



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:34 PM UTC

PDB ID : 7YE3 / pdb_00007ye3
Title : Crystal structure of Lactobacillus rhamnosus 4-deoxy-L-threo-5-hexosulose-urionate ketol-isomerase KduI complexed with MES
Authors : Yamamoto, Y.; Oiki, S.; Takase, R.; Mikami, B.; Hashimoto, W.
Deposited on : 2022-07-05
Resolution : 2.55 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

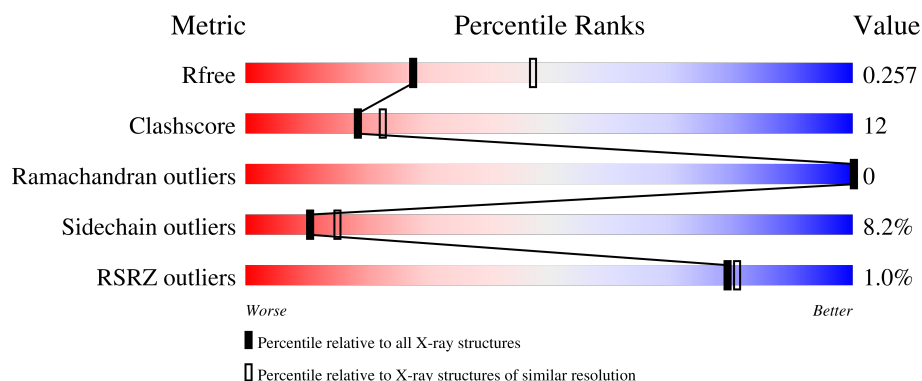
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	289	
1	B	289	
1	C	289	
1	D	289	
1	E	289	

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Mol	Chain	Length	Quality of chain
1	F	289	2% 62% 29% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13292 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 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2222	1409	375	421	17			
1	B	279	Total	C	N	O	S	0	0	0
			2243	1423	378	424	18			
1	C	279	Total	C	N	O	S	0	0	0
			2243	1423	378	424	18			
1	D	261	Total	C	N	O	S	0	0	0
			2104	1339	356	393	16			
1	E	271	Total	C	N	O	S	0	0	0
			2182	1386	369	410	17			
1	F	278	Total	C	N	O	S	0	0	0
			2235	1417	377	423	18			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	282	LEU	-	expression tag	UNP C2JUP1
A	283	GLU	-	expression tag	UNP C2JUP1
A	284	HIS	-	expression tag	UNP C2JUP1
A	285	HIS	-	expression tag	UNP C2JUP1
A	286	HIS	-	expression tag	UNP C2JUP1
A	287	HIS	-	expression tag	UNP C2JUP1
A	288	HIS	-	expression tag	UNP C2JUP1
A	289	HIS	-	expression tag	UNP C2JUP1
B	282	LEU	-	expression tag	UNP C2JUP1
B	283	GLU	-	expression tag	UNP C2JUP1
B	284	HIS	-	expression tag	UNP C2JUP1
B	285	HIS	-	expression tag	UNP C2JUP1
B	286	HIS	-	expression tag	UNP C2JUP1
B	287	HIS	-	expression tag	UNP C2JUP1
B	288	HIS	-	expression tag	UNP C2JUP1
B	289	HIS	-	expression tag	UNP C2JUP1
C	282	LEU	-	expression tag	UNP C2JUP1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	283	GLU	-	expression tag	UNP C2JUP1
C	284	HIS	-	expression tag	UNP C2JUP1
C	285	HIS	-	expression tag	UNP C2JUP1
C	286	HIS	-	expression tag	UNP C2JUP1
C	287	HIS	-	expression tag	UNP C2JUP1
C	288	HIS	-	expression tag	UNP C2JUP1
C	289	HIS	-	expression tag	UNP C2JUP1
D	282	LEU	-	expression tag	UNP C2JUP1
D	283	GLU	-	expression tag	UNP C2JUP1
D	284	HIS	-	expression tag	UNP C2JUP1
D	285	HIS	-	expression tag	UNP C2JUP1
D	286	HIS	-	expression tag	UNP C2JUP1
D	287	HIS	-	expression tag	UNP C2JUP1
D	288	HIS	-	expression tag	UNP C2JUP1
D	289	HIS	-	expression tag	UNP C2JUP1
E	282	LEU	-	expression tag	UNP C2JUP1
E	283	GLU	-	expression tag	UNP C2JUP1
E	284	HIS	-	expression tag	UNP C2JUP1
E	285	HIS	-	expression tag	UNP C2JUP1
E	286	HIS	-	expression tag	UNP C2JUP1
E	287	HIS	-	expression tag	UNP C2JUP1
E	288	HIS	-	expression tag	UNP C2JUP1
E	289	HIS	-	expression tag	UNP C2JUP1
F	282	LEU	-	expression tag	UNP C2JUP1
F	283	GLU	-	expression tag	UNP C2JUP1
F	284	HIS	-	expression tag	UNP C2JUP1
F	285	HIS	-	expression tag	UNP C2JUP1
F	286	HIS	-	expression tag	UNP C2JUP1
F	287	HIS	-	expression tag	UNP C2JUP1
F	288	HIS	-	expression tag	UNP C2JUP1
F	289	HIS	-	expression tag	UNP C2JUP1

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

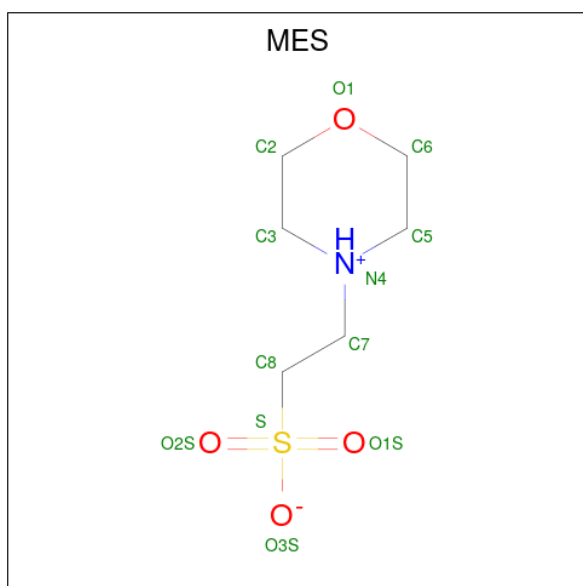
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	B	2	Total	O	0	0
			2	2		

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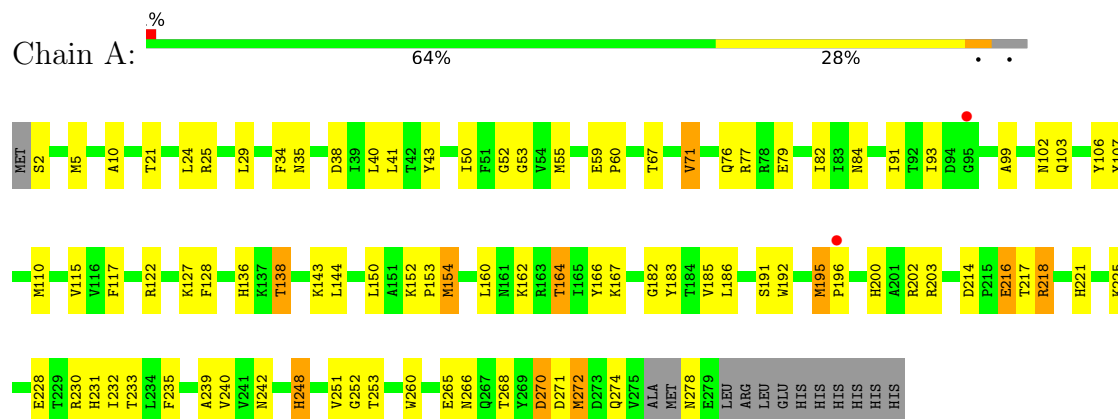
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	3	Total 3	O 3	0	0
4	E	1	Total 1	O 1	0	0

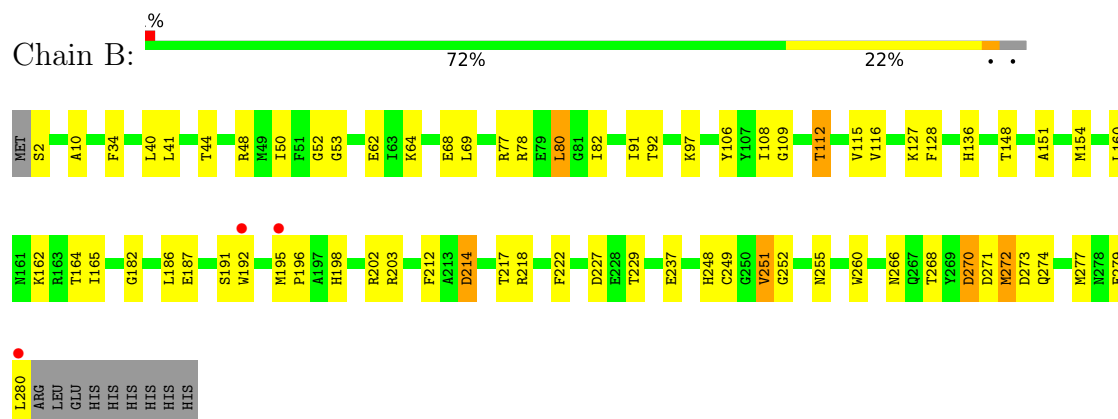
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

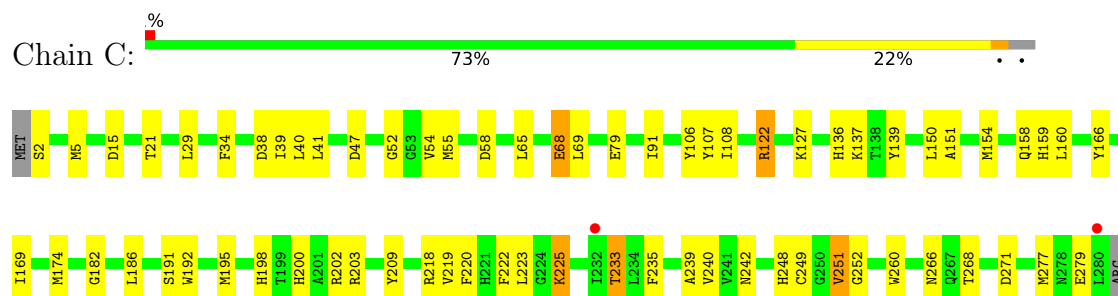
- Molecule 1: 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase



- Molecule 1: 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase



- Molecule 1: 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	93.03Å 189.10Å 114.85Å 90.00° 107.12° 90.00°	Depositor
Resolution (Å)	37.57 – 2.55 37.57 – 2.55	Depositor EDS
% Data completeness (in resolution range)	98.9 (37.57-2.55) 98.9 (37.57-2.55)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.10.1 _2155	Depositor
R, R_{free}	0.193 , 0.256 0.196 , 0.257	Depositor DCC
R_{free} test set	3038 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	66.8	Xtriage
Anisotropy	0.691	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 60.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13292	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MES, ZN

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	0.36	0/2281	0.61	0/3090
1	B	0.36	0/2303	0.65	0/3121
1	C	0.36	0/2303	0.66	0/3121
1	D	0.41	0/2159	0.66	0/2920
1	E	0.34	0/2238	0.62	0/3027
1	F	0.38	0/2295	0.69	2/3110 (0.1%)
All	All	0.37	0/13579	0.65	2/18389 (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	F	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	277	MET	CA-C-N	5.03	130.83	121.62
1	F	277	MET	C-N-CA	5.03	130.83	121.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	60	PRO	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	2222	0	2118	61	0
1	B	2243	0	2144	54	0
1	C	2243	0	2144	55	0
1	D	2104	0	2020	55	0
1	E	2182	0	2090	54	0
1	F	2235	0	2133	76	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	12	0	12	0	0
3	B	12	0	12	0	0
3	C	12	0	12	0	0
3	F	12	0	12	1	0
4	A	3	0	0	0	0
4	B	2	0	0	0	0
4	C	3	0	0	0	0
4	E	1	0	0	0	0
All	All	13292	0	12697	311	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 12.

