



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:41 AM UTC

PDB ID : 8UPQ / pdb_00008upq
Title : Campylobacter jejuni ketol-acid reductoisomerase in complex with 2,3-dihydroxy-3-isovalerate.
Authors : Lin, X.; Lonhienne, T.; Guddat, L.W.
Deposited on : 2023-10-23
Resolution : 2.45 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

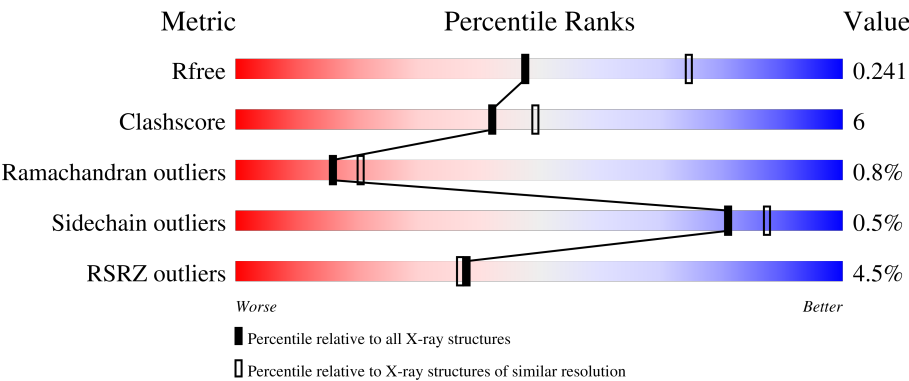
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	344	5% 86% 13% ..
1	B	344	% 88% 11% .
1	C	344	% 86% 13% .
1	D	344	2% 85% 13% .
1	E	344	8% 80% 18% ..

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Mol	Chain	Length	Quality of chain
1	F	344	10% 83% 16%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15985 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 Ketol-acid reductoisomerase (NADP(+)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	1	0
			2555	1612	434	493	16			
1	B	342	Total	C	N	O	S	0	0	0
			2581	1631	441	493	16			
1	C	341	Total	C	N	O	S	0	0	0
			2574	1628	439	491	16			
1	F	341	Total	C	N	O	S	0	1	0
			2563	1619	438	490	16			
1	E	340	Total	C	N	O	S	0	0	0
			2564	1619	442	486	17			
1	D	340	Total	C	N	O	S	0	0	0
			2544	1605	437	486	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	337	ALA	LYS	conflict	UNP A0A5T0UG45
B	337	ALA	LYS	conflict	UNP A0A5T0UG45
C	337	ALA	LYS	conflict	UNP A0A5T0UG45
F	337	ALA	LYS	conflict	UNP A0A5T0UG45
E	337	ALA	LYS	conflict	UNP A0A5T0UG45
D	337	ALA	LYS	conflict	UNP A0A5T0UG45

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

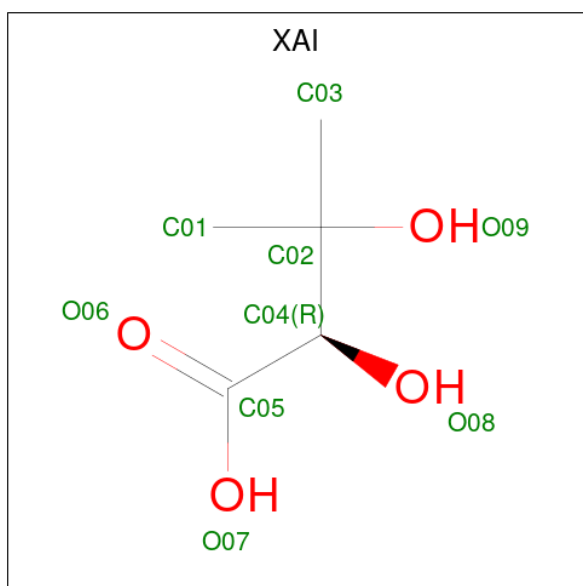
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

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

- Molecule 3 is (2R)-2,3-dihydroxy-3-methylbutanoic acid (CCD ID: XAI) (formula: C₅H₁₀O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	5	4		
3	B	1	Total	C	O	0	0
			9	5	4		
3	C	1	Total	C	O	0	0
			9	5	4		
3	F	1	Total	C	O	0	0
			9	5	4		
3	E	1	Total	C	O	0	0
			9	5	4		
3	D	1	Total	C	O	0	0
			9	5	4		

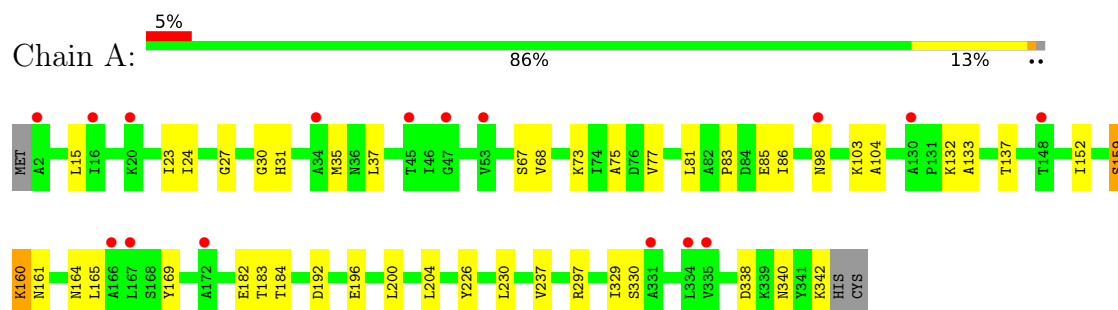
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	81	Total 81	O 81	0	0
4	B	118	Total 118	O 118	0	0
4	C	103	Total 103	O 103	0	0
4	F	77	Total 77	O 77	0	0
4	E	78	Total 78	O 78	0	0
4	D	87	Total 87	O 87	0	0

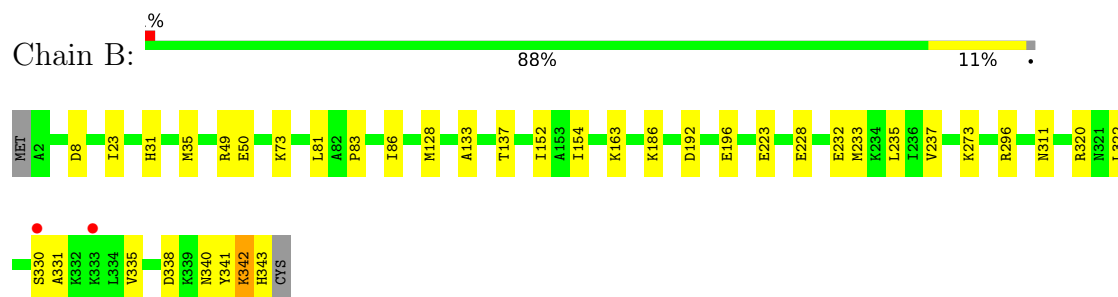
3 Residue-property plots [i](#)

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.

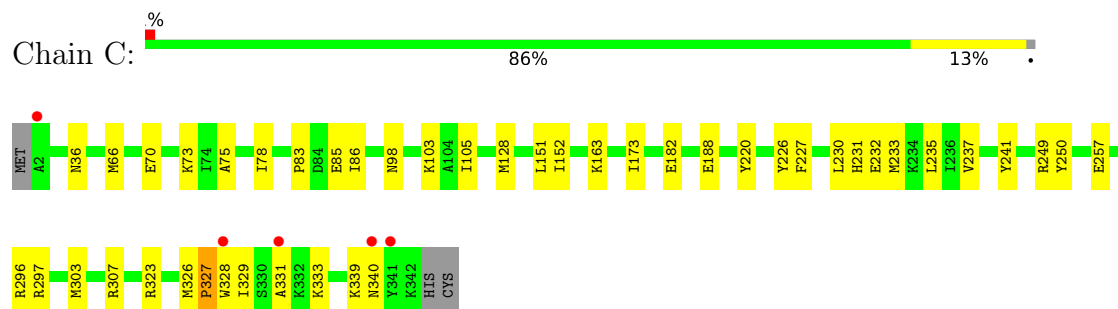
- Molecule 1: Ketol-acid reductoisomerase (NADP(+))



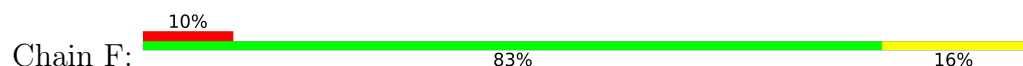
- Molecule 1: Ketol-acid reductoisomerase (NADP(+))

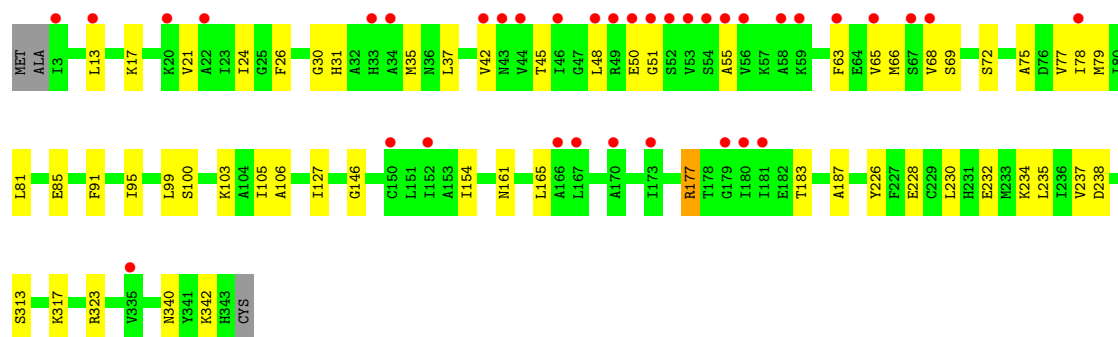


- Molecule 1: Ketol-acid reductoisomerase (NADP(+))

