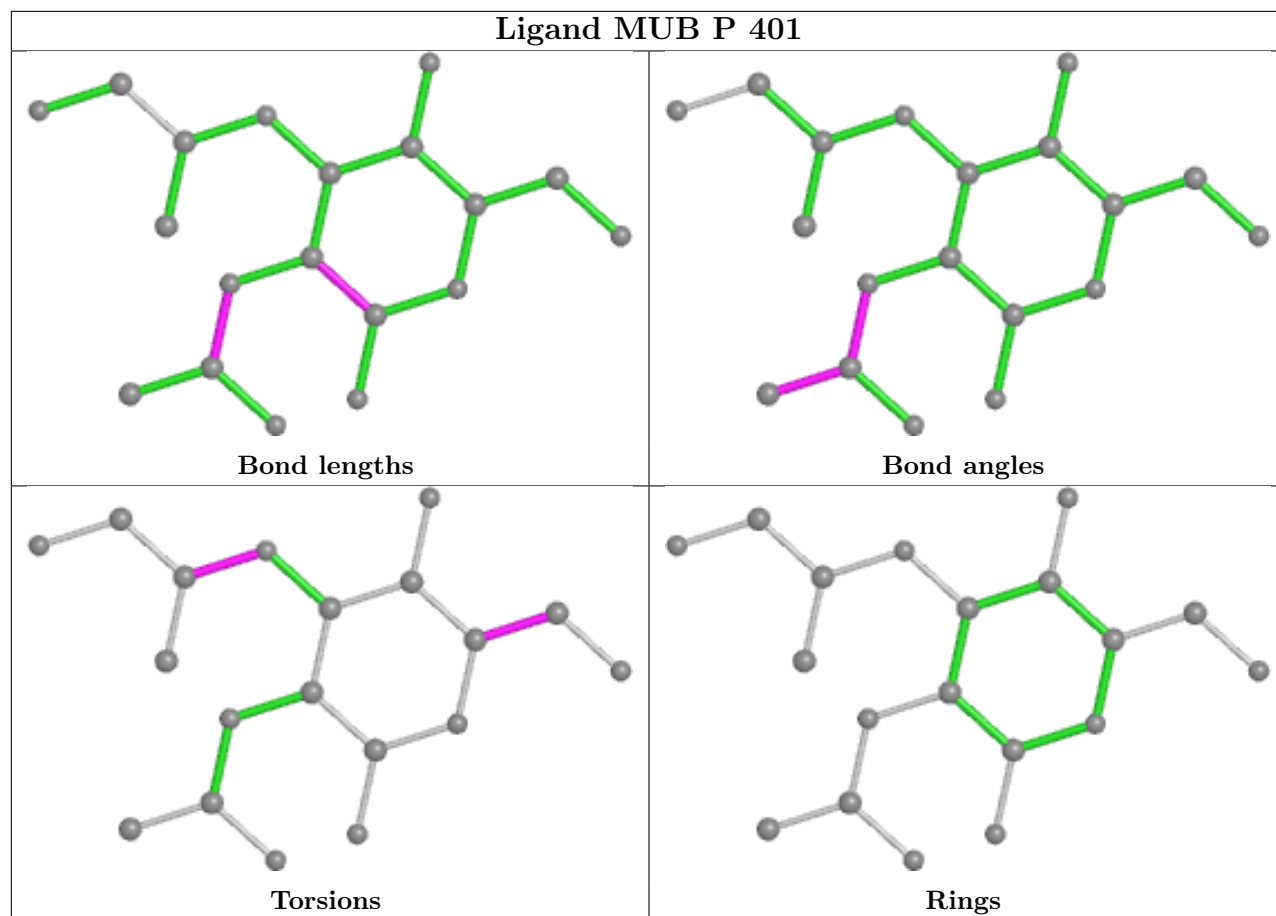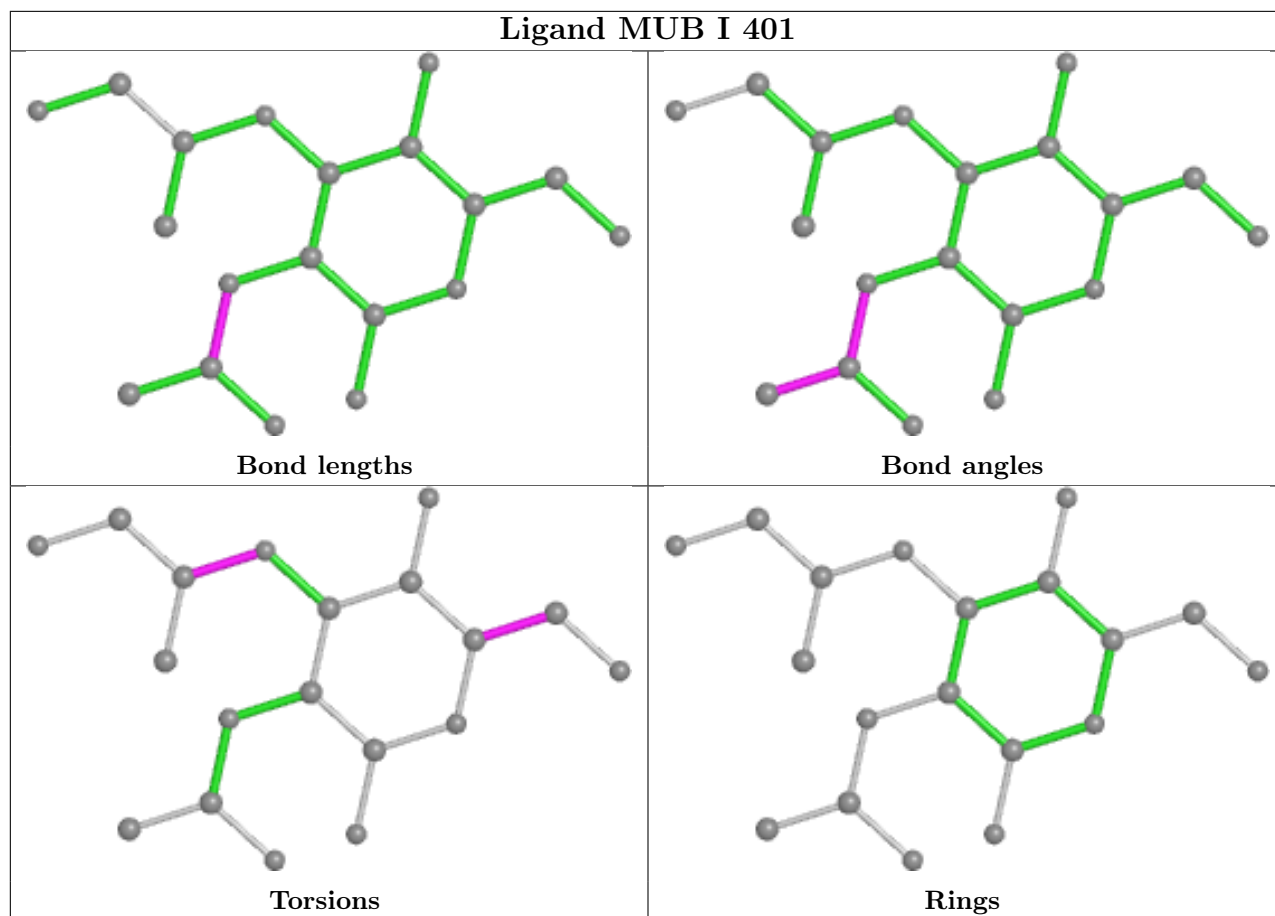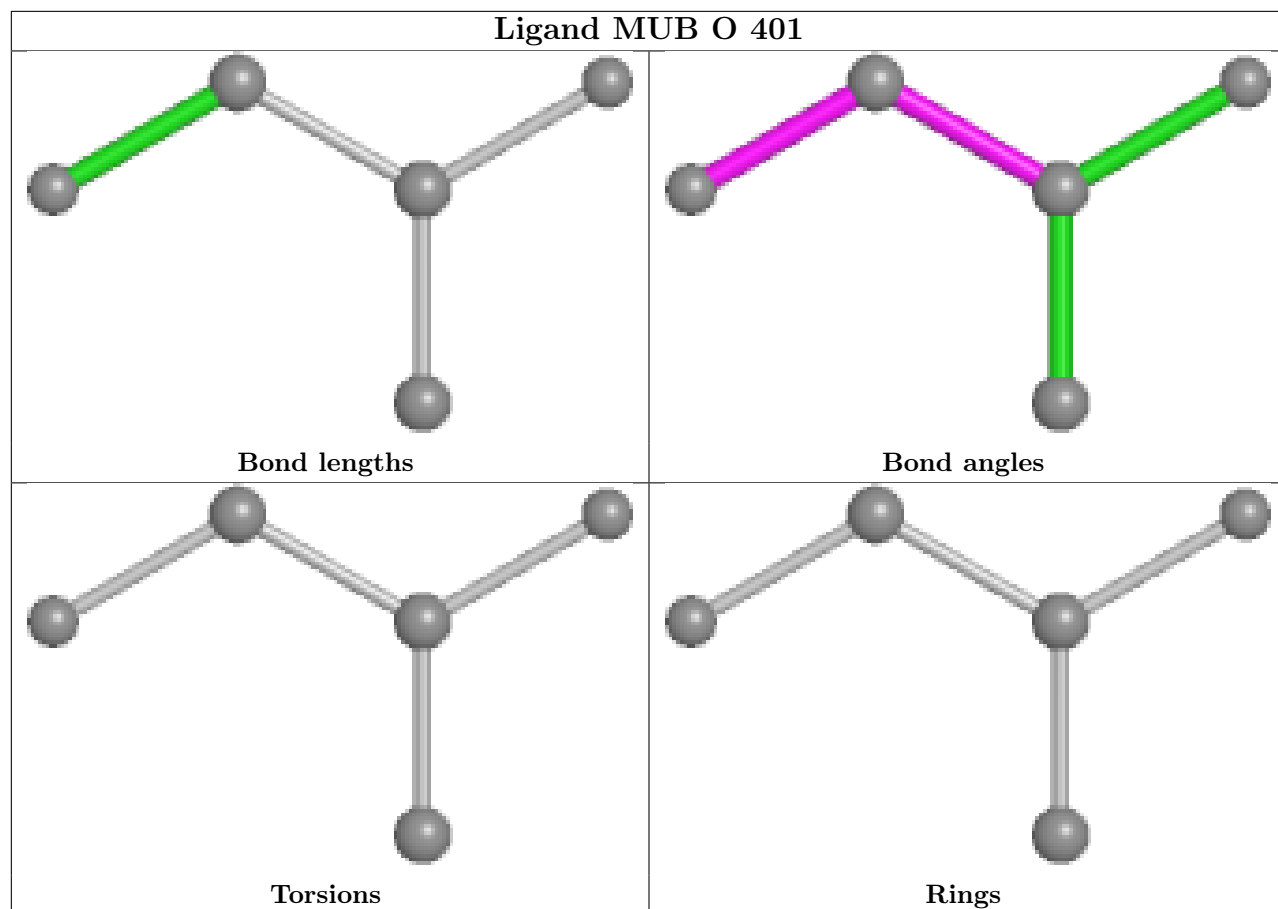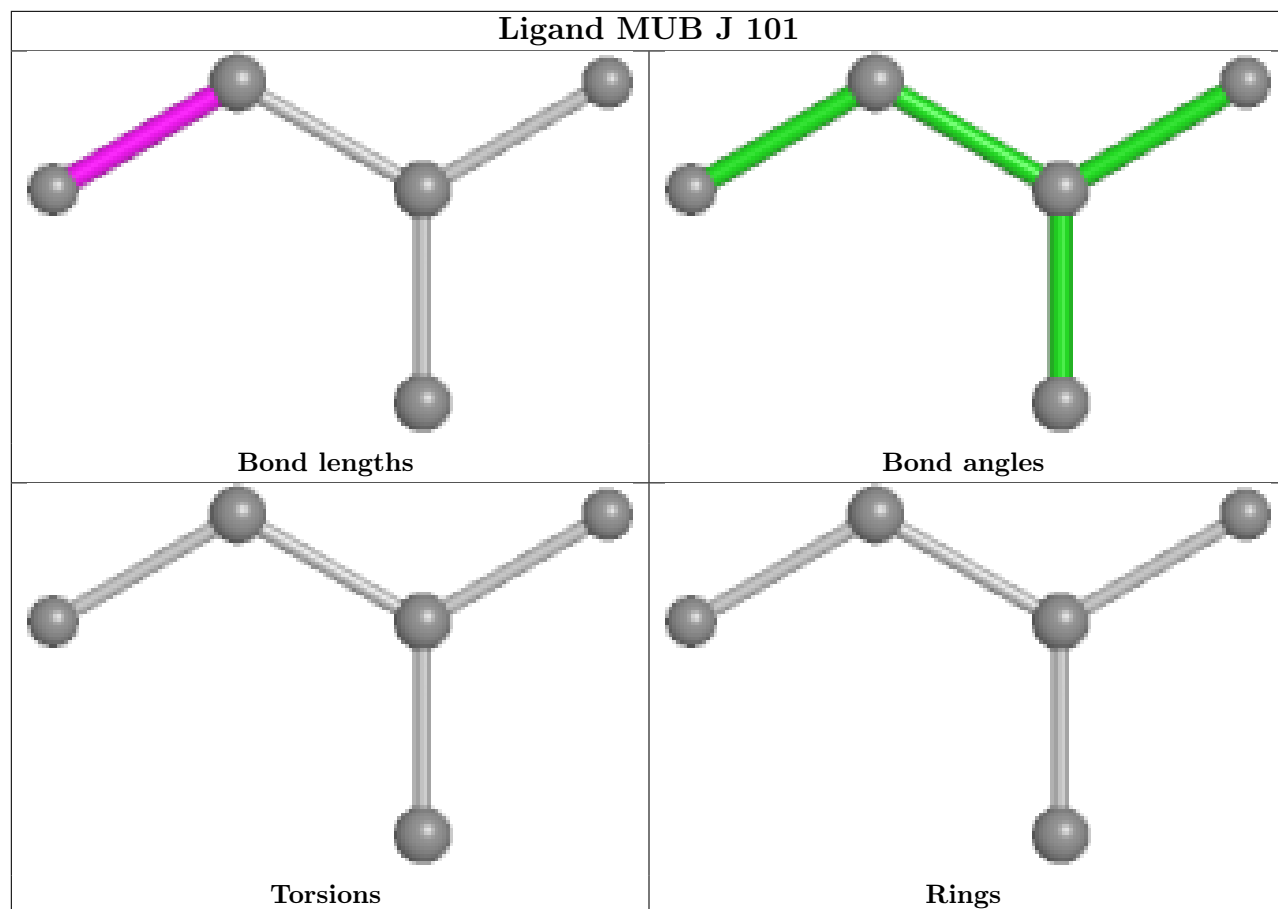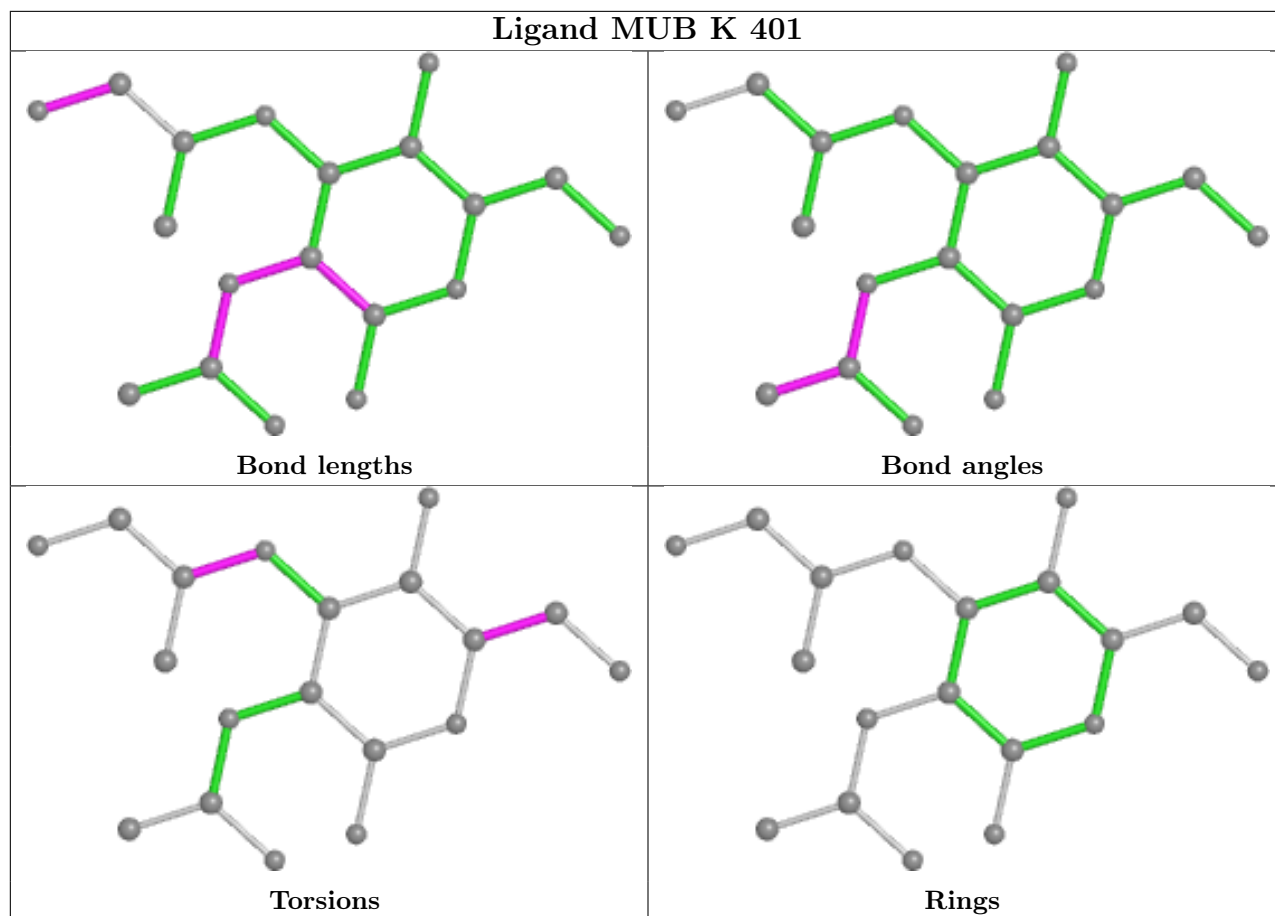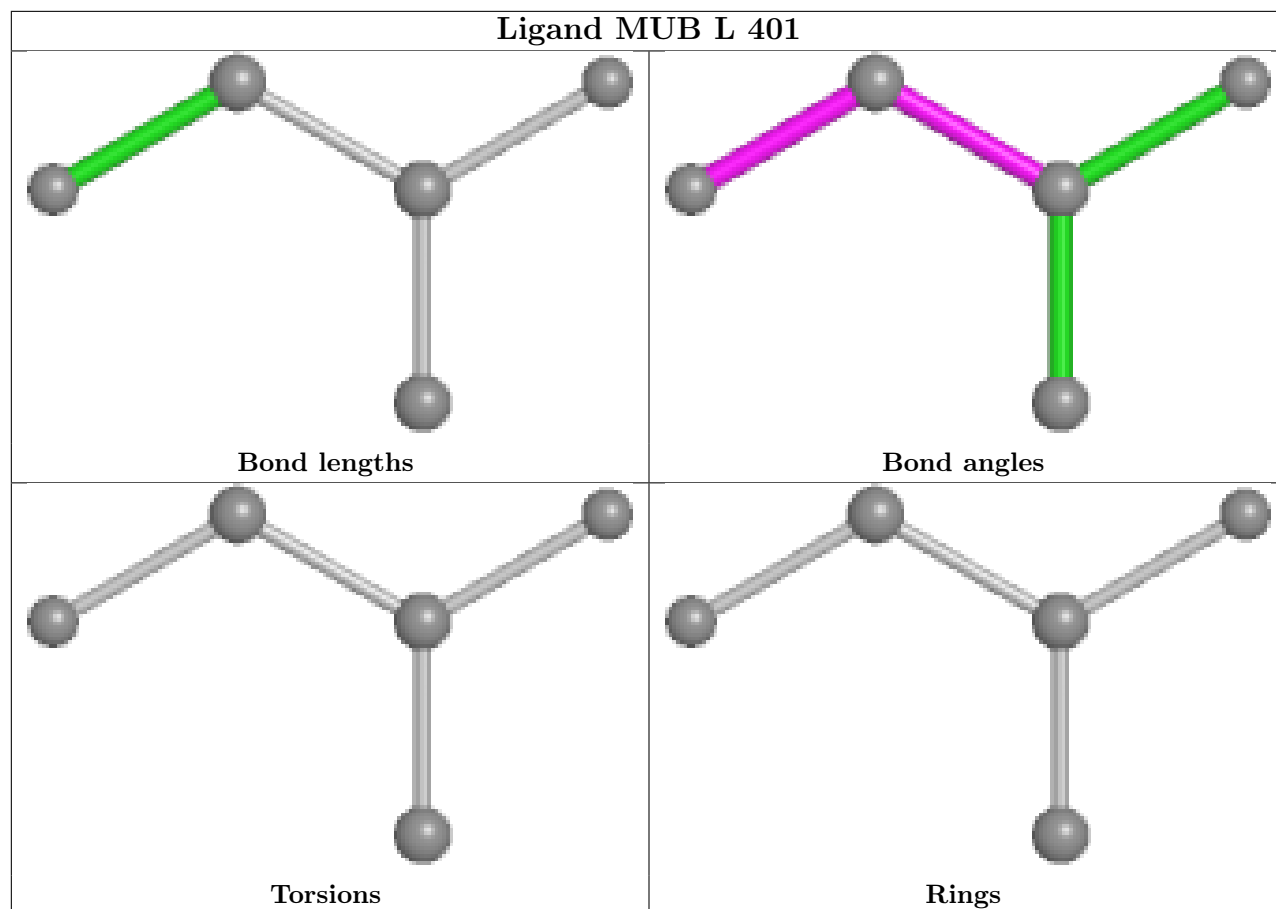
5.7 Other polymers ⓘ

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	197/219 (89%)	-0.12	0	100	100	21, 35, 51, 62	0
1	B	196/219 (89%)	0.24	4 (2%)	65	72	24, 38, 63, 73	0
1	C	196/219 (89%)	-0.08	0	100	100	19, 35, 48, 52	0
1	D	196/219 (89%)	0.30	6 (3%)	49	58	21, 36, 51, 57	0
1	E	196/219 (89%)	0.17	2 (1%)	82	86	22, 35, 48, 55	0