All (311) 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:F:63:ILE:HD13	1:F:63:ILE:H	1.33	0.93
1:D:5:MET:HE2	1:D:43:TYR:HB2	1.49	0.93
1:A:5:MET:HE2	1:A:43:TYR:HB2	1.53	0.88
1:A:55:MET:HE2	1:A:127:LYS:HG2	1.56	0.86
1:A:25:ARG:HH11	1:E:280:LEU:HD23	1.42	0.85
1:A:233:THR:H	1:E:280:LEU:HD22	1.41	0.84
1:F:54:VAL:HG23	1:F:128:PHE:HB2	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:154:MET:HG3	1:F:165:ILE:HD12	1.61	0.81
1:A:218:ARG:HH21	1:A:235:PHE:HE1	1.29	0.79
1:B:160:LEU:HD23	1:C:160:LEU:HD23	1.62	0.79
1:B:80:LEU:HD13	1:B:82:ILE:HD11	1.67	0.75
1:F:191:SER:HB2	1:F:252:GLY:H	1.52	0.75
1:F:178:GLN:HG2	1:F:263:CYS:HB2	1.69	0.75
1:A:164:THR:HB	1:A:166:TYR:HE1	1.51	0.74
1:C:191:SER:HB2	1:C:252:GLY:H	1.53	0.72
1:D:191:SER:HB2	1:D:252:GLY:H	1.52	0.72
1:E:150:LEU:HB2	1:E:167:LYS:HD2	1.71	0.72
1:D:161:ASN:O	1:D:163:ARG:HG3	1.90	0.72
1:F:65:LEU:HB3	1:F:69:LEU:HD22	1.72	0.72
1:E:191:SER:HB2	1:E:252:GLY:H	1.54	0.71
1:D:160:LEU:HD23	1:F:160:LEU:HD23	1.73	0.71
1:F:82:ILE:HG23	1:F:106:TYR:HB3	1.73	0.71
1:A:59:GLU:HG3	1:A:60:PRO:HD2	1.72	0.70
1:B:191:SER:HB2	1:B:252:GLY:H	1.56	0.70
1:F:96:ARG:NH2	1:F:97:LYS:O	2.25	0.70
1:C:55:MET:HE2	1:C:127:LYS:HG2	1.74	0.68
1:A:24:LEU:HB3	1:A:232:ILE:HD11	1.74	0.68
1:A:160:LEU:HD23	1:E:160:LEU:HD23	1.76	0.68
1:B:218:ARG:HG2	1:C:277:MET:HE3	1.76	0.68
1:B:280:LEU:HD22	1:C:21:THR:HG21	1.74	0.67
1:E:55:MET:HE2	1:E:127:LYS:HG2	1.77	0.67
1:A:152:LYS:HD3	1:A:167:LYS:HE2	1.75	0.67
1:D:251:VAL:HG21	1:F:251:VAL:HG21	1.76	0.67
1:E:39:ILE:HD13	1:E:63:ILE:HG12	1.75	0.67
1:B:270:ASP:OD1	1:B:270:ASP:N	2.28	0.66
1:B:277:MET:HB3	1:C:218:ARG:HD2	1.78	0.66
1:F:63:ILE:HD11	1:F:115:VAL:HG23	1.78	0.65
1:F:106:TYR:CE2	1:F:143:LYS:HD2	2.32	0.65
1:D:202:ARG:O	1:D:265:GLU:N	2.28	0.64
1:C:34:PHE:HB3	1:C:55:MET:CE	2.27	0.64
1:C:137:LYS:NZ	1:C:139:TYR:OH	2.31	0.64
1:B:62:GLU:HG3	1:B:115:VAL:O	1.98	0.64
1:F:39:ILE:HG22	1:F:61:LEU:HD22	1.78	0.64
1:A:34:PHE:HB3	1:A:55:MET:CE	2.28	0.64
1:D:58:ASP:HB3	1:D:122:ARG:HH22	1.62	0.63
1:D:65:LEU:HD22	1:D:68:GLU:HG3	1.81	0.63
1:A:270:ASP:OD1	1:A:270:ASP:N	2.31	0.62
1:F:39:ILE:HB	1:F:54:VAL:HG12	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:227:ASP:O	1:E:280:LEU:HA	2.00	0.61
1:F:84:ASN:HB2	1:F:100:MET:HE2	1.82	0.61
1:B:280:LEU:HG	1:C:233:THR:HG23	1.82	0.61
1:F:214:ASP:O	1:F:217:THR:HG23	2.01	0.61
1:C:39:ILE:HD12	1:C:54:VAL:HG22	1.82	0.61
1:E:15:ASP:OD2	1:F:11:HIS:ND1	2.22	0.61
1:B:92:THR:HA	1:B:97:LYS:HA	1.83	0.60
1:E:34:PHE:HB3	1:E:55:MET:CE	2.32	0.60
1:A:41:LEU:HD23	1:A:52:GLY:HA3	1.83	0.60
1:C:169:ILE:HA	1:C:174:MET:HE1	1.83	0.60
1:E:41:LEU:HD23	1:E:52:GLY:HA3	1.83	0.60
1:D:39:ILE:HG12	1:D:54:VAL:HB	1.84	0.59
1:D:167:LYS:HG2	1:D:170:ASP:HB2	1.83	0.59
1:E:90:ALA:HB3	1:E:97:LYS:HE2	1.82	0.59
1:A:77:ARG:HD3	1:B:266:ASN:HA	1.85	0.58
1:A:99:ALA:O	1:A:143:LYS:NZ	2.29	0.58
1:B:279:GLU:O	1:C:233:THR:OG1	2.22	0.58
1:E:11:HIS:ND1	1:F:15:ASP:OD2	2.32	0.58
1:D:6:VAL:HG22	1:D:42:THR:HG22	1.85	0.57
1:E:203:ARG:NH1	1:E:266:ASN:OD1	2.37	0.57
1:A:228:GLU:HA	1:E:21:THR:HG21	1.86	0.57
1:F:3:PHE:CD2	1:F:39:ILE:HG12	2.40	0.57
1:A:202:ARG:NE	1:B:68:GLU:O	2.38	0.57
1:F:93:ILE:HG22	1:F:115:VAL:HG12	1.86	0.57
1:F:108:ILE:HD13	1:F:115:VAL:HG11	1.87	0.57
1:F:195:MET:HB3	1:F:196:PRO:HD3	1.85	0.57
1:C:195:MET:HE2	1:C:277:MET:HE1	1.87	0.57
1:F:90:ALA:N	1:F:118:THR:O	2.29	0.57
1:D:182:GLY:HA3	1:D:260:TRP:CZ2	2.39	0.57
1:B:227:ASP:O	1:B:280:LEU:HA	2.04	0.56
1:F:197:ALA:HB1	1:F:247:ILE:HB	1.87	0.56
1:B:203:ARG:HH12	1:B:271:ASP:HB3	1.71	0.56
1:B:48:ARG:O	1:B:78:ARG:NH2	2.38	0.56
1:B:162:LYS:HE2	1:B:187:GLU:HG3	1.87	0.56
1:C:40:LEU:O	1:C:52:GLY:HA3	2.05	0.56
1:E:39:ILE:O	1:E:39:ILE:HG13	2.06	0.56
1:E:110:MET:HG2	1:E:111:GLY:N	2.19	0.56
1:B:218:ARG:NH1	1:C:277:MET:O	2.36	0.56
1:A:202:ARG:HD2	1:A:202:ARG:N	2.21	0.56
1:D:4:SER:HB3	1:D:40:LEU:HD23	1.88	0.56
1:C:34:PHE:CD1	1:C:127:LYS:HB3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:ASP:OD2	1:D:122:ARG:NH1	2.35	0.55
1:D:152:LYS:HB3	1:D:165:ILE:HG22	1.86	0.55
1:C:68:GLU:O	1:D:202:ARG:NH1	2.40	0.55
1:B:222:PHE:HB2	1:B:249:CYS:HB2	1.88	0.55
1:B:218:ARG:HH12	1:C:279:GLU:H	1.51	0.55
1:B:214:ASP:O	1:B:217:THR:HG22	2.06	0.55
1:D:102:ASN:OD1	1:D:103:GLN:HG2	2.07	0.55
1:E:200:HIS:ND1	1:E:200:HIS:O	2.39	0.54
1:F:25:ARG:O	1:F:29:LEU:HB3	2.06	0.54
1:E:92:THR:HA	1:E:97:LYS:HA	1.90	0.54
1:E:192:TRP:HB3	1:E:195:MET:HG2	1.89	0.54
1:A:191:SER:HB2	1:A:252:GLY:H	1.73	0.54
1:D:100:MET:SD	1:D:106:TYR:HD2	2.30	0.54
1:B:212:PHE:HB3	1:B:217:THR:CG2	2.38	0.54
1:F:74:PHE:HE2	1:F:80:LEU:HD12	1.73	0.53
1:F:63:ILE:H	1:F:63:ILE:CD1	2.07	0.53
1:C:202:ARG:NE	1:D:68:GLU:O	2.42	0.53
1:F:277:MET:HE2	1:F:277:MET:HA	1.91	0.53
1:A:150:LEU:HD11	1:A:167:LYS:HD2	1.91	0.53
1:B:229:THR:OG1	1:B:280:LEU:HD21	2.08	0.53
1:C:15:ASP:OD2	1:D:11:HIS:ND1	2.38	0.53
1:E:29:LEU:HD12	1:E:239:ALA:O	2.08	0.53
1:B:2:SER:OG	1:B:2:SER:O	2.23	0.52
1:D:2:SER:OG	1:D:38:ASP:OD1	2.22	0.52
1:C:2:SER:OG	1:C:38:ASP:OD1	2.25	0.52
1:F:198:HIS:H	1:F:275:VAL:HG13	1.74	0.52
1:B:151:ALA:HA	1:B:165:ILE:O	2.10	0.52
1:C:65:LEU:HB3	1:C:69:LEU:HD13	1.91	0.52
1:C:218:ARG:HH12	1:C:235:PHE:HD1	1.58	0.52
1:D:5:MET:HE3	1:D:50:ILE:HG23	1.90	0.52
1:F:58:ASP:HB2	1:F:59:GLU:CD	2.35	0.51
1:A:214:ASP:O	1:A:217:THR:HG23	2.10	0.51
1:C:191:SER:HB2	1:C:252:GLY:N	2.23	0.51
1:D:191:SER:HB2	1:D:252:GLY:N	2.25	0.51
1:D:40:LEU:O	1:D:52:GLY:HA3	2.10	0.51
1:D:21:THR:OG1	1:F:228:GLU:OE1	2.28	0.51
1:A:10:ALA:HB3	1:B:10:ALA:HB3	1.92	0.51
1:A:202:ARG:HD3	1:A:271:ASP:OD2	2.11	0.51
1:B:255:ASN:OD1	1:C:158:GLN:NE2	2.43	0.51
1:E:201:ALA:HB1	1:E:202:ARG:HH21	1.75	0.51
1:F:221:HIS:CD2	1:F:240:VAL:HG11	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:VAL:HG22	1:E:76:GLN:OE1	2.11	0.51
1:A:29:LEU:HD12	1:A:239:ALA:O	2.11	0.50
1:E:195:MET:N	1:E:196:PRO:HD2	2.26	0.50
1:B:202:ARG:HD2	1:B:202:ARG:N	2.27	0.50
1:C:220:PHE:HD1	1:C:233:THR:HG22	1.77	0.50
1:D:29:LEU:HD12	1:D:239:ALA:O	2.12	0.50
1:D:224:GLY:HA2	1:D:245:TRP:HZ3	1.76	0.50
1:B:41:LEU:HD23	1:B:52:GLY:HA3	1.94	0.49
1:A:272:MET:HE1	1:A:274:GLN:OE1	2.13	0.49
1:A:5:MET:HE3	1:A:50:ILE:HG23	1.93	0.49
1:A:2:SER:HB2	1:A:38:ASP:OD1	2.13	0.49
1:C:222:PHE:HB2	1:C:249:CYS:HB2	1.94	0.49
1:D:2:SER:OG	1:D:2:SER:O	2.30	0.48
1:F:157:GLN:CA	1:F:157:GLN:HE21	2.25	0.48
1:F:91:ILE:HG22	1:F:117:PHE:CD2	2.49	0.48
1:D:92:THR:HA	1:D:97:LYS:HA	1.96	0.48
1:F:220:PHE:O	1:F:250:GLY:HA2	2.14	0.48
1:B:160:LEU:HD23	1:C:160:LEU:CD2	2.38	0.48
1:F:191:SER:HB2	1:F:252:GLY:N	2.25	0.48
1:D:99:ALA:O	1:D:143:LYS:NZ	2.38	0.48
1:C:192:TRP:CD2	1:C:251:VAL:HG13	2.49	0.48
1:C:203:ARG:NH2	1:C:271:ASP:O	2.29	0.48
1:C:225:LYS:HB3	1:C:225:LYS:HE3	1.62	0.48
1:D:200:HIS:CD2	1:D:203:ARG:HB3	2.48	0.48
1:A:182:GLY:HA3	1:A:260:TRP:CZ2	2.49	0.48
1:C:39:ILE:CD1	1:C:54:VAL:HG13	2.44	0.48
1:F:110:MET:O	1:F:138:THR:OG1	2.19	0.48
1:F:200:HIS:O	1:F:200:HIS:ND1	2.46	0.48
1:B:108:ILE:HD13	1:B:115:VAL:HG21	1.96	0.47
1:F:82:ILE:HD11	1:F:128:PHE:HD1	1.79	0.47
1:A:265:GLU:O	1:B:77:ARG:HD3	2.14	0.47
1:E:103:GLN:O	1:E:168:TYR:OH	2.24	0.47
1:B:195:MET:HB3	1:B:196:PRO:HD3	1.96	0.47
