



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:50 AM UTC

PDB ID : 7JS3 / pdb\_00007js3  
Title : Structure of the Class II Fructose-1,6-Bisphosphatase from *Francisella tularensis*  
Authors : Abad-Zapatero, C.; Wolf, N.M.; Movahedzadeh, F.; Gutka, H.; Selezneva, A.  
Deposited on : 2020-08-13  
Resolution : 2.40 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](mailto: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>.

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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

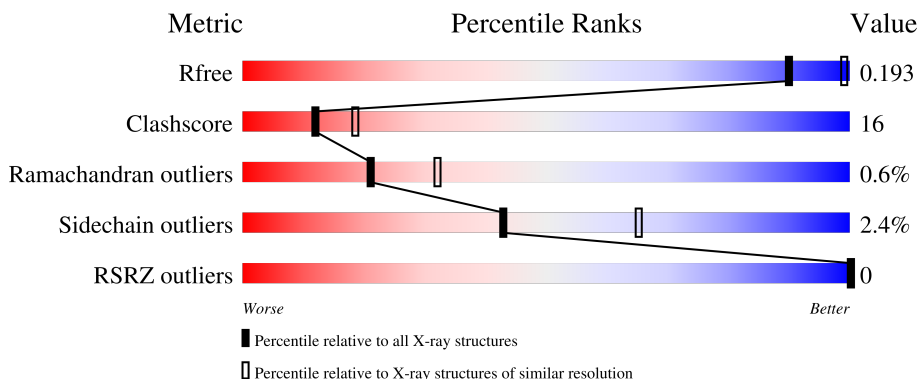
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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  $\geq 3$ , 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	348	 70% 22% • 7%
1	B	348	 71% 21% • 7%
1	C	348	 53% 39% • 7%
1	D	348	 65% 26% • 7%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9838 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 Fructose-1,6-bisphosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	325	2409	1494	425	474	16	0	1	0
1	B	325	2406	1492	425	474	15	0	0	0
1	C	325	2412	1496	425	476	15	0	1	0
1	D	325	2406	1492	425	474	15	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A0E2ZJY0
A	-18	GLY	-	expression tag	UNP A0A0E2ZJY0
A	-17	SER	-	expression tag	UNP A0A0E2ZJY0
A	-16	SER	-	expression tag	UNP A0A0E2ZJY0
A	-15	HIS	-	expression tag	UNP A0A0E2ZJY0
A	-14	HIS	-	expression tag	UNP A0A0E2ZJY0
A	-13	HIS	-	expression tag	UNP A0A0E2ZJY0
A	-12	HIS	-	expression tag	UNP A0A0E2ZJY0
A	-11	HIS	-	expression tag	UNP A0A0E2ZJY0
A	-10	HIS	-	expression tag	UNP A0A0E2ZJY0
A	-9	SER	-	expression tag	UNP A0A0E2ZJY0
A	-8	SER	-	expression tag	UNP A0A0E2ZJY0
A	-7	GLY	-	expression tag	UNP A0A0E2ZJY0
A	-6	LEU	-	expression tag	UNP A0A0E2ZJY0
A	-5	VAL	-	expression tag	UNP A0A0E2ZJY0
A	-4	PRO	-	expression tag	UNP A0A0E2ZJY0
A	-3	ARG	-	expression tag	UNP A0A0E2ZJY0
A	-2	GLY	-	expression tag	UNP A0A0E2ZJY0
A	-1	SER	-	expression tag	UNP A0A0E2ZJY0
A	0	HIS	-	expression tag	UNP A0A0E2ZJY0
B	-19	MET	-	initiating methionine	UNP A0A0E2ZJY0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP A0A0E2ZJY0
B	-17	SER	-	expression tag	UNP A0A0E2ZJY0
B	-16	SER	-	expression tag	UNP A0A0E2ZJY0
B	-15	HIS	-	expression tag	UNP A0A0E2ZJY0
B	-14	HIS	-	expression tag	UNP A0A0E2ZJY0
B	-13	HIS	-	expression tag	UNP A0A0E2ZJY0
B	-12	HIS	-	expression tag	UNP A0A0E2ZJY0
B	-11	HIS	-	expression tag	UNP A0A0E2ZJY0
B	-10	HIS	-	expression tag	UNP A0A0E2ZJY0
B	-9	SER	-	expression tag	UNP A0A0E2ZJY0
B	-8	SER	-	expression tag	UNP A0A0E2ZJY0
B	-7	GLY	-	expression tag	UNP A0A0E2ZJY0
B	-6	LEU	-	expression tag	UNP A0A0E2ZJY0
B	-5	VAL	-	expression tag	UNP A0A0E2ZJY0
B	-4	PRO	-	expression tag	UNP A0A0E2ZJY0
B	-3	ARG	-	expression tag	UNP A0A0E2ZJY0
B	-2	GLY	-	expression tag	UNP A0A0E2ZJY0
B	-1	SER	-	expression tag	UNP A0A0E2ZJY0
B	0	HIS	-	expression tag	UNP A0A0E2ZJY0
C	-19	MET	-	initiating methionine	UNP A0A0E2ZJY0
C	-18	GLY	-	expression tag	UNP A0A0E2ZJY0
C	-17	SER	-	expression tag	UNP A0A0E2ZJY0
C	-16	SER	-	expression tag	UNP A0A0E2ZJY0
C	-15	HIS	-	expression tag	UNP A0A0E2ZJY0
C	-14	HIS	-	expression tag	UNP A0A0E2ZJY0
C	-13	HIS	-	expression tag	UNP A0A0E2ZJY0
C	-12	HIS	-	expression tag	UNP A0A0E2ZJY0
C	-11	HIS	-	expression tag	UNP A0A0E2ZJY0
C	-10	HIS	-	expression tag	UNP A0A0E2ZJY0
C	-9	SER	-	expression tag	UNP A0A0E2ZJY0
C	-8	SER	-	expression tag	UNP A0A0E2ZJY0
C	-7	GLY	-	expression tag	UNP A0A0E2ZJY0
C	-6	LEU	-	expression tag	UNP A0A0E2ZJY0
C	-5	VAL	-	expression tag	UNP A0A0E2ZJY0
C	-4	PRO	-	expression tag	UNP A0A0E2ZJY0
C	-3	ARG	-	expression tag	UNP A0A0E2ZJY0
C	-2	GLY	-	expression tag	UNP A0A0E2ZJY0
C	-1	SER	-	expression tag	UNP A0A0E2ZJY0
C	0	HIS	-	expression tag	UNP A0A0E2ZJY0
D	-19	MET	-	initiating methionine	UNP A0A0E2ZJY0
D	-18	GLY	-	expression tag	UNP A0A0E2ZJY0
D	-17	SER	-	expression tag	UNP A0A0E2ZJY0