1	F	196/219 (89%)	0.06	1 (0%)	91	93	20, 31, 51, 58	0
1	G	196/219 (89%)	-0.07	1 (0%)	91	93	22, 34, 48, 51	0
1	H	196/219 (89%)	-0.09	0	100	100	21, 33, 49, 57	0
2	I	1/5 (20%)	0.52	0	100	100	45, 45, 45, 45	0
2	J	1/5 (20%)	0.17	0	100	100	45, 45, 45, 45	0
2	K	1/5 (20%)	-0.36	0	100	100	44, 44, 44, 44	0
2	L	1/5 (20%)	0.52	0	100	100	46, 46, 46, 46	0
2	M	1/5 (20%)	-0.30	0	100	100	44, 44, 44, 44	0
2	N	1/5 (20%)	-0.00	0	100	100	45, 45, 45, 45	0
2	O	1/5 (20%)	1.60	0	100	100	45, 45, 45, 45	0
2	P	1/5 (20%)	1.49	0	100	100	45, 45, 45, 45	0
All	All	1577/1792 (88%)	0.05	14 (0%)	84	88	19, 35, 51, 73	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	123	ILE	5.7
1	B	277	ALA	3.6
1	G	277	ALA	3.4
1	D	95	LYS	2.9
1	E	288	VAL	2.8

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

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
2	FGA	N	2	9/10	0.88	0.16	25,41,47,52	0
2	FGA	O	2	9/10	0.90	0.16	25,41,46,51	0
2	FGA	P	2	9/10	0.90	0.17	25,41,48,53	0
2	FGA	M	2	9/10	0.93	0.12	26,38,46,50	0
2	FGA	I	2	9/10	0.94	0.13	24,39,46,52	0
2	FGA	K	2	9/10	0.94	0.13	24,40,47,51	0
2	API	I	3	12/13	0.94	0.15	23,30,41,44	0
2	FGA	J	2	9/10	0.95	0.14	25,41,47,52	0
2	API	N	3	12/13	0.95	0.14	22,29,39,45	0
