



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2025 – 02:09 PM JST

PDB ID : 9KTK / pdb_00009ktk
Title : Crystal structure of human SIRT3 with its activator SKLB-11A
Authors : Ouyang, L.; Wu, C.Y.
Deposited on : 2024-12-02
Resolution : 2.49 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 Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

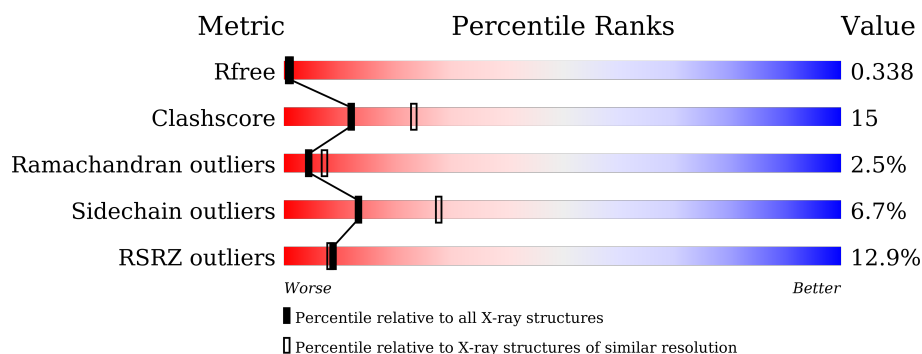
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	277	<div> <div>6%</div> <div>71%</div> <div>25%</div> <div>..</div> </div>
1	B	277	<div> <div>7%</div> <div>67%</div> <div>25%</div> <div>5% ..</div> </div>
1	C	277	<div> <div>18%</div> <div>61%</div> <div>34%</div> <div>..</div> </div>
1	D	277	<div> <div>18%</div> <div>60%</div> <div>32%</div> <div>6% .</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8634 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 NAD-dependent protein deacetylase sirtuin-3, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	32	0	0
			2132	1373	367	383	9			
1	B	271	Total	C	N	O	S	10	0	0
			2127	1370	366	382	9			
1	C	272	Total	C	N	O	S	76	0	0
			2132	1373	367	383	9			
1	D	272	Total	C	N	O	S	55	0	0
			2132	1373	367	383	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	SER	-	expression tag	UNP Q9NTG7
A	116	ASN	-	expression tag	UNP Q9NTG7
A	117	ALA	-	expression tag	UNP Q9NTG7
B	115	SER	-	expression tag	UNP Q9NTG7
B	116	ASN	-	expression tag	UNP Q9NTG7
B	117	ALA	-	expression tag	UNP Q9NTG7
C	115	SER	-	expression tag	UNP Q9NTG7
C	116	ASN	-	expression tag	UNP Q9NTG7
C	117	ALA	-	expression tag	UNP Q9NTG7
D	115	SER	-	expression tag	UNP Q9NTG7
D	116	ASN	-	expression tag	UNP Q9NTG7
D	117	ALA	-	expression tag	UNP Q9NTG7

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

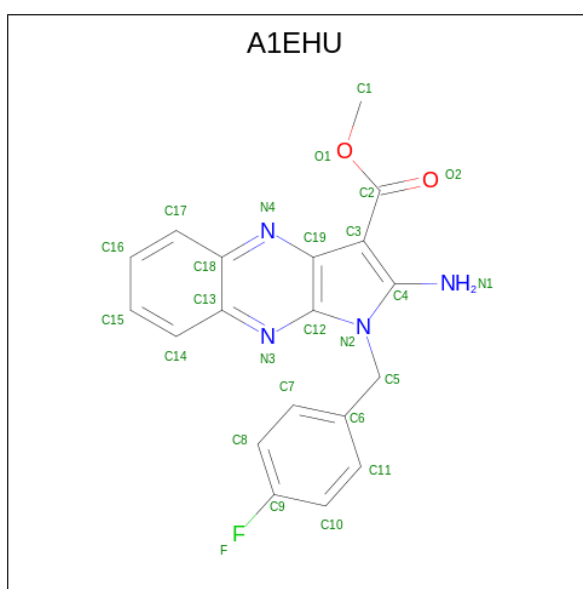
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	1	0
			1	1		

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

- Molecule 3 is methyl 2-azanyl-1-[(4-fluorophenyl)methyl]pyrrolo[3,2-b]quinoxaline-3-carboxylate (CCD ID: A1EHU) (formula: C₁₉H₁₅FN₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			26	19	1	4	2		
3	B	1	Total	C	F	N	O	0	0
			26	19	1	4	2		
3	C	1	Total	C	F	N	O	0	0
			26	19	1	4	2		
3	D	1	Total	C	F	N	O	0	0
			26	19	1	4	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

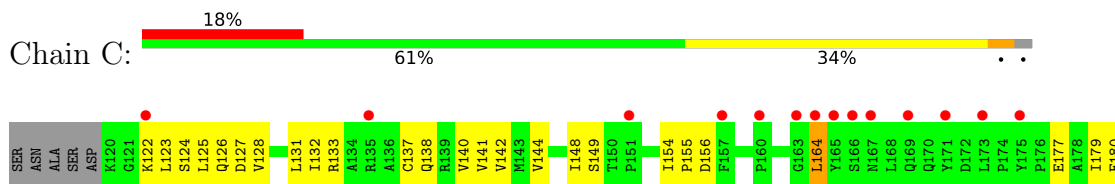
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	1	0
			1	1		

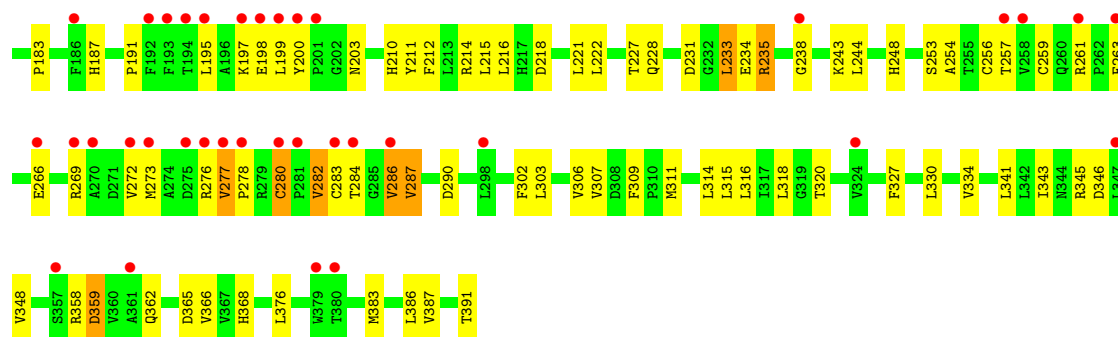
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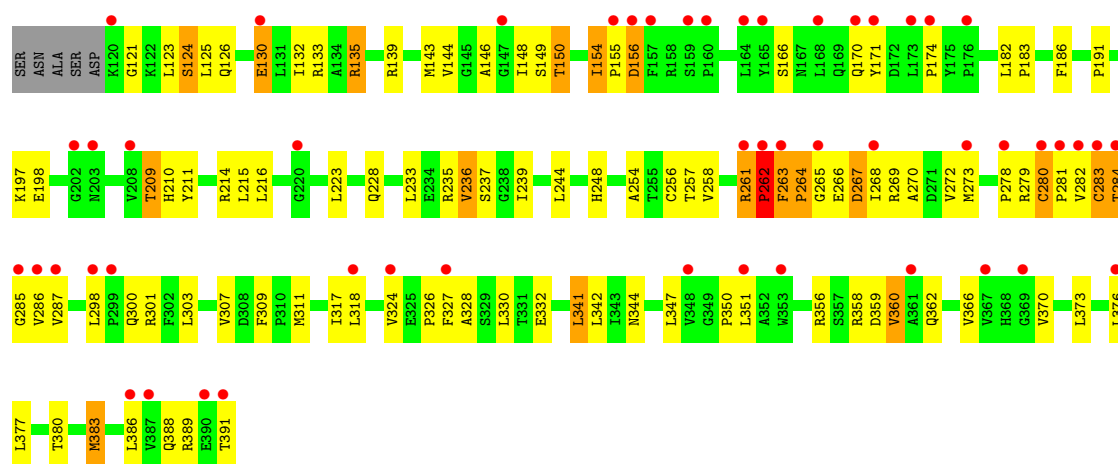
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total 1	Mg 1	1	0
4	D	1	Total 1	Mg 1	0	0

- Molecule 1: NAD-dependent protein deacetylase sirtuin-3, mitochondrial





- Molecule 1: NAD-dependent protein deacetylase sirtuin-3, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.58Å 120.36Å 134.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.47 – 2.49 45.47 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.47-2.49) 99.9 (45.47-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.48Å)	Xtriage
Refinement program	PHENIX (1.20_4459: ???)	Depositor
R, R_{free}	0.262 , 0.340 0.262 , 0.338	Depositor DCC
R_{free} test set	39544 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	57.4	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.5	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	0.92	EDS
Total number of atoms	8634	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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: ZN, MG, A1EHU

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	0.48	1/2187 (0.0%)	0.70	1/2981 (0.0%)
1	B	0.60	1/2182 (0.0%)	0.83	3/2974 (0.1%)
1	C	0.41	0/2187	0.68	0/2981
1	D	0.40	1/2187 (0.0%)	0.68	1/2981 (0.0%)
All	All	0.48	3/8743 (0.0%)	0.73	5/11917 (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	1
1	B	0	3
1	C	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	283	CYS	CB-SG	-9.02	1.51	1.81
1	A	277	VAL	N-CA	-6.21	1.41	1.46
1	D	150	THR	C-N	5.00	1.38	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	190	LYS	CG-CD-CE	-6.89	95.44	111.30
1	B	190	LYS	CA-CB-CG	-6.25	101.61	114.10
1	B	278	PRO	N-CA-C	5.40	123.59	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	HIS	CB-CA-C	-5.32	102.48	112.00
1	D	262	PRO	N-CA-C	5.25	123.30	112.47

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	PHE	Peptide
1	B	122	LYS	Peptide
1	B	276	ARG	Sidechain
1	B	278	PRO	Peptide
1	C	122	LYS	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	2132	0	2138	39	1
1	B	2127	0	2137	66	1
1	C	2132	0	2138	77	0
1	D	2132	0	2138	79	1
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
3	A	26	0	0	1	0
3	B	26	0	0	2	0
3	C	26	0	0	1	0
3	D	26	0	0	1	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	8634	0	8551	259	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 15.

