Full wwPDB X-ray Structure Validation Report (i)

Oct 30, 2023 – 01:31 PM JST

PDB ID	:	5B0I
Title	:	Structure of MoeN5-Sso7d fusion protein in complex with beta-octyl glucoside
Authors	:	Ko, T.-P.; Zhang, L.; Chen, C.-C.; Guo, R.-T.; Oldfield, E.O.
Deposited on	:	2015-10-30
Resolution	:	2.26 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

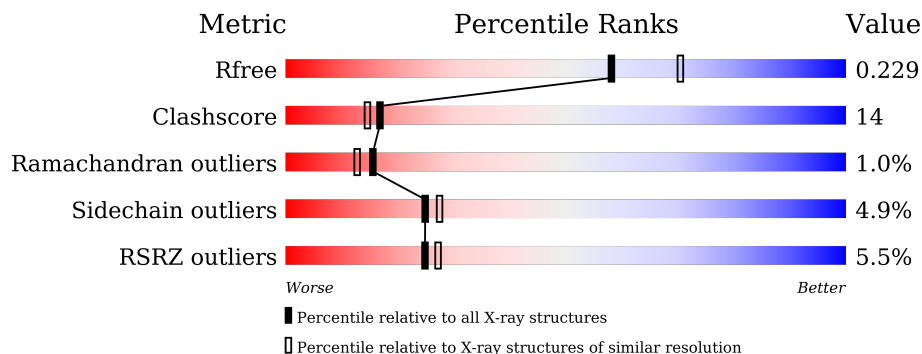|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.26 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.229
Clashscore		14
Ramachandran outliers		1.0%
Sidechain outliers		4.9%
RSRZ outliers		5.5%

Worse .... *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	343	4% / 63% / 12% · 22%
1	B	343	6% / 71% / 23% ··
1	C	343	% / 55% / 18% ·· 24%
1	D	343	8% / 70% / 25% ··

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 9876 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 MoeN5,DNA-binding protein 7d.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	0
			2026	1250	376	389	11			
1	B	332	Total	C	N	O	S	0	0	0
			2533	1571	463	485	14			
1	C	262	Total	C	N	O	S	0	0	0
			1998	1234	372	381	11			
1	D	333	Total	C	N	O	S	0	0	0
			2543	1579	466	484	14			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP A0A010
A	-12	ALA	-	expression tag	UNP A0A010
A	-11	HIS	-	expression tag	UNP A0A010
A	-10	HIS	-	expression tag	UNP A0A010
A	-9	HIS	-	expression tag	UNP A0A010
A	-8	HIS	-	expression tag	UNP A0A010
A	-7	HIS	-	expression tag	UNP A0A010
A	-6	HIS	-	expression tag	UNP A0A010
A	-5	VAL	-	expression tag	UNP A0A010
A	-4	ASP	-	expression tag	UNP A0A010
A	-3	ASP	-	expression tag	UNP A0A010
A	-2	ASP	-	expression tag	UNP A0A010
A	-1	ASP	-	expression tag	UNP A0A010
A	0	LYS	-	expression tag	UNP A0A010
A	261	ALA	-	linker	UNP A0A010
A	262	GLY	-	linker	UNP A0A010
A	263	ALA	-	linker	UNP A0A010
A	264	GLY	-	linker	UNP A0A010
A	265	ALA	-	linker	UNP A0A010
B	-13	MET	-	expression tag	UNP A0A010
B	-12	ALA	-	expression tag	UNP A0A010

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	expression tag	UNP A0A010
B	-10	HIS	-	expression tag	UNP A0A010
B	-9	HIS	-	expression tag	UNP A0A010
B	-8	HIS	-	expression tag	UNP A0A010
B	-7	HIS	-	expression tag	UNP A0A010
B	-6	HIS	-	expression tag	UNP A0A010
B	-5	VAL	-	expression tag	UNP A0A010
B	-4	ASP	-	expression tag	UNP A0A010
B	-3	ASP	-	expression tag	UNP A0A010
B	-2	ASP	-	expression tag	UNP A0A010
B	-1	ASP	-	expression tag	UNP A0A010
B	0	LYS	-	expression tag	UNP A0A010
B	261	ALA	-	linker	UNP A0A010
B	262	GLY	-	linker	UNP A0A010
B	263	ALA	-	linker	UNP A0A010
B	264	GLY	-	linker	UNP A0A010
B	265	ALA	-	linker	UNP A0A010
C	-13	MET	-	expression tag	UNP A0A010
C	-12	ALA	-	expression tag	UNP A0A010
C	-11	HIS	-	expression tag	UNP A0A010
C	-10	HIS	-	expression tag	UNP A0A010
C	-9	HIS	-	expression tag	UNP A0A010
C	-8	HIS	-	expression tag	UNP A0A010
C	-7	HIS	-	expression tag	UNP A0A010
C	-6	HIS	-	expression tag	UNP A0A010
C	-5	VAL	-	expression tag	UNP A0A010
C	-4	ASP	-	expression tag	UNP A0A010
C	-3	ASP	-	expression tag	UNP A0A010
C	-2	ASP	-	expression tag	UNP A0A010
C	-1	ASP	-	expression tag	UNP A0A010
C	0	LYS	-	expression tag	UNP A0A010
C	261	ALA	-	linker	UNP A0A010
C	262	GLY	-	linker	UNP A0A010
C	263	ALA	-	linker	UNP A0A010
C	264	GLY	-	linker	UNP A0A010
C	265	ALA	-	linker	UNP A0A010
D	-13	MET	-	expression tag	UNP A0A010
D	-12	ALA	-	expression tag	UNP A0A010
D	-11	HIS	-	expression tag	UNP A0A010
D	-10	HIS	-	expression tag	UNP A0A010
D	-9	HIS	-	expression tag	UNP A0A010
D	-8	HIS	-	expression tag	UNP A0A010