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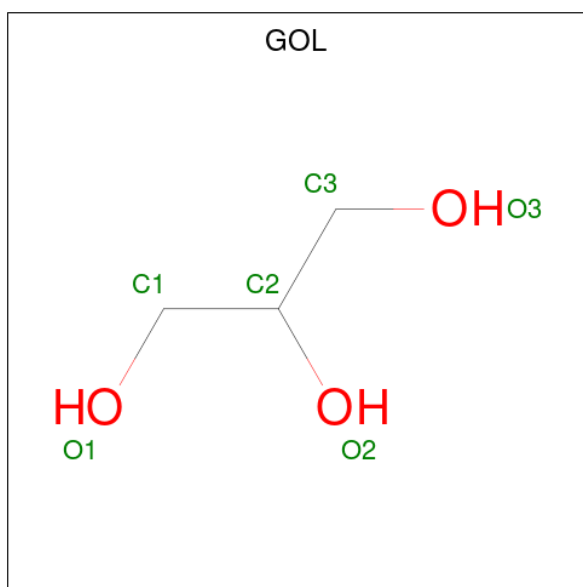
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP A0A0E2ZJY0
D	-15	HIS	-	expression tag	UNP A0A0E2ZJY0
D	-14	HIS	-	expression tag	UNP A0A0E2ZJY0
D	-13	HIS	-	expression tag	UNP A0A0E2ZJY0
D	-12	HIS	-	expression tag	UNP A0A0E2ZJY0
D	-11	HIS	-	expression tag	UNP A0A0E2ZJY0
D	-10	HIS	-	expression tag	UNP A0A0E2ZJY0
D	-9	SER	-	expression tag	UNP A0A0E2ZJY0
D	-8	SER	-	expression tag	UNP A0A0E2ZJY0
D	-7	GLY	-	expression tag	UNP A0A0E2ZJY0
D	-6	LEU	-	expression tag	UNP A0A0E2ZJY0
D	-5	VAL	-	expression tag	UNP A0A0E2ZJY0
D	-4	PRO	-	expression tag	UNP A0A0E2ZJY0
D	-3	ARG	-	expression tag	UNP A0A0E2ZJY0
D	-2	GLY	-	expression tag	UNP A0A0E2ZJY0
D	-1	SER	-	expression tag	UNP A0A0E2ZJY0
D	0	HIS	-	expression tag	UNP A0A0E2ZJY0

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).

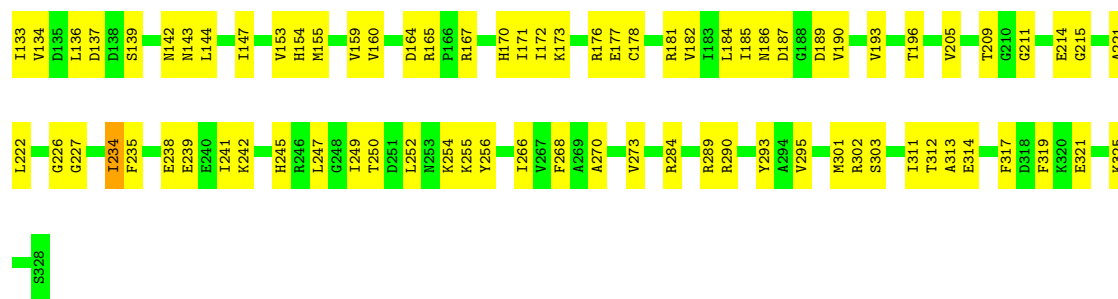


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

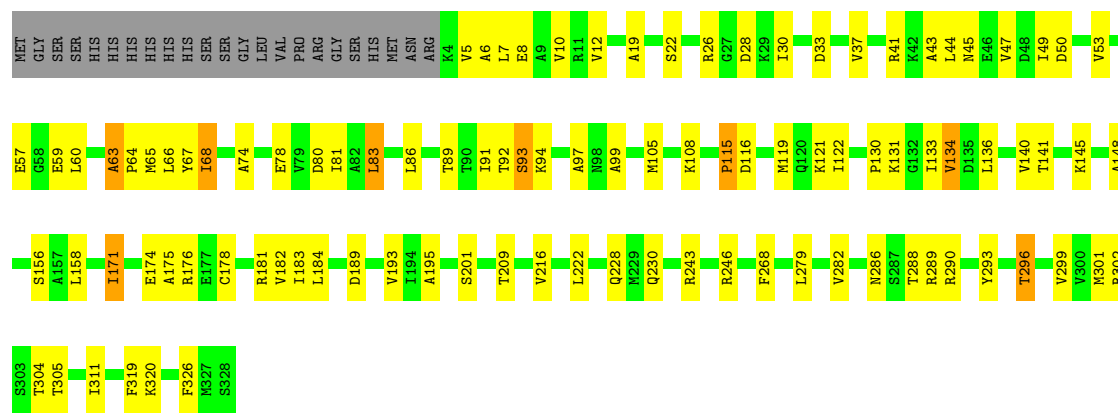
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	59	Total O 59 59	0	0
4	B	55	Total O 55 55	0	0
4	C	21	Total O 21 21	0	0
4	D	30	Total O 30 30	0	0





- Molecule 1: Fructose-1,6-bisphosphatase

Chain D: 65% 26% 7%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.30Å 100.17Å 92.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.11 – 2.40 38.11 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.7 (38.11-2.40) 98.9 (38.11-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.92 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.8.0258, PHENIX 1.16-3549	Depositor
R, $R_{free}$	0.153 , 0.193 0.153 , 0.193	Depositor DCC
$R_{free}$ test set	2732 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.8	Xtrriage
Anisotropy	0.149	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 37.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	0.417 for h,-k,-l	Xtrriage
Reported twinning fraction	0.568 for H, K, L 0.432 for -h,-k,l	Depositor
Outliers	0 of 53663 reflections	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9838	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, GOL

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	1.12	1/2438 (0.0%)	1.06	0/3290
1	B	1.05	1/2432 (0.0%)	1.05	0/3282
1	C	0.98	0/2441	1.10	1/3294 (0.0%)
1	D	1.01	1/2432 (0.0%)	1.10	0/3282
All	All	1.04	3/9743 (0.0%)	1.08	1/13148 (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	A	0	2
1	C	0	3
1	D	0	1
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	193	VAL	C-O	5.26	1.30	1.24
1	B	162	THR	C-O	5.11	1.30	1.23
1	D	296	THR	C-O	5.01	1.30	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	187	ASP	O-C-N	5.24	124.71	120.83

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	ASN	Peptide
1	A	83	LEU	Peptide
1	C	109	GLY	Peptide
1	C	186	ASN	Peptide
1	C	83	LEU	Peptide
1	D	83	LEU	Peptide

## 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	2409	0	2430	60	0
1	B	2406	0	2425	73	0
1	C	2412	0	2431	114	0
1	D	2406	0	2425	74	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	6	0	8	1	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	18	0	24	2	0
4	A	59	0	0	4	0
4	B	55	0	0	2	0
4	C	21	0	0	1	0
4	D	30	0	0	3	0
All	All	9838	0	9759	305	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 16.