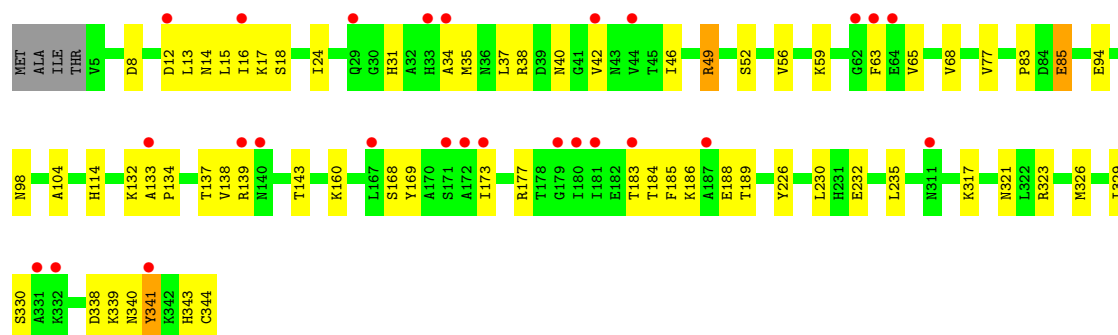


- Molecule 1: Ketol-acid reductoisomerase (NADP(+))

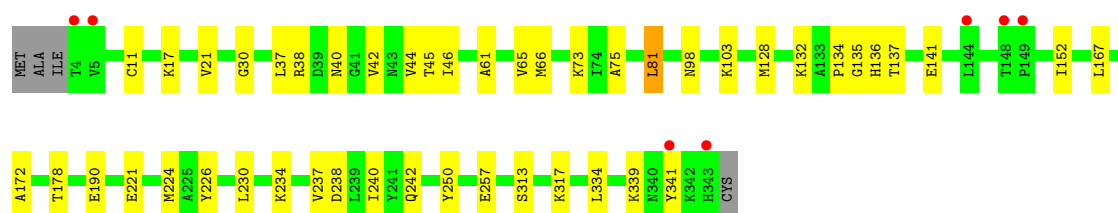
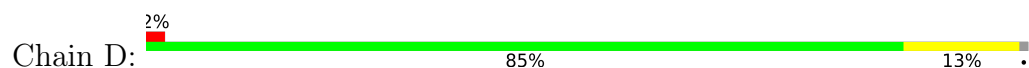




- Molecule 1: Ketol-acid reductoisomerase (NADP(+))



- Molecule 1: Ketol-acid reductoisomerase (NADP(+))



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	179.82Å 134.13Å 126.86Å 90.00° 134.83° 90.00°	Depositor
Resolution (Å)	42.19 – 2.45 42.19 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.1 (42.19-2.45) 97.3 (42.19-2.45)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.193 , 0.240 0.198 , 0.241	Depositor DCC
R_{free} test set	2019 reflections (2.57%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h+2*k,-h-l 0.004 for h,-k,-h-l 0.016 for -h-2*k,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15985	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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: MG, XAI

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	0.15	0/2598	0.33	0/3507
1	B	0.18	0/2622	0.36	0/3536
1	C	0.17	0/2615	0.35	0/3525
1	D	0.20	0/2584	0.32	0/3488
1	E	0.23	0/2606	0.43	0/3513
1	F	0.27	2/2607 (0.1%)	0.37	0/3519
All	All	0.21	2/15632 (0.0%)	0.36	0/21088

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	E	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	85	GLU	CD-OE1	-7.19	1.11	1.25
1	F	85	GLU	CD-OE2	-6.02	1.14	1.25

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	12	ASP	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	2555	0	2515	29	0
1	B	2581	0	2572	28	0
1	C	2574	0	2569	35	0
1	D	2544	0	2517	33	0
1	E	2564	0	2551	52	0
1	F	2563	0	2534	34	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	9	0	0	0	0
3	B	9	0	0	1	0
3	C	9	0	0	0	0
3	D	9	0	0	0	0
3	E	9	0	0	0	0
3	F	9	0	0	0	0
4	A	81	0	0	0	0
4	B	118	0	0	5	0
4	C	103	0	0	1	0
4	D	87	0	0	1	0
4	E	78	0	0	1	0
4	F	77	0	0	4	0
All	All	15985	0	15258	192	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 6.