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-7	HIS	-	expression tag	UNP A0A010
D	-6	HIS	-	expression tag	UNP A0A010
D	-5	VAL	-	expression tag	UNP A0A010
D	-4	ASP	-	expression tag	UNP A0A010
D	-3	ASP	-	expression tag	UNP A0A010
D	-2	ASP	-	expression tag	UNP A0A010
D	-1	ASP	-	expression tag	UNP A0A010
D	0	LYS	-	expression tag	UNP A0A010
D	261	ALA	-	linker	UNP A0A010
D	262	GLY	-	linker	UNP A0A010
D	263	ALA	-	linker	UNP A0A010
D	264	GLY	-	linker	UNP A0A010
D	265	ALA	-	linker	UNP A0A010

- Molecule 2 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).
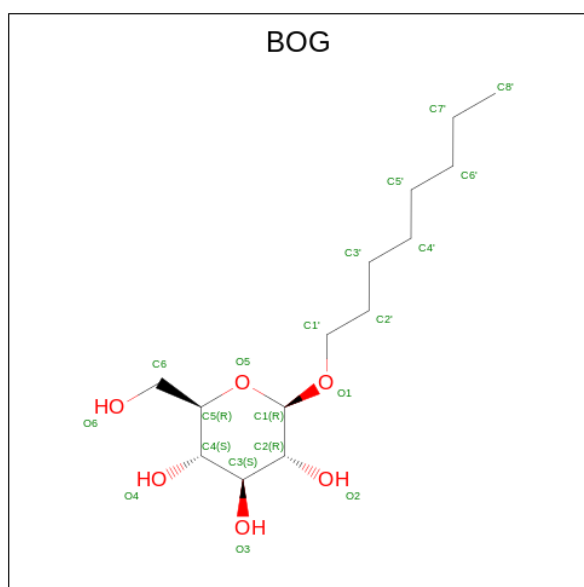
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			20	14	6		
2	B	1	Total	C	O	0	0
			20	14	6		
2	C	1	Total	C	O	0	0
			20	14	6		
2	D	1	Total	C	O	0	0
			20	14	6		

- Molecule 3 is water.

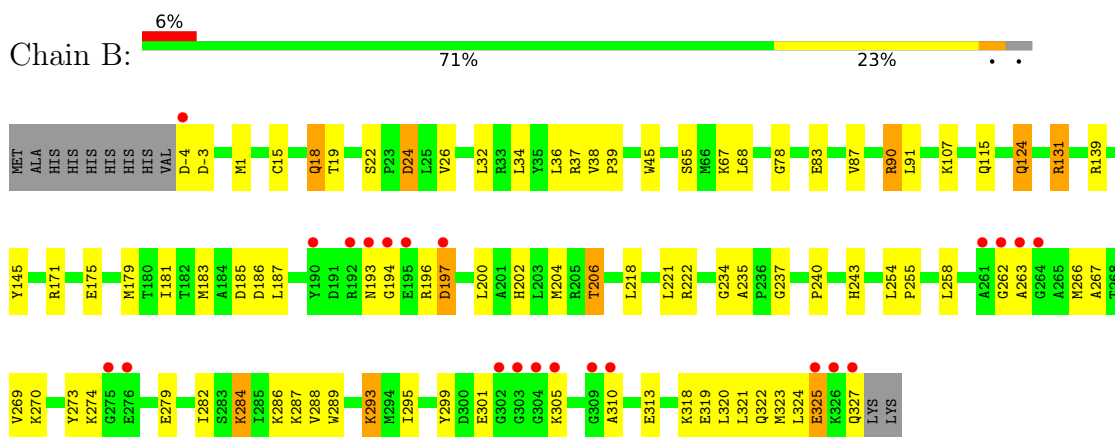| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	164	Total 164	O 164	0	0
3	B	187	Total 187	O 187	0	0
3	C	157	Total 157	O 157	0	0
3	D	168	Total 168	O 168	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
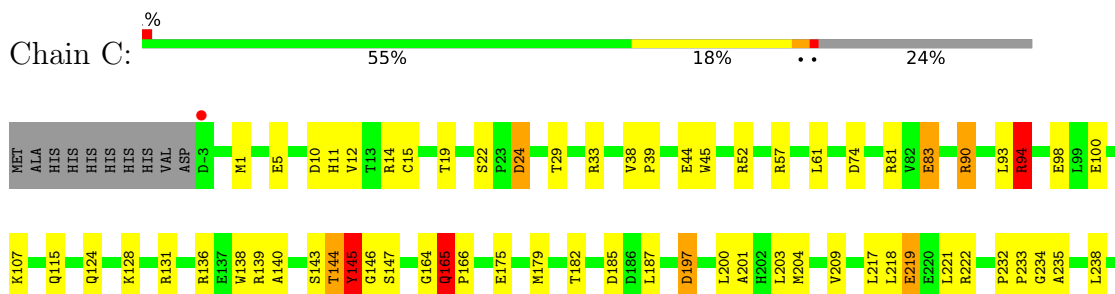
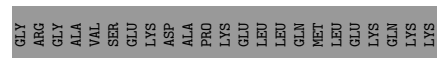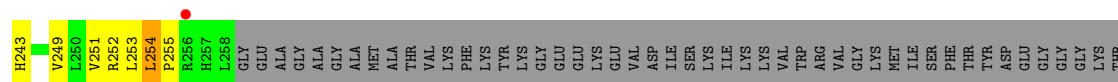• Molecule 1: MoeN5,DNA-binding protein 7d