All (259) 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:D:279:ARG:HE	1:D:284:THR:HB	1.17	1.08
1:B:271:ASP:HB2	1:B:276:ARG:HG3	1.42	1.02
1:B:272:VAL:HA	1:B:276:ARG:HH21	1.36	0.90
1:B:272:VAL:HA	1:B:276:ARG:NH2	1.86	0.90
1:B:193:PHE:CD1	1:B:276:ARG:NH1	2.44	0.86
1:A:125:LEU:HD21	1:A:362:GLN:HB2	1.61	0.82
1:B:259:CYS:HB3	1:B:282:VAL:C	2.05	0.81
1:D:280:CYS:N	1:D:284:THR:O	2.16	0.79
1:B:197:LYS:HG3	1:B:272:VAL:O	1.82	0.79
1:D:256:CYS:HB2	1:D:262:PRO:HG2	1.64	0.78
1:C:197:LYS:NZ	1:C:273:MET:O	2.15	0.78
1:C:200:TYR:O	1:C:203:ASN:ND2	2.16	0.78
1:B:268:ILE:HB	1:B:276:ARG:HG2	1.64	0.77
1:B:158:ARG:HH12	1:B:324:VAL:HG12	1.47	0.77
1:C:343:ILE:HG22	1:C:366:VAL:HG13	1.68	0.76
1:A:316:LEU:HD22	1:A:318:LEU:HD11	1.68	0.76
1:B:259:CYS:SG	1:B:283:CYS:SG	2.84	0.75
1:D:317:ILE:HD12	1:D:351:LEU:HD11	1.68	0.75
1:C:214:ARG:NH1	1:C:218:ASP:OD2	2.21	0.74
1:C:123:LEU:HD23	1:C:358:ARG:HA	1.69	0.73
1:C:183:PRO:HB3	1:D:283:CYS:O	1.89	0.73
1:C:214:ARG:HE	1:C:238:GLY:HA3	1.55	0.71
1:C:278:PRO:HB2	1:C:287:VAL:HG23	1.72	0.71
1:D:130:GLU:OE1	1:D:133:ARG:NH1	2.23	0.71
1:D:324:VAL:HG11	3:D:403:A1EHU:C16	2.20	0.71
1:B:209:THR:HG23	1:B:370:VAL:HG21	1.73	0.70
1:B:298:LEU:H	1:B:298:LEU:HD23	1.56	0.69
1:C:259:CYS:SG	1:C:261:ARG:HG2	2.33	0.68
1:A:164:LEU:HD21	1:A:195:LEU:HD12	1.76	0.67
1:B:149:SER:HB3	1:B:154:ILE:HD13	1.76	0.67
1:C:222:LEU:O	1:C:243:LYS:NZ	2.27	0.66
1:D:383:MET:O	1:D:386:LEU:N	2.30	0.65
1:B:271:ASP:CB	1:B:276:ARG:HG3	2.22	0.65
1:A:190:LYS:O	1:A:194:THR:HG23	1.96	0.65
1:D:146:ALA:O	1:D:150:THR:HG23	1.97	0.64
1:C:125:LEU:HD23	1:C:376:LEU:HD22	1.80	0.64
1:D:261:ARG:H	1:D:262:PRO:HD2	1.61	0.64
1:C:365:ASP:HB3	1:C:368:HIS:CD2	2.34	0.63
1:C:138:GLN:HA	1:C:221:LEU:HD12	1.79	0.63
1:B:164:LEU:HD21	1:B:195:LEU:HA	1.81	0.62
1:C:132:ILE:HD13	1:C:137:CYS:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:THR:OG1	1:D:285:GLY:N	2.32	0.62
1:C:144:VAL:HB	1:C:148:ILE:HG12	1.80	0.62
1:C:302:PHE:CZ	1:C:330:LEU:HD11	2.34	0.61
1:B:276:ARG:N	1:B:276:ARG:HD2	2.14	0.61
1:C:128:VAL:HG21	1:C:341:LEU:HD12	1.82	0.61
1:D:144:VAL:HB	1:D:148:ILE:HD13	1.82	0.61
1:B:271:ASP:C	1:B:273:MET:H	2.09	0.61
1:B:279:ARG:HD2	1:B:279:ARG:N	2.16	0.60
1:D:279:ARG:HB3	1:D:284:THR:HA	1.83	0.60
1:A:321:SER:HB3	1:A:323:GLU:HG3	1.84	0.60
1:C:215:LEU:HG	1:C:386:LEU:HD22	1.84	0.60
1:D:143:MET:HE2	1:D:309:PHE:HE2	1.67	0.59
1:B:271:ASP:O	1:B:273:MET:N	2.35	0.59
1:A:169:GLN:OE1	1:A:169:GLN:HA	2.03	0.58
1:B:181:GLU:HG2	1:B:184:PHE:HB2	1.83	0.58
1:D:283:CYS:O	1:D:285:GLY:N	2.36	0.58
1:A:149:SER:OG	1:A:231:ASP:OD2	2.21	0.58
1:D:326:PRO:O	1:D:330:LEU:HG	2.03	0.57
1:D:366:VAL:O	1:D:370:VAL:HG13	2.04	0.57
1:C:327:PHE:O	1:C:330:LEU:HD12	2.04	0.57
1:B:259:CYS:HB2	1:B:282:VAL:HB	1.86	0.57
1:C:341:LEU:HD21	1:C:343:ILE:HD13	1.85	0.57
1:B:124:SER:OG	1:B:127:ASP:OD1	2.19	0.57
1:B:272:VAL:HA	1:B:276:ARG:CZ	2.34	0.56
1:C:149:SER:HB3	1:C:154:ILE:HG13	1.88	0.56
1:C:280:CYS:O	1:C:284:THR:HA	2.06	0.56
1:C:211:TYR:HA	1:C:214:ARG:HB3	1.88	0.56
1:D:228:GLN:HG2	1:D:248:HIS:CE1	2.41	0.56
1:B:341:LEU:HD13	1:B:360:VAL:HB	1.87	0.56
1:A:203:ASN:HB3	1:A:204:TYR:CD2	2.40	0.55
1:D:209:THR:HG23	1:D:370:VAL:HG11	1.87	0.55
1:A:342:LEU:HD13	1:A:351:LEU:HD12	1.89	0.55
1:C:215:LEU:HD12	1:C:383:MET:SD	2.47	0.55
1:A:197:LYS:HE2	1:A:272:VAL:O	2.06	0.55
1:A:322:LEU:HD12	1:A:348:VAL:HG23	1.88	0.55
1:B:278:PRO:HG2	1:B:287:VAL:HG11	1.88	0.55
1:C:133:ARG:HH11	1:C:133:ARG:HB3	1.71	0.55
1:B:193:PHE:CG	1:B:276:ARG:NH1	2.75	0.55
1:C:278:PRO:O	1:C:286:VAL:HA	2.07	0.54
1:D:235:ARG:HG2	1:D:244:LEU:HD22	1.88	0.54
1:B:381:GLU:O	1:B:384:ARG:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:VAL:HG11	1:C:341:LEU:HD13	1.89	0.54
1:A:128:VAL:HG21	1:A:341:LEU:HD12	1.89	0.54
1:B:259:CYS:SG	1:B:261:ARG:HB2	2.47	0.54
1:A:196:ALA:O	1:A:200:TYR:HD1	1.91	0.54
1:B:144:VAL:HG12	1:B:318:LEU:HB2	1.90	0.53
1:D:307:VAL:O	1:D:311:MET:HG3	2.07	0.53
1:C:315:LEU:HB2	1:C:334:VAL:HG11	1.91	0.53
1:B:177:GLU:HG2	3:B:403:A1EHU:C14	2.38	0.53
1:A:310:PRO:HG3	1:D:298:LEU:HD11	1.90	0.53
1:C:314:LEU:HD12	1:C:315:LEU:N	2.24	0.53
1:D:362:GLN:HE21	1:D:362:GLN:HA	1.72	0.53
1:B:276:ARG:HD2	1:B:276:ARG:H	1.74	0.53
1:C:346:ASP:O	1:C:348:VAL:HG13	2.09	0.53
1:A:374:VAL:HG13	1:A:379:TRP:HB2	1.90	0.52
1:A:385:ASP:O	1:A:389:ARG:HG3	2.08	0.52
1:B:230:ILE:HD12	1:B:251:PHE:CE2	2.45	0.52
1:C:200:TYR:CZ	1:C:269:ARG:HB2	2.43	0.52
1:D:356:ARG:N	1:D:359:ASP:OD1	2.31	0.52
1:A:187:HIS:O	1:A:189:PRO:HD3	2.08	0.52
1:C:269:ARG:HA	1:C:272:VAL:HG12	1.92	0.52
1:B:293:PHE:HB2	1:B:296:GLU:HG3	1.92	0.52
1:B:259:CYS:CB	1:B:282:VAL:HB	2.40	0.52
1:C:200:TYR:OH	1:C:269:ARG:HB2	2.09	0.52
1:B:256:CYS:HA	1:B:287:VAL:HA	1.92	0.51
1:A:197:LYS:HZ3	1:A:273:MET:HA	1.74	0.51
1:D:279:ARG:NE	1:D:284:THR:HB	2.02	0.51
1:B:347:LEU:HG	1:B:352:ALA:HB2	1.92	0.51
1:C:133:ARG:HB3	1:C:133:ARG:NH1	2.26	0.51
1:D:244:LEU:O	1:D:301:ARG:NH2	2.41	0.51
1:C:278:PRO:HB2	1:C:287:VAL:CG2	2.41	0.51
1:D:197:LYS:HD3	1:D:272:VAL:HG12	1.92	0.51
1:B:219:LYS:HD2	1:B:379:TRP:CZ2	2.47	0.50
1:C:345:ARG:HE	1:C:365:ASP:HA	1.76	0.50
1:B:279:ARG:HD2	1:B:279:ARG:H	1.75	0.50
1:C:343:ILE:HG22	1:C:343:ILE:O	2.10	0.50
1:B:272:VAL:O	1:B:272:VAL:HG12	2.12	0.50
1:D:125:LEU:HD21	1:D:373:LEU:HB2	1.92	0.50
1:D:223:LEU:HD21	1:D:311:MET:HE2	1.93	0.50
1:A:182:LEU:HD11	1:A:186:PHE:CZ	2.47	0.50
1:A:255:THR:HG23	1:A:290:ASP:OD1	2.12	0.50
1:C:387:VAL:O	1:C:391:THR:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:VAL:HG12	1:D:318:LEU:HB2	1.94	0.49
1:D:228:GLN:NE2	1:D:327:PHE:HB2	2.27	0.49
1:A:211:TYR:CD2	1:A:387:VAL:HG22	2.46	0.49
1:B:155:PRO:O	1:B:156:ASP:HB3	2.12	0.49
1:A:315:LEU:HB2	1:A:334:VAL:HG11	1.95	0.49
1:B:275:ASP:C	1:B:275:ASP:OD1	2.55	0.49
1:C:149:SER:OG	1:C:231:ASP:OD2	2.16	0.49
1:D:228:GLN:HE22	1:D:327:PHE:HB2	1.77	0.49
1:D:342:LEU:HB2	1:D:351:LEU:HD12	1.95	0.49
1:D:362:GLN:HA	1:D:362:GLN:NE2	2.27	0.49
1:A:189:PRO:HB2	1:A:193:PHE:CD2	2.48	0.49
1:A:266:GLU:N	1:A:266:GLU:CD	2.71	0.49
1:C:212:PHE:O	1:C:216:LEU:HD12	2.13	0.48
1:D:132:ILE:HB	1:D:377:LEU:HD11	1.94	0.48
1:D:214:ARG:NH1	1:D:237:SER:O	2.45	0.48
1:D:341:LEU:HA	1:D:360:VAL:O	2.12	0.48
1:C:154:ILE:HG23	1:C:199:LEU:HD21	1.94	0.48
1:A:144:VAL:HG12	1:A:318:LEU:HB2	1.96	0.48
1:A:189:PRO:HB2	1:A:193:PHE:HD2	1.78	0.48
1:C:253:SER:OG	1:C:290:ASP:OD2	2.27	0.48
1:D:133:ARG:C	1:D:135:ARG:H	2.20	0.48
1:D:123:LEU:HD13	1:D:358:ARG:HA	1.96	0.48
1:D:342:LEU:HD22	1:D:351:LEU:HD12	1.96	0.48
1:B:124:SER:O	1:B:128:VAL:HG23	2.14	0.48
1:A:317:ILE:HD13	1:A:351:LEU:HD11	1.96	0.48
1:C:266:GLU:HA	1:C:269:ARG:HB3	1.95	0.47
1:D:342:LEU:HD21	1:D:347:LEU:HA	1.96	0.47
1:C:314:LEU:HD12	1:C:315:LEU:H	1.78	0.47
1:D:126:GLN:O	1:D:130:GLU:HG2	2.14	0.47
1:D:211:TYR:HB3	1:D:383:MET:HE1	1.96	0.47
1:A:128:VAL:HG21	1:A:341:LEU:CD1	2.44	0.47
1:A:122:LYS:HG3	1:A:123:LEU:H	1.79	0.47
1:C:141:VAL:HG13	1:C:315:LEU:HD13	1.97	0.47
1:D:269:ARG:HD3	1:D:270:ALA:N	2.29	0.47
1:D:303:LEU:HD23	1:D:303:LEU:HA	1.58	0.47
1:C:210:HIS:CE1	1:C:233:LEU:HD23	2.49	0.47
1:C:254:ALA:HB3	1:C:263:PHE:HB2	1.95	0.47
1:C:276:ARG:HG2	1:C:277:VAL:H	1.79	0.47
1:C:124:SER:O	1:C:127:ASP:N	2.48	0.47
1:D:278:PRO:C	1:D:279:ARG:HG2	2.40	0.47
1:A:142:VAL:HG13	1:A:316:LEU:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:LEU:HD12	1:B:318:LEU:HG	1.97	0.47
1:C:235:ARG:HG2	1:C:244:LEU:CD1	2.45	0.47
1:A:292:VAL:O	3:A:402:A1EHU:N1	2.47	0.47
1:C:303:LEU:HD23	1:C:303:LEU:HA	1.75	0.47
1:D:186:PHE:HE2	1:D:257:THR:HB	1.80	0.47
1:B:178:ALA:O	1:B:181:GLU:HB3	2.15	0.46
1:D:266:GLU:H	1:D:266:GLU:CD	2.22	0.46
1:C:256:CYS:HA	1:C:287:VAL:HG12	1.97	0.46
1:C:248:HIS:HB3	3:C:403:A1EHU:O2	2.15	0.46
1:A:266:GLU:N	1:A:266:GLU:OE1	2.44	0.46
1:C:142:VAL:HG22	1:C:316:LEU:HB3	1.96	0.46
1:C:126:GLN:HA	1:C:376:LEU:HD23	1.98	0.46
1:C:343:ILE:HD12	1:C:362:GLN:HB3	1.98	0.46
1:D:155:PRO:O	1:D:156:ASP:HB3	2.16	0.46
1:D:285:GLY:O	1:D:286:VAL:C	2.58	0.46
1:B:318:LEU:HD23	1:B:343:ILE:HB	1.97	0.46
1:D:269:ARG:HG3	1:D:269:ARG:HH11	1.81	0.46
1:B:196:ALA:O	1:B:200:TYR:HB2	2.16	0.46
1:D:215:LEU:CD2	1:D:386:LEU:HD22	2.46	0.45
1:B:226:TYR:CE2	1:B:245:VAL:HG21	2.51	0.45
1:D:170:GLN:OE1	1:D:170:GLN:HA	2.17	0.45
1:D:182:LEU:HB3	1:D:183:PRO:HD3	1.98	0.45
1:B:158:ARG:O	1:B:160:PRO:HD3	2.17	0.45
1:B:177:GLU:HG2	3:B:403:A1EHU:C15	2.47	0.45
1:D:233:LEU:HA	1:D:236:VAL:HB	1.99	0.45
1:D:235:ARG:HD2	1:D:239:ILE:O	2.17	0.45
1:D:254:ALA:O	1:D:263:PHE:HA	2.17	0.45
1:B:298:LEU:H	1:B:298:LEU:CD2	2.26	0.44
1:C:256:CYS:CA	1:C:287:VAL:HG12	2.47	0.44
1:A:122:LYS:HA	1:A:122:LYS:HD3	1.79	0.44
1:C:127:ASP:O	1:C:131:LEU:HD22	2.18	0.44
1:C:155:PRO:HG2	1:C:164:LEU:HD23	1.98	0.44
1:D:261:ARG:N	1:D:262:PRO:HD2	2.32	0.44
1:D:124:SER:OG	1:D:125:LEU:N	2.50	0.44
1:D:235:ARG:HG2	1:D:244:LEU:CD2	2.48	0.44
1:B:122:LYS:HD3	1:B:122:LYS:HA	1.82	0.44
1:B:217:HIS:CE1	1:B:240:PRO:HG2	2.52	0.44
1:B:318:LEU:CD2	1:B:343:ILE:HB	2.47	0.44
1:C:141:VAL:HG21	1:C:309:PHE:CE1	2.53	0.44
1:D:279:ARG:HB3	1:D:284:THR:CA	2.48	0.43
1:D:328:ALA:O	1:D:350:PRO:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:VAL:N	1:B:278:PRO:HD2	2.33	0.43
1:B:124:SER:OG	1:B:126:GLN:HG3	2.19	0.43
1:A:243:LYS:HD3	1:A:243:LYS:HA	1.71	0.43
1:C:187:HIS:C	1:C:187:HIS:CD2	2.96	0.43
1:C:195:LEU:HD21	1:C:199:LEU:HD12	2.00	0.43
1:B:145:GLY:HA3	1:B:320:THR:HB	2.00	0.43
1:C:199:LEU:HD23	1:C:199:LEU:HA	1.83	0.43
1:D:342:LEU:HB2	1:D:351:LEU:CD1	2.49	0.43
1:A:188:ASN:O	1:A:191:PRO:HD2	2.18	0.43
1:B:150:THR:N	1:B:151:PRO:HD2	2.34	0.43
1:C:211:TYR:C	1:C:383:MET:HE1	2.43	0.43
1:B:215:LEU:HD13	1:B:386:LEU:HD22	2.01	0.43
1:D:171:TYR:CD1	1:D:191:PRO:HG3	2.54	0.43
1:D:309:PHE:CE2	1:D:330:LEU:HB3	2.54	0.43
1:C:179:ILE:HG13	1:C:180:PHE:N	2.33	0.42
1:C:256:CYS:SG	1:C:257:THR:N	2.92	0.42
1:C:256:CYS:HA	1:C:287:VAL:HA	2.02	0.42
1:D:210:HIS:CE1	1:D:233:LEU:HD12	2.54	0.42
1:B:215:LEU:HD12	1:B:215:LEU:HA	1.80	0.42
1:B:271:ASP:C	1:B:273:MET:N	2.74	0.42
1:C:227:THR:OG1	1:C:234:GLU:OE2	2.29	0.42
1:C:307:VAL:O	1:C:311:MET:HG2	2.19	0.42
1:D:342:LEU:HD11	1:D:344:ASN:HB3	2.00	0.42
1:B:211:TYR:HA	1:B:214:ARG:HB3	2.01	0.42
1:D:216:LEU:HD23	1:D:216:LEU:HA	1.91	0.42
1:D:300:GLN:CD	1:D:300:GLN:H	2.27	0.42
1:B:179:ILE:HG22	1:B:191:PRO:HB2	2.01	0.42
1:A:377:LEU:HD13	1:A:379:TRP:CZ3	2.54	0.42
1:C:140:VAL:HG12	1:C:142:VAL:HG23	2.01	0.42
1:C:195:LEU:HD23	1:C:195:LEU:C	2.45	0.42
1:D:258:VAL:HG23	1:D:285:GLY:HA2	2.00	0.42
1:B:268:ILE:O	1:B:272:VAL:HG23	2.20	0.41
1:C:359:ASP:OD1	1:C:359:ASP:N	2.52	0.41
1:C:278:PRO:O	1:C:287:VAL:N	2.49	0.41
1:D:133:ARG:HG3	1:D:377:LEU:HD13	2.03	0.41
1:B:152:SER:HB2	1:B:154:ILE:HD12	2.00	0.41
1:C:228:GLN:HB3	1:C:248:HIS:CE1	2.55	0.41
1:D:197:LYS:NZ	1:D:273:MET:HB2	2.35	0.41
1:C:144:VAL:HG12	1:C:318:LEU:HB2	2.02	0.41
1:C:303:LEU:HD22	1:C:306:VAL:CG2	2.51	0.41
1:D:139:ARG:HB3	1:D:223:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:VAL:HG12	1:B:282:VAL:O	2.20	0.41
1:D:311:MET:HE3	1:D:311:MET:HB3	1.72	0.41
1:A:152:SER:OG	1:A:207:ASN:ND2	2.49	0.41
1:B:179:ILE:HD12	1:B:195:LEU:HD13	2.03	0.41
1:C:303:LEU:HD22	1:C:306:VAL:HG23	2.01	0.41
1:D:332:GLU:OE2	1:D:350:PRO:HB3	2.20	0.41
1:B:135:ARG:HB3	1:B:138:GLN:HG2	2.03	0.40
1:A:173:LEU:HG	1:A:178:ALA:HB3	2.04	0.40
1:D:166:SER:O	1:D:170:GLN:HG2	2.20	0.40
1:D:125:LEU:HB2	1:D:362:GLN:OE1	2.22	0.40
1:D:342:LEU:CD2	1:D:347:LEU:HA	2.51	0.40
1:A:266:GLU:HG3	1:A:269:ARG:NH2	2.36	0.40
1:D:149:SER:HB2	1:D:154:ILE:HD13	2.03	0.40