All (192) 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:79:MET:HA	1:F:106:ALA:HB3	1.55	0.86
1:E:132:LYS:NZ	1:E:188:GLU:OE2	2.13	0.82
1:F:45:THR:HG21	1:F:66:MET:HE3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:SER:HB3	1:B:331:ALA:HA	1.68	0.75
1:F:340:ASN:ND2	1:F:342:LYS:O	2.20	0.75
1:A:77:VAL:HG22	1:A:104:ALA:HB3	1.70	0.74
1:A:297:ARG:O	1:C:297:ARG:NH1	2.22	0.73
1:F:161:ASN:O	4:F:501:HOH:O	2.06	0.73
1:B:186:LYS:NZ	4:B:501:HOH:O	2.21	0.72
1:D:30:GLY:HA2	1:D:81:LEU:HD23	1.70	0.72
1:E:16:ILE:HD13	1:E:169:TYR:HA	1.72	0.72
1:E:13:LEU:O	1:E:15:LEU:N	2.20	0.72
1:A:83:PRO:HG3	1:A:338:ASP:HB3	1.70	0.72
1:E:8:ASP:OD2	1:E:177:ARG:NH1	2.25	0.70
1:E:17:LYS:HD2	1:E:17:LYS:H	1.56	0.70
1:D:234:LYS:NZ	1:D:238:ASP:OD2	2.24	0.69
1:E:38:ARG:CZ	1:E:63:PHE:HZ	2.05	0.69
1:D:17:LYS:HE2	1:D:40:ASN:O	1.92	0.69
1:A:75:ALA:O	1:A:103:LYS:NZ	2.26	0.68
1:F:228:GLU:OE2	4:F:502:HOH:O	2.10	0.68
1:A:24:ILE:HD12	1:A:68:VAL:HG13	1.76	0.67
1:E:38:ARG:NH1	1:E:63:PHE:HZ	1.95	0.65
1:C:66:MET:HE2	1:C:70:GLU:HB3	1.77	0.65
1:F:165:LEU:N	4:F:501:HOH:O	2.30	0.64
1:F:30:GLY:HA2	1:F:81:LEU:HD12	1.80	0.62
1:F:100:SER:H	1:F:103:LYS:HD2	1.65	0.62
1:E:49:ARG:NH2	1:E:52:SER:O	2.32	0.62
1:B:273:LYS:NZ	4:B:507:HOH:O	2.31	0.61
1:F:323:ARG:NH2	4:F:507:HOH:O	2.31	0.61
1:B:311:ASN:O	1:B:320:ARG:NH2	2.34	0.61
1:F:234:LYS:NZ	1:F:238:ASP:OD2	2.34	0.60
1:E:38:ARG:NH2	1:E:63:PHE:HZ	1.99	0.60
1:A:161:ASN:OD1	1:A:164:ASN:ND2	2.32	0.60
1:D:38:ARG:NH2	1:D:61:ALA:O	2.34	0.59
1:A:23:ILE:HG23	1:A:81:LEU:HD12	1.85	0.59
1:C:329:ILE:O	1:D:242:GLN:NE2	2.32	0.59
1:E:35:MET:O	1:E:38:ARG:HD2	2.04	0.58
1:C:163:LYS:NZ	1:C:182:GLU:OE1	2.37	0.57
1:E:326:MET:HB2	1:E:329:ILE:HG12	1.86	0.57
1:E:24:ILE:HD12	1:E:68:VAL:HG13	1.87	0.57
1:E:34:ALA:HB1	1:E:38:ARG:NH2	2.20	0.57
1:B:340:ASN:O	1:B:342:LYS:N	2.34	0.56
1:D:45:THR:HG21	1:D:66:MET:HE3	1.88	0.56
1:A:192:ASP:O	1:A:196:GLU:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:TYR:OH	1:D:190:GLU:OE1	2.24	0.56
1:A:137:THR:HG21	1:B:235:LEU:HB3	1.87	0.55
1:F:99:LEU:HD21	1:F:105:ILE:HD11	1.88	0.55
1:F:313:SER:O	1:F:317:LYS:HG2	2.05	0.55
1:E:37:LEU:HB3	1:E:42:VAL:CG2	2.37	0.55
1:F:127:ILE:HG22	1:F:154:ILE:CD1	2.36	0.55
1:E:183:THR:HG22	1:E:184:THR:H	1.71	0.55
1:C:241:TYR:CD2	1:D:234:LYS:HD3	2.41	0.54
1:B:232:GLU:OE2	3:B:402:XAI:O09	2.25	0.54
1:C:250:TYR:HA	1:D:339:LYS:HE2	1.89	0.54
1:E:16:ILE:HG23	1:E:168:SER:HB3	1.90	0.54
1:E:38:ARG:NH2	1:E:63:PHE:CZ	2.76	0.53
1:D:221:GLU:HB2	1:D:224:MET:HG3	1.90	0.53
1:F:24:ILE:HD12	1:F:68:VAL:HG13	1.90	0.52
1:F:146:GLY:O	1:F:177[B]:ARG:NH1	2.38	0.52
1:E:13:LEU:C	1:E:15:LEU:H	2.13	0.52
1:A:30:GLY:HA2	1:A:81:LEU:HD13	1.91	0.51
1:A:31:HIS:NE2	1:A:35:MET:HE2	2.25	0.51
1:A:132:LYS:HD2	1:B:228:GLU:OE2	2.10	0.51
1:F:26:PHE:HB2	1:F:48:LEU:HD11	1.93	0.51
1:E:16:ILE:HG12	1:E:168:SER:OG	2.11	0.51
1:F:127:ILE:HG22	1:F:154:ILE:HD12	1.93	0.51
1:E:38:ARG:NH1	1:E:63:PHE:CZ	2.77	0.50
1:E:94:GLU:O	1:E:98:ASN:ND2	2.44	0.50
1:C:83:PRO:HD2	1:C:86:ILE:HD11	1.94	0.50
1:C:329:ILE:C	1:D:242:GLN:HE22	2.19	0.50
1:F:75:ALA:O	1:F:103:LYS:NZ	2.35	0.50
1:F:78:ILE:O	1:F:106:ALA:N	2.37	0.50
1:D:75:ALA:O	1:D:103:LYS:NZ	2.37	0.50
1:D:73:LYS:HG2	1:D:98:ASN:HB3	1.94	0.50
1:D:313:SER:O	1:D:317:LYS:HG3	2.10	0.50
1:F:55:ALA:HB1	1:F:65:VAL:HG21	1.94	0.50
1:E:232:GLU:HG3	1:E:235:LEU:HD12	1.94	0.50
1:E:37:LEU:HD11	1:E:169:TYR:CZ	2.47	0.50
1:C:241:TYR:CG	1:D:234:LYS:HD3	2.47	0.49
1:F:79:MET:CA	1:F:106:ALA:HB3	2.36	0.49
1:F:232:GLU:HA	1:F:235:LEU:HD23	1.93	0.49
1:C:327:PRO:HD2	1:C:328:TRP:CZ3	2.48	0.49
1:B:341:TYR:O	1:B:343:HIS:N	2.45	0.49
1:F:31:HIS:CD2	1:F:35:MET:HE1	2.48	0.48
1:F:35:MET:HG3	1:F:63:PHE:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:133:ALA:HB1	1:E:137:THR:CG2	2.43	0.48
1:E:185:PHE:O	1:E:189:THR:HG23	2.13	0.48
1:F:13:LEU:HD13	1:F:17:LYS:HE2	1.96	0.48
1:E:77:VAL:HG22	1:E:104:ALA:HB3	1.95	0.48
1:D:21:VAL:HG11	1:D:37:LEU:HD13	1.94	0.48
1:A:237:VAL:HG11	1:B:233:MET:HG2	1.94	0.48
1:F:106:ALA:HA	1:F:127:ILE:HD12	1.96	0.48
1:E:34:ALA:HB1	1:E:38:ARG:HH22	1.77	0.48
1:E:17:LYS:HA	1:E:42:VAL:HG12	1.95	0.47
1:E:133:ALA:HB1	1:E:137:THR:HG23	1.96	0.47
1:C:307:ARG:HD3	1:D:257:GLU:OE2	2.13	0.47
1:F:91:PHE:HA	1:F:95:ILE:HB	1.97	0.47
1:E:37:LEU:HB3	1:E:42:VAL:HG21	1.96	0.47
1:E:15:LEU:O	1:E:18:SER:OG	2.26	0.47
1:E:339:LYS:O	1:E:341:TYR:N	2.47	0.47
1:E:134:PRO:O	1:E:138:VAL:HG23	2.14	0.47
1:B:133:ALA:HB1	1:B:137:THR:OG1	2.15	0.47
1:D:134:PRO:O	1:D:137:THR:HG22	2.14	0.46
1:D:137:THR:O	1:D:141:GLU:HG2	2.15	0.46
1:A:183:THR:OG1	1:A:184:THR:N	2.45	0.46
1:C:75:ALA:O	1:C:103:LYS:NZ	2.36	0.46
1:B:192:ASP:O	1:B:196:GLU:HG3	2.16	0.46
1:C:235:LEU:HD13	1:D:137:THR:HG21	1.96	0.46
1:C:303:MET:O	1:C:307:ARG:HG3	2.16	0.46
1:F:13:LEU:CD1	1:F:17:LYS:HE2	2.46	0.46
1:C:233:MET:O	1:C:237:VAL:HG23	2.15	0.46
1:E:139:ARG:HH11	1:E:143:THR:HG21	1.81	0.46
1:A:15:LEU:HD21	1:A:165:LEU:HD12	1.98	0.46
1:E:17:LYS:HD2	1:E:17:LYS:N	2.28	0.46
1:E:31:HIS:O	1:E:35:MET:HG2	2.15	0.46
1:A:85:GLU:HG2	1:A:86:ILE:HG23	1.97	0.45
1:A:226:TYR:CZ	1:A:230:LEU:HD22	2.51	0.45
1:E:46:ILE:HB	1:E:65:VAL:HG22	1.97	0.45
1:A:37:LEU:HD11	1:A:169:TYR:CZ	2.51	0.45
1:B:83:PRO:HG3	1:B:338:ASP:HB3	1.99	0.45
1:A:159:SER:OG	1:A:160:LYS:N	2.49	0.45
1:B:31:HIS:O	1:B:35:MET:HG2	2.16	0.45
1:C:128:MET:O	1:C:152:ILE:HA	2.16	0.45
1:E:56:VAL:HA	1:E:59:LYS:HG2	1.98	0.45
1:C:328:TRP:HH2	1:D:178:THR:HB	1.82	0.45
1:F:37:LEU:HB3	1:F:42:VAL:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:LEU:HD11	1:E:169:TYR:OH	2.17	0.44
1:F:183:THR:OG1	1:F:187:ALA:HB3	2.17	0.44
1:C:85:GLU:HB3	1:C:296:ARG:HD2	2.00	0.44
1:D:128:MET:O	1:D:152:ILE:HA	2.17	0.44
1:B:86:ILE:HG22	1:B:296:ARG:NH1	2.31	0.44
1:B:73:LYS:NZ	4:B:520:HOH:O	2.50	0.44
1:B:330:SER:HB3	1:B:331:ALA:CA	2.45	0.44
1:F:226:TYR:CZ	1:F:230:LEU:HD22	2.53	0.44
1:E:226:TYR:CZ	1:E:230:LEU:HD22	2.53	0.44
1:D:46:ILE:HB	1:D:65:VAL:HG22	2.00	0.44
1:A:133:ALA:HB1	1:A:137:THR:OG1	2.17	0.44
1:C:232:GLU:CD	1:D:132:LYS:HB3	2.43	0.43
1:E:37:LEU:HG	1:E:173:ILE:HD11	2.00	0.43
1:E:343:HIS:N	1:E:344:CYS:HA	2.32	0.43
1:C:226:TYR:OH	4:C:501:HOH:O	2.20	0.43
1:E:83:PRO:HG3	1:E:338:ASP:HB3	1.99	0.43
1:E:85:GLU:H	1:E:85:GLU:CD	2.26	0.43
1:A:73:LYS:HG2	1:A:98:ASN:HB3	1.99	0.43
1:C:235:LEU:HD23	1:C:235:LEU:HA	1.89	0.43
1:C:230:LEU:HD21	1:D:240:ILE:HG22	2.01	0.42
1:F:21:VAL:HA	1:F:77:VAL:HG22	2.00	0.42
1:C:152:ILE:HG13	1:C:182:GLU:HA	2.00	0.42
1:C:227:PHE:HA	1:C:231:HIS:HB3	2.00	0.42
1:A:152:ILE:HG13	1:A:182:GLU:HA	2.01	0.42
1:B:273:LYS:HB3	1:B:273:LYS:HE2	1.80	0.42
1:C:323:ARG:HA	1:C:326:MET:HE2	1.99	0.42
1:A:204:LEU:HD21	1:B:237:VAL:HG22	2.02	0.42
1:B:49:ARG:HD2	1:B:50:GLU:O	2.19	0.42
1:C:151:LEU:HD12	1:C:188:GLU:HG2	2.02	0.42
1:A:27:GLY:O	1:A:31:HIS:HB3	2.20	0.42
1:E:114:HIS:CD2	1:E:186:LYS:HA	2.55	0.42
1:B:23:ILE:HG23	1:B:81:LEU:HD12	2.01	0.42
1:B:128:MET:O	1:B:152:ILE:HA	2.20	0.42
1:C:73:LYS:HG3	1:C:98:ASN:HB3	2.02	0.42
1:C:339:LYS:HE2	1:D:250:TYR:HA	2.02	0.42
1:A:196:GLU:HG2	4:B:535:HOH:O	2.20	0.42
1:E:323:ARG:NH2	4:E:507:HOH:O	2.47	0.42
1:C:340:ASN:O	1:C:340:ASN:OD1	2.38	0.41
1:A:200:LEU:HA	1:B:233:MET:HE2	2.02	0.41
1:B:223:GLU:HG3	1:B:322:LEU:HD11	2.03	0.41
1:E:160:LYS:HA	1:E:160:LYS:HD3	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:ASN:HB3	1:C:173:ILE:HA	2.02	0.41
1:D:134:PRO:O	1:D:136:HIS:N	2.53	0.41
1:A:340:ASN:C	1:A:342:LYS:H	2.28	0.41
1:C:78:ILE:HB	1:C:105:ILE:HD13	2.02	0.41
1:E:13:LEU:C	1:E:15:LEU:N	2.77	0.41
1:E:329:ILE:HD13	1:E:329:ILE:HA	1.96	0.41
1:D:226:TYR:CZ	1:D:230:LEU:HD22	2.56	0.41
1:B:8:ASP:OD2	4:B:502:HOH:O	2.21	0.41
1:E:317:LYS:NZ	1:E:321:ASN:HD21	2.19	0.41
1:C:249:ARG:HB3	1:C:257:GLU:HG3	2.02	0.41
1:E:8:ASP:CG	1:E:177:ARG:NH1	2.78	0.41
1:B:233:MET:HB2	1:B:233:MET:HE3	1.82	0.41
1:F:69:SER:O	1:F:72:SER:OG	2.34	0.41
1:C:333:LYS:HD3	1:C:333:LYS:H	1.86	0.41
1:E:59:LYS:HB3	1:E:59:LYS:HE2	1.78	0.41
1:D:40:ASN:ND2	4:D:503:HOH:O	2.38	0.41
1:D:40:ASN:ND2	1:D:172:ALA:O	2.46	0.41
1:A:196:GLU:HG3	1:A:196:GLU:H	1.62	0.41
1:B:233:MET:O	1:B:237:VAL:HG23	2.21	0.41
1:D:11:CYS:SG	1:D:167:LEU:HB3	2.61	0.40
1:A:226:TYR:CE2	1:A:230:LEU:HD13	2.57	0.40
1:F:35:MET:HE3	1:F:35:MET:HB2	1.56	0.40
1:C:237:VAL:HG21	1:D:237:VAL:HG21	2.04	0.40
1:D:42:VAL:O	1:D:44:VAL:HG23	2.21	0.40
1:B:154:ILE:HD11	1:B:163:LYS:HA	2.02	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	340/344 (99%)	320 (94%)	18 (5%)	2 (1%)	21 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	340/344 (99%)	324 (95%)	14 (4%)	2 (1%)	21	27
1	C	339/344 (98%)	324 (96%)	13 (4%)	2 (1%)	21	27
1	D	338/344 (98%)	326 (96%)	9 (3%)	3 (1%)	14	17
1	E	338/344 (98%)	316 (94%)	17 (5%)	5 (2%)	8	7
1	F	340/344 (99%)	325 (96%)	13 (4%)	2 (1%)	21	27
All	All	2035/2064 (99%)	1935 (95%)	84 (4%)	16 (1%)	16	20