Chain A:

• Molecule 1: MoeN5,DNA-binding protein 7d

Chain B:

• Molecule 1: MoeN5,DNA-binding protein 7d

Chain C:

H243 V249 L250 V251 R252 L253 L254 P255 R256 H257 L258 GLY GLU ALA GLY ALA GLY ALA MET ALA THR VAL LYS PHE LYS TYR LYS GLY GLU GLU LYS GLU VAL ASP ILE SER LYS ILE LYS LYS VAL TRP ARG VAL GLY LYS MET ILE SER PHE THR TYR ASP GLU GLY GLY LYS THR

GLY ARG GLY ALA VAL SER GLU LYS ASP ALA PRO LYS GLU LEU LEU GLN MET LEU GLU GLU LYS GLN LYS LYS

• Molecule 1: MoeN5,DNA-binding protein 7d

8%

Chain D:

70% 25%

MET ALA HIS HIS HIS HIS HIS VAL ASP D-3 D-2 D10 T19 L34 V38 P39 E44 W45 R52 L61 D75 R81 V87 R90 L91 R94 E98 L99 E100 S101 L102 A103 R104 K107 L113 D116 Q124 R131 N134 L135

R136 E137 W138 A142 F149 Y153 V170 R171 E175 I181 T182 D185 R192 R196 D197 H202 L203 T206 G207 A208 V209 R222 L238 V242 H243 R252 L253 L254 P255 R256 H257 L258 G259 E260 A263 G264 A265 M266 A267 T268 V269 K270 F271 K272

Y273 K274 G275 E276 E277 K278 E279 V280 D281 I282 S283 K284 I285 Y299 D300 E301 G302 G303 G304 K305 T306 G307 R308 V311 S312 E313 K314 P317 K318 E319 L320 L321 E325 K326 Q327 K328 K329

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	137.53Å 218.39Å 104.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.26 24.99 – 2.26	Depositor EDS
% Data completeness (in resolution range)	97.0 (25.00-2.26) 96.9 (24.99-2.26)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.81 (at 2.26Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.183 , 0.229 0.183 , 0.229	Depositor DCC
R_{free} test set	3626 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	40.9	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 44.6	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9876	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.81	0/2058	0.91	3/2797 (0.1%)
1	B	0.77	1/2572 (0.0%)	0.87	0/3478
1	C	0.86	3/2030 (0.1%)	0.93	3/2759 (0.1%)
1	D	0.74	0/2582	0.85	4/3489 (0.1%)
All	All	0.79	4/9242 (0.0%)	0.89	10/12523 (0.1%)

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	D	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	83	GLU	CB-CG	-5.58	1.41	1.52
1	C	219	GLU	CG-CD	5.45	1.60	1.51
1	B	15	CYS	CB-SG	-5.21	1.73	1.81
1	C	15	CYS	CB-SG	-5.14	1.73	1.81

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	94	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	D	52	ARG	NE-CZ-NH1	-8.09	116.26	120.30
1	C	94	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	A	94	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	A	37	ARG	NE-CZ-NH2	7.13	123.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	94	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	D	-2	ASP	N-CA-C	-5.36	96.53	111.00
1	D	222	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	C	145	TYR	N-CA-C	-5.09	97.26	111.00
1	A	171	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	153	TYR	Sidechain

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	2026	0	2005	51	0
1	B	2533	0	2532	67	0
1	C	1998	0	1983	61	0
1	D	2543	0	2554	80	0
2	A	40	0	56	5	0
2	B	20	0	28	1	0
2	C	20	0	28	5	0
2	D	20	0	28	4	0
3	A	164	0	0	4	0
3	B	187	0	0	5	0
3	C	157	0	0	9	0
3	D	168	0	0	4	0
All	All	9876	0	9214	259	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 14.