1:C:58:ASP:OD1	1:C:122:ARG:HD2	2.14	0.47
1:D:78:ARG:HG2	1:D:134:PRO:HA	1.97	0.47
1:C:91:ILE:HD12	1:C:108:ILE:HD11	1.94	0.47
1:A:195:MET:HB3	1:A:196:PRO:HD3	1.96	0.47
1:B:109:GLY:O	1:B:112:THR:HG23	2.15	0.47
1:B:191:SER:HB2	1:B:252:GLY:N	2.27	0.47
1:B:192:TRP:CZ3	1:B:251:VAL:HG22	2.49	0.47
1:E:182:GLY:HA3	1:E:260:TRP:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:266:ASN:ND2	1:F:69:LEU:O	2.46	0.47
1:A:218:ARG:HH12	1:E:279:GLU:CB	2.27	0.47
1:C:202:ARG:N	1:C:202:ARG:HD2	2.29	0.47
1:E:3:PHE:CE2	1:E:39:ILE:HD11	2.50	0.47
1:F:39:ILE:HB	1:F:54:VAL:CG1	2.45	0.47
1:F:54:VAL:HB	1:F:61:LEU:HD13	1.97	0.47
1:F:105:GLY:HA3	1:F:144:LEU:HB2	1.96	0.47
1:A:34:PHE:CD1	1:A:127:LYS:HB3	2.50	0.47
1:B:50:ILE:HG13	1:B:78:ARG:NH2	2.30	0.47
1:A:251:VAL:HG21	1:E:251:VAL:HG11	1.97	0.47
1:B:62:GLU:OE1	1:B:64:LYS:NZ	2.47	0.47
1:F:154:MET:HE2	1:F:154:MET:HA	1.97	0.47
1:F:5:MET:HE1	1:F:50:ILE:HD13	1.97	0.47
1:D:200:HIS:O	1:D:202:ARG:N	2.48	0.46
1:E:92:THR:OG1	1:E:116:VAL:HG22	2.15	0.46
1:A:53:GLY:HA2	1:A:128:PHE:O	2.15	0.46
1:A:218:ARG:HH12	1:E:279:GLU:HB2	1.79	0.46
1:A:266:ASN:HA	1:B:77:ARG:HD3	1.96	0.46
1:B:198:HIS:CD2	1:B:272:MET:HE2	2.50	0.46
1:B:280:LEU:HD22	1:C:21:THR:CG2	2.44	0.46
1:A:153:PRO:O	1:A:154:MET:HG2	2.16	0.46
1:C:159:HIS:C	1:C:160:LEU:HD12	2.41	0.46
1:D:30:MET:SD	1:D:42:THR:HG23	2.56	0.46
3:F:302:MES:H51	3:F:302:MES:H82	1.54	0.46
1:B:182:GLY:HA3	1:B:260:TRP:CE2	2.51	0.46
1:E:69:LEU:HD22	1:F:265:GLU:OE1	2.16	0.46
1:F:91:ILE:HA	1:F:116:VAL:O	2.16	0.46
1:E:203:ARG:HA	1:E:264:GLY:HA3	1.97	0.46
1:A:230:ARG:HH12	1:E:21:THR:CG2	2.27	0.46
1:D:150:LEU:HD13	1:D:173:GLN:OE1	2.16	0.46
1:A:242:ASN:CG	1:A:248:HIS:HB3	2.41	0.46
1:E:244:SER:HB2	1:F:45:TYR:HE2	1.81	0.46
1:F:170:ASP:OD1	1:F:172:SER:OG	2.31	0.46
1:D:218:ARG:HH21	1:D:233:THR:HG22	1.80	0.45
1:F:209:TYR:OH	1:F:221:HIS:ND1	2.31	0.45
1:B:280:LEU:HG	1:C:233:THR:CG2	2.46	0.45
1:C:79:GLU:OE2	1:C:107:TYR:OH	2.30	0.45
1:D:200:HIS:CE1	1:D:203:ARG:O	2.69	0.45
1:A:40:LEU:O	1:A:52:GLY:HA3	2.16	0.45
1:F:242:ASN:OD1	1:F:248:HIS:HB3	2.16	0.45
1:A:216:GLU:H	1:A:216:GLU:HG3	1.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ILE:HA	1:B:116:VAL:O	2.17	0.45
1:E:104:ASP:OD1	1:E:145:PRO:HA	2.17	0.45
1:E:110:MET:HE1	1:E:136:HIS:C	2.42	0.45
1:A:84:ASN:O	1:A:103:GLN:N	2.45	0.44
1:C:136:HIS:ND1	1:D:177:CYS:HB3	2.32	0.44
1:F:82:ILE:CG2	1:F:106:TYR:HB3	2.44	0.44
1:D:80:LEU:HD11	1:D:130:VAL:HB	1.99	0.44
1:E:19:TYR:CD1	1:E:23:LYS:HD3	2.52	0.44
1:F:39:ILE:O	1:F:39:ILE:HG13	2.11	0.44
1:F:53:GLY:HA2	1:F:128:PHE:O	2.17	0.44
1:F:182:GLY:HA3	1:F:260:TRP:CE2	2.52	0.44
1:A:150:LEU:HD12	1:A:150:LEU:O	2.17	0.44
1:E:200:HIS:CE1	1:E:248:HIS:NE2	2.85	0.44
1:A:192:TRP:CE3	1:A:251:VAL:HB	2.53	0.44
1:C:182:GLY:HA3	1:C:260:TRP:CZ2	2.53	0.44
1:A:192:TRP:CZ3	1:A:251:VAL:HB	2.53	0.44
1:B:53:GLY:HA2	1:B:128:PHE:O	2.17	0.44
1:C:266:ASN:HA	1:D:77:ARG:HD3	2.00	0.44
1:B:44:THR:O	1:B:48:ARG:HA	2.19	0.43
1:A:253:THR:HB	1:E:195:MET:HE1	2.00	0.43
1:A:34:PHE:HB3	1:A:55:MET:HE3	1.99	0.43
1:C:198:HIS:HD2	1:C:200:HIS:CD2	2.37	0.43
1:D:54:VAL:HG22	1:D:128:PHE:HB2	2.00	0.43
1:C:2:SER:OG	1:C:2:SER:O	2.36	0.43
1:E:54:VAL:HG12	1:E:56:PRO:HD3	1.99	0.43
1:E:91:ILE:HD11	1:E:93:ILE:HD11	2.00	0.43
1:A:102:ASN:OD1	1:A:103:GLN:HG2	2.19	0.43
1:C:5:MET:HA	1:C:41:LEU:O	2.18	0.43
1:D:234:LEU:HD23	1:D:234:LEU:HA	1.64	0.43
1:B:91:ILE:HG13	1:B:91:ILE:O	2.17	0.43
1:D:41:LEU:HD23	1:D:52:GLY:HA3	1.99	0.43
1:A:79:GLU:OE2	1:A:107:TYR:OH	2.33	0.43
1:A:110:MET:O	1:A:138:THR:HB	2.19	0.43
1:B:272:MET:HE3	1:B:272:MET:HB3	1.75	0.43
1:E:222:PHE:HB2	1:E:249:CYS:HB2	2.01	0.43
1:A:136:HIS:HB2	1:B:136:HIS:HB2	1.99	0.43
1:D:174:MET:HE2	1:D:174:MET:HB3	1.65	0.43
1:F:11:HIS:NE2	1:F:27:GLU:OE2	2.52	0.43
1:E:25:ARG:O	1:E:29:LEU:HB3	2.18	0.43
1:F:2:SER:O	1:F:38:ASP:HA	2.19	0.43
1:F:157:GLN:HE21	1:F:157:GLN:HA	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:150:LEU:HD12	1:F:150:LEU:O	2.18	0.42
1:F:202:ARG:NH2	1:F:271:ASP:OD1	2.52	0.42
1:A:35:ASN:ND2	1:A:38:ASP:OD2	2.50	0.42
1:A:166:TYR:HB2	1:A:183:TYR:HB3	2.02	0.42
1:B:40:LEU:O	1:B:52:GLY:HA3	2.20	0.42
1:C:220:PHE:CD1	1:C:233:THR:HG22	2.54	0.42
1:D:169:ILE:HA	1:D:174:MET:HE3	2.02	0.42
1:E:136:HIS:ND1	1:F:177:CYS:HB3	2.34	0.42
1:E:191:SER:HB2	1:E:252:GLY:N	2.29	0.42
1:F:198:HIS:CG	1:F:198:HIS:O	2.72	0.42
1:A:228:GLU:OE2	1:E:21:THR:HG23	2.19	0.42
1:B:127:LYS:NZ	1:B:237:GLU:OE2	2.41	0.42
1:C:240:VAL:HG12	1:C:242:ASN:OD1	2.20	0.42
1:E:61:LEU:HD23	1:E:61:LEU:HA	1.90	0.42
1:E:198:HIS:HB2	1:E:273:ASP:O	2.18	0.42
1:A:152:LYS:HB2	1:A:152:LYS:HE3	1.90	0.42
1:C:200:HIS:ND1	1:C:203:ARG:O	2.52	0.42
1:D:203:ARG:HD2	1:D:262:MET:SD	2.60	0.42
1:F:89:GLY:HA2	1:F:119:SER:HA	2.01	0.42
1:F:143:LYS:HD3	1:F:143:LYS:HA	1.73	0.42
1:D:48:ARG:O	1:D:78:ARG:NH2	2.41	0.42
1:D:91:ILE:HD11	1:D:106:TYR:CD2	2.54	0.42
1:F:56:PRO:HB3	1:F:61:LEU:HG	2.01	0.42
1:F:91:ILE:HG23	1:F:100:MET:SD	2.59	0.42
1:F:234:LEU:HD23	1:F:234:LEU:HA	1.70	0.42
1:D:182:GLY:HA3	1:D:260:TRP:CE2	2.54	0.42
1:B:229:THR:H	1:B:280:LEU:HD21	1.85	0.41
1:B:229:THR:HG1	1:B:280:LEU:HD21	1.85	0.41
1:C:151:ALA:HB2	1:C:166:TYR:CE1	2.55	0.41
1:C:209:TYR:CE2	1:C:219:VAL:HG11	2.55	0.41
1:D:75:LEU:HB2	1:D:112:THR:O	2.19	0.41
1:F:139:TYR:CE1	1:F:175:ASP:HB3	2.55	0.41
1:A:21:THR:HG23	1:E:228:GLU:OE2	2.20	0.41
1:C:198:HIS:CD2	1:C:200:HIS:CD2	3.09	0.41
1:C:29:LEU:HD12	1:C:239:ALA:O	2.20	0.41
1:E:265:GLU:OE2	1:F:69:LEU:HG	2.19	0.41
1:F:82:ILE:HD11	1:F:128:PHE:CD1	2.56	0.41
1:A:242:ASN:OD1	1:A:248:HIS:HB3	2.21	0.41
1:C:47:ASP:OD1	1:D:48:ARG:NE	2.31	0.41
1:C:182:GLY:HA3	1:C:260:TRP:CE2	2.55	0.41
1:C:169:ILE:HA	1:C:174:MET:CE	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:HIS:CE1	1:D:248:HIS:HE2	2.37	0.41
1:D:218:ARG:HE	1:D:233:THR:CG2	2.34	0.41
1:A:200:HIS:ND1	1:A:203:ARG:O	2.54	0.41
1:D:91:ILE:HA	1:D:116:VAL:O	2.21	0.41
1:A:221:HIS:O	1:A:231:HIS:HA	2.22	0.40
1:F:56:PRO:HG2	1:F:119:SER:OG	2.21	0.40
1:F:74:PHE:CE2	1:F:80:LEU:HD12	2.53	0.40
1:F:150:LEU:HD21	1:F:167:LYS:HD2	2.03	0.40
1:A:71:VAL:CG2	1:A:76:GLN:HB3	2.51	0.40
1:B:34:PHE:CD1	1:B:127:LYS:HB3	2.56	0.40
1:F:63:ILE:HG12	1:F:63:ILE:O	2.20	0.40
1:A:82:ILE:HD13	1:A:117:PHE:CE2	2.56	0.40
1:F:198:HIS:HA	1:F:273:ASP:O	2.21	0.40
1:E:169:ILE:HA	1:E:174:MET:HE3	2.03	0.40
1:F:174:MET:HE2	1:F:174:MET:HB3	1.67	0.40
1:D:56:PRO:HG2	1:D:119:SER:OG	2.22	0.40
1:E:73:PHE:CZ	1:E:113:GLN:HG2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	272/289 (94%)	266 (98%)	6 (2%)	0	100	100
1	B	277/289 (96%)	272 (98%)	5 (2%)	0	100	100
1	C	277/289 (96%)	270 (98%)	7 (2%)	0	100	100
1	D	256/289 (89%)	250 (98%)	6 (2%)	0	100	100
1	E	263/289 (91%)	257 (98%)	6 (2%)	0	100	100
1	F	276/289 (96%)	266 (96%)	10 (4%)	0	100	100
All	All	1621/1734 (94%)	1581 (98%)	40 (2%)	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	241/253 (95%)	217 (90%)	24 (10%)	7	9
1	B	243/253 (96%)	227 (93%)	16 (7%)	15	21
1	C	243/253 (96%)	231 (95%)	12 (5%)	22	33
1	D	228/253 (90%)	207 (91%)	21 (9%)	8	11
1	E	237/253 (94%)	219 (92%)	18 (8%)	12	17
1	F	242/253 (96%)	216 (89%)	26 (11%)	6	7
All	All	1434/1518 (94%)	1317 (92%)	117 (8%)	10	15