All (305) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:LEU:HD12	1:B:85:PRO:HD3	1.43	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ARG:HD3	1:A:65:MET:HE2	1.47	0.97
1:A:127:ILE:HG12	1:A:226:GLY:HA3	1.50	0.93
1:B:83:LEU:CD1	1:B:85:PRO:HD3	1.99	0.91
1:C:121:LYS:NZ	1:C:189:ASP:OD2	2.06	0.89
1:B:22:SER:OG	1:B:323:ILE:HG22	1.73	0.88
1:C:222:LEU:HD22	1:C:227:GLY:HA3	1.55	0.88
1:C:37:VAL:HB	1:C:66:LEU:HD12	1.55	0.87
1:B:127:ILE:HD13	1:B:306:LYS:HE3	1.54	0.87
1:A:100:LEU:HD11	1:A:278:MET:HE1	1.59	0.84
1:B:127:ILE:CD1	1:B:306:LYS:HE3	2.10	0.81
1:D:289:ARG:NH1	4:D:502:HOH:O	2.11	0.81
1:D:148:ALA:HB2	1:D:158:LEU:HD11	1.62	0.81
1:A:290:ARG:NH1	1:A:314:GLU:OE2	2.11	0.81
1:C:119:MET:HE2	1:C:121:LYS:HE2	1.64	0.80
1:C:94:LYS:HB2	1:D:184:LEU:HD23	1.64	0.78
1:A:131:LYS:HD2	1:A:132:GLY:H	1.51	0.76
1:D:7:LEU:O	1:D:10:VAL:HG12	1.86	0.76
1:C:29:LYS:HD3	1:C:90:THR:HG22	1.67	0.75
1:C:19:ALA:O	1:C:22:SER:OG	2.04	0.75
1:B:197:ALA:HA	1:C:289:ARG:HD3	1.68	0.75
1:C:40:MET:HE3	1:C:83:LEU:HD23	1.69	0.73
1:A:100:LEU:HD11	1:A:278:MET:CE	2.18	0.73
1:D:130:PRO:HD2	1:D:133:ILE:HD12	1.72	0.72
1:A:121:LYS:NZ	1:A:189:ASP:OD2	2.23	0.72
1:D:33:ASP:HB2	1:D:89:THR:HG21	1.71	0.71
1:C:81:ILE:HD12	1:C:105:MET:HE2	1.72	0.71
1:D:279:LEU:HD21	1:D:299:VAL:HG23	1.72	0.71
1:A:50:ASP:OD1	1:A:71:LYS:NZ	2.15	0.70
1:C:193:VAL:O	1:C:196:THR:OG1	2.04	0.70
1:C:160:VAL:HB	1:C:182:VAL:HG12	1.74	0.69
1:C:94:LYS:HB2	1:D:184:LEU:CD2	2.23	0.69
1:C:127:ILE:HB	1:C:226:GLY:HA3	1.76	0.68
1:C:290:ARG:HH12	1:C:314:GLU:HB2	1.59	0.67
1:B:37:VAL:HG22	1:B:85:PRO:HG3	1.76	0.67
1:C:25:GLY:HA2	1:C:94:LYS:HA	1.76	0.67
1:C:37:VAL:HB	1:C:66:LEU:CD1	2.23	0.67
1:C:290:ARG:NH1	1:C:314:GLU:HB2	2.10	0.67
1:A:91:ILE:HD11	1:A:187:ASP:HB3	1.78	0.65
1:A:292:SER:OG	1:A:317:PHE:O	2.14	0.65
1:B:130:PRO:O	1:B:228:GLN:NE2	2.30	0.65
1:C:54:VAL:HG23	1:C:55:ILE:HG13	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:VAL:HG23	1:D:8:GLU:HB2	1.76	0.65
1:C:133:ILE:HG13	1:C:134:VAL:N	2.12	0.65
1:A:83:LEU:HD23	1:A:103:LEU:HD13	1.78	0.64
1:A:148:ALA:HB2	1:A:158:LEU:HD11	1.79	0.64
1:C:33:ASP:O	1:C:37:VAL:HG13	1.98	0.64
1:D:243:ARG:HG2	1:D:246:ARG:HH21	1.63	0.63
1:C:124:VAL:HG11	1:C:133:ILE:HD11	1.79	0.63
1:C:239:GLU:O	1:C:242:LYS:HB2	1.99	0.63
1:C:41:ARG:HD2	1:C:65:MET:HE2	1.80	0.63
1:B:128:ASN:HB2	1:B:150:PHE:HE1	1.65	0.62
1:C:37:VAL:HG12	1:C:85:PRO:CG	2.29	0.62
1:C:50:ASP:HB3	1:C:78:GLU:HG2	1.81	0.62
1:C:290:ARG:O	1:C:290:ARG:HG3	1.99	0.62
1:A:234:ILE:HG22	1:A:236:ASN:ND2	2.14	0.61
1:A:234:ILE:CG2	1:A:236:ASN:ND2	2.64	0.60
1:A:41:ARG:NH2	1:A:70:GLU:OE2	2.33	0.60
1:D:53:VAL:HG13	1:D:83:LEU:HD13	1.81	0.60
1:D:122:ILE:HG12	1:D:134:VAL:HG21	1.84	0.60
1:B:121:LYS:NZ	1:B:189:ASP:OD2	2.34	0.60
1:D:91:ILE:HA	1:D:94:LYS:HB3	1.83	0.59
1:C:103:LEU:HD21	1:C:105:MET:HE3	1.84	0.59
1:D:47:VAL:HG12	1:D:49:ILE:HG12	1.84	0.59
1:D:63:ALA:HB3	1:D:64:PRO:HD3	1.83	0.59
1:C:113:ASN:O	1:C:247:LEU:HD21	2.02	0.59
1:B:169:GLU:O	1:B:173:LYS:HG2	2.03	0.59
1:C:153:VAL:HG23	1:D:319:PHE:HB3	1.85	0.59
1:D:59:GLU:O	1:D:67:TYR:HB2	2.03	0.59
1:A:235:PHE:CE1	1:A:244:ALA:HB2	2.37	0.58
1:B:164:ASP:O	1:B:165:ARG:HD3	2.03	0.58
1:A:180:ALA:O	1:B:26:ARG:NH1	2.35	0.58
1:D:41:ARG:NH2	1:D:65:MET:O	2.37	0.58
1:C:79:VAL:HG23	1:C:81:ILE:HD11	1.84	0.58
1:A:133:ILE:HG23	1:A:134:VAL:HG13	1.86	0.58
1:C:266:ILE:HB	1:C:303:SER:HB3	1.85	0.58
1:B:22:SER:OG	1:B:323:ILE:O	2.22	0.57
1:D:326:PHE:O	4:D:503:HOH:O	2.17	0.57
1:D:57:GLU:O	1:D:64:PRO:HG3	2.05	0.57
1:C:49:ILE:HD11	1:C:77:CYS:HB2	1.87	0.57
1:D:53:VAL:O	1:D:68:ILE:HA	2.04	0.57
1:B:128:ASN:HB2	1:B:150:PHE:CE1	2.39	0.57
1:A:126:GLY:HA2	1:D:289:ARG:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:PRO:O	1:B:117:VAL:HG12	2.05	0.57
1:B:7:LEU:HD12	1:C:11:ARG:HE	1.70	0.56
1:B:22:SER:HA	1:B:323:ILE:CG2	2.36	0.56
1:C:54:VAL:HG11	1:C:80:ASP:HB3	1.87	0.56
1:D:108:LYS:HD3	1:D:108:LYS:C	2.30	0.56
1:C:144:LEU:CB	1:C:155:MET:HE3	2.35	0.56
1:B:229:MET:HB3	1:B:258:ILE:HG13	1.88	0.56
1:C:164:ASP:N	1:C:185:ILE:O	2.35	0.56
1:A:127:ILE:O	1:A:127:ILE:HG22	2.06	0.55
1:C:95:GLY:HA3	1:D:183:ILE:HB	1.87	0.55
1:C:235:PHE:CE2	1:C:252:LEU:HG	2.41	0.55
1:C:155:MET:HE2	1:C:178:CYS:SG	2.47	0.55
1:A:131:LYS:N	4:A:506:HOH:O	2.37	0.55
1:D:81:ILE:HD12	1:D:105:MET:HG2	1.89	0.54
1:B:302:ARG:O	1:B:306:LYS:HA	2.06	0.54
1:B:21:TRP:HD1	1:B:24:MET:CE	2.20	0.54
1:C:165:ARG:HG3	1:C:167:ARG:CZ	2.38	0.54
1:B:33:ASP:O	1:B:37:VAL:HG23	2.08	0.54
1:B:106:ALA:HB2	1:B:266:ILE:HD13	1.89	0.54