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:B:1:MET:SD	1:B:1:MET:CE	2.05	1.43
2:D:401:BOG:H2	3:D:583:HOH:O	1.62	0.98
1:D:131:ARG:HG2	1:D:131:ARG:HH11	1.30	0.96
2:D:401:BOG:H4	3:D:524:HOH:O	1.66	0.94
1:D:325:GLU:HB2	1:D:329:LYS:HD2	1.52	0.90
1:D:192:ARG:HG2	1:D:192:ARG:HH11	1.39	0.87
1:C:219:GLU:OE1	1:C:222:ARG:NE	2.08	0.86
1:B:318:LYS:HG3	1:B:319:GLU:OE2	1.77	0.84
1:D:282:ILE:HA	1:D:285:ILE:HD13	1.59	0.83
1:C:145:TYR:CE1	2:C:401:BOG:H61	2.14	0.83
1:A:150:LEU:HD13	2:A:501:BOG:H8'1	1.62	0.81
1:A:193:ASN:HB3	1:A:195:GLU:HG3	1.62	0.81
1:D:192:ARG:HH11	1:D:192:ARG:CG	1.94	0.79
1:C:136:ARG:HB3	1:C:136:ARG:NH1	1.98	0.78
1:B:1:MET:HG2	1:B:37:ARG:HD3	1.65	0.78
1:B:179:MET:HE3	1:B:221:LEU:HD21	1.67	0.77
1:D:131:ARG:HG2	1:D:131:ARG:NH1	2.00	0.76
1:D:222:ARG:HH11	1:D:243:HIS:HD2	1.34	0.76
1:B:22:SER:O	1:B:26:VAL:HG23	1.85	0.76
1:B:222:ARG:HH11	1:B:243:HIS:HD2	1.34	0.74
1:A:200:LEU:HG	1:A:204:MET:CE	2.17	0.74
1:A:38:VAL:HG12	1:A:39:PRO:HD3	1.69	0.73
1:A:94:ARG:HD2	1:A:98:GLU:OE2	1.87	0.73
1:B:124:GLN:HE21	1:B:124:GLN:HA	1.54	0.72
1:D:301:GLU:HG3	1:D:305:LYS:HB3	1.72	0.71
1:A:195:GLU:C	1:A:196:ARG:HH11	1.95	0.70
1:C:124:GLN:NE2	2:C:401:BOG:H5'2	2.07	0.70
1:C:131:ARG:HH11	1:C:131:ARG:HG2	1.57	0.70
1:C:139:ARG:HG3	1:C:179:MET:HE3	1.74	0.69
1:D:203:LEU:HA	1:D:206:THR:HG22	1.74	0.69
1:D:142:ALA:HB1	1:D:182:THR:HG21	1.73	0.69
1:B:22:SER:OG	1:B:24:ASP:HB2	1.93	0.69
1:C:22:SER:N	1:C:83:GLU:OE1	2.26	0.69
1:C:179:MET:HE2	1:C:217:LEU:HD11	1.75	0.69
1:D:94:ARG:HD2	1:D:98:GLU:OE2	1.93	0.69
1:C:187:LEU:HD21	1:C:204:MET:HE3	1.75	0.68
1:A:131:ARG:HG3	1:A:197:ASP:HB3	1.75	0.68
1:D:252:ARG:O	1:D:255:PRO:HD2	1.93	0.67
1:A:192:ARG:HA	1:A:192:ARG:NE	2.09	0.67
1:B:131:ARG:HG3	1:B:197:ASP:HB3	1.77	0.66
1:A:61:LEU:HD13	1:A:94:ARG:HG3	1.77	0.66
1:B:179:MET:CE	1:B:221:LEU:HD21	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:TYR:CE2	1:B:274:LYS:HD2	2.30	0.66
1:D:203:LEU:HA	1:D:206:THR:CG2	2.26	0.65
1:B:301:GLU:OE2	1:B:305:LYS:HE3	1.98	0.64
1:D:135:LEU:HB2	1:D:209:VAL:HG22	1.80	0.63
1:A:131:ARG:HG3	1:A:197:ASP:CB	2.29	0.63
1:D:124:GLN:HG2	2:D:401:BOG:H7'1	1.81	0.63
1:C:200:LEU:HG	1:C:204:MET:HE2	1.80	0.63
1:D:267:ALA:HB1	1:D:282:ILE:HG13	1.81	0.62
1:A:104:ARG:HD2	3:A:688:HOH:O	1.99	0.62
1:C:140:ALA:O	1:C:144:THR:HG23	2.00	0.62
1:A:195:GLU:O	1:A:196:ARG:NH1	2.29	0.61
1:D:280:VAL:HG21	1:D:299:TYR:CZ	2.36	0.61
1:D:134:ASN:HD21	1:D:136:ARG:NH2	1.98	0.60
1:B:323:MET:O	1:B:327:GLN:HB2	2.01	0.60
1:A:189:ASP:O	1:A:193:ASN:HB2	2.02	0.60
1:C:218:LEU:HD11	1:C:249:VAL:HG11	1.83	0.60
1:B:179:MET:HG2	1:B:221:LEU:HD11	1.84	0.60
1:C:94:ARG:HD2	1:C:98:GLU:OE2	2.00	0.60
1:A:38:VAL:CG1	1:A:39:PRO:HD3	2.33	0.59
1:D:149:PHE:CD1	2:D:401:BOG:H2'2	2.38	0.58
1:D:138:TRP:HH2	1:D:182:THR:HG22	1.69	0.58
1:D:34:LEU:HD21	1:D:181:ILE:HG21	1.84	0.58
1:D:238:LEU:O	1:D:242:VAL:HG23	2.04	0.58