2	DAL	I	5	6/6	0.95	0.11	23,28,33,35	0
2	FGA	L	2	9/10	0.96	0.11	23,39,46,51	0
2	API	K	3	12/13	0.96	0.12	23,31,40,45	0
2	API	J	3	12/13	0.97	0.12	22,29,39,45	0
2	API	O	3	12/13	0.97	0.10	23,29,39,45	0
2	API	P	3	12/13	0.97	0.11	22,30,40,45	0
2	DAL	I	4	5/6	0.97	0.12	22,26,28,31	0
2	DAL	K	4	5/6	0.97	0.08	22,27,28,32	0
2	DAL	O	4	5/6	0.97	0.09	22,25,28,30	0
2	API	M	3	12/13	0.97	0.11	22,29,39,43	0
2	DAL	K	5	6/6	0.97	0.11	25,30,32,36	0
2	DAL	O	5	6/6	0.97	0.12	26,30,33,36	0
2	DAL	N	4	5/6	0.98	0.14	22,24,28,29	0
2	DAL	J	4	5/6	0.98	0.11	22,25,27,30	0
2	API	L	3	12/13	0.98	0.14	20,28,39,43	0
2	DAL	J	5	6/6	0.98	0.10	26,30,33,36	0
2	DAL	L	4	5/6	0.98	0.11	21,26,27,30	0
2	DAL	L	5	6/6	0.98	0.10	25,30,32,36	0
2	DAL	M	5	6/6	0.98	0.12	25,29,32,35	0
2	DAL	N	5	6/6	0.98	0.12	25,30,32,36	0
2	DAL	M	4	5/6	0.98	0.15	21,25,28,31	0
2	DAL	P	4	5/6	0.99	0.10	20,25,29,30	0
2	DAL	P	5	6/6	0.99	0.09	26,30,34,36	0

6.3 Carbohydrates ⓘ

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	MUB	K	401	19/20	0.71	0.23	43,57,69,78	0
4	MUB	N	401	19/20	0.74	0.23	43,56,69,77	0
4	MUB	P	401	19/20	0.76	0.28	41,56,70,78	0
4	MUB	I	401	19/20	0.77	0.23	44,56,70,77	0
4	MUB	J	101	5/20	0.79	0.21	43,44,53,53	0