1:B:127:ILE:HD11	1:B:306:LYS:HZ1	1.72	0.54
1:A:131:LYS:HD2	1:A:132:GLY:N	2.21	0.54
1:B:5:VAL:HG21	1:B:105:MET:HE1	1.90	0.54
1:D:45:ASN:O	1:D:74:ALA:HB2	2.08	0.54
1:A:290:ARG:NH2	4:A:510:HOH:O	2.41	0.54
1:B:90:THR:O	1:B:94:LYS:HG3	2.08	0.54
1:B:257:ASP:OD1	1:B:257:ASP:N	2.41	0.54
1:B:54:VAL:HG12	1:B:81:ILE:O	2.07	0.54
1:D:176:ARG:HE	1:D:182:VAL:HB	1.73	0.54
1:C:290:ARG:NH1	1:C:314:GLU:CB	2.70	0.53
1:B:224:CYS:HB2	1:B:301:MET:HE3	1.90	0.53
1:C:221:ALA:HB2	1:C:268:PHE:CE2	2.43	0.53
1:D:80:ASP:CG	1:D:108:LYS:HA	2.33	0.53
1:D:304:THR:OG1	1:D:305:THR:N	2.40	0.53
1:C:137:ASP:OD2	1:C:255:LYS:NZ	2.30	0.53
1:B:83:LEU:HD12	1:B:85:PRO:CD	2.27	0.53
1:A:21:TRP:CZ3	1:A:323:ILE:HD11	2.43	0.53
1:B:21:TRP:HD1	1:B:24:MET:HE3	1.73	0.53
1:B:171:ILE:HG13	1:B:172:ILE:N	2.25	0.52
1:C:144:LEU:HB2	1:C:155:MET:HE3	1.91	0.52
1:C:222:LEU:HD22	1:C:227:GLY:CA	2.34	0.52
1:A:135:ASP:OD1	1:A:255:LYS:NZ	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ILE:CD1	1:B:306:LYS:CE	2.87	0.52
1:C:37:VAL:HG12	1:C:85:PRO:HG2	1.90	0.52
1:A:195:ALA:HB1	1:A:201:SER:OG	2.09	0.52
1:C:147:ILE:HD11	1:C:205:VAL:HG21	1.91	0.52
1:A:242:LYS:O	1:A:246:ARG:HG2	2.10	0.52
1:B:42:LYS:HD3	1:B:328:SER:HB3	1.92	0.52
1:C:12:VAL:HG11	1:C:103:LEU:HD13	1.92	0.52
1:C:80:ASP:O	1:C:105:MET:HA	2.08	0.52
1:A:127:ILE:CG1	1:A:226:GLY:HA3	2.32	0.51
1:C:40:MET:HE3	1:C:83:LEU:CD2	2.39	0.51
1:C:176:ARG:HD3	1:D:26:ARG:HA	1.92	0.51
1:D:286:ASN:HB2	4:D:505:HOH:O	2.09	0.51
1:A:41:ARG:NH1	1:A:65:MET:HA	2.24	0.51
1:C:21:TRP:O	1:D:181:ARG:NH2	2.43	0.51
1:C:190:VAL:HG22	1:C:214:GLU:HB3	1.92	0.51
1:C:173:LYS:O	1:C:177:GLU:HG3	2.11	0.51
1:D:30:ILE:HD12	1:D:30:ILE:H	1.76	0.51
1:C:254:LYS:HD3	1:C:256:TYR:CE2	2.45	0.51
1:D:268:PHE:HD2	1:D:301:MET:HE3	1.75	0.51
1:B:156:SER:O	1:B:181:ARG:HD2	2.11	0.51
1:A:81:ILE:HD13	1:A:105:MET:HG2	1.93	0.50
1:D:156:SER:O	1:D:181:ARG:HD2	2.12	0.50
1:D:279:LEU:HD21	1:D:299:VAL:CG2	2.40	0.50
1:C:30:ILE:HG13	1:C:31:ALA:N	2.26	0.50
1:C:44:LEU:O	1:C:73:GLY:HA2	2.11	0.50
1:D:86:LEU:HD21	1:D:92:THR:OG1	2.10	0.50
1:D:86:LEU:HD23	1:D:89:THR:HA	1.92	0.50
1:C:143:ASN:O	1:C:147:ILE:HG23	2.11	0.50
1:D:171:ILE:HG21	3:D:403:GOL:O3	2.12	0.50
1:B:122:ILE:HG12	1:B:134:VAL:CG2	2.42	0.50
1:C:119:MET:HE1	1:C:215:GLY:HA3	1.94	0.50
1:D:41:ARG:HE	1:D:66:LEU:HD12	1.77	0.50
1:D:268:PHE:CD2	1:D:301:MET:HE3	2.46	0.50
1:D:175:ALA:O	1:D:178:CYS:HB2	2.12	0.50
1:A:30:ILE:HD12	4:A:531:HOH:O	2.11	0.49
1:B:37:VAL:HG22	1:B:85:PRO:CG	2.40	0.49
1:A:143:ASN:OD1	1:A:146:ARG:NH2	2.46	0.49
1:B:88:GLY:HA2	4:B:547:HOH:O	2.12	0.49
1:B:127:ILE:HD11	1:B:306:LYS:CE	2.42	0.49
1:D:53:VAL:HG13	1:D:83:LEU:CD1	2.42	0.49
1:C:184:LEU:HD13	4:C:510:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:VAL:HB	1:D:174:GLU:OE2	2.12	0.49
1:D:37:VAL:HG21	1:D:65:MET:HB2	1.95	0.48
1:A:234:ILE:HG22	1:A:236:ASN:HD22	1.79	0.48
1:A:253:ASN:N	1:A:253:ASN:OD1	2.46	0.48
1:B:129:ALA:N	1:B:130:PRO:CD	2.76	0.48
1:C:57:GLU:HB2	1:C:66:LEU:HB3	1.94	0.48
1:B:91:ILE:HD11	1:B:187:ASP:HB3	1.95	0.48
1:C:245:HIS:HA	1:C:249:ILE:O	2.14	0.48
1:C:266:ILE:O	1:C:302:ARG:HA	2.13	0.48
1:B:127:ILE:HD12	1:C:290:ARG:O	2.14	0.48
1:C:165:ARG:HB3	1:C:167:ARG:HG2	1.96	0.48
1:D:91:ILE:HG13	1:D:99:ALA:HB2	1.95	0.48
1:A:19:ALA:O	1:A:22:SER:HB2	2.14	0.48
1:C:159:VAL:CG2	1:C:181:ARG:NH2	2.77	0.48
1:A:181:ARG:HG2	1:B:24:MET:O	2.14	0.48
1:B:41:ARG:NH1	1:B:65:MET:HG2	2.28	0.48
1:B:226:GLY:O	4:B:503:HOH:O	2.20	0.48
1:B:22:SER:HA	1:B:323:ILE:HG21	1.94	0.48
1:C:238:GLU:HG3	1:C:241:ILE:HB	1.96	0.48
1:A:234:ILE:CG2	1:A:236:ASN:HD22	2.27	0.47
1:B:163:MET:HB2	1:B:168:HIS:CE1	2.50	0.47
1:D:41:ARG:HB2	1:D:66:LEU:HD13	1.97	0.47
1:D:130:PRO:O	1:D:228:GLN:HG3	2.14	0.47
1:B:41:ARG:HH11	1:B:65:MET:HE2	1.78	0.47
1:B:131:LYS:HG2	1:B:132:GLY:H	1.80	0.47
1:B:33:ASP:CG	1:B:89:THR:HG21	2.40	0.47
1:C:295:VAL:HA	1:C:313:ALA:O	2.14	0.47
1:A:230:GLN:OE1	1:A:255:LYS:HD2	2.15	0.47
1:B:209:THR:HG21	1:B:234:ILE:HD11	1.97	0.47
1:C:234:ILE:HG22	1:C:235:PHE:H	1.79	0.47
1:C:122:ILE:HD13	1:C:134:VAL:HB	1.97	0.47
1:C:211:GLY:HA3	1:C:214:GLU:OE1	2.14	0.47
1:B:4:LYS:HZ2	1:B:4:LYS:N	2.13	0.46
1:B:229:MET:HB3	1:B:258:ILE:CG1	2.45	0.46
1:C:120:GLN:OE1	1:C:136:LEU:HB3	2.15	0.46
1:D:290:ARG:HD3	1:D:293:TYR:CE1	2.51	0.46
1:B:163:MET:HB2	1:B:168:HIS:HE1	1.81	0.46
1:D:115:PRO:O	1:D:116:ASP:C	2.59	0.46
1:D:131:LYS:HE3	1:D:131:LYS:HB2	1.81	0.46
1:C:325:LYS:HG2	1:C:325:LYS:O	2.16	0.45
1:A:41:ARG:CZ	1:A:70:GLU:OE2	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:SER:HA	1:B:323:ILE:HG22	1.99	0.45