1:D:61:LEU:HD13	1:D:94:ARG:HG3	1.86	0.58
1:D:313:GLU:HG2	1:D:314:LYS:N	2.19	0.58
1:D:269:VAL:HG22	1:D:317:PRO:HG3	1.86	0.57
1:D:192:ARG:NH1	1:D:192:ARG:HB3	2.19	0.57
1:D:203:LEU:CA	1:D:206:THR:HG22	2.34	0.57
1:D:259:GLY:C	1:D:260:GLU:HG2	2.26	0.56
1:B:243:HIS:HE1	3:B:626:HOH:O	1.88	0.56
1:C:187:LEU:HD21	1:C:204:MET:CE	2.36	0.56
1:B:287:LYS:HG3	1:B:288:VAL:N	2.20	0.56
1:C:139:ARG:HG3	1:C:179:MET:CE	2.34	0.55
1:D:272:LYS:HA	1:D:276:GLU:O	2.07	0.55
1:B:301:GLU:HB3	1:B:305:LYS:HD3	1.89	0.55
1:A:90:ARG:C	1:A:90:ARG:HD3	2.27	0.55
1:B:200:LEU:HG	1:B:204:MET:HE2	1.89	0.55
1:B:266:MET:HE3	1:B:266:MET:HA	1.88	0.55
1:C:81:ARG:HD3	1:D:81:ARG:NH2	2.21	0.55
1:B:267:ALA:O	1:B:282:ILE:HG12	2.07	0.54
1:C:61:LEU:HD13	1:C:94:ARG:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:584:HOH:O	1:D:107:LYS:HD3	2.06	0.54
1:C:81:ARG:NH2	3:C:501:HOH:O	2.40	0.54
1:C:136:ARG:HB3	1:C:136:ARG:CZ	2.37	0.54
1:C:10:ASP:CG	1:C:14:ARG:HH22	2.11	0.54
1:A:107:LYS:O	1:A:107:LYS:HD3	2.08	0.54
1:A:200:LEU:HG	1:A:204:MET:HE2	1.90	0.54
1:B:19:THR:HG22	1:B:19:THR:O	2.07	0.53
1:C:11:HIS:CD2	1:C:57:ARG:HD2	2.43	0.53
1:A:182:THR:HG23	2:A:502:BOG:O6	2.09	0.53
1:C:74:ASP:OD1	1:C:128:LYS:NZ	2.41	0.53
1:A:192:ARG:HG3	3:C:617:HOH:O	2.09	0.53
1:D:268:THR:HG22	1:D:281:ASP:HA	1.90	0.53
1:C:218:LEU:HD11	1:C:249:VAL:CG1	2.39	0.53
1:B:284:LYS:HE3	1:B:284:LYS:HA	1.91	0.52
1:C:147:SER:O	1:C:175:GLU:HG2	2.08	0.52
1:D:325:GLU:O	1:D:329:LYS:HB3	2.09	0.52
1:A:259:GLY:O	1:D:131:ARG:NH2	2.41	0.52
1:D:192:ARG:HH11	1:D:192:ARG:CB	2.21	0.52
1:B:266:MET:HE2	1:B:267:ALA:N	2.25	0.52
1:C:219:GLU:CD	1:C:222:ARG:HH21	2.13	0.52
1:A:61:LEU:CD1	1:A:94:ARG:HG3	2.40	0.52
1:A:187:LEU:HD21	1:A:204:MET:CE	2.40	0.52
1:B:321:LEU:O	1:B:324:LEU:HB2	2.10	0.51
1:A:139:ARG:HD3	1:A:179:MET:HE1	1.91	0.51
1:C:179:MET:HG2	1:C:221:LEU:HD11	1.93	0.51
1:B:270:LYS:HE2	1:B:279:GLU:OE2	2.10	0.51
1:D:259:GLY:O	1:D:260:GLU:HG2	2.11	0.51
1:B:266:MET:CE	1:B:267:ALA:H	2.23	0.51
1:C:38:VAL:N	1:C:39:PRO:CD	2.74	0.51
1:D:269:VAL:HG22	1:D:317:PRO:CG	2.40	0.50
1:B:286:LYS:HE2	1:B:299:TYR:O	2.10	0.50
1:C:164:GLY:N	3:C:503:HOH:O	2.44	0.50
1:B:266:MET:CE	1:B:267:ALA:N	2.74	0.50
1:C:19:THR:O	1:C:19:THR:HG22	2.11	0.50
1:D:192:ARG:HH11	1:D:192:ARG:HB3	1.76	0.50
1:C:145:TYR:HE1	2:C:401:BOG:H61	1.72	0.50
1:A:200:LEU:HG	1:A:204:MET:HE1	1.93	0.50
1:B:115:GLN:HG2	3:B:643:HOH:O	2.10	0.50
1:B:301:GLU:CD	1:B:305:LYS:HE3	2.31	0.50
1:D:90:ARG:HD3	1:D:90:ARG:C	2.32	0.50
1:C:11:HIS:CG	1:C:57:ARG:HD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ARG:HG2	1:C:131:ARG:NH1	2.25	0.49
1:A:131:ARG:CG	1:A:197:ASP:HB3	2.43	0.49
1:D:202:HIS:O	1:D:206:THR:HG22	2.12	0.49
1:B:90:ARG:HD3	1:B:90:ARG:C	2.33	0.49
1:A:179:MET:HE2	1:A:221:LEU:HD21	1.94	0.49
1:B:318:LYS:O	1:B:322:GLN:HG3	2.12	0.48
1:D:280:VAL:HG21	1:D:299:TYR:CE1	2.48	0.48
1:B:266:MET:HE3	1:B:267:ALA:H	1.78	0.48