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	SER
1	E	330	SER
1	E	340	ASN
1	E	341	TYR
1	B	342	LYS
1	C	331	ALA
1	F	50	GLU
1	F	51	GLY
1	E	14	ASN
1	D	135	GLY
1	D	341	TYR
1	D	334	LEU
1	C	327	PRO
1	A	160	LYS
1	E	49	ARG
1	B	335	VAL

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	260/275 (94%)	257 (99%)	3 (1%)	63	74
1	B	266/275 (97%)	266 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	265/275 (96%)	265 (100%)	0	100	100
1	D	260/275 (94%)	259 (100%)	1 (0%)	84	89
1	E	264/275 (96%)	262 (99%)	2 (1%)	73	83
1	F	262/275 (95%)	259 (99%)	3 (1%)	65	76
All	All	1577/1650 (96%)	1568 (99%)	9 (1%)	81	86

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	SER
1	A	329	ILE
1	A	330	SER
1	F	177[A]	ARG
1	F	177[B]	ARG
1	F	237	VAL
1	E	40	ASN
1	E	85	GLU
1	D	81	LEU

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	33	HIS
1	A	242	GLN
1	B	43	ASN
1	F	14	ASN
1	F	92	ASN
1	F	197	GLN
1	E	33	HIS
1	E	60	ASN
1	E	321	ASN
1	D	60	ASN
1	D	311	ASN

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 12 ligands modelled in this entry, 6 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	XAI	E	402	2	7,8,8	1.27	1 (14%)	9,12,12	1.10	1 (11%)
3	XAI	F	402	2	7,8,8	1.25	1 (14%)	9,12,12	1.27	1 (11%)
3	XAI	C	402	2	7,8,8	1.27	1 (14%)	9,12,12	1.14	2 (22%)
3	XAI	D	402	2	7,8,8	1.30	1 (14%)	9,12,12	1.11	1 (11%)
3	XAI	A	402	2	7,8,8	1.24	1 (14%)	9,12,12	1.15	1 (11%)
3	XAI	B	402	2	7,8,8	1.32	1 (14%)	9,12,12	1.11	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	XAI	E	402	2	-	4/10/10/10	-
3	XAI	F	402	2	-	5/10/10/10	-
3	XAI	C	402	2	-	4/10/10/10	-
3	XAI	D	402	2	-	2/10/10/10	-
3	XAI	A	402	2	-	9/10/10/10	-
3	XAI	B	402	2	-	4/10/10/10	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	XAI	O09-C02	-2.67	1.40	1.44
3	E	402	XAI	O09-C02	-2.49	1.40	1.44
3	D	402	XAI	O09-C02	-2.49	1.40	1.44
3	A	402	XAI	O09-C02	-2.45	1.40	1.44
3	C	402	XAI	O09-C02	-2.40	1.40	1.44
3	F	402	XAI	O09-C02	-2.35	1.40	1.44

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	XAI	O07-C05-O06	-2.33	118.80	124.08
3	A	402	XAI	O07-C05-O06	-2.25	118.97	124.08
3	D	402	XAI	O07-C05-O06	-2.23	119.02	124.08
3	E	402	XAI	O07-C05-C04	2.11	121.17	112.80
3	C	402	XAI	O07-C05-C04	2.06	120.95	112.80
3	F	402	XAI	O07-C05-C04	2.02	120.79	112.80

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	XAI	C03-C02-C04-C05
3	A	402	XAI	C03-C02-C04-O08
3	A	402	XAI	C02-C04-C05-O06
3	A	402	XAI	C02-C04-C05-O07
3	C	402	XAI	C02-C04-C05-O06
3	C	402	XAI	C02-C04-C05-O07
3	F	402	XAI	C03-C02-C04-C05
3	D	402	XAI	C02-C04-C05-O06
3	D	402	XAI	C02-C04-C05-O07
3	A	402	XAI	C01-C02-C04-O08
3	F	402	XAI	C01-C02-C04-O08
3	B	402	XAI	C03-C02-C04-C05
3	B	402	XAI	C02-C04-C05-O07
3	A	402	XAI	O09-C02-C04-O08
3	C	402	XAI	O09-C02-C04-O08
3	E	402	XAI	O09-C02-C04-O08
3	B	402	XAI	C03-C02-C04-O08
3	C	402	XAI	C03-C02-C04-O08
3	F	402	XAI	C03-C02-C04-O08
3	E	402	XAI	C01-C02-C04-O08

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Mol	Chain	Res	Type	Atoms
3	A	402	XAI	O09-C02-C04-C05
3	F	402	XAI	O09-C02-C04-C05
3	A	402	XAI	C01-C02-C04-C05
3	F	402	XAI	C01-C02-C04-C05
3	E	402	XAI	C01-C02-C04-C05
3	A	402	XAI	O08-C04-C05-O07
3	B	402	XAI	C02-C04-C05-O06
3	E	402	XAI	C02-C04-C05-O07

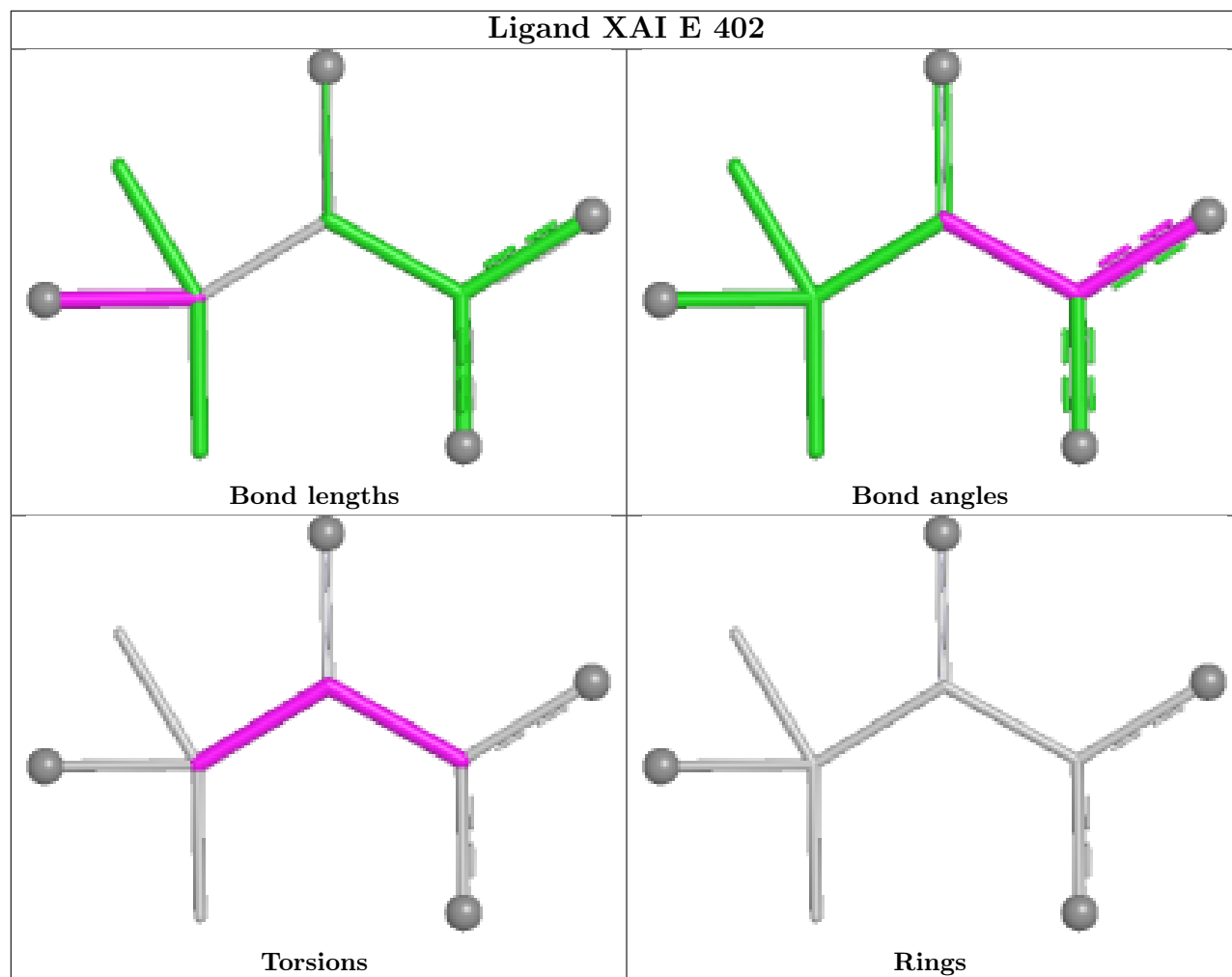
There are no ring outliers.