1:B:286:ASN:HA	1:B:292:SER:HA	1.98	0.45
1:C:139:SER:OG	1:C:142:ASN:HB2	2.16	0.45
1:A:254:LYS:HA	3:A:403:GOL:H31	1.98	0.45
1:A:195:ALA:HB2	1:A:277:ASN:HB3	1.97	0.45
1:A:254:LYS:HD3	1:A:256:TYR:CE2	2.52	0.45
1:C:159:VAL:CG2	1:C:181:ARG:HH21	2.30	0.45
1:A:4:LYS:HD3	1:D:8:GLU:HG3	1.98	0.45
1:A:34:GLN:HG3	4:A:558:HOH:O	2.16	0.45
1:C:102:VAL:HG12	1:C:270:ALA:HB2	1.97	0.45
1:B:127:ILE:HG13	1:C:290:ARG:HA	1.99	0.44
1:B:224:CYS:HB2	1:B:301:MET:CE	2.47	0.44
1:C:119:MET:O	1:C:209:THR:HA	2.16	0.44
1:C:139:SER:O	1:C:143:ASN:ND2	2.45	0.44
1:C:317:PHE:CE2	1:C:319:PHE:HA	2.53	0.44
1:B:115:PRO:HG2	1:B:117:VAL:HG11	1.99	0.44
1:D:289:ARG:HE	1:D:289:ARG:HB3	1.57	0.44
1:A:123:ALA:CB	1:A:193:VAL:HG13	2.48	0.44
1:B:67:TYR:CE1	1:B:70:GLU:HB2	2.53	0.44
1:B:194:ILE:HG21	1:B:278:MET:HE3	1.98	0.44
1:B:296:THR:HG23	1:B:315:HIS:CD2	2.53	0.44
1:C:49:ILE:O	1:C:73:GLY:HA3	2.18	0.44
1:C:129:ALA:HA	1:C:131:LYS:HE2	1.99	0.44
1:C:124:VAL:HG11	1:C:133:ILE:CD1	2.47	0.44
1:C:144:LEU:HB3	1:C:155:MET:HE3	1.99	0.44
1:B:131:LYS:HG2	1:B:132:GLY:N	2.32	0.43
1:C:155:MET:CE	1:C:178:CYS:SG	3.06	0.43
1:D:189:ASP:O	1:D:193:VAL:HG23	2.18	0.43
1:A:189:ASP:OD1	1:A:189:ASP:N	2.51	0.43
1:A:262:ALA:HB1	1:A:266:ILE:HD13	1.99	0.43
1:D:141:THR:O	1:D:145:LYS:HG3	2.18	0.43
1:A:156:SER:O	1:A:181:ARG:HD2	2.18	0.43
1:C:317:PHE:HE2	1:C:319:PHE:HA	1.84	0.43
1:B:127:ILE:HG12	1:B:226:GLY:HA3	2.00	0.43
1:C:57:GLU:HG3	1:C:66:LEU:HD13	1.99	0.43
1:D:44:LEU:HD23	1:D:44:LEU:HA	1.79	0.43
1:C:159:VAL:HG22	1:C:181:ARG:NH2	2.34	0.43
1:A:246:ARG:HA	1:A:246:ARG:NE	2.33	0.43
1:C:293:TYR:CE2	1:C:314:GLU:HG2	2.53	0.43
1:D:50:ASP:HB3	1:D:78:GLU:HA	2.01	0.43
1:D:91:ILE:HD12	1:D:97:ALA:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:VAL:HG12	1:C:85:PRO:HG3	1.99	0.43
1:C:235:PHE:CZ	1:C:252:LEU:HG	2.53	0.43
1:D:28:ASP:N	1:D:93:SER:OG	2.51	0.43
1:B:21:TRP:CD1	1:B:24:MET:HE3	2.53	0.43
1:C:284:ARG:HG3	1:C:319:PHE:CE2	2.53	0.43
1:D:86:LEU:HD23	1:D:89:THR:CA	2.49	0.43
1:C:10:VAL:HG11	1:C:311:ILE:HD12	2.01	0.43
1:C:222:LEU:O	1:C:226:GLY:N	2.47	0.43
1:D:136:LEU:HD12	1:D:230:GLN:HG2	2.01	0.43
1:A:317:PHE:CZ	1:A:325:LYS:HB2	2.54	0.42
1:C:147:ILE:HD11	1:C:205:VAL:CG2	2.49	0.42
1:C:28:ASP:HB3	1:C:31:ALA:HB3	2.01	0.42
1:D:282:VAL:HG22	1:D:296:THR:HG22	2.01	0.42
1:B:131:LYS:C	1:B:133:ILE:H	2.28	0.42
1:C:120:GLN:HG2	1:C:136:LEU:HD13	2.01	0.42
1:C:129:ALA:N	1:C:130:PRO:HD3	2.34	0.42
1:A:112:LEU:HD22	1:A:261:LEU:HD23	2.02	0.42
1:A:4:LYS:HG2	1:D:8:GLU:HB3	2.02	0.42
1:A:140:VAL:HB	1:A:174:GLU:CD	2.45	0.42
1:A:10:VAL:HG21	1:A:311:ILE:HD12	2.02	0.42
1:B:105:MET:HE2	1:B:267:VAL:HG11	2.01	0.42
1:D:121:LYS:NZ	1:D:189:ASP:OD2	2.53	0.42
1:C:133:ILE:HG13	1:C:134:VAL:H	1.81	0.42
1:D:12:VAL:HG13	1:D:43:ALA:HB3	2.01	0.42
1:A:120:GLN:O	1:A:231:ALA:HA	2.20	0.42
1:B:301:MET:HE2	1:B:301:MET:HB2	1.81	0.42
1:A:296:THR:OG1	1:A:313:ALA:HB3	2.20	0.41
1:C:268:PHE:HB3	1:C:301:MET:HG3	2.01	0.41
1:D:122:ILE:HG12	1:D:134:VAL:CG2	2.49	0.41
1:C:170:HIS:CG	1:C:171:ILE:N	2.89	0.41
1:A:268:PHE:HB3	1:A:301:MET:HG3	2.02	0.41
1:C:49:ILE:O	1:C:74:ALA:N	2.45	0.41
1:A:189:ASP:O	1:A:193:VAL:HG23	2.20	0.41
1:D:59:GLU:C	1:D:67:TYR:HB2	2.45	0.41
1:C:154:HIS:HB2	1:D:320:LYS:O	2.21	0.41
1:B:127:ILE:HD11	1:B:306:LYS:NZ	2.36	0.41
1:A:41:ARG:HH11	1:A:65:MET:HA	1.86	0.41
1:B:129:ALA:H	1:B:130:PRO:HD3	1.85	0.41
1:C:100:LEU:HA	1:C:273:VAL:HG23	2.02	0.41
1:C:8:GLU:OE1	1:C:11:ARG:NH2	2.53	0.41
1:C:36:ALA:HB1	1:C:85:PRO:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87[A]:GLU:HG2	1:C:214:GLU:HG2	2.03	0.41
1:D:6:ALA:HB2	1:D:302:ARG:NH1	2.36	0.41
1:A:282:VAL:HA	1:A:295:VAL:O	2.21	0.41
1:B:115:PRO:HG2	1:B:117:VAL:CG1	2.51	0.41
1:C:86:LEU:HD21	1:C:92:THR:OG1	2.20	0.41
1:C:88:GLY:CA	1:C:91:ILE:HG12	2.51	0.40
1:B:168:HIS:O	1:B:169:GLU:C	2.63	0.40
1:C:91:ILE:HD12	1:C:97:ALA:O	2.20	0.40
1:D:136:LEU:HA	3:D:403:GOL:H12	2.03	0.40
1:C:51:GLY:O	1:C:71:LYS:HA	2.20	0.40
1:D:119:MET:O	1:D:209:THR:HA	2.21	0.40
1:C:65:MET:HG2	1:C:65:MET:O	2.21	0.40
1:C:120:GLN:HB3	1:C:234:ILE:HD11	2.03	0.40
1:D:19:ALA:O	1:D:22:SER:HB2	2.21	0.40
1:D:195:ALA:O	1:D:201:SER:OG	2.23	0.40
1:B:94:LYS:HE2	1:B:94:LYS:HB3	1.93	0.40
1:D:290:ARG:HD3	1:D:293:TYR:CD1	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	324/348 (93%)	307 (95%)	17 (5%)	0	100	100
1	B	323/348 (93%)	298 (92%)	23 (7%)	2 (1%)	21	32
1	C	324/348 (93%)	287 (89%)	34 (10%)	3 (1%)	14	22
1	D	323/348 (93%)	296 (92%)	24 (7%)	3 (1%)	14	22
All	All	1294/1392 (93%)	1188 (92%)	98 (8%)	8 (1%)	21	32