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)
1:B:190:LYS:NZ	1:D:170:GLN:O[3_545]	1.86	0.34
1:A:283:CYS:O	1:A:388:GLN:NE2[4_455]	2.18	0.02

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	270/277 (98%)	249 (92%)	19 (7%)	2 (1%)	19	35
1	B	269/277 (97%)	248 (92%)	13 (5%)	8 (3%)	3	5
1	C	270/277 (98%)	239 (88%)	27 (10%)	4 (2%)	8	16
1	D	270/277 (98%)	236 (87%)	21 (8%)	13 (5%)	2	2
All	All	1079/1108 (97%)	972 (90%)	80 (7%)	27 (2%)	4	7

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	272	VAL
1	B	278	PRO
1	B	280	CYS
1	B	365	ASP
1	D	174	PRO
1	D	262	PRO
1	D	263	PHE
1	D	267	ASP
1	B	187	HIS
1	B	281	PRO
1	B	282	VAL
1	D	284	THR
1	A	174	PRO
1	B	156	ASP
1	D	135	ARG
1	D	261	ARG
1	D	265	GLY
1	D	383	MET
1	A	156	ASP
1	D	156	ASP
1	D	264	PRO
1	C	156	ASP
1	C	282	VAL
1	D	281	PRO
1	C	286	VAL
1	D	121	GLY
1	C	191	PRO

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	235/240 (98%)	219 (93%)	16 (7%)	13	27
1	B	235/240 (98%)	220 (94%)	15 (6%)	14	30
1	C	235/240 (98%)	223 (95%)	12 (5%)	20	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	235/240 (98%)	215 (92%)	20 (8%)	8	18
All	All	940/960 (98%)	877 (93%)	63 (7%)	13	28

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	GLN
1	A	149	SER
1	A	150	THR
1	A	165	TYR
1	A	172	ASP
1	A	173	LEU
1	A	181	GLU
1	A	208	VAL
1	A	223	LEU
1	A	255	THR
1	A	259	CYS
1	A	307	VAL
1	A	316	LEU
1	A	320	THR
1	A	329	SER
1	A	372	SER
1	B	122	LYS
1	B	133	ARG
1	B	150	THR
1	B	181	GLU
1	B	194	THR
1	B	195	LEU
1	B	203	ASN
1	B	244	LEU
1	B	280	CYS
1	B	298	LEU
1	B	316	LEU
1	B	320	THR
1	B	321	SER
1	B	323	GLU
1	B	324	VAL
1	C	164	LEU
1	C	177	GLU
1	C	198	GLU
1	C	233	LEU
1	C	235	ARG