4	MUB	L	401	5/20	0.87	0.16	44,44,45,51	0
4	MUB	M	401	5/20	0.90	0.14	43,43,45,51	0
4	MUB	O	401	5/20	0.91	0.16	43,44,53,53	0
3	GOL	F	401	6/6	0.94	0.09	43,51,57,59	0
3	GOL	H	401	6/6	0.95	0.09	40,48,52,58	0
3	GOL	C	401	6/6	0.95	0.23	38,47,57,57	0
3	GOL	G	401	6/6	0.95	0.12	38,47,53,63	0
3	GOL	A	401	6/6	0.96	0.10	39,47,53,63	0
3	GOL	E	401	6/6	0.97	0.10	32,42,51,60	0
3	GOL	D	401	6/6	0.97	0.15	33,42,54,61	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.
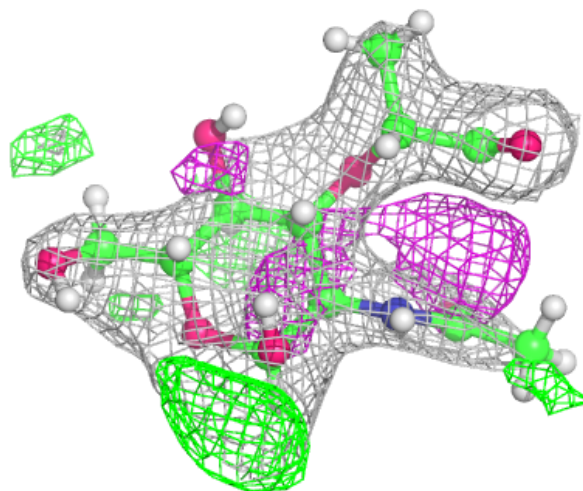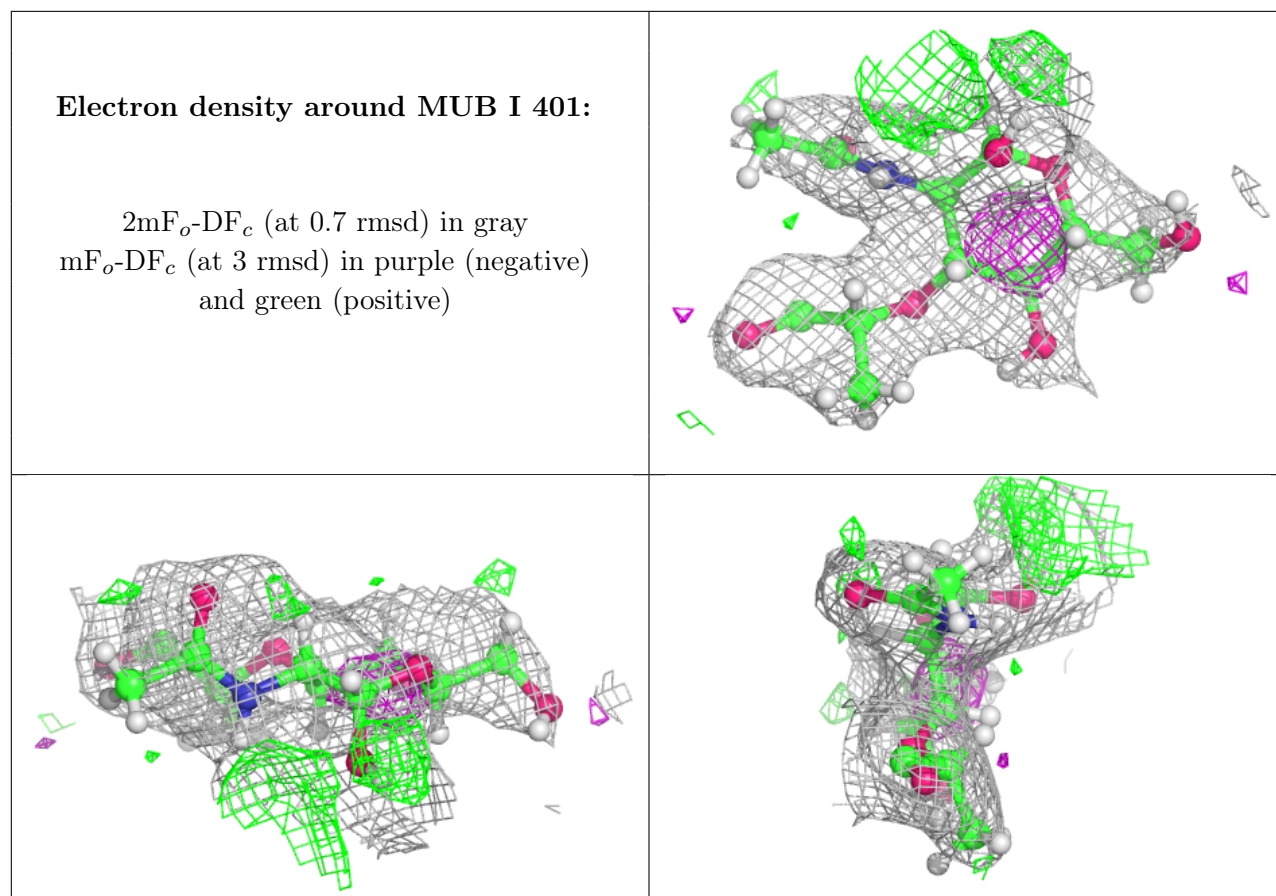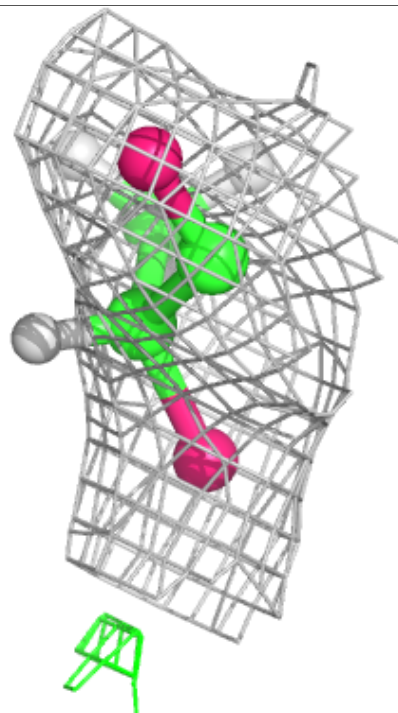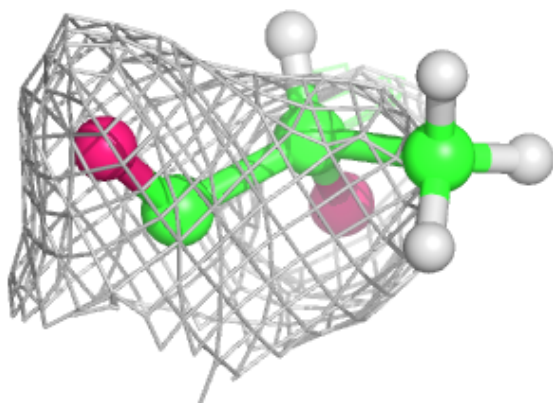