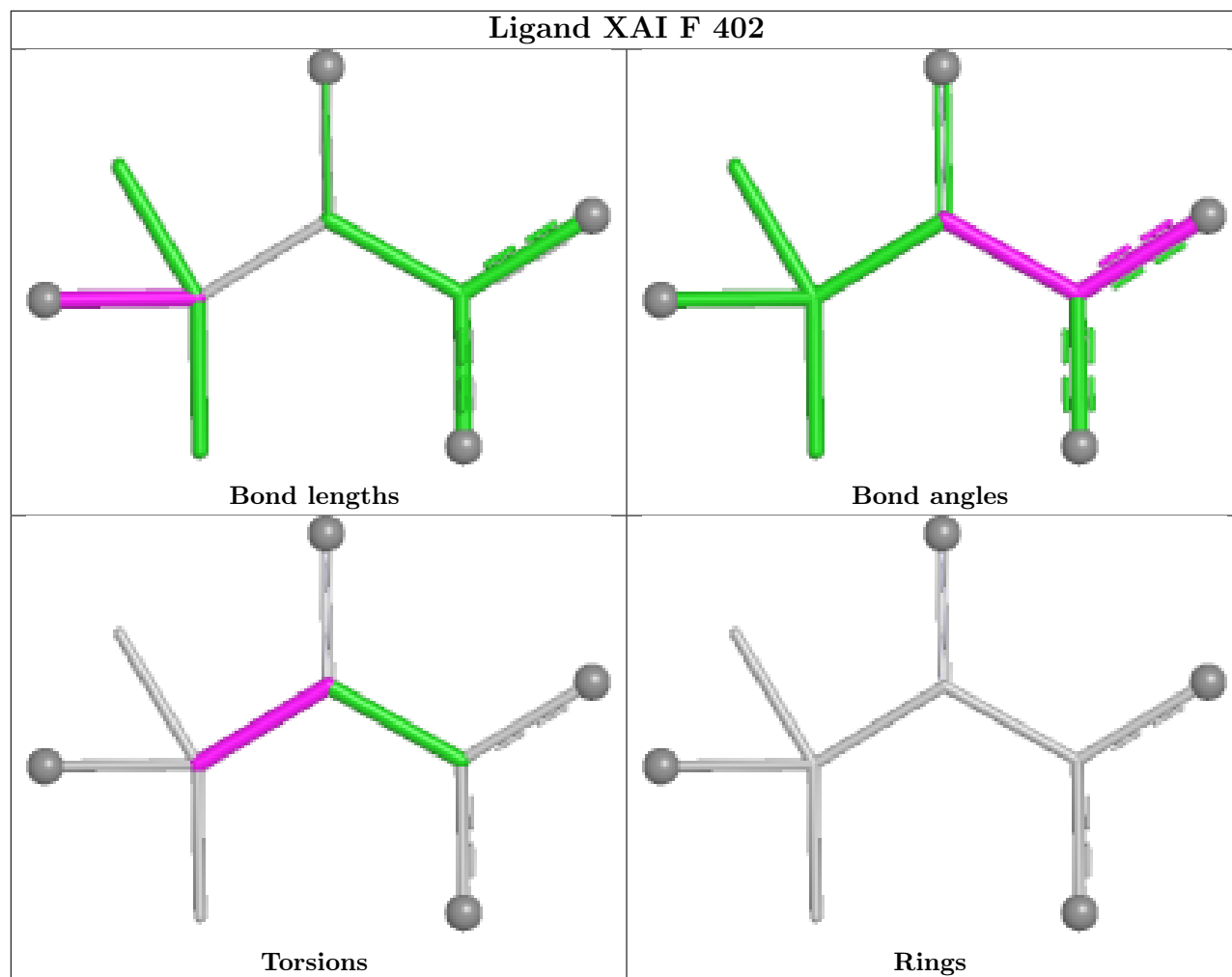
1 monomer is involved in 1 short contact:

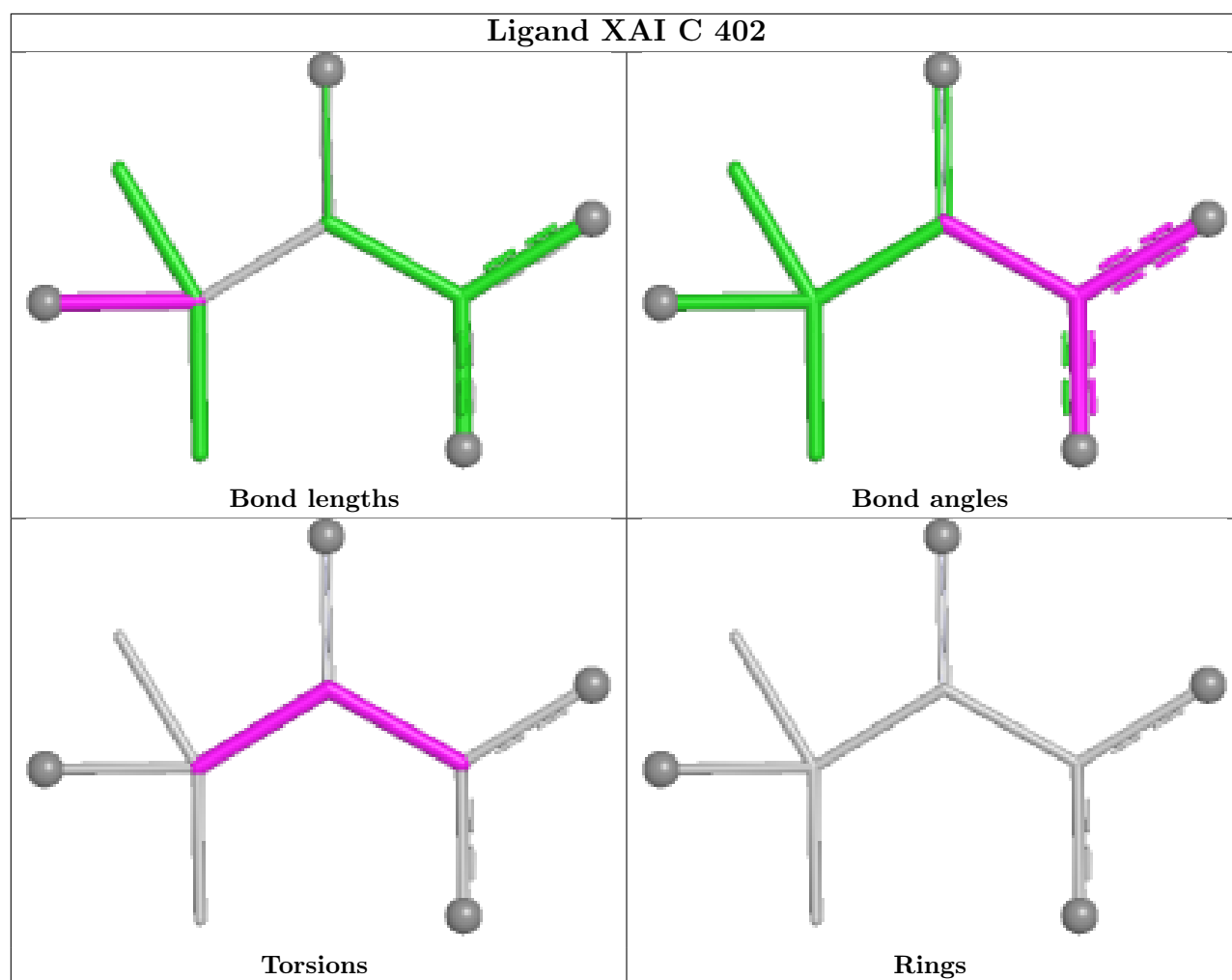
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	XAI	1	0