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Mol	Chain	Res	Type
1	C	277	VAL
1	C	280	CYS
1	C	282	VAL
1	C	283	CYS
1	C	287	VAL
1	C	320	THR
1	C	359	ASP
1	D	124	SER
1	D	130	GLU
1	D	154	ILE
1	D	198	GLU
1	D	209	THR
1	D	236	VAL
1	D	264	PRO
1	D	267	ASP
1	D	268	ILE
1	D	280	CYS
1	D	282	VAL
1	D	283	CYS
1	D	287	VAL
1	D	341	LEU
1	D	360	VAL
1	D	376	LEU
1	D	380	THR
1	D	388	GLN
1	D	389	ARG
1	D	391	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	ASN
1	A	300	GLN
1	A	362	GLN
1	B	248	HIS
1	B	354	HIS
1	C	203	ASN
1	C	217	HIS
1	C	368	HIS
1	D	126	GLN
1	D	167	ASN
1	D	203	ASN

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Mol	Chain	Res	Type
1	D	210	HIS
1	D	228	GLN
1	D	260	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 7 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	A1EHU	D	403	-	26,29,29	1.08	2 (7%)	31,42,42	1.62	5 (16%)
3	A1EHU	C	403	-	26,29,29	1.15	2 (7%)	31,42,42	1.50	4 (12%)
3	A1EHU	B	403	-	26,29,29	1.01	2 (7%)	31,42,42	1.68	9 (29%)
3	A1EHU	A	402	-	26,29,29	1.13	2 (7%)	31,42,42	1.63	6 (19%)

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	A1EHU	D	403	-	-	3/10/10/10	0/4/4/4
3	A1EHU	C	403	-	-	4/10/10/10	0/4/4/4
3	A1EHU	B	403	-	-	2/10/10/10	0/4/4/4
3	A1EHU	A	402	-	-	4/10/10/10	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	403	A1EHU	C3-C2	-3.43	1.41	1.50
3	A	402	A1EHU	C3-C2	-3.38	1.41	1.50
3	D	403	A1EHU	C3-C2	-3.06	1.42	1.50
3	A	402	A1EHU	C19-C12	2.82	1.48	1.40
3	D	403	A1EHU	C19-C12	2.75	1.48	1.40
3	B	403	A1EHU	C3-C2	-2.63	1.43	1.50
3	B	403	A1EHU	C19-C12	2.55	1.47	1.40
3	C	403	A1EHU	C19-C12	2.52	1.47	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	A1EHU	C3-C19-N4	4.61	135.78	127.15
3	D	403	A1EHU	C3-C19-N4	4.37	135.33	127.15
3	B	403	A1EHU	C3-C19-N4	4.01	134.65	127.15
3	C	403	A1EHU	O1-C2-C3	3.86	120.00	111.90
3	B	403	A1EHU	O1-C2-C3	3.83	119.95	111.90
3	C	403	A1EHU	C3-C19-N4	3.41	133.54	127.15
3	B	403	A1EHU	C6-C5-N2	3.22	117.62	112.63
3	B	403	A1EHU	C19-N4-C18	2.91	120.34	117.02
3	A	402	A1EHU	O1-C2-C3	2.88	117.94	111.90
3	D	403	A1EHU	O1-C2-C3	2.83	117.84	111.90
3	A	402	A1EHU	C13-N3-C12	2.74	120.66	116.90
3	D	403	A1EHU	C19-N4-C18	2.71	120.11	117.02
3	D	403	A1EHU	C13-N3-C12	2.64	120.52	116.90
3	B	403	A1EHU	C11-C10-C9	2.63	121.09	118.36
3	D	403	A1EHU	C1-O1-C2	2.50	120.65	115.83
3	C	403	A1EHU	C13-N3-C12	2.45	120.26	116.90
3	A	402	A1EHU	C6-C5-N2	2.32	116.22	112.63
3	A	402	A1EHU	C17-C18-N4	2.31	122.00	119.09
3	C	403	A1EHU	C19-N4-C18	2.25	119.58	117.02
3	B	403	A1EHU	C10-C9-C8	-2.22	119.88	122.83
3	B	403	A1EHU	C13-N3-C12	2.22	119.94	116.90
3	B	403	A1EHU	O1-C2-O2	-2.11	119.33	123.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	A1EHU	C11-C6-C7	2.04	121.37	118.17
3	B	403	A1EHU	C13-C18-N4	-2.03	119.74	121.42

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	403	A1EHU	C3-C2-O1-C1
3	C	403	A1EHU	O2-C2-O1-C1
3	A	402	A1EHU	C3-C2-O1-C1
3	B	403	A1EHU	N2-C5-C6-C11
3	D	403	A1EHU	O2-C2-O1-C1
3	B	403	A1EHU	N2-C5-C6-C7
3	D	403	A1EHU	N2-C5-C6-C7
3	A	402	A1EHU	N2-C5-C6-C7
3	A	402	A1EHU	O2-C2-O1-C1
3	D	403	A1EHU	N2-C5-C6-C11
3	A	402	A1EHU	N2-C5-C6-C11
3	C	403	A1EHU	N2-C5-C6-C11
3	C	403	A1EHU	N2-C5-C6-C7

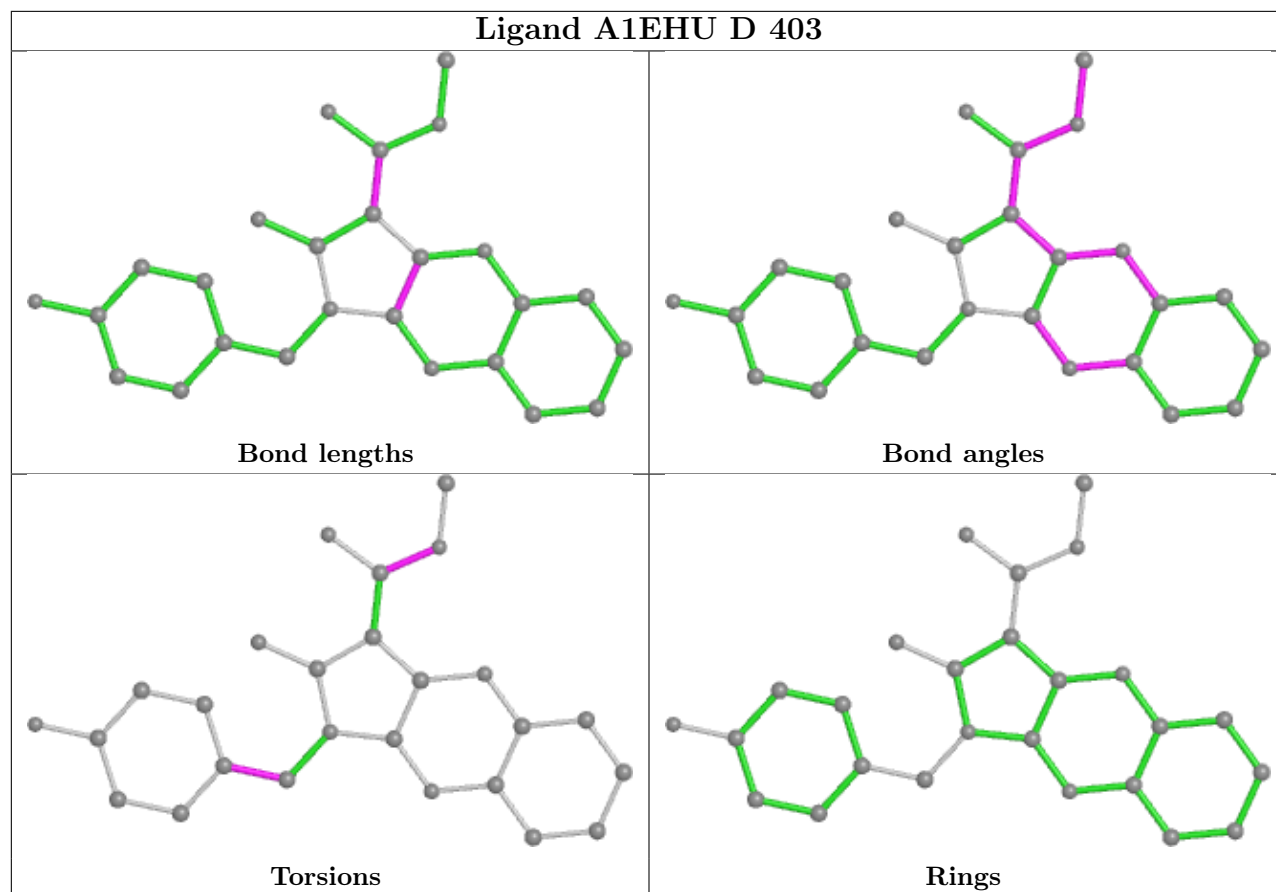
There are no ring outliers.

4 monomers are involved in 5 short contacts:

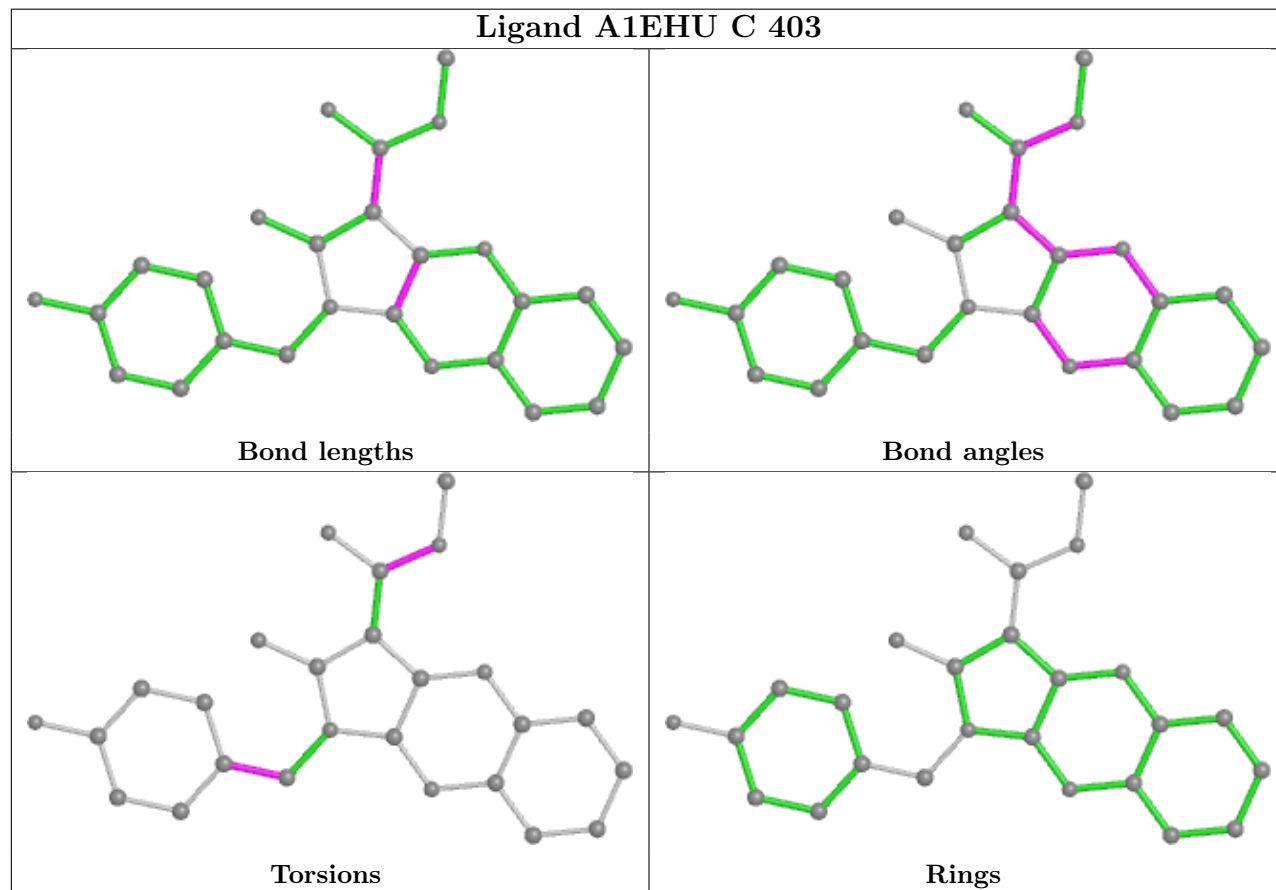
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	403	A1EHU	1	0
3	C	403	A1EHU	1	0
3	B	403	A1EHU	2	0
3	A	402	A1EHU	1	0

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.