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	THR
1	A	71	VAL
1	A	91	ILE
1	A	93	ILE
1	A	106	TYR
1	A	115	VAL
1	A	122	ARG
1	A	138	THR
1	A	144	LEU
1	A	154	MET
1	A	162	LYS
1	A	164	THR
1	A	185	VAL
1	A	186	LEU
1	A	195	MET
1	A	216	GLU
1	A	218	ARG
1	A	225	LYS
1	A	240	VAL

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Mol	Chain	Res	Type
1	A	248	HIS
1	A	268	THR
1	A	270	ASP
1	A	272	MET
1	A	278	ASN
1	B	69	LEU
1	B	80	LEU
1	B	106	TYR
1	B	112	THR
1	B	148	THR
1	B	154	MET
1	B	164	THR
1	B	186	LEU
1	B	214	ASP
1	B	248	HIS
1	B	251	VAL
1	B	268	THR
1	B	270	ASP
1	B	272	MET
1	B	273	ASP
1	B	274	GLN
1	C	68	GLU
1	C	106	TYR
1	C	122	ARG
1	C	150	LEU
1	C	154	MET
1	C	186	LEU
1	C	223	LEU
1	C	225	LYS
1	C	233	THR
1	C	248	HIS
1	C	251	VAL
1	C	268	THR
1	D	21	THR
1	D	27	GLU
1	D	54	VAL
1	D	58	ASP
1	D	68	GLU
1	D	93	ILE
1	D	106	TYR
1	D	110	MET
1	D	158	GLN

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Mol	Chain	Res	Type
1	D	163	ARG
1	D	164	THR
1	D	165	ILE
1	D	167	LYS
1	D	174	MET
1	D	193	ASN
1	D	195	MET
1	D	200	HIS
1	D	202	ARG
1	D	203	ARG
1	D	223	LEU
1	D	265	GLU
1	E	39	ILE
1	E	71	VAL
1	E	116	VAL
1	E	163	ARG
1	E	164	THR
1	E	167	LYS
1	E	185	VAL
1	E	195	MET
1	E	200	HIS
1	E	218	ARG
1	E	223	LEU
1	E	225	LYS
1	E	233	THR
1	E	240	VAL
1	E	251	VAL
1	E	272	MET
1	E	273	ASP
1	E	280	LEU
1	F	6	VAL
1	F	7	THR
1	F	39	ILE
1	F	44	THR
1	F	54	VAL
1	F	55	MET
1	F	58	ASP
1	F	63	ILE
1	F	69	LEU
1	F	82	ILE
1	F	114	LYS
1	F	118	THR

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Mol	Chain	Res	Type
1	F	119	SER
1	F	143	LYS
1	F	157	GLN
1	F	185	VAL
1	F	195	MET
1	F	217	THR
1	F	225	LYS
1	F	240	VAL
1	F	244	SER
1	F	248	HIS
1	F	268	THR
1	F	274	GLN
1	F	275	VAL
1	F	279	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	124	HIS
1	A	198	HIS
1	A	236	ASN
1	B	26	HIS
1	B	46	ASN
1	B	124	HIS
1	B	242	ASN
1	D	200	HIS
1	D	242	ASN
1	E	26	HIS
1	E	200	HIS
1	E	242	ASN
1	F	46	ASN
1	F	198	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	MES	B	302	-	12,12,12	2.42	1 (8%)	15,16,16	2.62	6 (40%)
3	MES	C	302	-	12,12,12	2.12	1 (8%)	15,16,16	2.24	6 (40%)
3	MES	A	302	-	12,12,12	2.35	1 (8%)	15,16,16	2.39	7 (46%)
3	MES	F	302	-	12,12,12	2.29	1 (8%)	15,16,16	1.78	4 (26%)