1:B:139:ARG:NH1	3:B:503:HOH:O	2.34	0.48
1:D:269:VAL:HG21	1:D:320:LEU:HD22	1.96	0.48
1:C:219:GLU:HG3	3:C:515:HOH:O	2.14	0.48
1:A:260:GLU:HG3	1:D:131:ARG:HH21	1.78	0.48
2:C:401:BOG:H1'2	2:C:401:BOG:O2	2.14	0.48
1:B:171:ARG:O	1:B:175:GLU:HG3	2.14	0.47
1:B:293:LYS:HG2	1:B:313:GLU:OE2	2.14	0.47
1:D:301:GLU:CG	1:D:305:LYS:HB3	2.42	0.47
1:D:192:ARG:CG	1:D:192:ARG:NH1	2.64	0.47
1:B:202:HIS:O	1:B:206:THR:HB	2.15	0.47
1:D:45:TRP:CE3	1:D:170:VAL:HG22	2.49	0.47
1:D:267:ALA:HB1	1:D:282:ILE:CG1	2.44	0.47
1:C:232:PRO:HA	1:C:233:PRO:C	2.34	0.47
1:D:192:ARG:HG2	1:D:192:ARG:NH1	2.17	0.47
1:D:196:ARG:O	1:D:197:ASP:C	2.53	0.47
1:D:267:ALA:HA	1:D:319:GLU:OE1	2.15	0.47
1:C:83:GLU:HG3	3:C:565:HOH:O	2.13	0.47
1:D:87:VAL:O	1:D:91:LEU:HG	2.14	0.47
1:A:134:ASN:OD1	1:A:137:GLU:HG3	2.15	0.47
1:C:187:LEU:CD2	1:C:204:MET:HE3	2.43	0.47
1:A:150:LEU:HD13	2:A:501:BOG:C8'	2.42	0.46
1:B:183:MET:HE1	1:B:218:LEU:HG	1.97	0.46
1:B:287:LYS:HG3	1:B:288:VAL:H	1.79	0.46
1:B:107:LYS:NZ	3:B:508:HOH:O	2.49	0.46
1:A:192:ARG:HD2	3:C:532:HOH:O	2.15	0.46
1:D:254:LEU:CD1	1:D:258:LEU:HD13	2.45	0.46
1:B:254:LEU:HB2	1:B:255:PRO:HD3	1.98	0.46
1:D:271:PHE:HB3	1:D:311:VAL:CG1	2.44	0.46
1:A:181:ILE:HD11	2:A:501:BOG:H8'3	1.98	0.46
1:B:67:LYS:NZ	2:B:401:BOG:O2	2.50	0.45
1:B:287:LYS:HG2	1:B:289:TRP:CE3	2.51	0.45
1:C:1:MET:HE2	3:C:589:HOH:O	2.16	0.45
1:D:75:ASP:HB2	1:D:81:ARG:NH1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:LYS:HA	1:D:321:LEU:HD12	1.98	0.45
1:A:131:ARG:HB3	1:A:198:GLY:N	2.31	0.45
1:D:270:LYS:HG3	1:D:279:GLU:HG3	1.98	0.45
1:A:75:ASP:CG	1:A:81:ARG:NH1	2.71	0.45
1:C:143:SER:O	1:C:147:SER:HB2	2.17	0.44
1:D:10:ASP:HB2	3:D:594:HOH:O	2.17	0.44
1:D:45:TRP:CD2	1:D:170:VAL:HG22	2.52	0.44
1:A:187:LEU:HD21	1:A:204:MET:HE3	1.99	0.44
1:A:192:ARG:HA	1:A:192:ARG:CZ	2.47	0.44
1:D:277:GLU:OE1	1:D:277:GLU:HA	2.18	0.44
1:A:244:LEU:HD12	3:A:651:HOH:O	2.18	0.44
1:A:196:ARG:HD2	1:A:202:HIS:ND1	2.33	0.44
1:D:281:ASP:O	1:D:284:LYS:HB2	2.17	0.44
1:B:1:MET:CG	1:B:37:ARG:HD3	2.43	0.44
1:D:252:ARG:NH1	1:D:253:LEU:HD21	2.33	0.44
1:B:187:LEU:HD21	1:B:204:MET:CE	2.48	0.43
1:D:171:ARG:O	1:D:175:GLU:HG3	2.17	0.43
1:D:192:ARG:NH1	1:D:192:ARG:CB	2.80	0.43
1:D:307:GLY:C	1:D:308:ARG:HG3	2.37	0.43
1:C:165:GLN:HA	1:C:166:PRO:HD2	1.87	0.43
1:C:232:PRO:HA	1:C:234:GLY:N	2.32	0.43
1:C:252:ARG:NH1	1:C:253:LEU:HD21	2.32	0.43
1:B:187:LEU:HD21	1:B:204:MET:HE1	1.99	0.43
2:C:401:BOG:H2'2	2:C:401:BOG:H5'1	1.59	0.43
1:C:90:ARG:HD3	1:C:90:ARG:C	2.39	0.43
1:A:179:MET:CE	1:A:221:LEU:HD21	2.49	0.43
1:B:237:GLY:O	1:B:240:PRO:HD2	2.18	0.43
1:D:138:TRP:CH2	1:D:182:THR:HG22	2.50	0.43
1:A:131:ARG:HG2	1:A:131:ARG:HH11	1.83	0.43
1:A:165:GLN:HA	1:A:166:PRO:HD2	1.90	0.43
1:B:269:VAL:HG21	1:B:320:LEU:HD22	2.01	0.43
1:C:93:LEU:HD22	1:D:113:LEU:HB3	2.01	0.43
1:D:38:VAL:N	1:D:39:PRO:CD	2.82	0.43
1:B:194:GLY:C	1:B:196:ARG:NH1	2.72	0.42