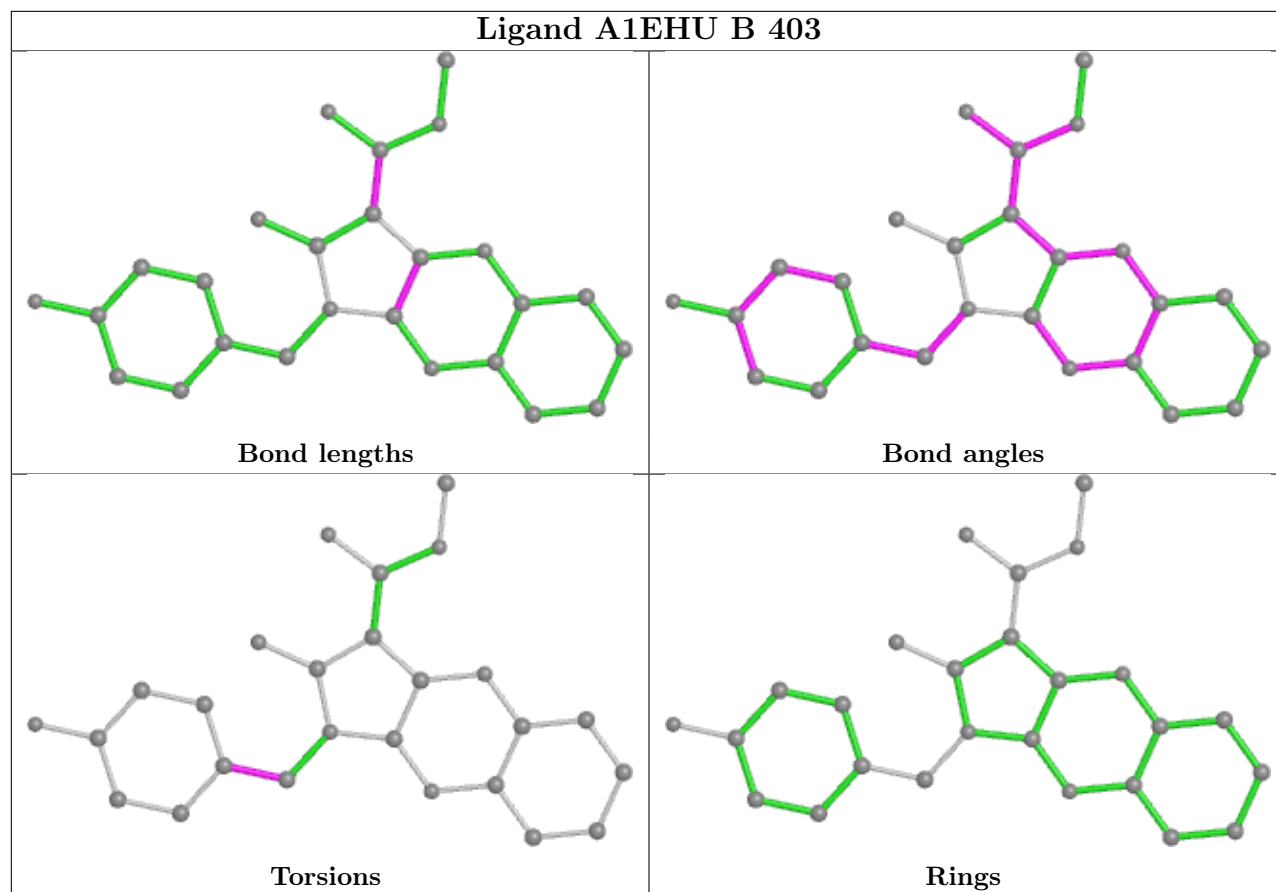
Ligand A1EHU D 403



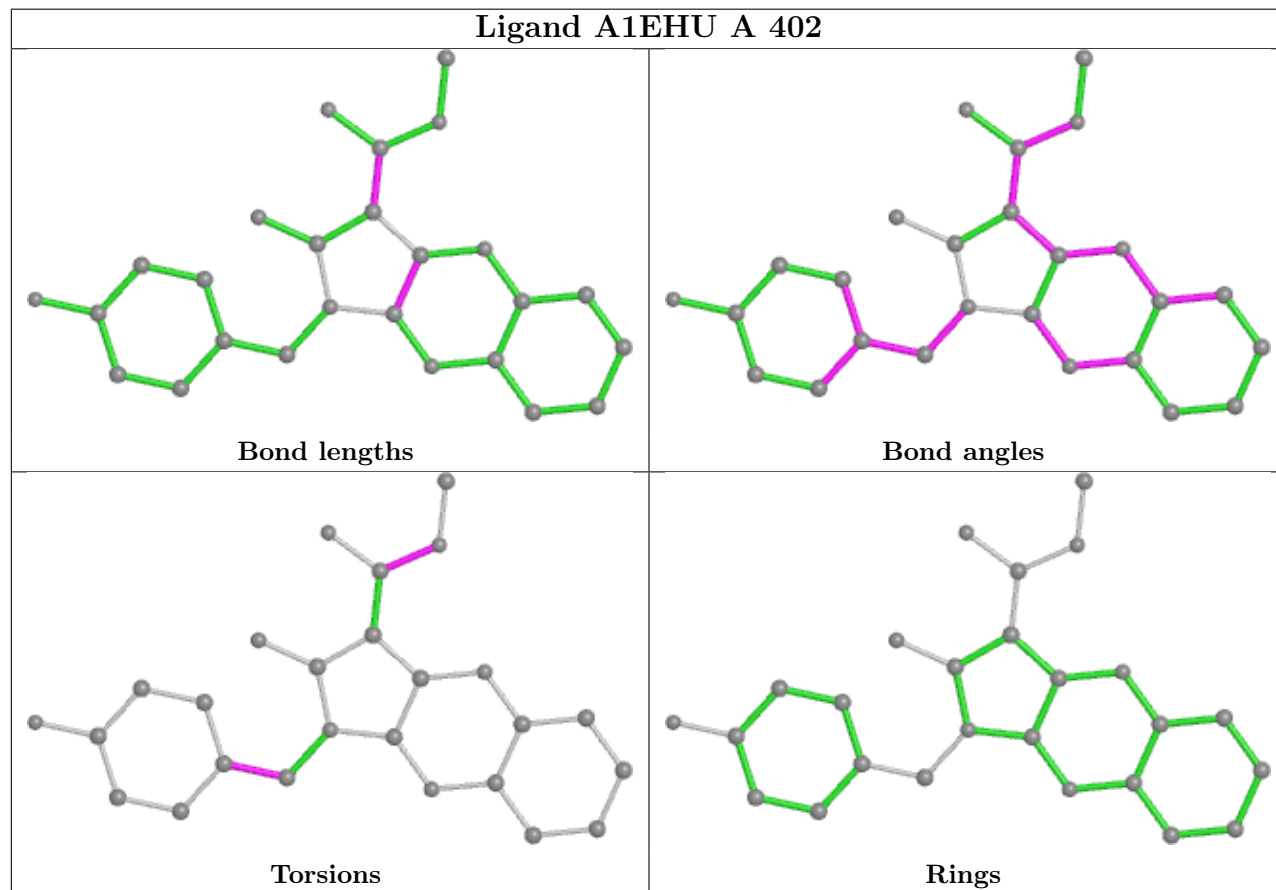
Ligand A1EHU C 403



Ligand A1EHU B 403



Ligand A1EHU A 402



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	267/277 (96%)	0.39	17 (6%) 27 25	38, 54, 77, 91	0
1	B	269/277 (97%)	0.36	19 (7%) 23 22	33, 47, 73, 91	0
1	C	261/277 (94%)	1.25	50 (19%) 4 4	46, 73, 107, 121	0
1	D	265/277 (95%)	1.22	51 (19%) 4 4	43, 73, 102, 119	0
All	All	1062/1108 (95%)	0.80	137 (12%) 9 8	33, 62, 98, 121	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	164	LEU	7.3
1	B	282	VAL	7.3
1	D	286	VAL	7.0
1	D	265	GLY	6.3
1	B	281	PRO	5.7
1	C	167	ASN	5.4
1	B	283	CYS	5.2
1	D	263	PHE	5.0
1	D	282	VAL	4.9
1	D	262	PRO	4.6
1	B	274	ALA	4.5
1	D	353	TRP	4.3
1	D	203	ASN	4.3
1	B	276	ARG	4.2
1	D	261	ARG	4.2
1	C	175	TYR	4.2
1	A	187	HIS	4.1
1	C	284	THR	4.0
1	C	157	PHE	4.0
1	C	347	LEU	3.9
1	C	281	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	175	TYR	3.9
1	B	279	ARG	3.9
1	C	277	VAL	3.9
1	B	278	PRO	3.9
1	D	283	CYS	3.8
1	B	273	MET	3.8
1	D	147	GLY	3.7
1	D	165	TYR	3.7
1	C	272	VAL	3.6
1	B	353	TRP	3.6
1	D	170	GLN	3.6
1	C	193	PHE	3.6
1	C	278	PRO	3.5
1	D	324	VAL	3.5
1	B	275	ASP	3.5
1	D	174	PRO	3.5
1	D	285	GLY	3.5
1	A	168	LEU	3.4
1	C	160	PRO	3.4
1	D	176	PRO	3.4
1	B	187	HIS	3.4
1	D	168	LEU	3.3
1	C	258	VAL	3.3
1	C	270	ALA	3.3
1	C	380	THR	3.3
1	C	280	CYS	3.3
1	D	157	PHE	3.3
1	D	284	THR	3.2
1	C	194	THR	3.2
1	D	298	LEU	3.1
1	D	386	LEU	3.1
1	C	286	VAL	3.1
1	D	160	PRO	3.1
1	D	156	ASP	3.1
1	B	272	VAL	3.1
1	D	369	GLY	3.0
1	C	197	LYS	3.0
1	C	379	TRP	3.0
1	D	390	GLU	3.0
1	C	166	SER	2.9
1	D	299	PRO	2.9
1	A	165	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	280	CYS	2.9
1	A	122	LYS	2.8
1	D	281	PRO	2.8
1	C	283	CYS	2.8
1	D	120	LYS	2.8
1	D	164	LEU	2.8
1	D	273	MET	2.8
1	B	277	VAL	2.7
1	D	171	TYR	2.7
1	C	361	ALA	2.7
1	B	284	THR	2.7
1	C	324	VAL	2.6
1	D	387	VAL	2.6
1	C	163	GLY	2.6
1	C	186	PHE	2.6
1	C	135	ARG	2.6
1	C	199	LEU	2.6
1	D	361	ALA	2.6
1	C	257	THR	2.6
1	C	275	ASP	2.6
1	A	274	ALA	2.6
1	C	201	PRO	2.6
1	B	299	PRO	2.5
1	C	195	LEU	2.5
1	D	351	LEU	2.5
1	D	268	ILE	2.5
1	A	276	ARG	2.5
1	A	169	GLN	2.5
1	C	165	TYR	2.5
1	A	200	TYR	2.4
1	D	348	VAL	2.4
1	A	391	THR	2.4
1	C	357	SER	2.4
1	D	155	PRO	2.4
1	C	273	MET	2.4
1	D	220	GLY	2.4
1	C	173	LEU	2.3
1	A	332	GLU	2.3
1	D	173	LEU	2.3
1	C	198	GLU	2.3
1	B	161	GLY	2.3
1	C	238	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	298	LEU	2.3
1	A	353	TRP	2.3
1	B	164	LEU	2.2
1	D	202	GLY	2.2
1	D	208	VAL	2.2
1	D	287	VAL	2.2
1	C	122	LYS	2.2
1	D	318	LEU	2.2
1	C	192	PHE	2.2
1	C	263	PHE	2.2
1	C	151	PRO	2.2
1	C	266	GLU	2.2
1	C	261	ARG	2.1
1	D	391	THR	2.1
1	A	259	CYS	2.1
1	A	203	ASN	2.1
1	B	163	GLY	2.1
1	C	200	TYR	2.1
1	D	376	LEU	2.1
1	D	278	PRO	2.1
1	D	130	GLU	2.1
1	C	269	ARG	2.1
1	C	171	TYR	2.0
1	B	122	LYS	2.0
1	D	327	PHE	2.0
1	A	325	GLU	2.0
1	D	159	SER	2.0
1	A	167	ASN	2.0
1	C	276	ARG	2.0
1	D	367	VAL	2.0
1	C	169	GLN	2.0
1	A	269	ARG	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