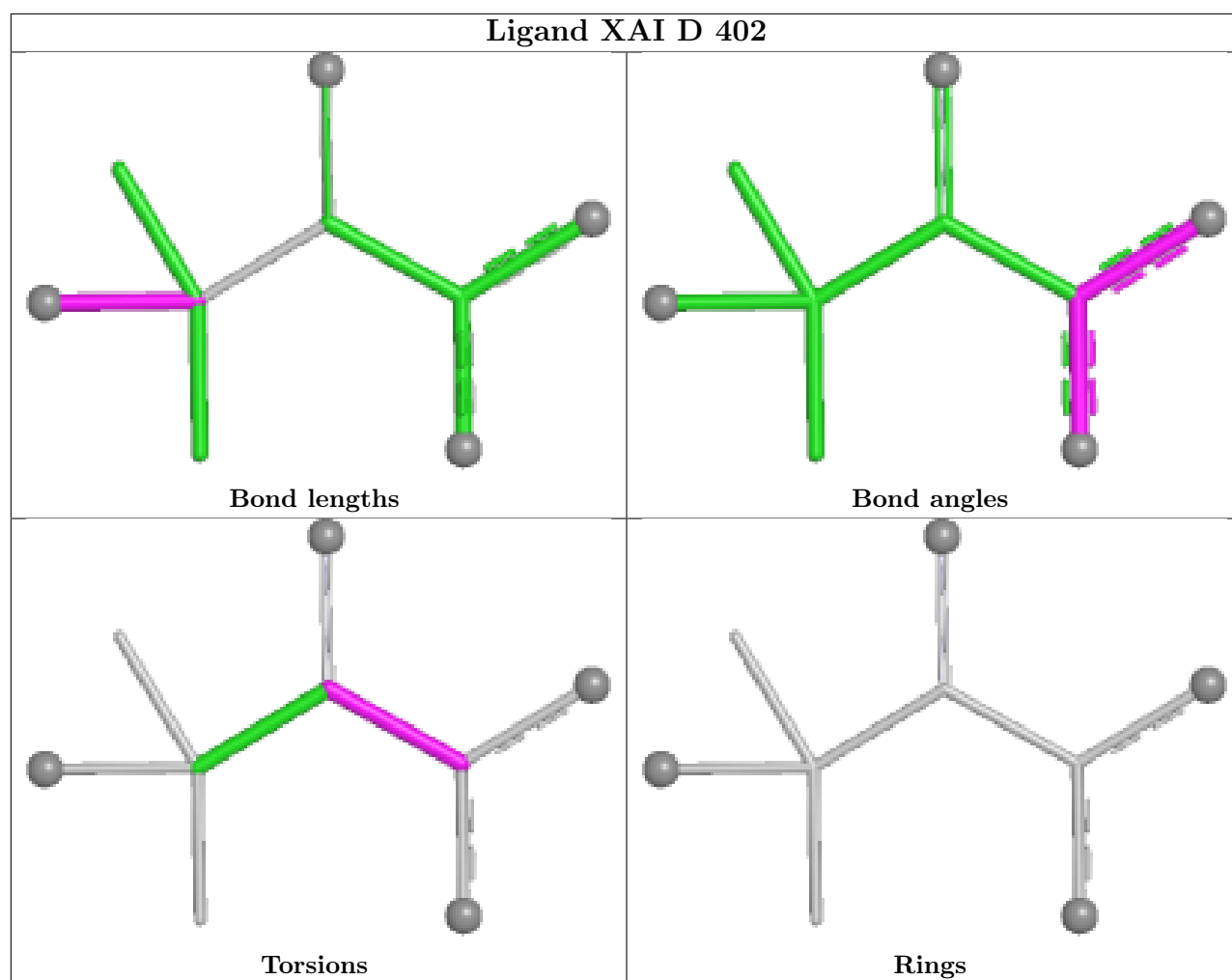
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