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	MES	B	302	-	-	5/6/14/14	0/1/1/1
3	MES	C	302	-	-	1/6/14/14	0/1/1/1
3	MES	A	302	-	-	3/6/14/14	0/1/1/1
3	MES	F	302	-	-	4/6/14/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	MES	C8-S	-8.04	1.66	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	MES	C8-S	-7.79	1.66	1.77
3	F	302	MES	C8-S	-7.59	1.66	1.77
3	C	302	MES	C8-S	-7.04	1.67	1.77

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	MES	C6-C5-N4	-5.85	101.23	110.12
3	B	302	MES	C5-N4-C3	5.69	121.10	108.84
3	A	302	MES	C5-N4-C3	5.65	121.02	108.84
3	C	302	MES	C5-N4-C3	5.41	120.49	108.84
3	F	302	MES	C5-N4-C3	4.19	117.87	108.84
3	A	302	MES	C6-C5-N4	-3.13	105.37	110.12
3	A	302	MES	C2-C3-N4	-3.09	105.43	110.12
3	C	302	MES	O2S-S-C8	3.04	111.32	106.73
3	A	302	MES	C7-N4-C5	2.96	119.12	111.24
3	C	302	MES	C7-N4-C3	2.81	118.74	111.24
3	A	302	MES	C7-N4-C3	2.80	118.70	111.24
3	F	302	MES	C7-N4-C5	2.74	118.53	111.24
3	C	302	MES	C7-N4-C5	2.63	118.23	111.24
3	F	302	MES	O2S-S-C8	2.56	110.60	106.73
3	B	302	MES	O1S-S-C8	2.53	110.55	106.73
3	B	302	MES	C7-N4-C5	2.51	117.93	111.24
3	A	302	MES	O2S-S-C8	2.39	110.35	106.73
3	B	302	MES	C7-N4-C3	2.34	117.47	111.24
3	F	302	MES	C6-C5-N4	-2.27	106.67	110.12
3	C	302	MES	C2-C3-N4	-2.17	106.82	110.12
3	C	302	MES	O3S-S-C8	2.09	110.10	106.00
3	A	302	MES	C8-C7-N4	-2.09	104.46	112.36
3	B	302	MES	O2S-S-O1S	-2.01	107.30	113.82

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	302	MES	C7-C8-S-O2S
3	B	302	MES	C7-C8-S-O3S
3	F	302	MES	C8-C7-N4-C5
3	F	302	MES	C7-C8-S-O1S
3	F	302	MES	C7-C8-S-O3S
3	A	302	MES	C8-C7-N4-C5
3	B	302	MES	C8-C7-N4-C3

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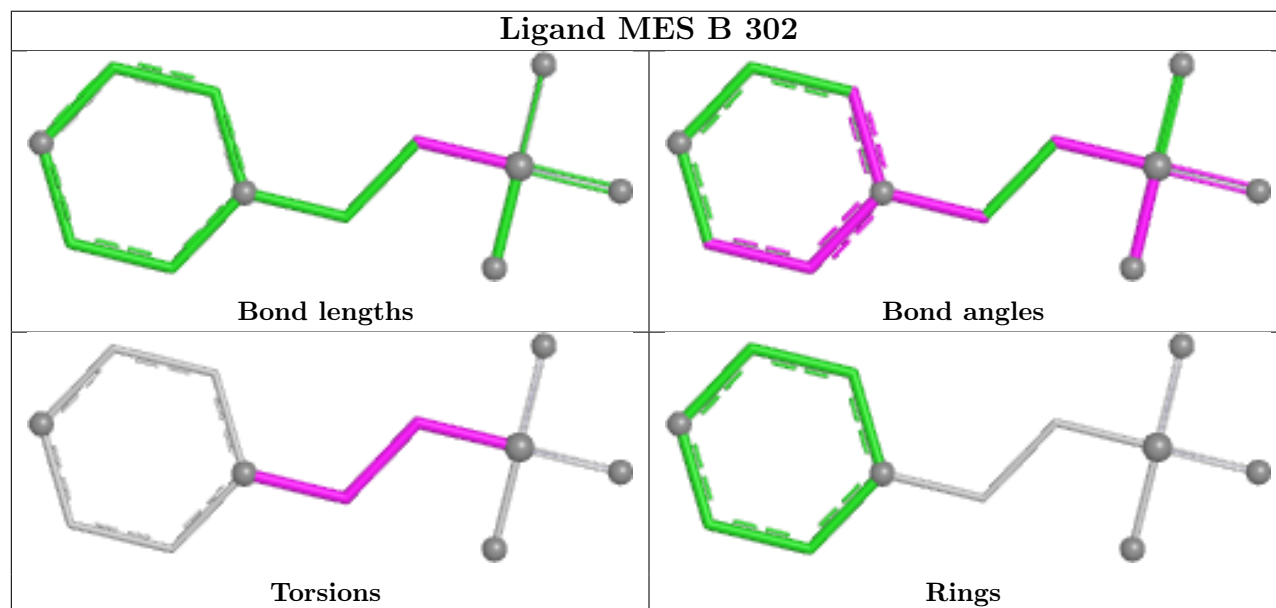
Mol	Chain	Res	Type	Atoms
3	C	302	MES	C8-C7-N4-C3
3	B	302	MES	C7-C8-S-O1S
3	F	302	MES	C7-C8-S-O2S
3	B	302	MES	N4-C7-C8-S
3	A	302	MES	C7-C8-S-O2S
3	A	302	MES	C7-C8-S-O3S

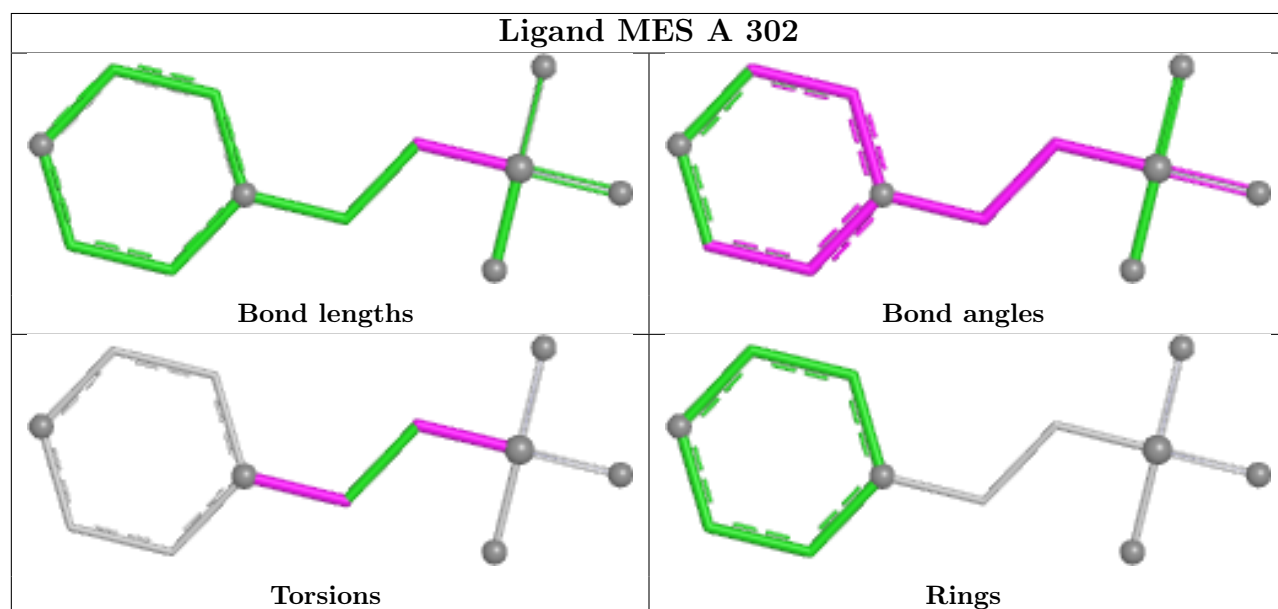
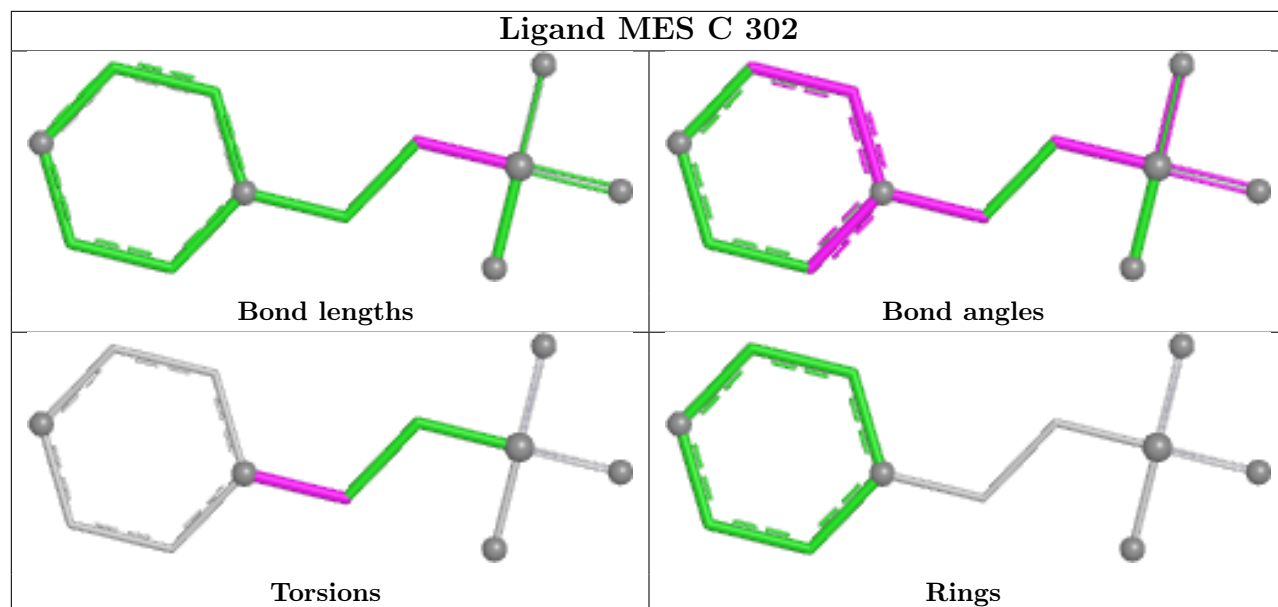
There are no ring outliers.