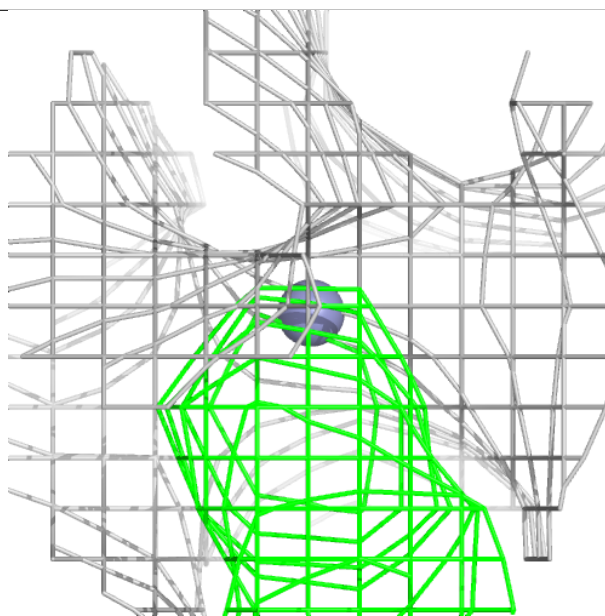
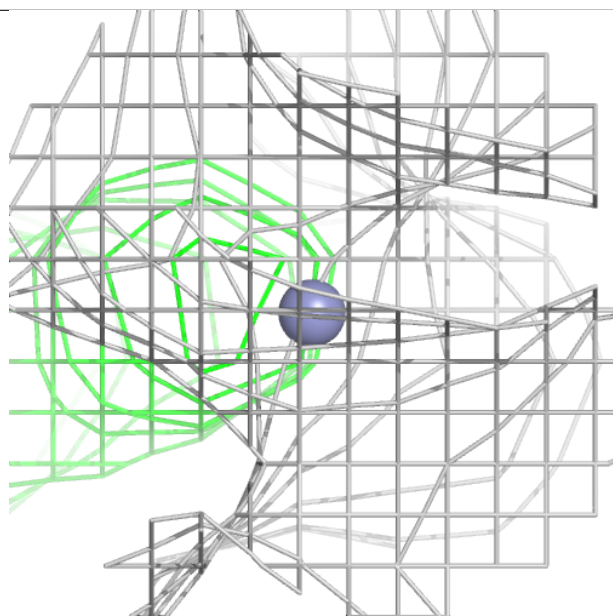
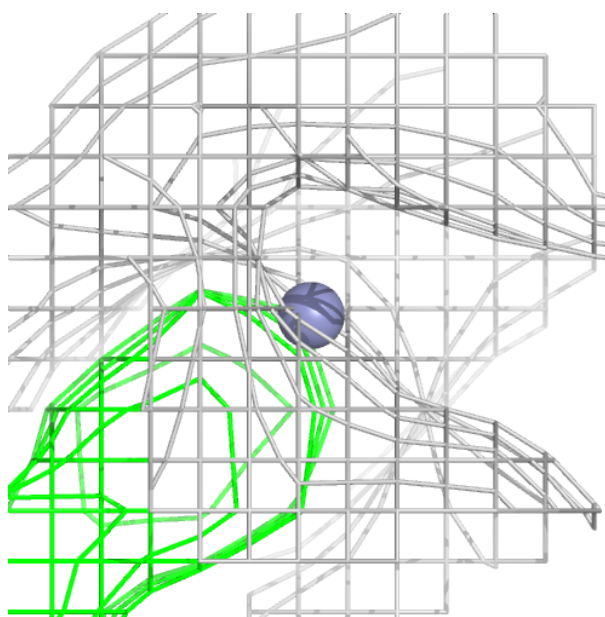
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	A	401	1/1	-	-	53,53,53,53	1
2	ZN	B	401	1/1	-	-	68,68,68,68	1
2	ZN	C	401	1/1	-	-	95,95,95,95	1
2	ZN	D	401	1/1	-	-	84,84,84,84	1
4	MG	D	402	1/1	0.64	0.21	78,78,78,78	0
3	A1EHU	C	403	26/26	0.89	0.11	57,66,76,81	0
3	A1EHU	A	402	26/26	0.91	0.10	43,52,56,58	0
3	A1EHU	D	403	26/26	0.93	0.09	42,47,55,55	0
4	MG	B	402	1/1	-	-	76,76,76,76	1
4	MG	C	402	1/1	-	-	87,87,87,87	1
3	A1EHU	B	403	26/26	0.94	0.08	32,39,42,45	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.

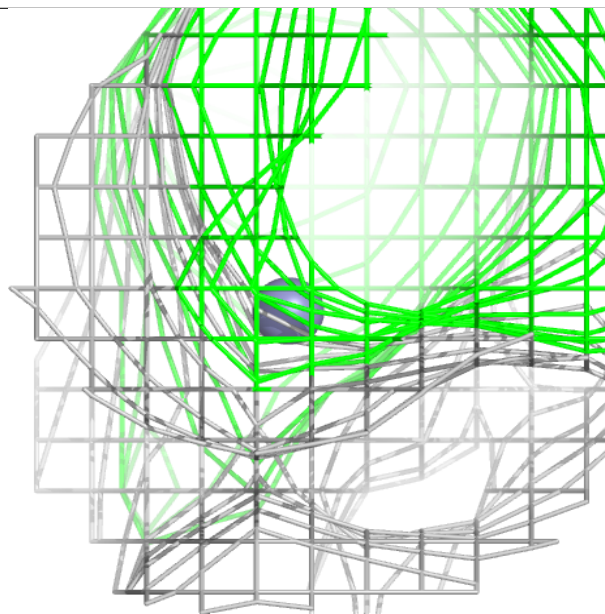
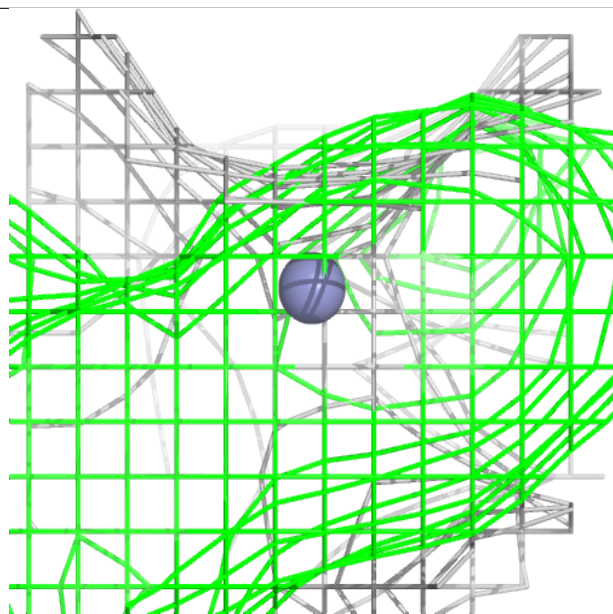
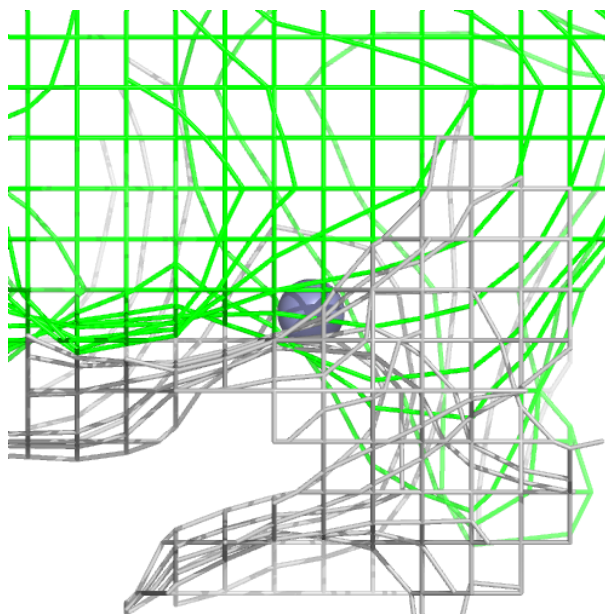
Electron density around ZN A 401:

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



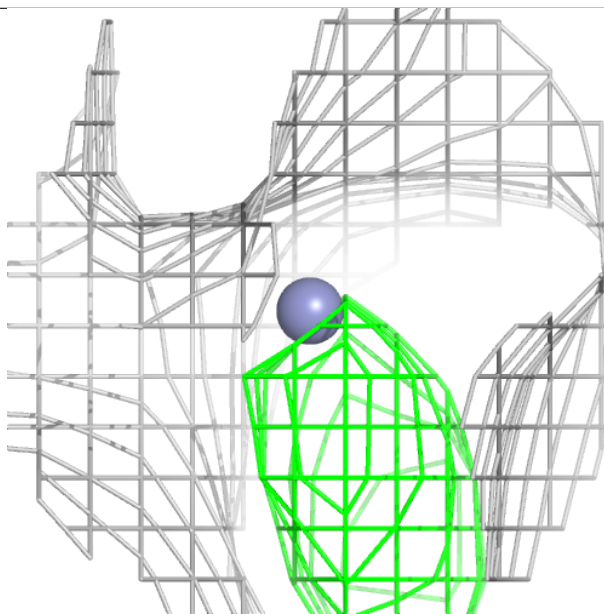
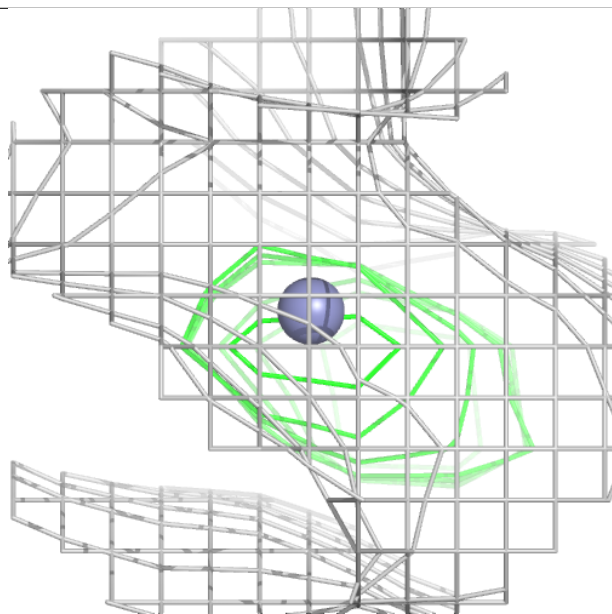
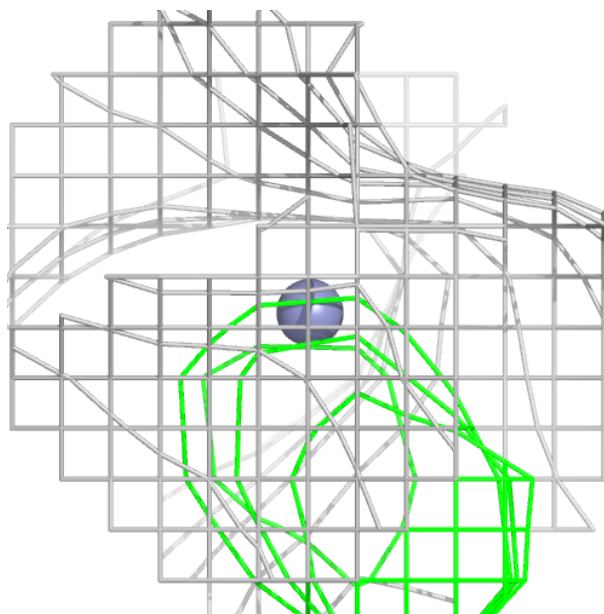
Electron density around ZN B 401:

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



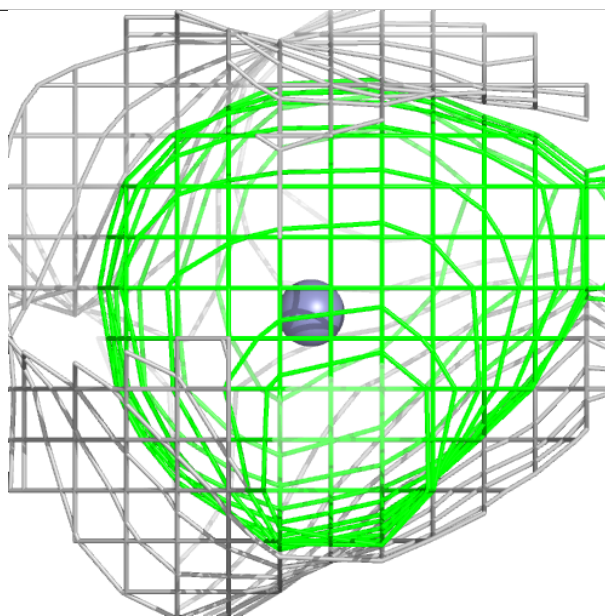
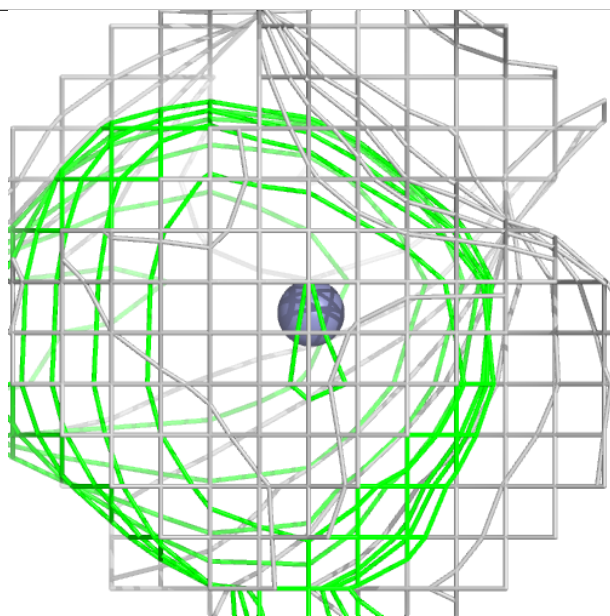
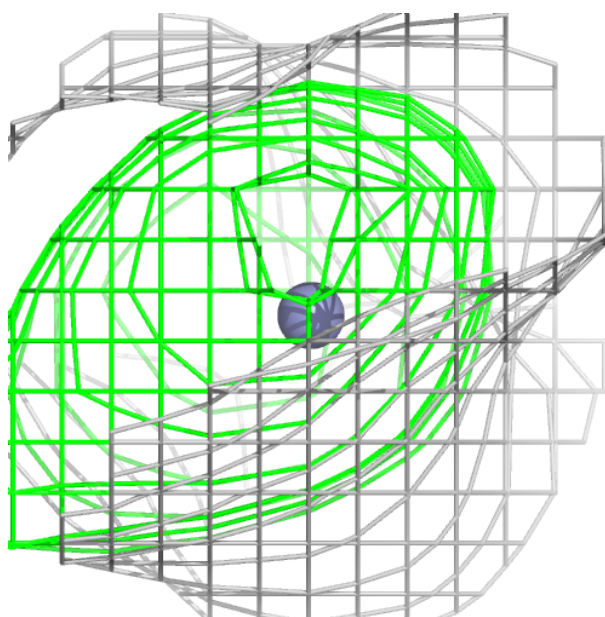
Electron density around ZN C 401:

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



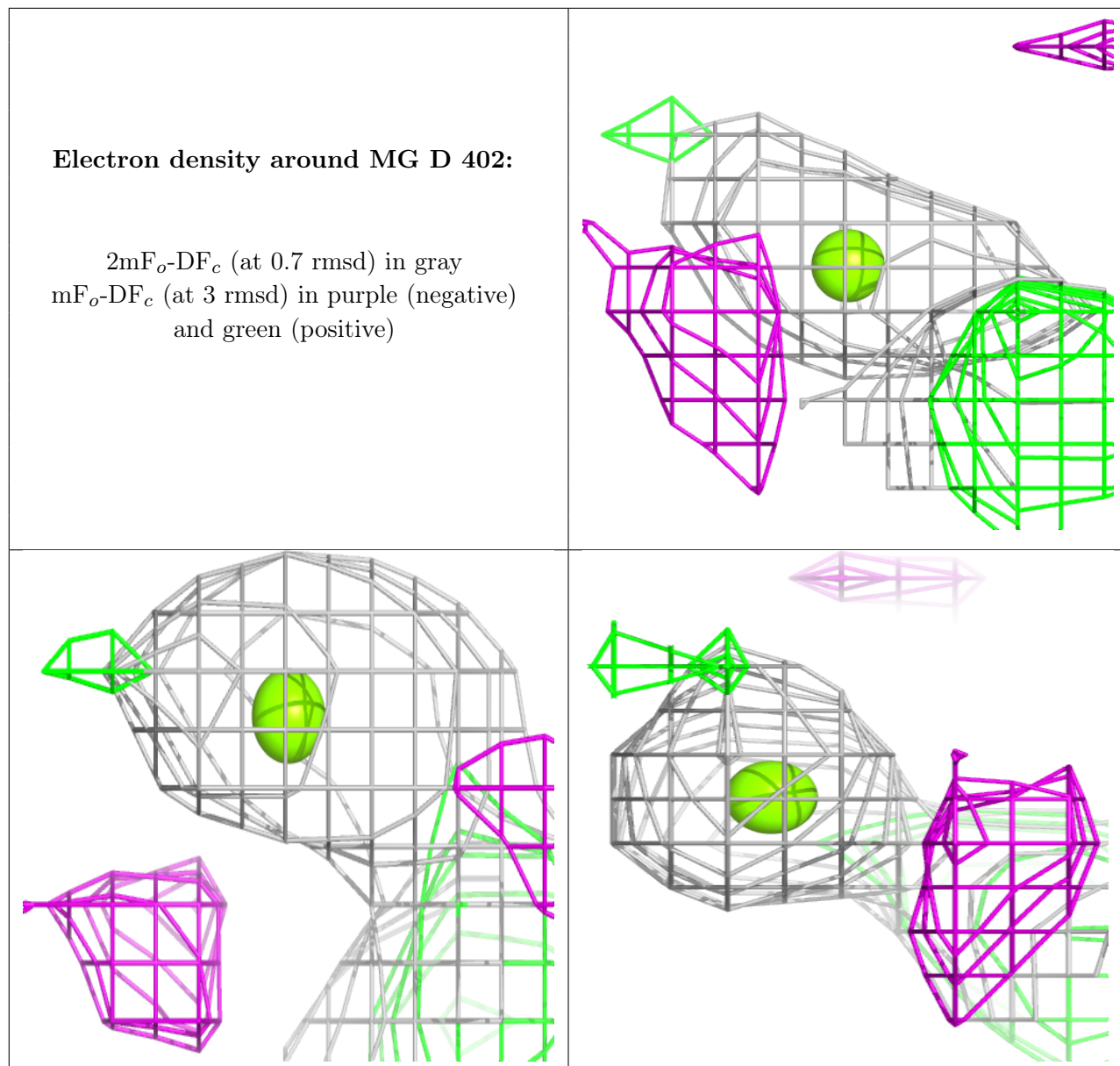
Electron density around ZN D 401:

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



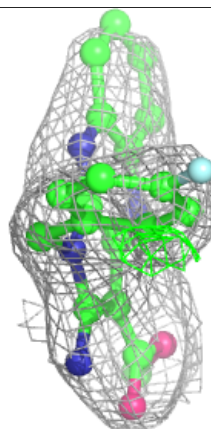
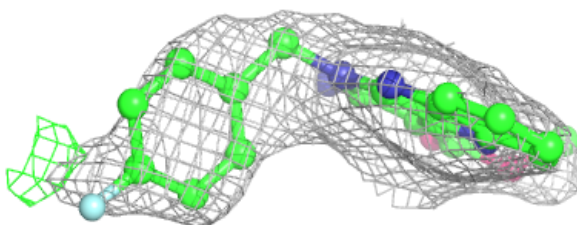
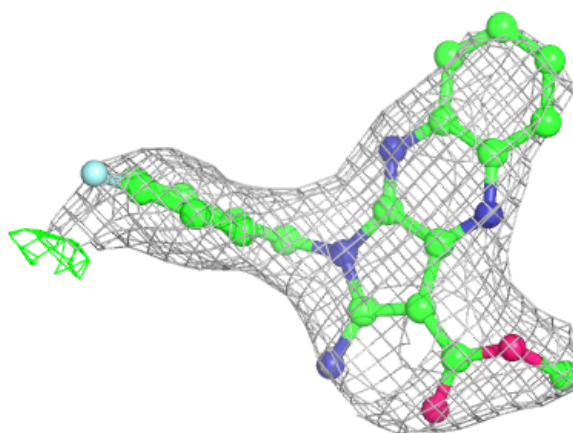
Electron density around MG D 402:

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



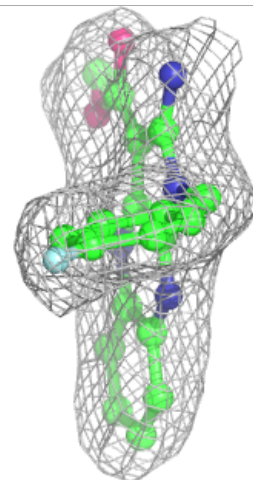
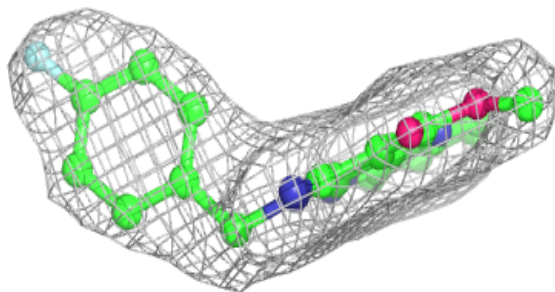
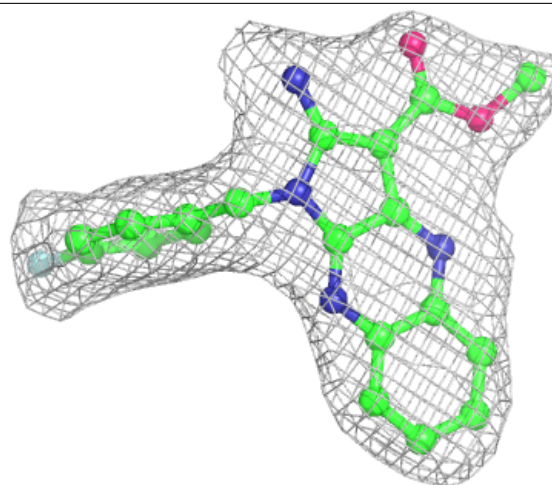
Electron density around A1EHU C 403:

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



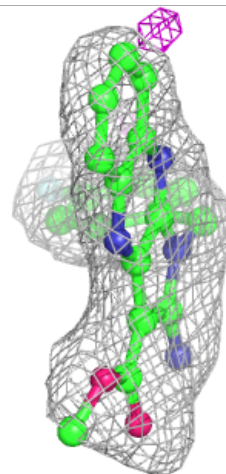
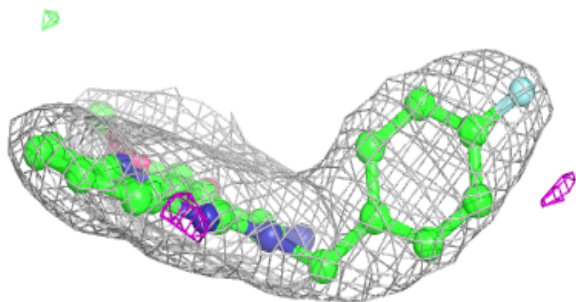
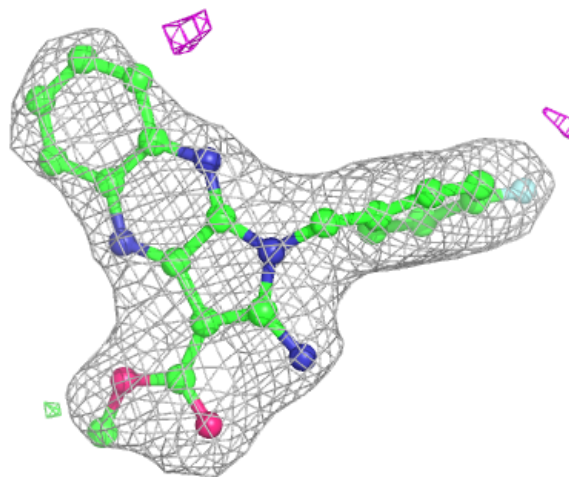
Electron density around A1EHU A 402:

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



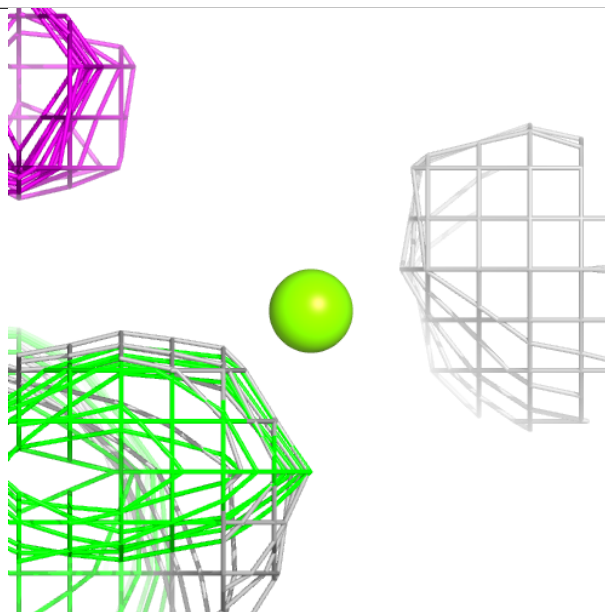
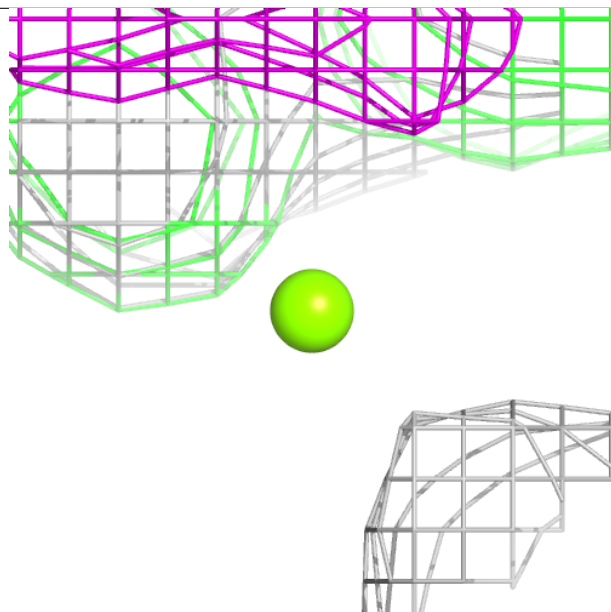
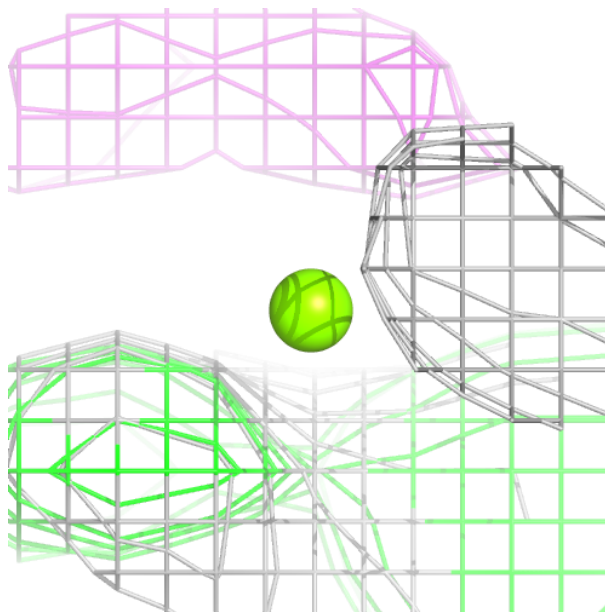
Electron density around A1EHU D 403:

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



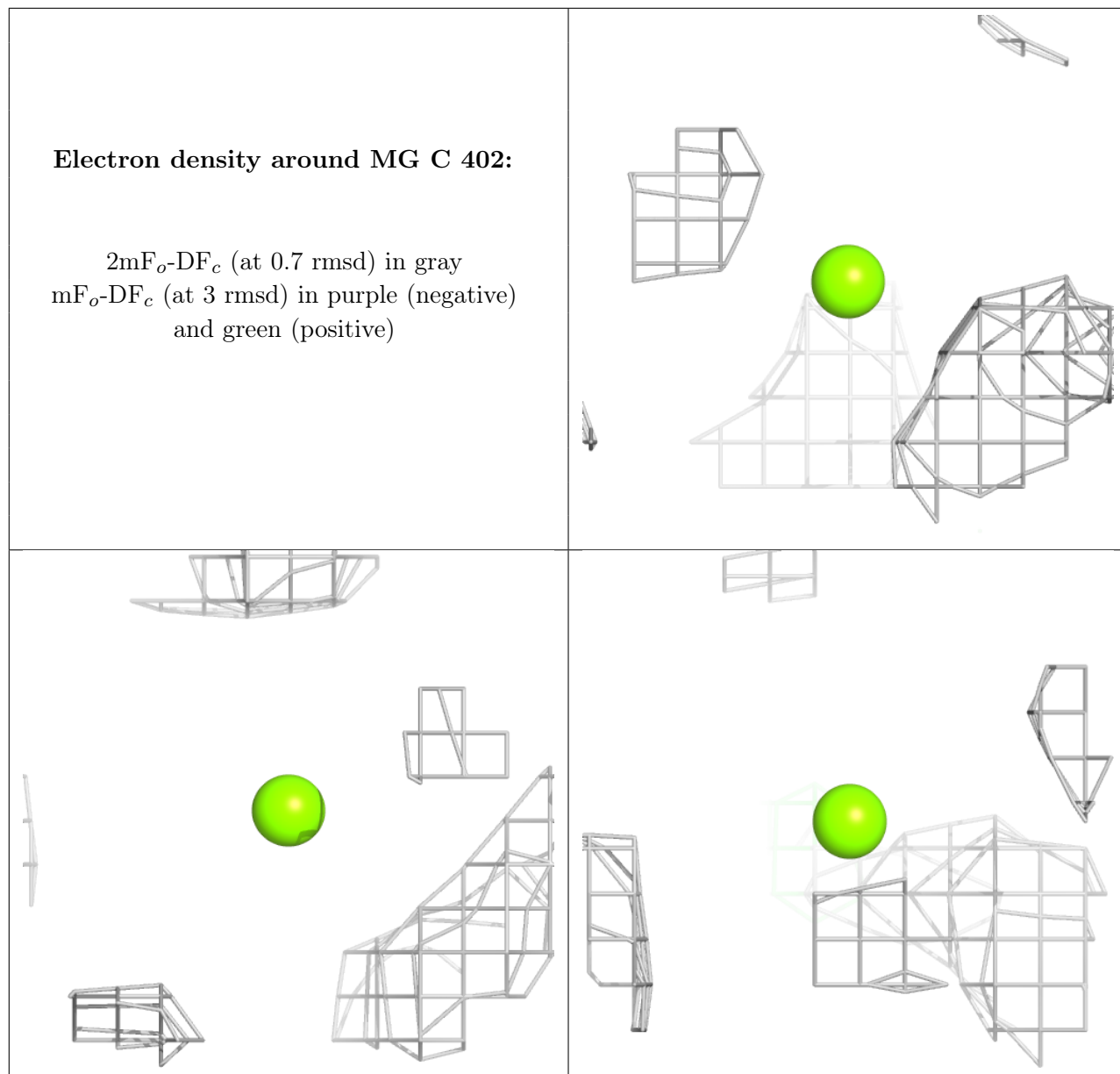
Electron density around MG B 402:

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and green (positive)



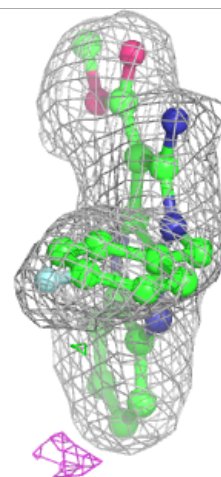
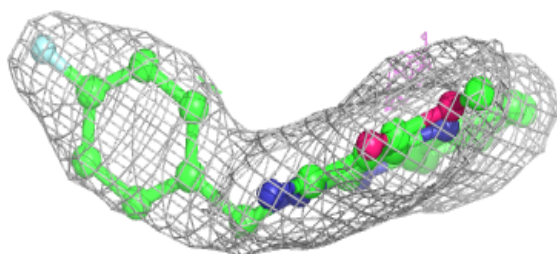
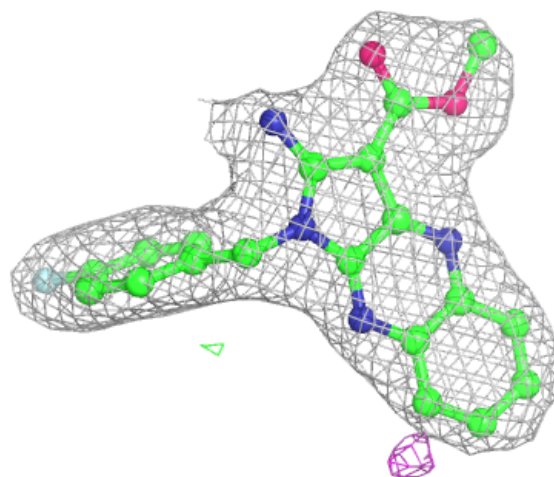
Electron density around MG C 402:

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



Electron density around A1EHU B 403:

$2mF_o-DF_c$ (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.