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	116	ASP
1	C	60	LEU
1	D	63	ALA
1	C	6	ALA
1	C	172	ILE
1	D	115	PRO
1	B	129	ALA
1	D	60	LEU

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	252/271 (93%)	245 (97%)	7 (3%)	38	60
1	B	251/271 (93%)	245 (98%)	6 (2%)	43	65
1	C	252/271 (93%)	248 (98%)	4 (2%)	55	76
1	D	251/271 (93%)	243 (97%)	8 (3%)	34	56
All	All	1006/1084 (93%)	981 (98%)	25 (2%)	43	64

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	77[A]	CYS
1	A	77[B]	CYS
1	A	90	THR
1	A	153	VAL
1	A	171	ILE
1	A	298	SER
1	B	18	LEU
1	B	171	ILE
1	B	178	CYS
1	B	257	ASP
1	B	265	ASP
1	B	267	VAL
1	C	234	ILE

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Mol	Chain	Res	Type
1	C	250	THR
1	C	312	THR
1	C	321	GLU
1	D	68	ILE
1	D	93	SER
1	D	134	VAL
1	D	171	ILE
1	D	216	VAL
1	D	222	LEU
1	D	288	THR
1	D	311	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	200	ASN
1	A	236	ASN
1	A	280	GLN
1	B	34	GLN
1	B	236	ASN
1	C	45	ASN
1	C	120	GLN
1	C	186	ASN
1	C	277	ASN
1	D	128	ASN
1	D	253	ASN

### 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

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	D	402	-	5,5,5	0.19	0	5,5,5	0.52	0
3	GOL	D	401	-	5,5,5	0.11	0	5,5,5	0.27	0
3	GOL	D	403	-	5,5,5	0.11	0	5,5,5	0.34	0
3	GOL	C	402	-	5,5,5	0.08	0	5,5,5	0.32	0
3	GOL	A	403	-	5,5,5	0.25	0	5,5,5	0.90	0
3	GOL	B	402	-	5,5,5	0.16	0	5,5,5	0.33	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	402	-	-	2/4/4/4	-
3	GOL	D	401	-	-	2/4/4/4	-
3	GOL	D	403	-	-	1/4/4/4	-
3	GOL	C	402	-	-	0/4/4/4	-
3	GOL	A	403	-	-	0/4/4/4	-
3	GOL	B	402	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	401	GOL	O1-C1-C2-C3
3	D	402	GOL	C1-C2-C3-O3
3	B	402	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	D	401	GOL	O1-C1-C2-O2
3	D	402	GOL	O2-C2-C3-O3
3	B	402	GOL	O1-C1-C2-O2
3	D	403	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	403	GOL	2	0
3	A	403	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	325/348 (93%)	-1.37	0 100 100	19, 33, 72, 94	1 (0%)
1	B	325/348 (93%)	-1.28	0 100 100	23, 41, 71, 109	0
1	C	325/348 (93%)	-1.02	0 100 100	33, 65, 118, 149	1 (0%)
1	D	325/348 (93%)	-1.17	0 100 100	26, 52, 87, 169	0
All	All	1300/1392 (93%)	-1.21	0 100 100	19, 47, 98, 169	2 (0%)

There are no RSRZ outliers to report.

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	GOL	C	402	6/6	0.94	0.05	65,73,76,78	0
3	GOL	D	402	6/6	0.94	0.08	60,72,81,88	0
3	GOL	D	401	6/6	0.97	0.06	74,84,85,87	0
3	GOL	B	402	6/6	0.97	0.06	102,109,109,112	0