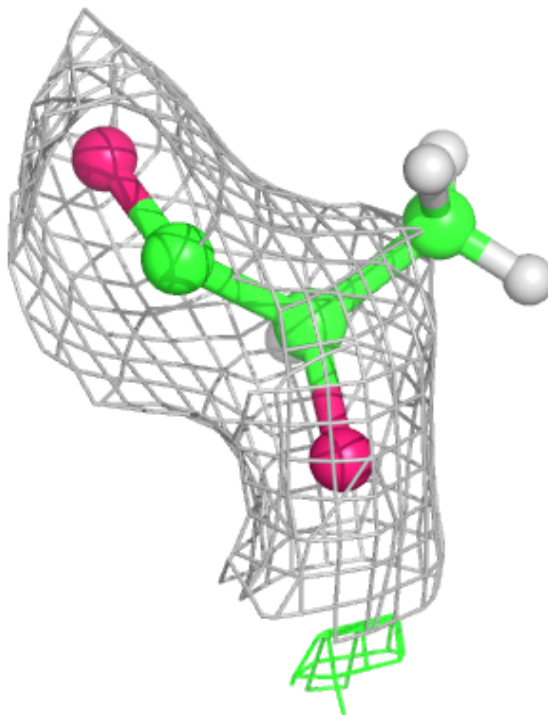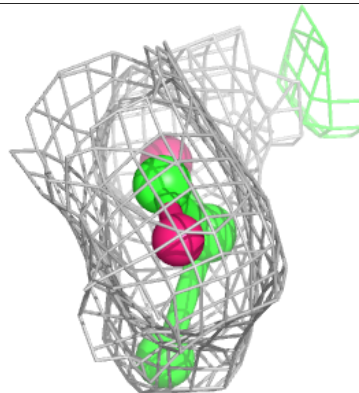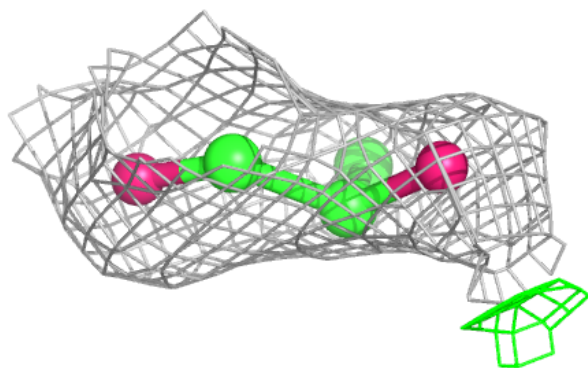
Electron density around MUB K 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
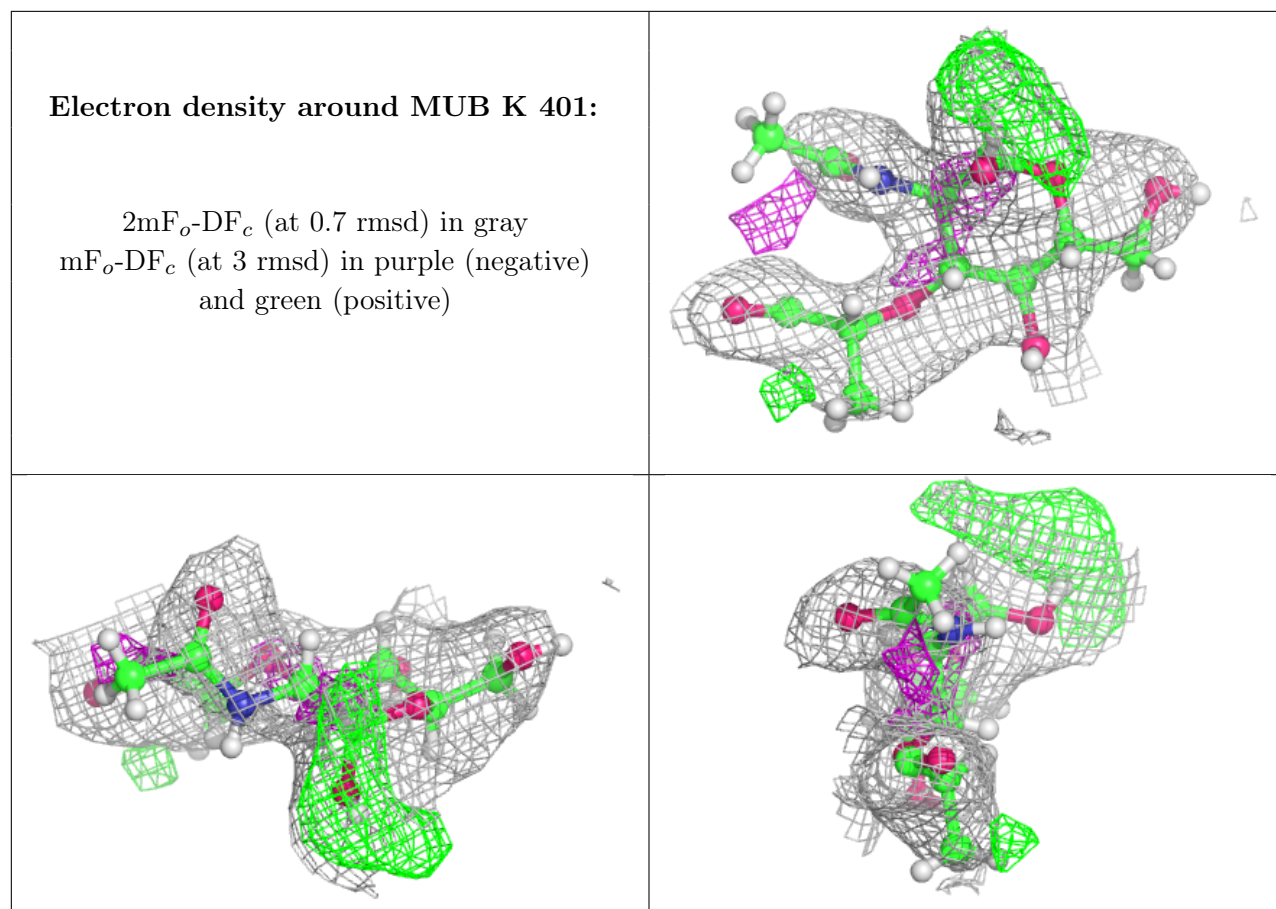
Electron density around MUB N 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
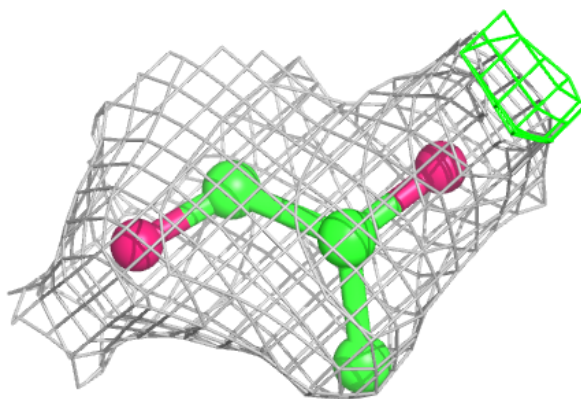and green (positive)
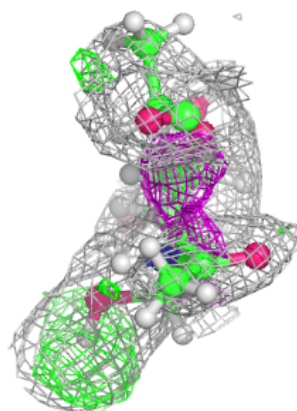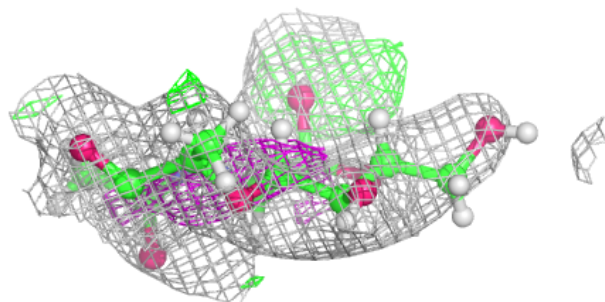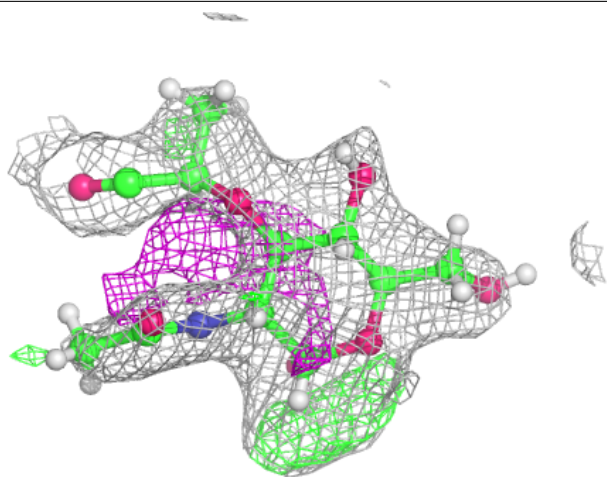
Electron density around MUB P 401:

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