1:C:44:GLU:HG2	1:C:238:LEU:HG	2.01	0.42
1:B:32:LEU:O	1:B:36:LEU:HD12	2.18	0.42
1:C:222:ARG:NH1	1:C:243:HIS:HD2	2.17	0.42
1:B:131:ARG:HA	1:B:131:ARG:HD2	1.72	0.42
1:C:131:ARG:HD2	1:C:197:ASP:OD1	2.19	0.42
1:C:136:ARG:HB3	1:C:136:ARG:HH11	1.77	0.42
1:B:322:GLN:HA	1:B:325:GLU:OE2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:THR:HG23	1:D:208:ALA:H	1.85	0.42
1:A:165:GLN:H	1:A:165:GLN:HG2	1.77	0.42
1:C:166:PRO:HD3	1:C:233:PRO:HD2	2.00	0.42
1:C:187:LEU:HD23	1:C:201:ALA:HB2	2.01	0.42
1:D:276:GLU:HA	1:D:276:GLU:OE1	2.19	0.42
1:A:75:ASP:CG	1:A:81:ARG:HH11	2.23	0.42
1:A:116:ASP:OD1	1:A:116:ASP:N	2.51	0.42
1:B:258:LEU:HB3	1:B:262:GLY:HA3	2.01	0.42
1:C:179:MET:CE	1:C:217:LEU:HD11	2.47	0.42
1:D:273:TYR:O	1:D:274:LYS:C	2.57	0.42
1:A:187:LEU:HD21	1:A:204:MET:HE1	2.01	0.42
1:C:203:LEU:HB3	1:C:209:VAL:HG23	2.01	0.42
1:A:187:LEU:CD2	1:A:204:MET:HE3	2.50	0.42
1:D:61:LEU:CD1	1:D:94:ARG:HG3	2.49	0.42
1:C:5:GLU:OE2	1:C:33:ARG:HG2	2.18	0.42
1:C:100:GLU:OE1	1:D:100:GLU:OE1	2.37	0.42
1:D:269:VAL:O	1:D:279:GLU:HA	2.20	0.41
2:A:502:BOG:H2'2	2:A:502:BOG:H5'1	1.80	0.41
1:A:76:ASP:OD1	1:A:76:ASP:N	2.53	0.41
1:B:34:LEU:HD21	1:B:181:ILE:HD12	2.02	0.41
1:B:78:GLY:N	3:B:501:HOH:O	2.21	0.41
1:B:124:GLN:NE2	1:B:145:TYR:HB3	2.35	0.41
1:A:81:ARG:HD2	3:A:713:HOH:O	2.19	0.41
1:C:24:ASP:HB2	3:C:554:HOH:O	2.20	0.41
1:C:251:VAL:HG13	1:C:252:ARG:N	2.36	0.41
1:D:256:ARG:HE	1:D:256:ARG:HB2	1.59	0.41
1:C:1:MET:SD	1:C:1:MET:C	2.98	0.41
1:C:12:VAL:HG12	1:C:29:THR:HG21	2.02	0.41
1:A:201:ALA:HB1	1:A:257:HIS:CE1	2.56	0.41
1:B:65:SER:HB2	1:B:91:LEU:HB2	2.01	0.41
1:B:83:GLU:O	1:B:87:VAL:HG23	2.21	0.41
1:B:194:GLY:C	1:B:196:ARG:HH12	2.24	0.41
1:C:136:ARG:HH11	1:C:136:ARG:CB	2.33	0.41
1:B:68:LEU:HD23	1:B:68:LEU:HA	1.89	0.41
1:B:295:ILE:O	1:B:310:ALA:HA	2.21	0.41
1:B:319:GLU:CD	1:B:319:GLU:H	2.23	0.41
1:D:44:GLU:HG2	1:D:238:LEU:HG	2.03	0.41
1:D:116:ASP:HA	3:D:584:HOH:O	2.21	0.41
1:B:18:GLN:HE21	1:B:18:GLN:HB2	1.65	0.41
1:A:150:LEU:HD12	1:A:150:LEU:HA	1.84	0.41
1:B:269:VAL:O	1:B:279:GLU:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:LEU:N	1:C:255:PRO:CD	2.84	0.41
1:A:11:HIS:CE1	1:A:57:ARG:CZ	3.03	0.41
1:B:38:VAL:N	1:B:39:PRO:CD	2.84	0.40
1:B:45:TRP:CE2	1:B:235:ALA:HB2	2.56	0.40
1:C:138:TRP:CZ2	1:C:182:THR:HG22	2.56	0.40
1:D:203:LEU:C	1:D:206:THR:HG22	2.41	0.40
1:D:273:TYR:C	1:D:275:GLY:N	2.74	0.40
1:B:273:TYR:O	1:B:274:LYS:HB2	2.21	0.40
1:D:254:LEU:N	1:D:255:PRO:CD	2.84	0.40
1:A:33:ARG:HD3	3:A:627:HOH:O	2.21	0.40
1:C:45:TRP:CE2	1:C:235:ALA:HB2	2.56	0.40
1:D:252:ARG:CZ	1:D:253:LEU:HD21	2.52	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	264/343 (77%)	248 (94%)	13 (5%)	3 (1%)	14	10
1	B	330/343 (96%)	307 (93%)	21 (6%)	2 (1%)	25	25
1	C	260/343 (76%)	251 (96%)	6 (2%)	3 (1%)	13	9
1	D	331/343 (96%)	307 (93%)	20 (6%)	4 (1%)	13	9
All	All	1185/1372 (86%)	1113 (94%)	60 (5%)	12 (1%)	15	13