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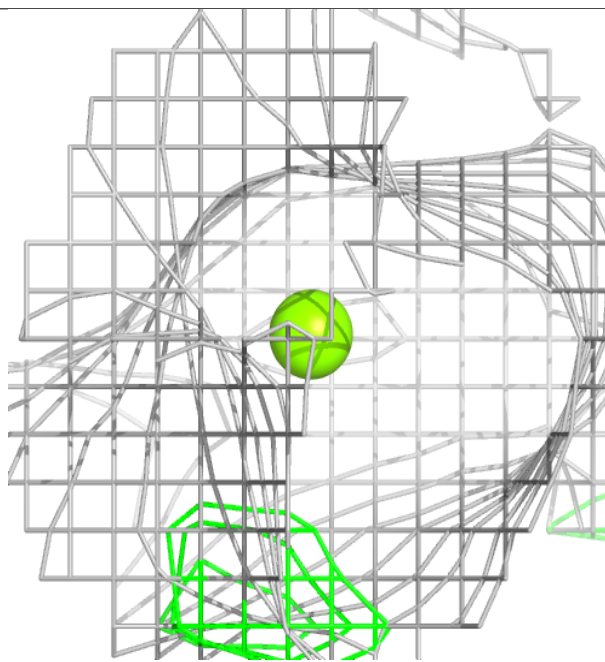
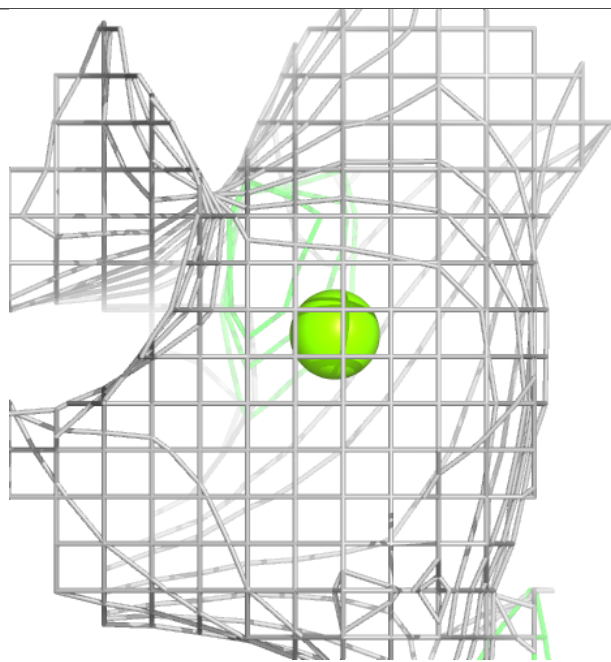
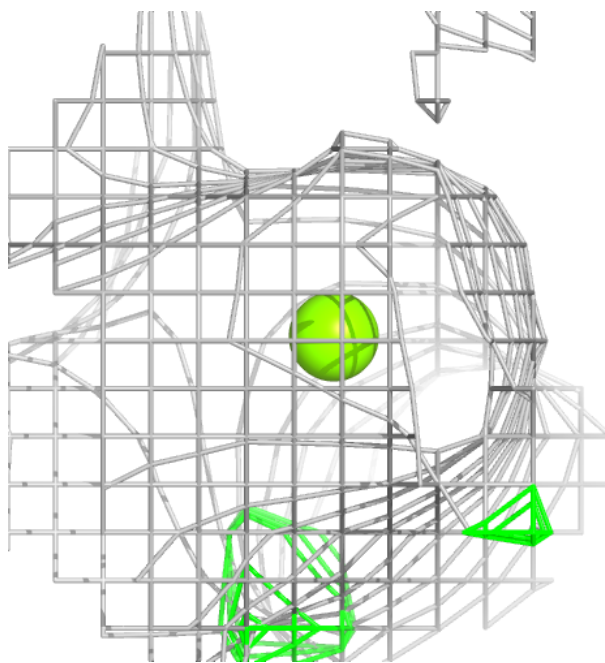
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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Atoms</b>	<b>RSCC</b>	<b>RSR</b>	<b>B-factors(<math>\text{\AA}^2</math>)</b>	<b>Q&lt;0.9</b>
3	GOL	A	403	6/6	0.98	0.04	38,43,45,47	0
3	GOL	D	403	6/6	0.98	0.05	63,65,67,71	0
2	MG	B	401	1/1	0.99	0.03	39,39,39,39	0
2	MG	C	401	1/1	0.99	0.05	68,68,68,68	0
2	MG	A	401	1/1	1.00	0.01	31,31,31,31	0
2	MG	A	402	1/1	1.00	0.03	27,27,27,27	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.

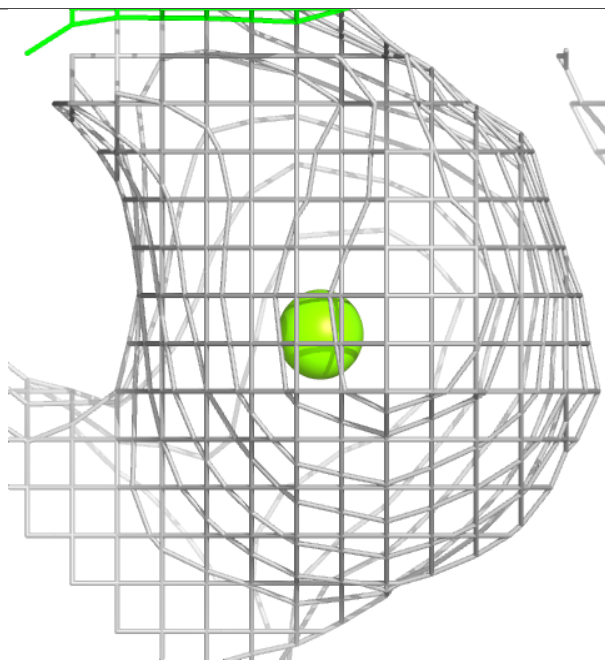
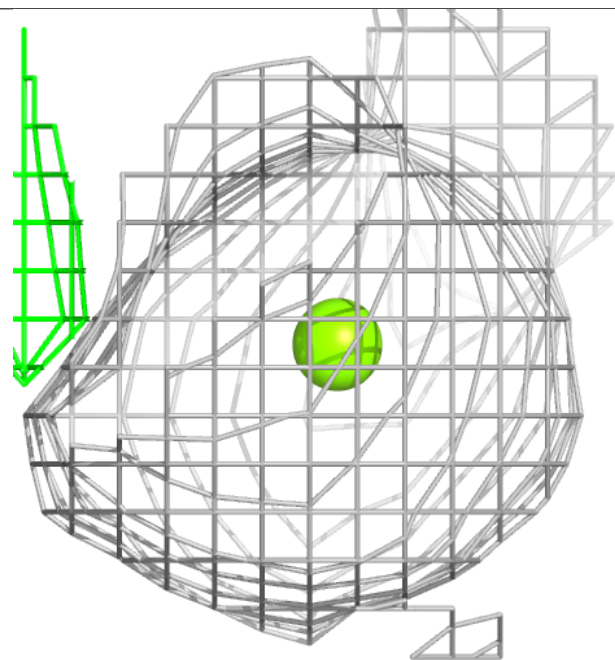
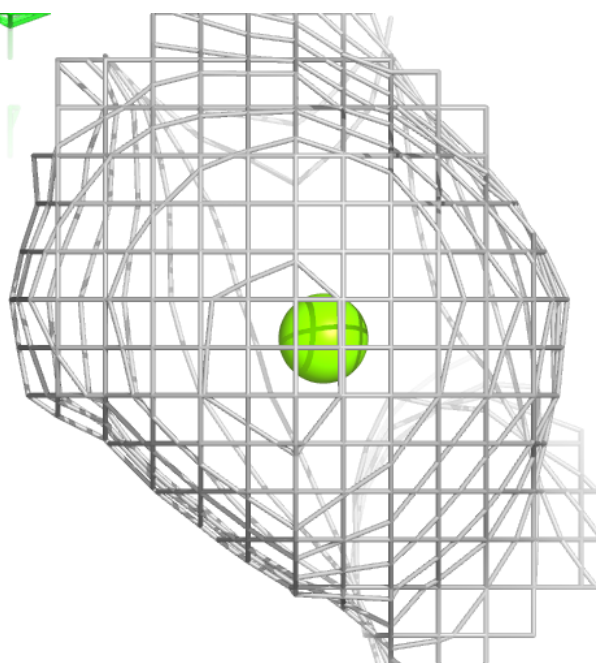
**Electron density around MG B 401:**