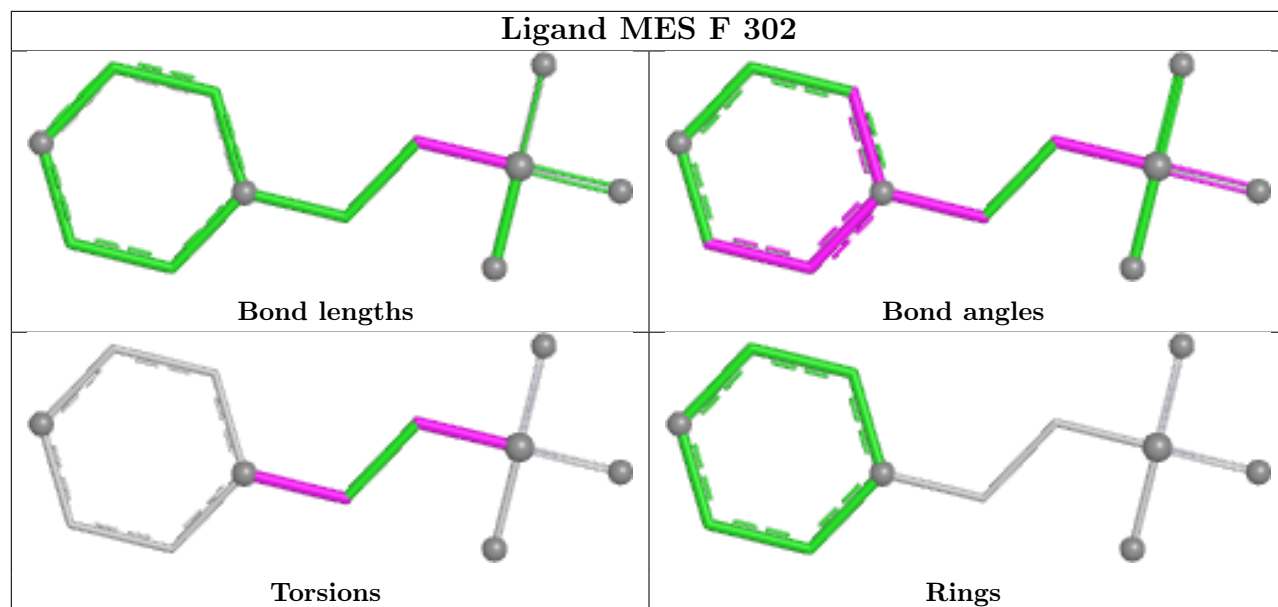
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	302	MES	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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	276/289 (95%)	-0.15	2 (0%) 84 86	56, 83, 122, 162	0
1	B	279/289 (96%)	-0.10	3 (1%) 78 80	51, 79, 118, 177	0
1	C	279/289 (96%)	-0.25	2 (0%) 84 86	56, 77, 119, 143	0
1	D	261/289 (90%)	-0.14	1 (0%) 88 90	56, 80, 120, 173	0
1	E	271/289 (93%)	-0.15	3 (1%) 78 80	55, 82, 130, 182	0
1	F	278/289 (96%)	0.10	6 (2%) 62 63	53, 91, 148, 196	0
All	All	1644/1734 (94%)	-0.12	17 (1%) 79 81	51, 82, 128, 196	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	195	MET	3.2
1	A	95	GLY	3.1
1	F	196	PRO	2.8
1	C	232	ILE	2.6
1	C	280	LEU	2.6
1	F	59	GLU	2.4
1	F	61	LEU	2.3
1	F	195	MET	2.3
1	B	280	LEU	2.2
1	E	130	VAL	2.2
1	D	150	LEU	2.1
1	A	196	PRO	2.1
1	F	117	PHE	2.1
1	F	197	ALA	2.1
1	E	196	PRO	2.1
1	B	192	TRP	2.1
1	E	268	THR	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](#)

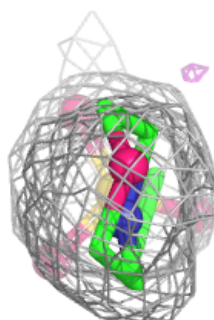
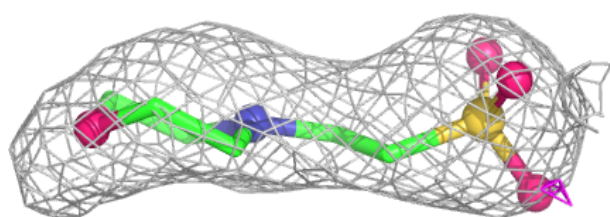
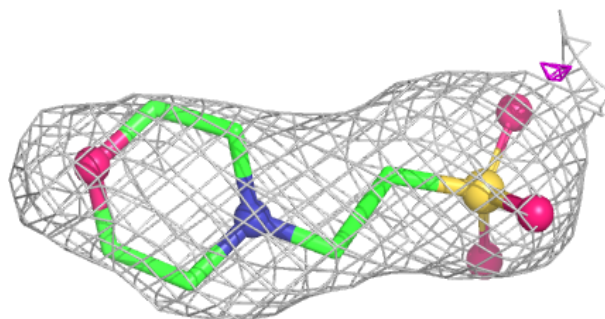
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MES	F	302	12/12	0.89	0.14	108,110,124,125	0
3	MES	C	302	12/12	0.90	0.13	111,122,140,146	0
3	MES	B	302	12/12	0.90	0.13	101,113,123,128	0
3	MES	A	302	12/12	0.91	0.12	125,131,134,134	0
2	ZN	D	301	1/1	0.94	0.05	129,129,129,129	0
2	ZN	E	301	1/1	0.97	0.04	126,126,126,126	0
2	ZN	B	301	1/1	0.98	0.04	105,105,105,105	0
2	ZN	F	301	1/1	0.98	0.04	100,100,100,100	0
2	ZN	C	301	1/1	0.99	0.04	97,97,97,97	0
2	ZN	A	301	1/1	1.00	0.03	88,88,88,88	0

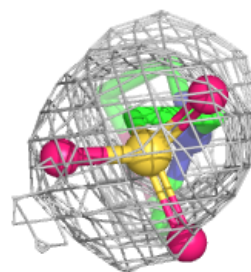
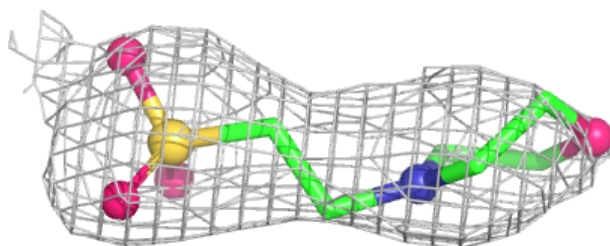
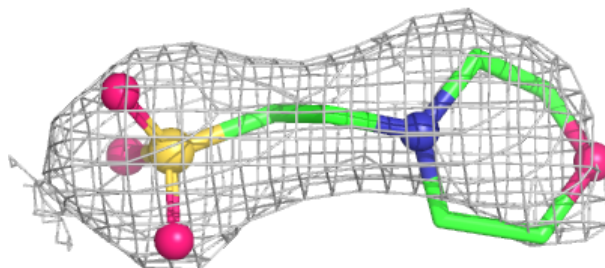
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around MES F 302:

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

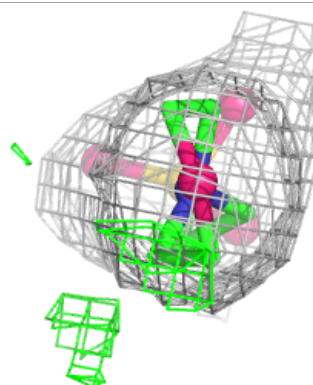
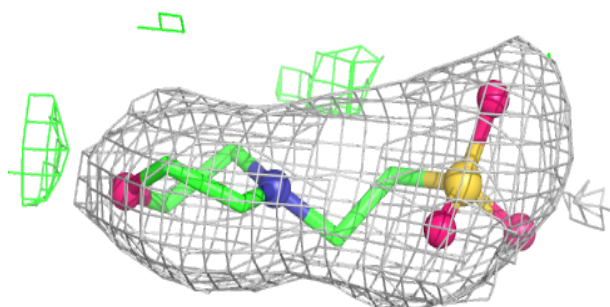
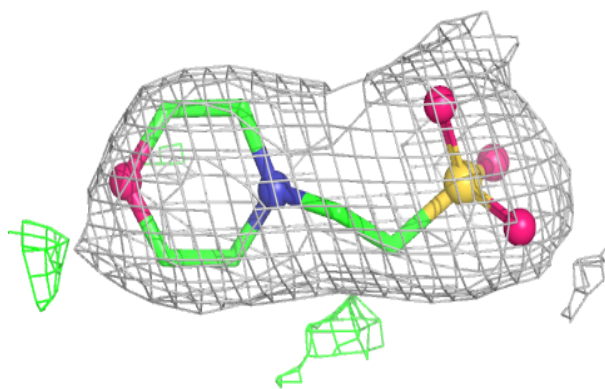
**Electron density around MES C 302:**

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

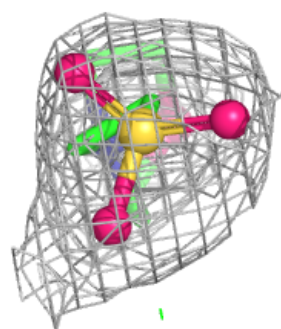
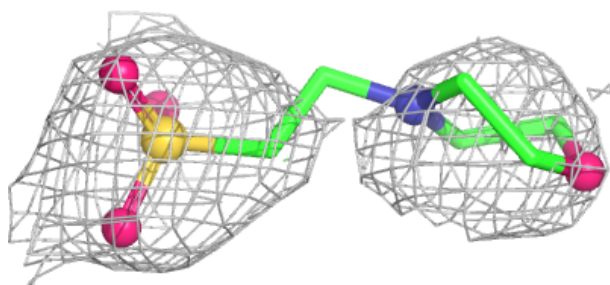
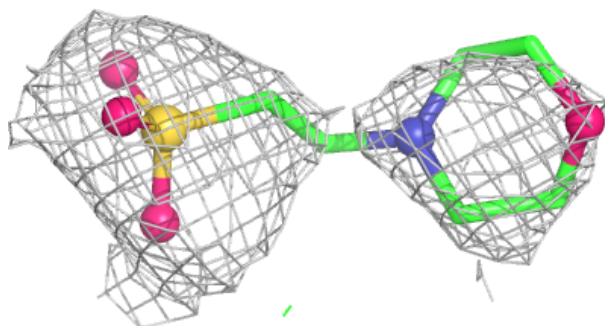


Electron density around MES B 302:

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and green (positive)