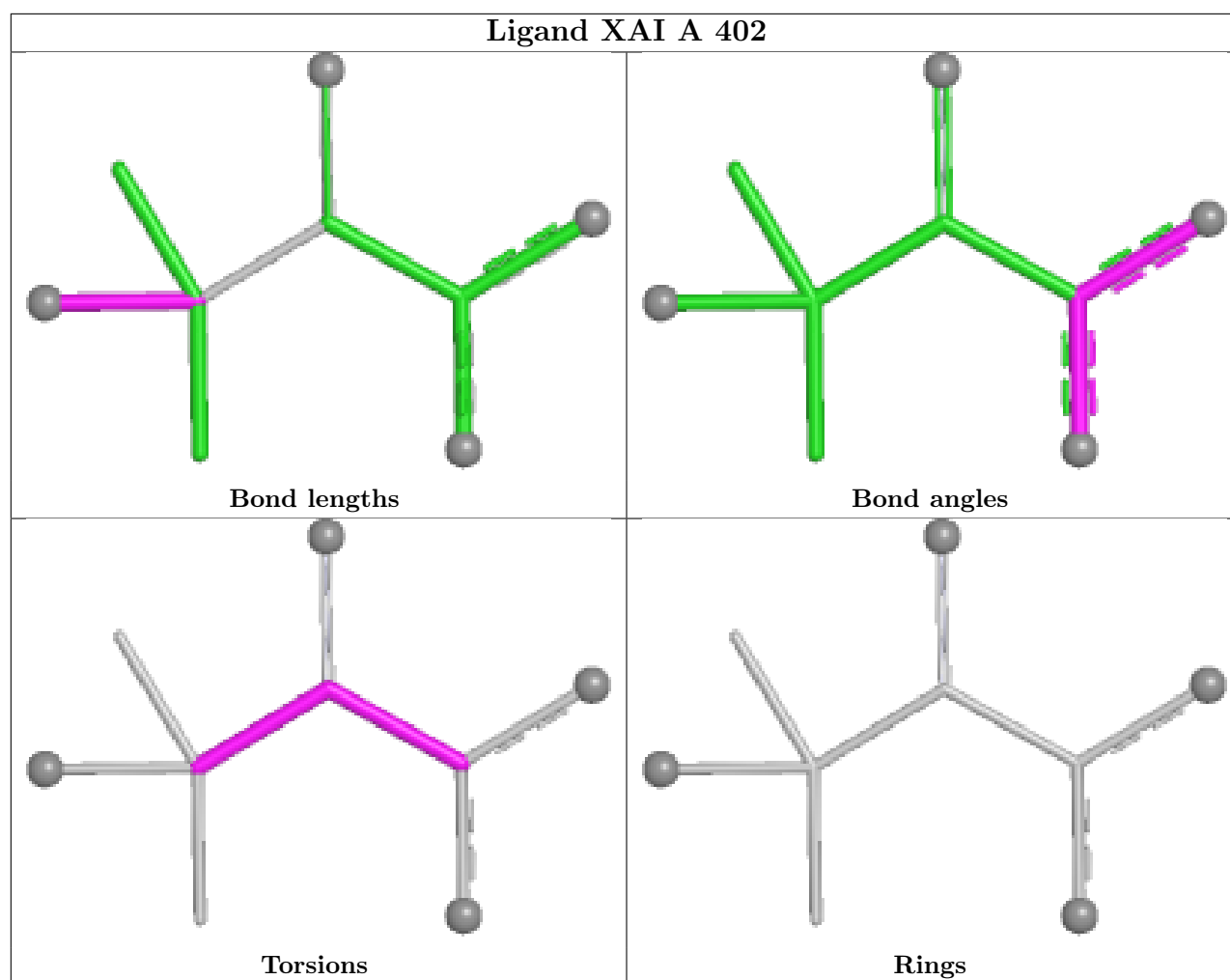
Ligand XAI E 402

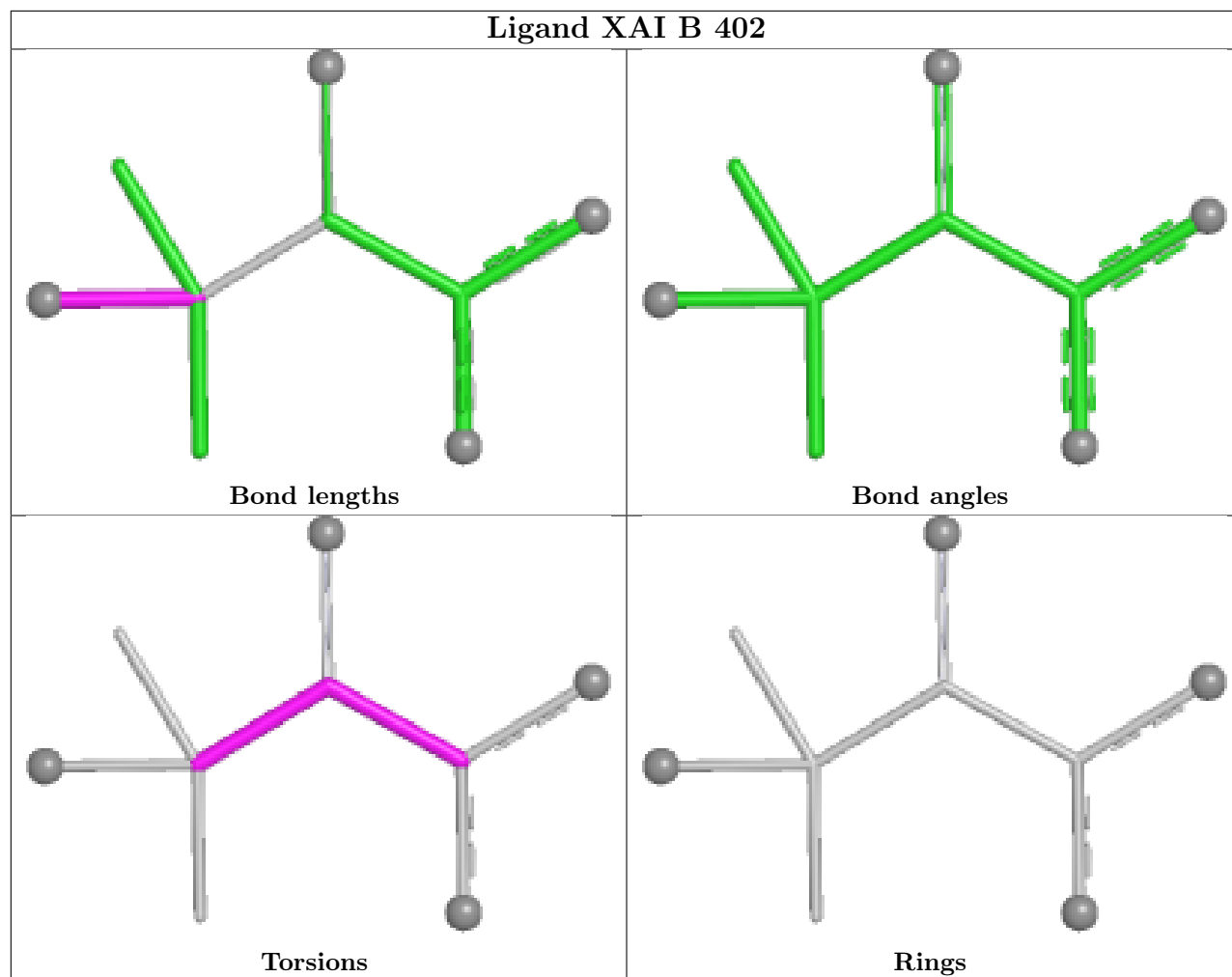












5.7 Other polymers [i](#)

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	341/344 (99%)	0.15	16 (4%) 36 35	18, 37, 71, 90	1 (0%)
1	B	342/344 (99%)	-0.48	2 (0%) 85 87	18, 27, 52, 97	0
1	C	341/344 (99%)	-0.42	5 (1%) 72 74	18, 28, 54, 99	0
1	D	340/344 (98%)	-0.14	7 (2%) 63 65	17, 33, 63, 74	0
1	E	340/344 (98%)	0.25	26 (7%) 20 17	18, 35, 69, 79	0
1	F	341/344 (99%)	0.44	36 (10%) 11 9	18, 42, 72, 89	1 (0%)
All	All	2045/2064 (99%)	-0.03	92 (4%) 38 37	17, 31, 66, 99	2 (0%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	179	GLY	5.3
1	F	54	SER	4.3
1	F	68	VAL	4.3
1	F	166	ALA	3.8
1	F	34	ALA	3.7
1	E	341	TYR	3.6
1	F	58	ALA	3.5
1	D	341	TYR	3.5
1	C	341	TYR	3.4
1	F	50	GLU	3.4
1	A	331	ALA	3.3
1	D	148	THR	3.2
1	F	44	VAL	3.2
1	F	179	GLY	3.2
1	F	42	VAL	3.1
1	F	170	ALA	3.0
1	F	55	ALA	3.0
1	F	65	VAL	3.0
1	F	53	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	173	ILE	3.0
1	A	34	ALA	3.0
1	F	167	LEU	3.0
1	A	167	LEU	2.9
1	E	171	SER	2.8
1	D	343	HIS	2.8
1	E	140	ASN	2.8
1	F	13	LEU	2.7
1	E	167	LEU	2.7
1	A	53	VAL	2.7
1	B	330	SER	2.7
1	C	328	TRP	2.7
1	E	12	ASP	2.6
1	E	16	ILE	2.6
1	F	46	ILE	2.6
1	F	49	ARG	2.6
1	E	63	PHE	2.6
1	B	333	LYS	2.6
1	A	2	ALA	2.5
1	E	133	ALA	2.5
1	C	331	ALA	2.5
1	E	172	ALA	2.5
1	E	331	ALA	2.5
1	F	22	ALA	2.5
1	E	181	ILE	2.4
1	A	172	ALA	2.4
1	F	181	ILE	2.4
1	D	144	LEU	2.4
1	F	56	VAL	2.4
1	A	20	LYS	2.4
1	A	16	ILE	2.4
1	E	33	HIS	2.4
1	E	187	ALA	2.4
1	F	3	ILE	2.4
1	E	44	VAL	2.4
1	F	20	LYS	2.4
1	A	47	GLY	2.3
1	E	34	ALA	2.3
1	F	152	ILE	2.3
1	D	5	VAL	2.3
1	E	139	ARG	2.3
1	A	45	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	130	ALA	2.2
1	A	166	ALA	2.2
1	E	311	ASN	2.2
1	A	334	LEU	2.2
1	D	4	THR	2.2
1	F	59	LYS	2.2
1	F	43	ASN	2.2
1	F	48	LEU	2.2
1	F	52	SER	2.2
1	E	180	ILE	2.2
1	F	63	PHE	2.2
1	F	33	HIS	2.1
1	F	173	ILE	2.1
1	F	51	GLY	2.1
1	F	180	ILE	2.1
1	F	67	SER	2.1
1	C	340	ASN	2.1
1	F	78	ILE	2.1
1	F	150	CYS	2.1
1	C	2	ALA	2.1
1	E	62	GLY	2.1
1	E	64	GLU	2.1
1	E	183	THR	2.1
1	E	332	LYS	2.1
1	E	29	GLN	2.0
1	A	335	VAL	2.0
1	F	335	VAL	2.0
1	D	149	PRO	2.0
1	E	42	VAL	2.0
1	A	98	ASN	2.0
1	A	148	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

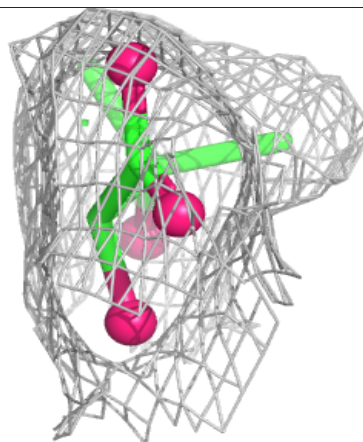
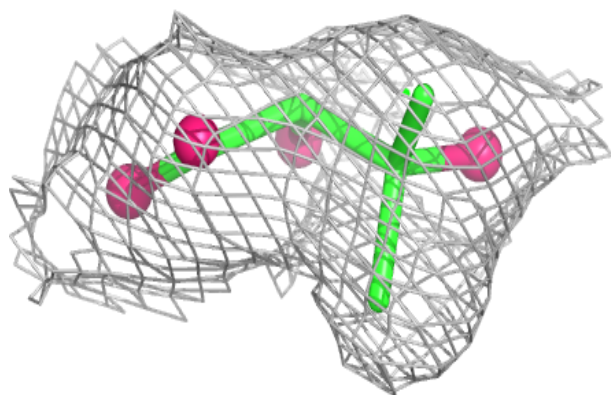
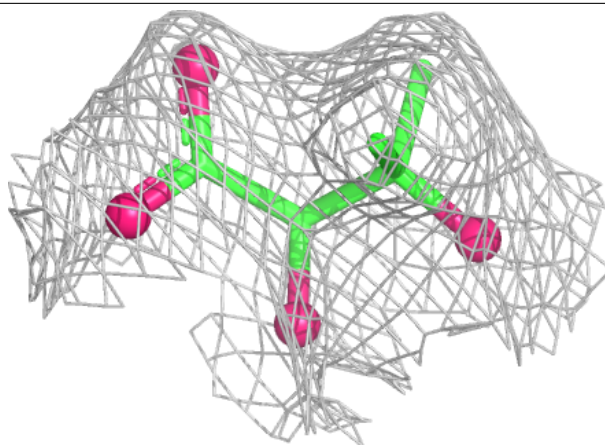
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	XAI	B	402	9/9	0.93	0.08	24,26,33,33	0
3	XAI	E	402	9/9	0.93	0.08	27,30,34,34	0
3	XAI	C	402	9/9	0.95	0.06	22,25,32,34	0
3	XAI	D	402	9/9	0.96	0.07	20,21,24,26	0
3	XAI	A	402	9/9	0.97	0.06	18,21,22,23	0
3	XAI	F	402	9/9	0.97	0.05	24,25,30,32	0
2	MG	F	401	1/1	0.98	0.02	28,28,28,28	0
2	MG	E	401	1/1	0.99	0.03	27,27,27,27	0
2	MG	D	401	1/1	0.99	0.02	24,24,24,24	0
2	MG	C	401	1/1	0.99	0.02	24,24,24,24	0
2	MG	B	401	1/1	0.99	0.02	21,21,21,21	0
2	MG	A	401	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.

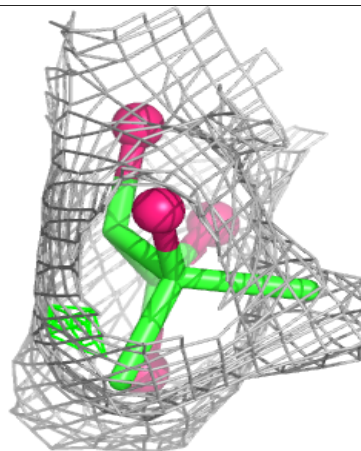
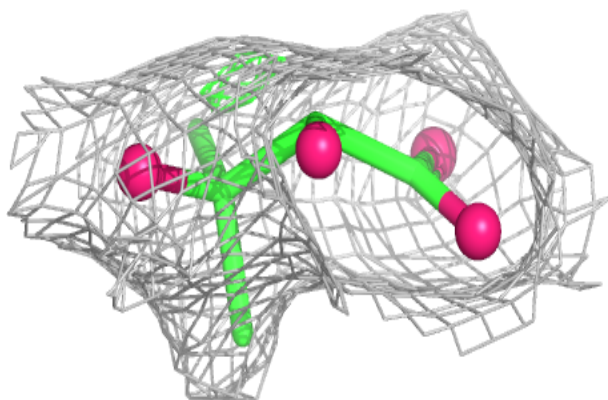
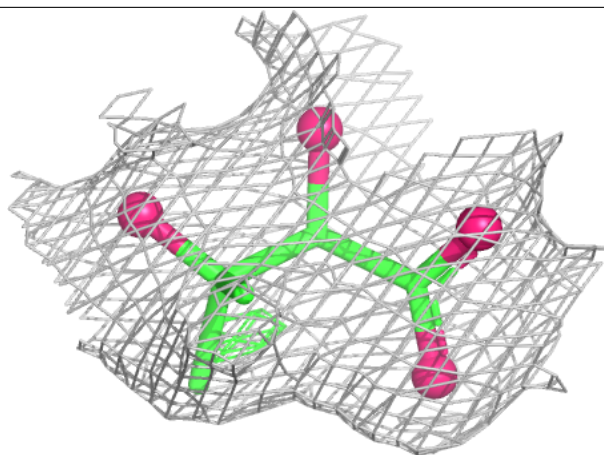
Electron density around XAI B 402:

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



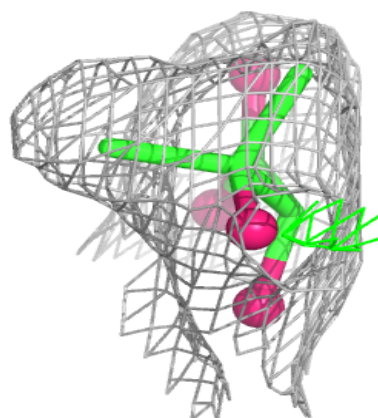
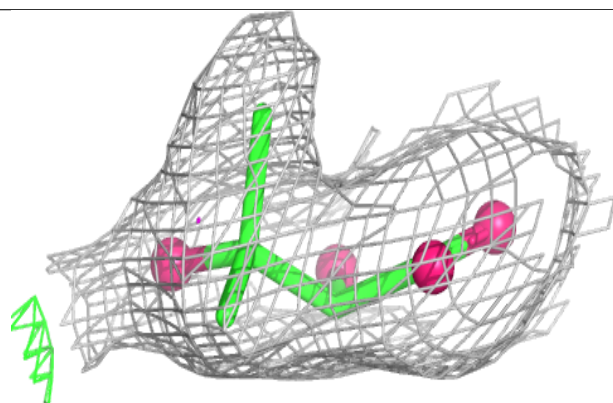
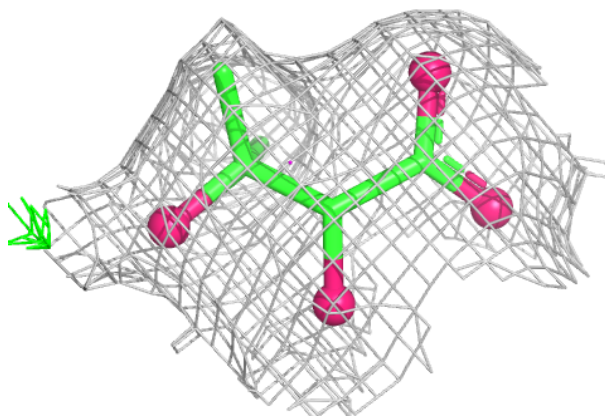
Electron density around XAI E 402:

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



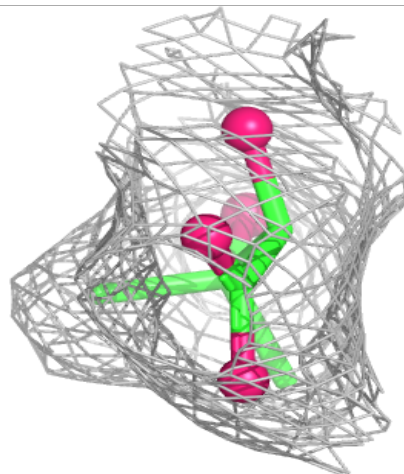
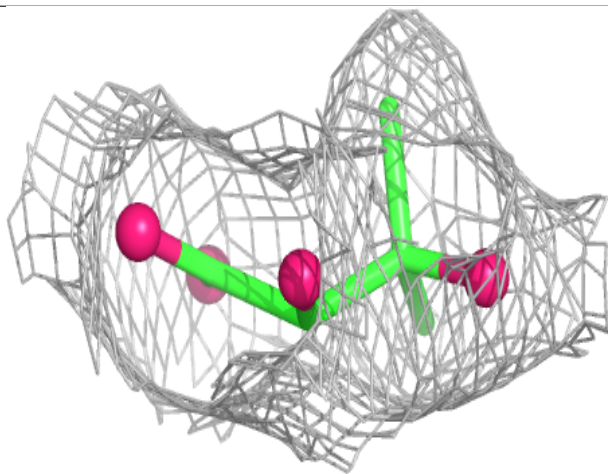
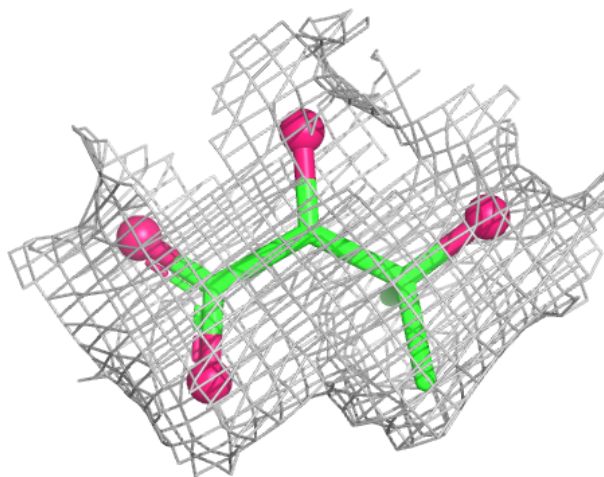
Electron density around XAI C 402:

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



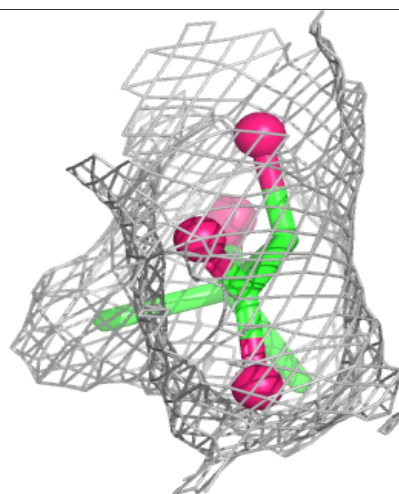
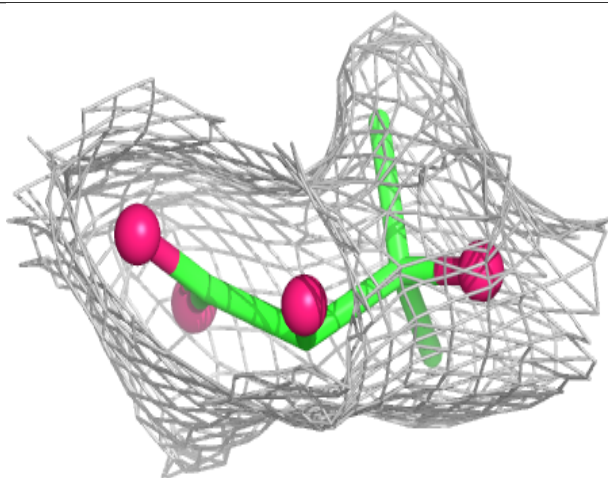
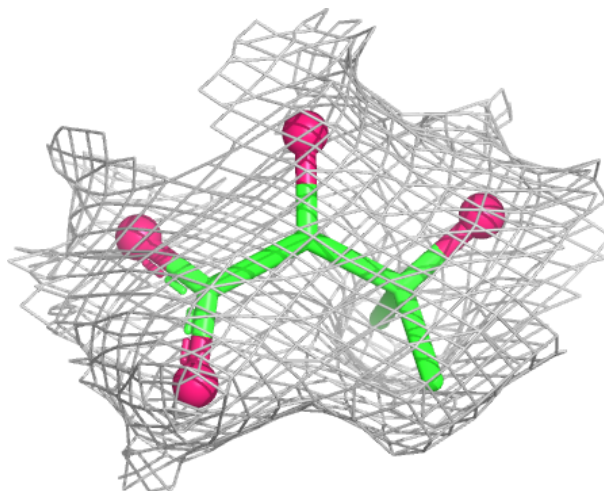
Electron density around XAI D 402:

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



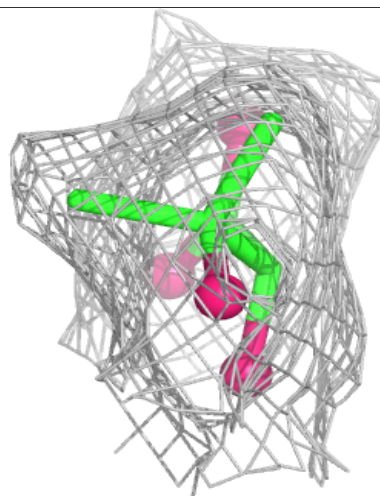
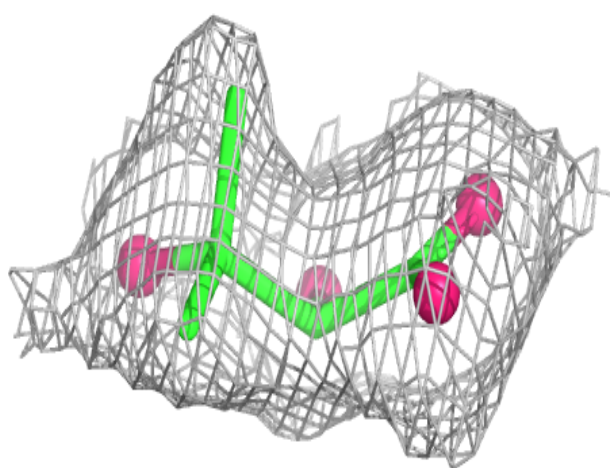
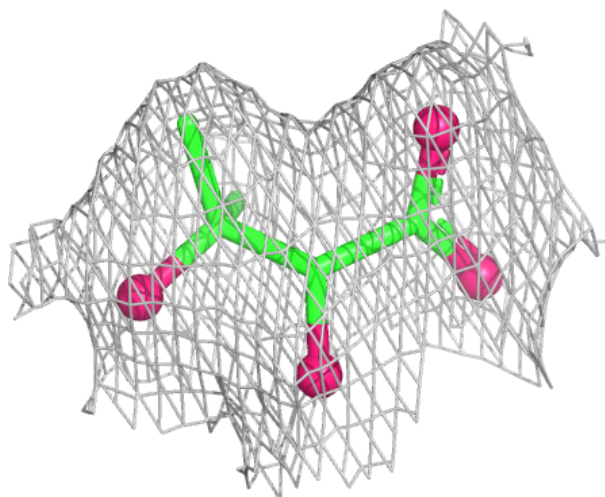
Electron density around XAI A 402:

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



Electron density around XAI F 402:

$2mF_o-DF_c$ (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.