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



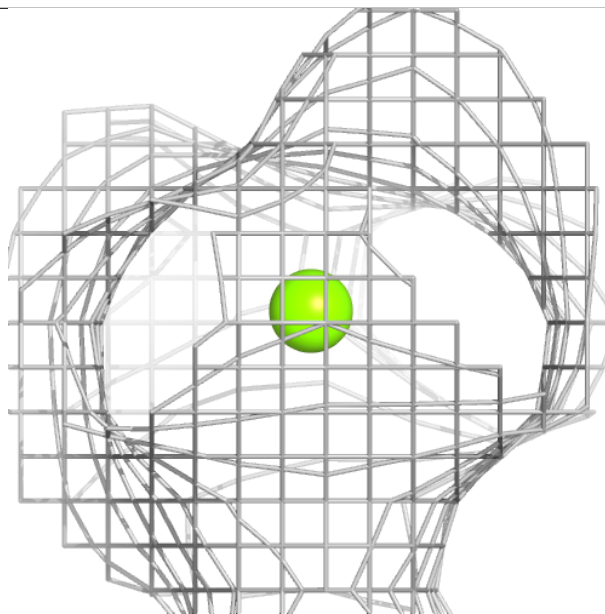
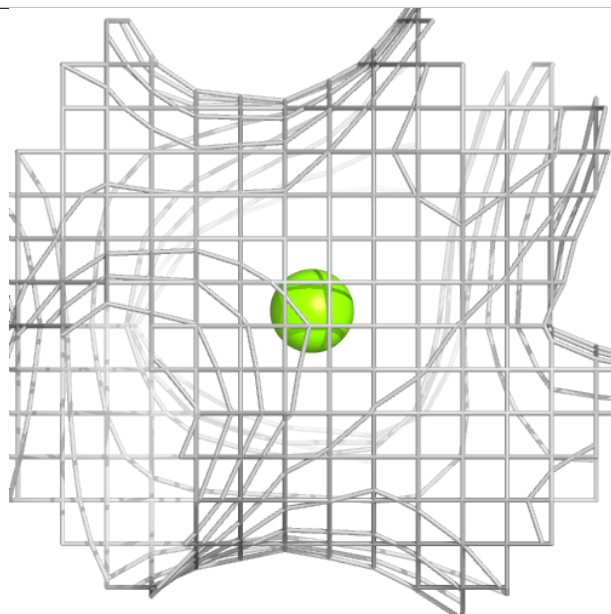
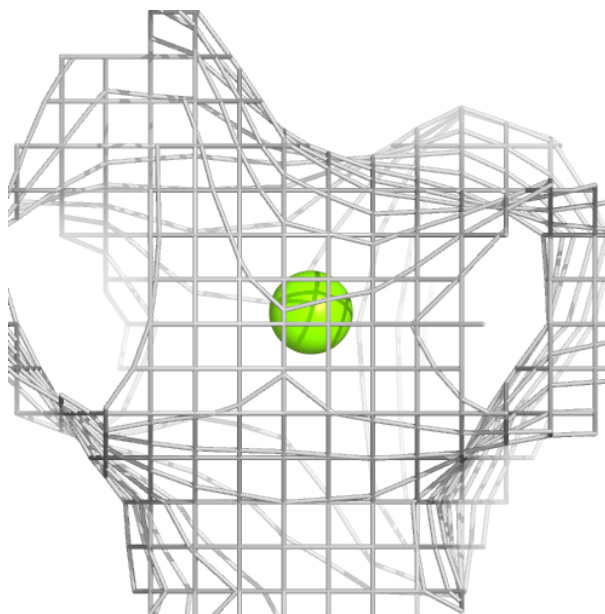
**Electron density around MG C 401:**

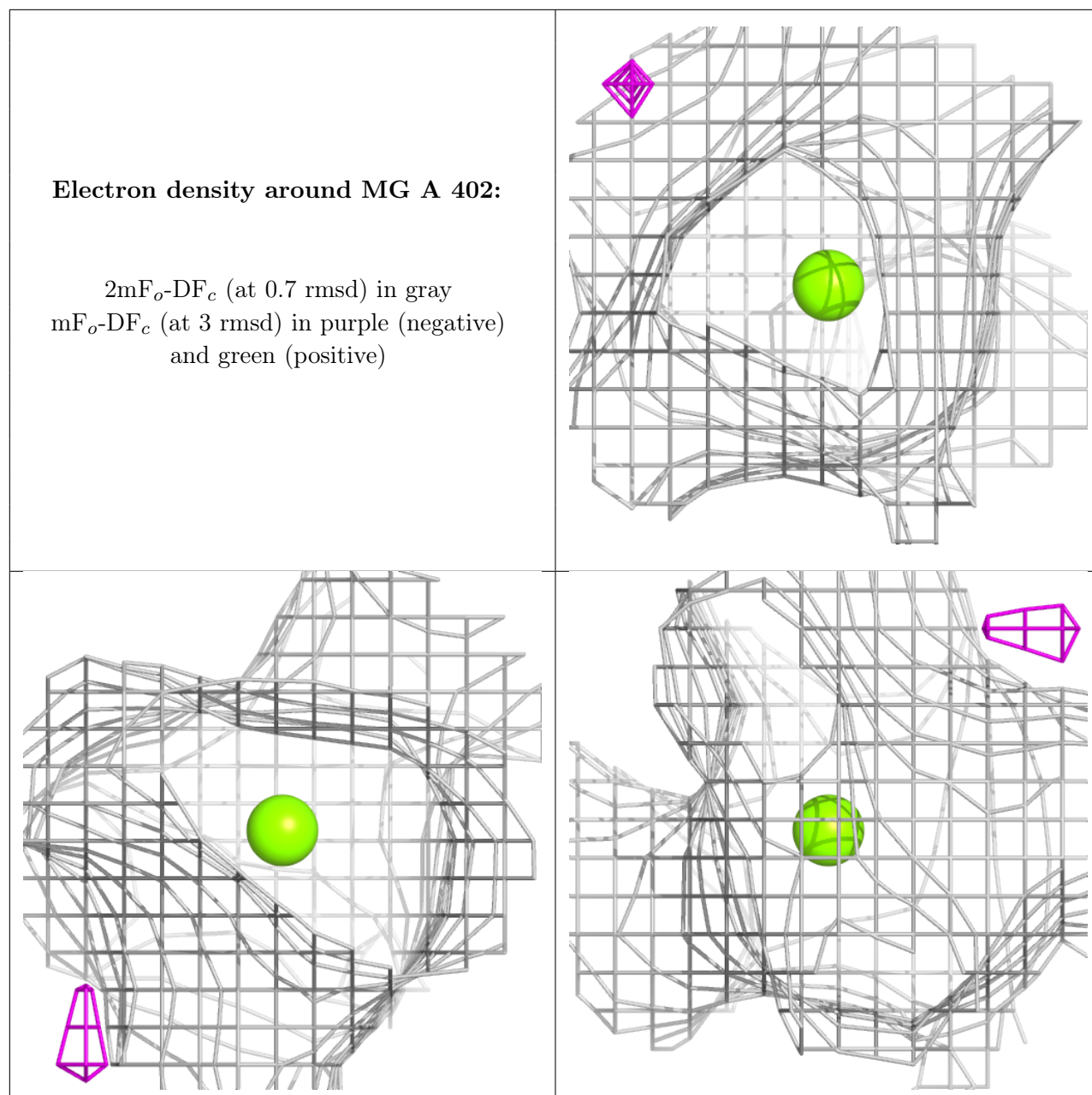
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around MG A 401:**

$2mF_o-DF_c$  (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.