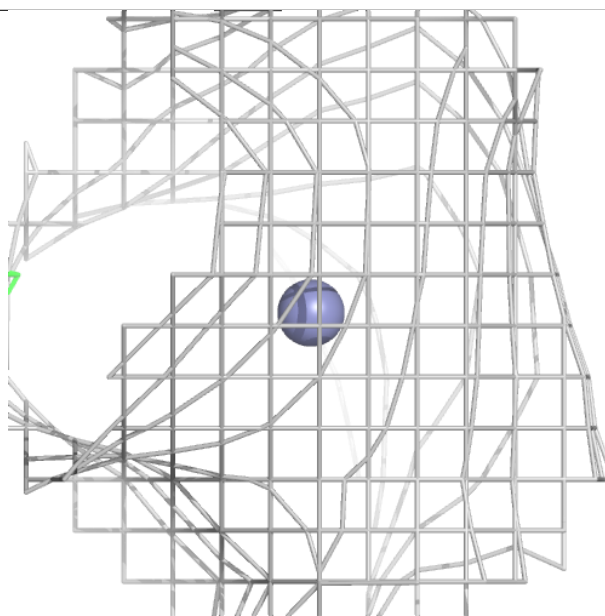
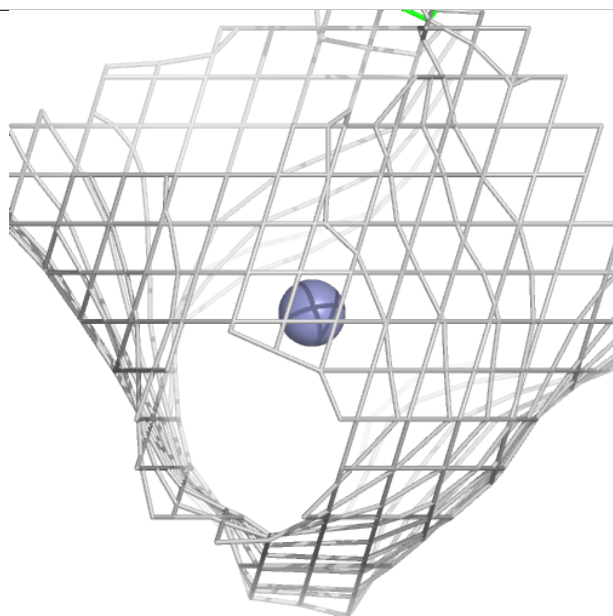
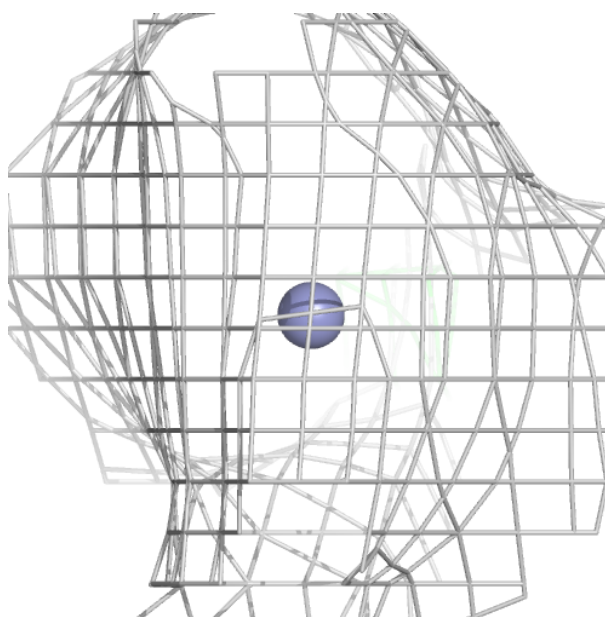
**Electron density around MES A 302:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



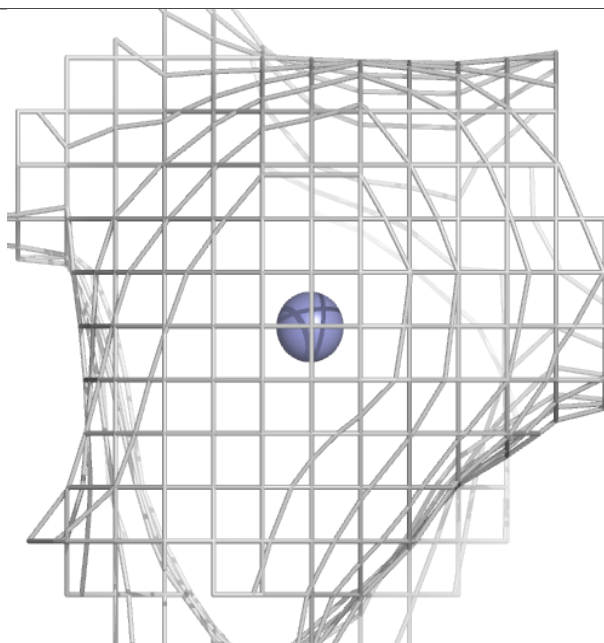
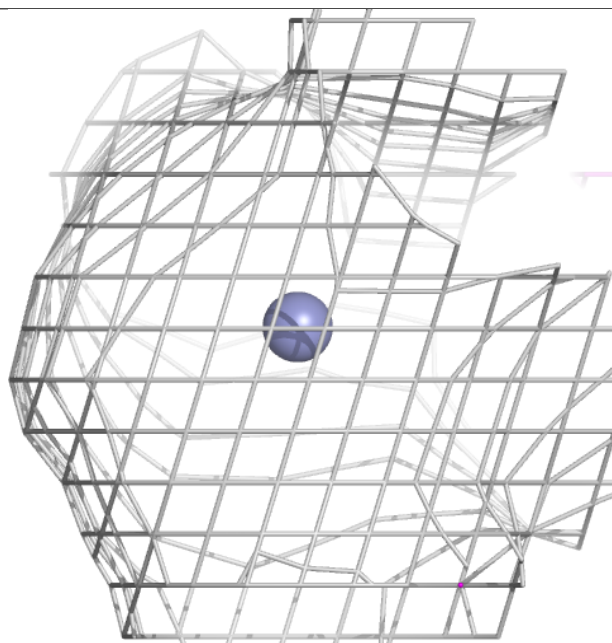
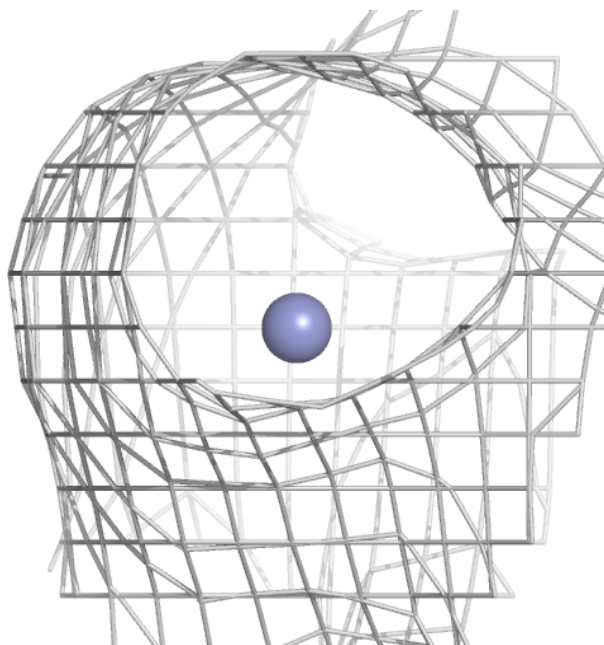
Electron density around ZN D 301:

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and green (positive)



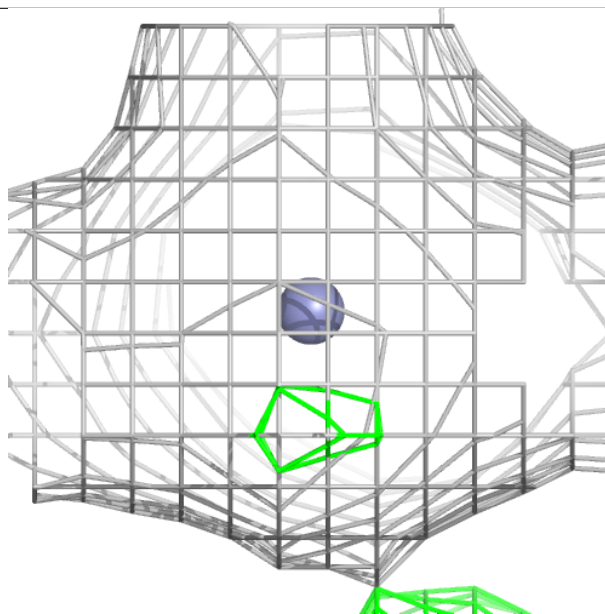
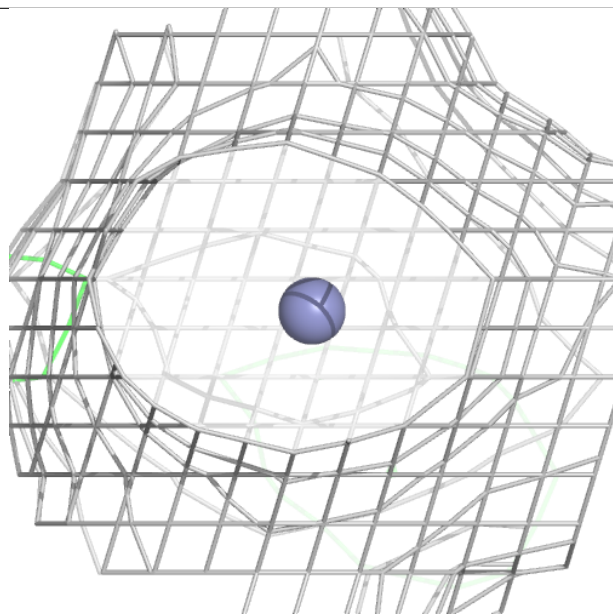
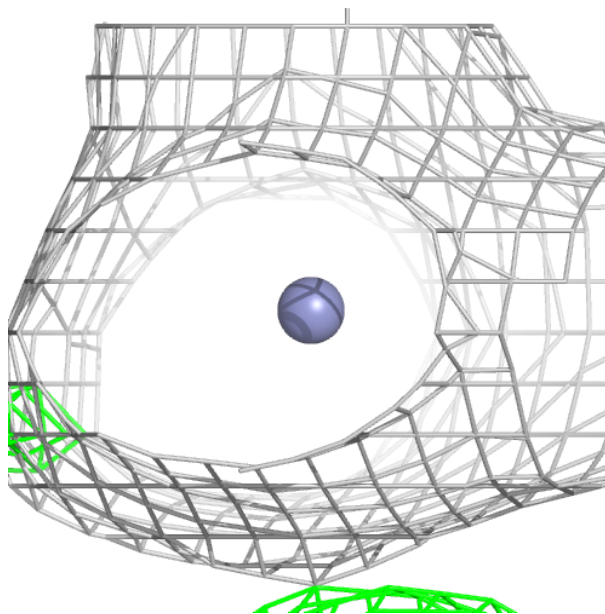
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and green (positive)