Electron density around MUB I 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
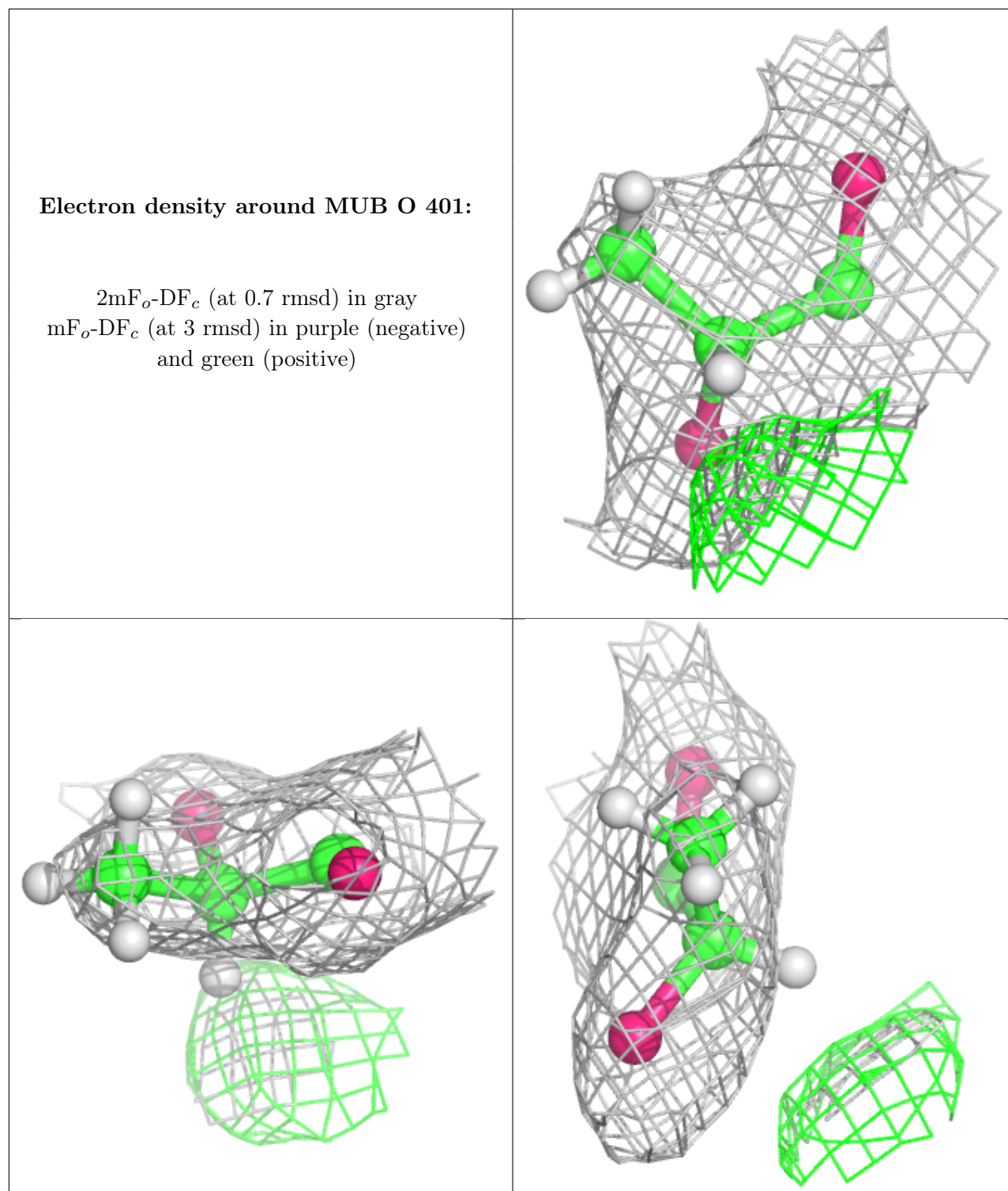and green (positive)
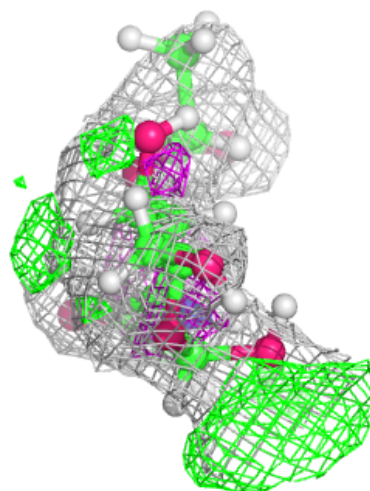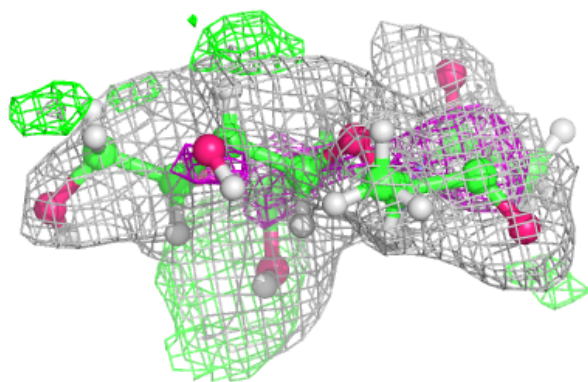
Electron density around MUB J 101:

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

Electron density around MUB L 401:

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

Electron density around MUB O 401:

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

6.5   Other polymers ⓘ

There are no such residues in this entry.