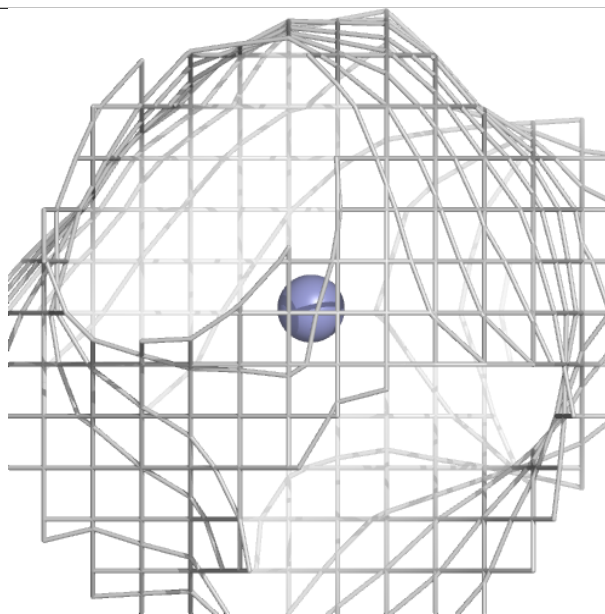
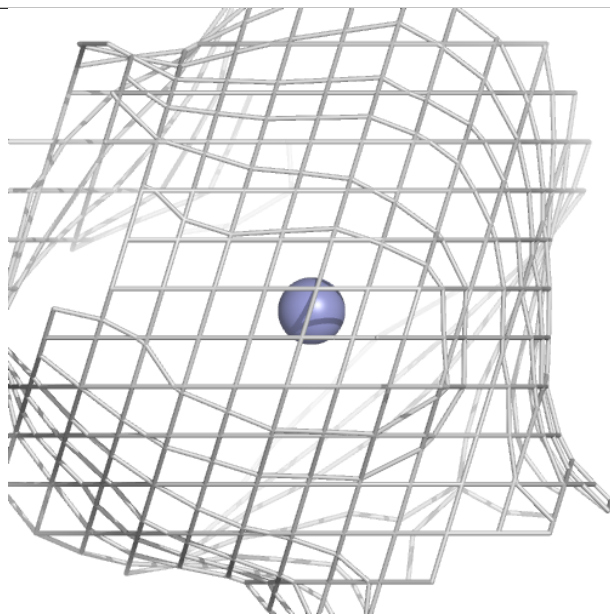
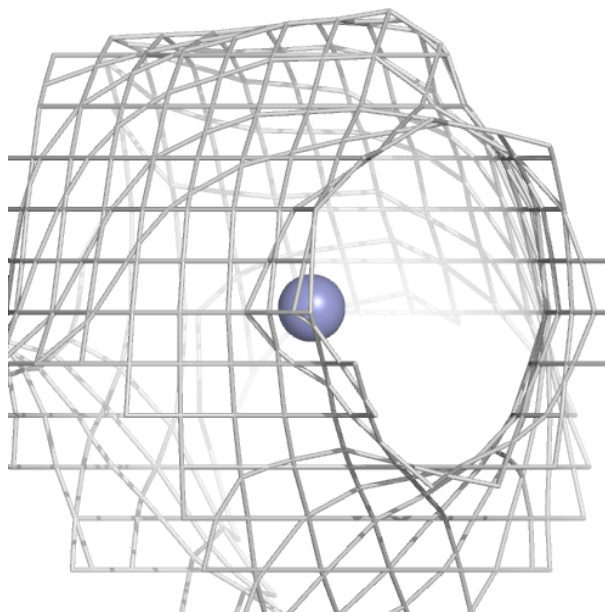
Electron density around ZN B 301:

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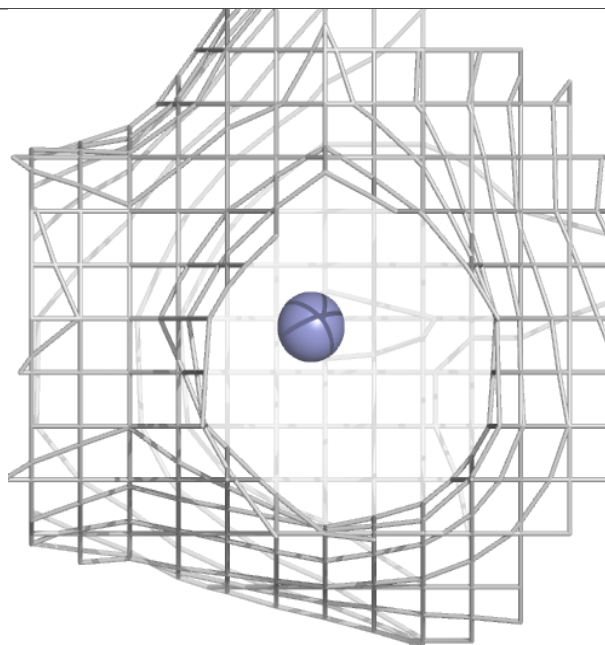
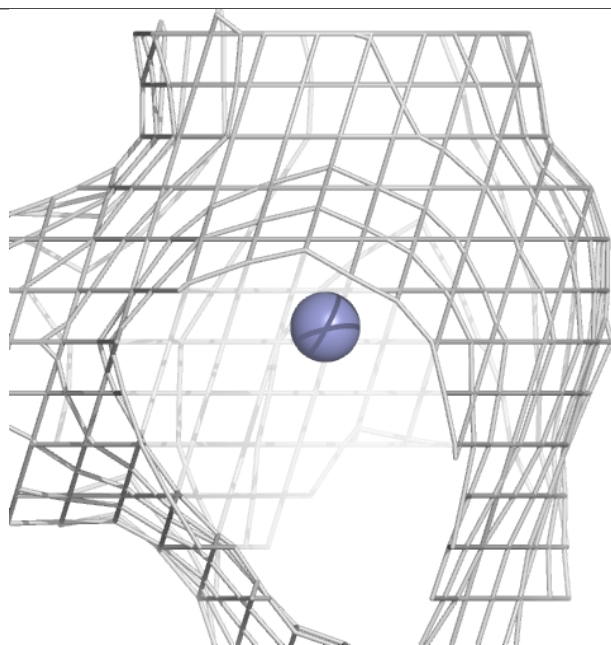
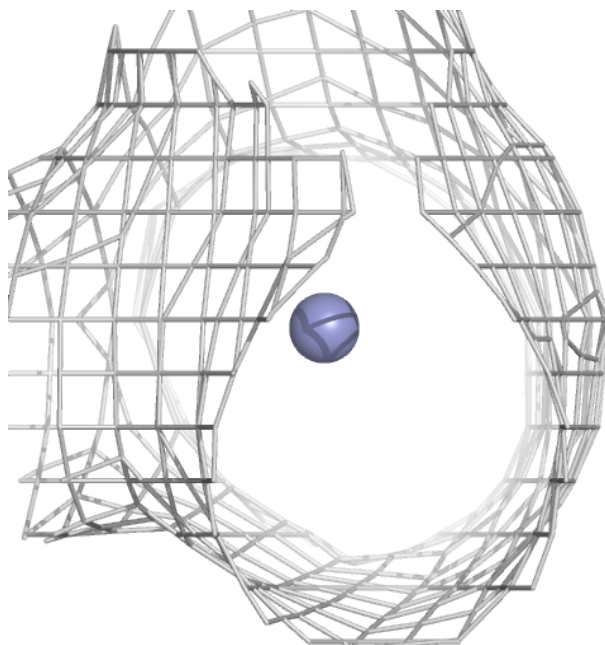
Electron density around ZN F 301:

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and green (positive)



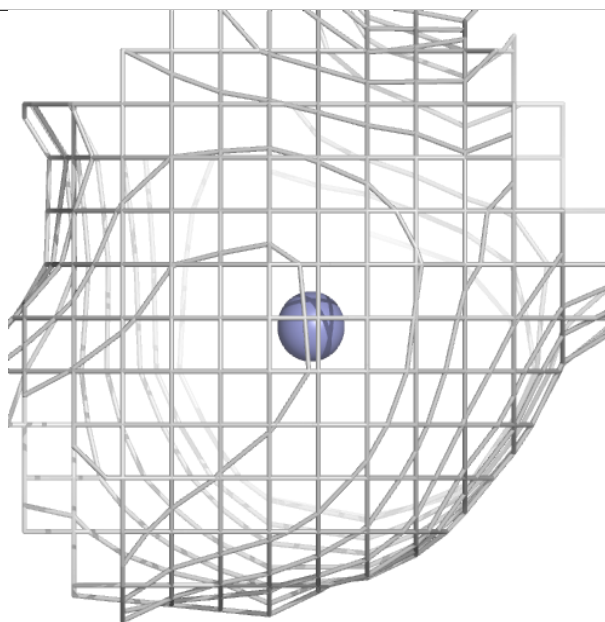
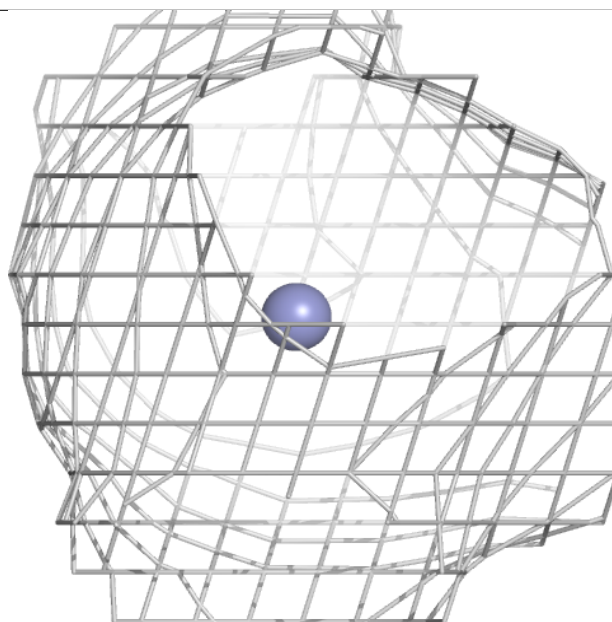
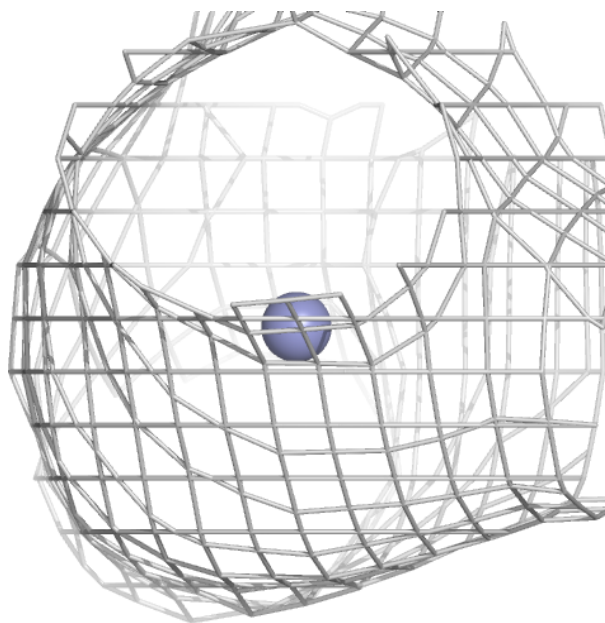
Electron density around ZN C 301:

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



Electron density around ZN A 301:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.