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	263	ALA
1	C	165	GLN
1	D	263	ALA

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Mol	Chain	Res	Type
1	D	264	GLY
1	A	165	GLN
1	A	259	GLY
1	C	146	GLY
1	A	193	ASN
1	D	197	ASP
1	C	145	TYR
1	D	302	GLY
1	B	234	GLY

5.3.2   Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/270 (77%)	196 (94%)	13 (6%)	18	17
1	B	260/270 (96%)	245 (94%)	15 (6%)	20	20
1	C	206/270 (76%)	195 (95%)	11 (5%)	22	23
1	D	261/270 (97%)	254 (97%)	7 (3%)	44	54
All	All	936/1080 (87%)	890 (95%)	46 (5%)	25	27

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-5	VAL
1	A	18	GLN
1	A	47	THR
1	A	90	ARG
1	A	107	LYS
1	A	115	GLN
1	A	139	ARG
1	A	163	GLU
1	A	189	ASP
1	A	191	ASP
1	A	192	ARG
1	A	197	ASP

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Mol	Chain	Res	Type
1	A	258	LEU
1	B	-4	ASP
1	B	-3	ASP
1	B	18	GLN
1	B	24	ASP
1	B	90	ARG
1	B	124	GLN
1	B	131	ARG
1	B	185	ASP
1	B	186	ASP
1	B	193	ASN
1	B	197	ASP
1	B	206	THR
1	B	284	LYS
1	B	293	LYS
1	B	325	GLU
1	C	24	ASP
1	C	52	ARG
1	C	90	ARG
1	C	94	ARG
1	C	107	LYS
1	C	115	GLN
1	C	144	THR
1	C	165	GLN
1	C	185	ASP
1	C	197	ASP
1	C	254	LEU
1	D	19	THR
1	D	90	ARG
1	D	104	ARG
1	D	182	THR
1	D	185	ASP
1	D	192	ARG
1	D	314	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	HIS
1	B	18	GLN
1	B	124	GLN
1	B	243	HIS

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Mol	Chain	Res	Type
1	C	115	GLN
1	C	124	GLN
1	C	243	HIS
1	D	243	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	BOG	A	501	-	20,20,20	1.05	1 (5%)	25,25,25	0.65	0
2	BOG	A	502	-	20,20,20	0.85	1 (5%)	25,25,25	0.95	1 (4%)
2	BOG	B	401	-	20,20,20	0.94	1 (5%)	25,25,25	1.01	1 (4%)
2	BOG	D	401	-	20,20,20	0.96	1 (5%)	25,25,25	0.75	1 (4%)
2	BOG	C	401	-	20,20,20	0.92	1 (5%)	25,25,25	0.65	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
2	BOG	A	501	-	-	5/11/31/31	0/1/1/1
2	BOG	A	502	-	-	4/11/31/31	0/1/1/1
2	BOG	B	401	-	-	5/11/31/31	0/1/1/1
2	BOG	D	401	-	-	4/11/31/31	0/1/1/1
2	BOG	C	401	-	-	8/11/31/31	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	BOG	O1-C1'	3.70	1.53	1.43
2	D	401	BOG	O1-C1'	3.65	1.53	1.43
2	B	401	BOG	O1-C1'	3.64	1.53	1.43
2	C	401	BOG	O1-C1'	3.44	1.52	1.43
2	A	502	BOG	O1-C1'	3.15	1.51	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	BOG	C1'-O1-C1	-2.87	109.08	113.84
2	A	502	BOG	C1'-O1-C1	-2.52	109.67	113.84
2	D	401	BOG	C1-C2-C3	2.08	114.32	110.00

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	BOG	C2'-C1'-O1-C1
2	B	401	BOG	C2'-C1'-O1-C1
2	C	401	BOG	O5-C1-O1-C1'
2	A	502	BOG	O5-C5-C6-O6
2	B	401	BOG	O1-C1'-C2'-C3'
2	C	401	BOG	O5-C5-C6-O6
2	C	401	BOG	C2-C1-O1-C1'
2	D	401	BOG	C4'-C5'-C6'-C7'
2	C	401	BOG	C4-C5-C6-O6
2	A	502	BOG	C4-C5-C6-O6
2	B	401	BOG	C3'-C4'-C5'-C6'
2	C	401	BOG	O1-C1'-C2'-C3'
2	B	401	BOG	C1'-C2'-C3'-C4'

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Mol	Chain	Res	Type	Atoms
2	A	501	BOG	C4'-C5'-C6'-C7'
2	C	401	BOG	C2'-C3'-C4'-C5'
2	A	501	BOG	C1'-C2'-C3'-C4'
2	B	401	BOG	C4'-C5'-C6'-C7'
2	A	501	BOG	C5'-C6'-C7'-C8'
2	D	401	BOG	C2'-C3'-C4'-C5'
2	D	401	BOG	O5-C5-C6-O6
2	A	502	BOG	C5'-C6'-C7'-C8'
2	A	501	BOG	C2'-C3'-C4'-C5'
2	D	401	BOG	C5'-C6'-C7'-C8'
2	C	401	BOG	C3'-C4'-C5'-C6'
2	A	502	BOG	C4'-C5'-C6'-C7'
2	C	401	BOG	C5'-C6'-C7'-C8'

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	BOG	3	0
2	A	502	BOG	2	0
2	B	401	BOG	1	0
2	D	401	BOG	4	0
2	C	401	BOG	5	0

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

Ligand BOG A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand BOG A 502

Bond lengths

Bond angles

Torsions

Rings

Ligand BOG B 401

Bond lengths

Bond angles

Torsions

Rings

Ligand BOG D 401

Bond lengths

Bond angles

Torsions

Rings

Ligand BOG C 401

Bond lengths

Bond angles

Torsions

Rings
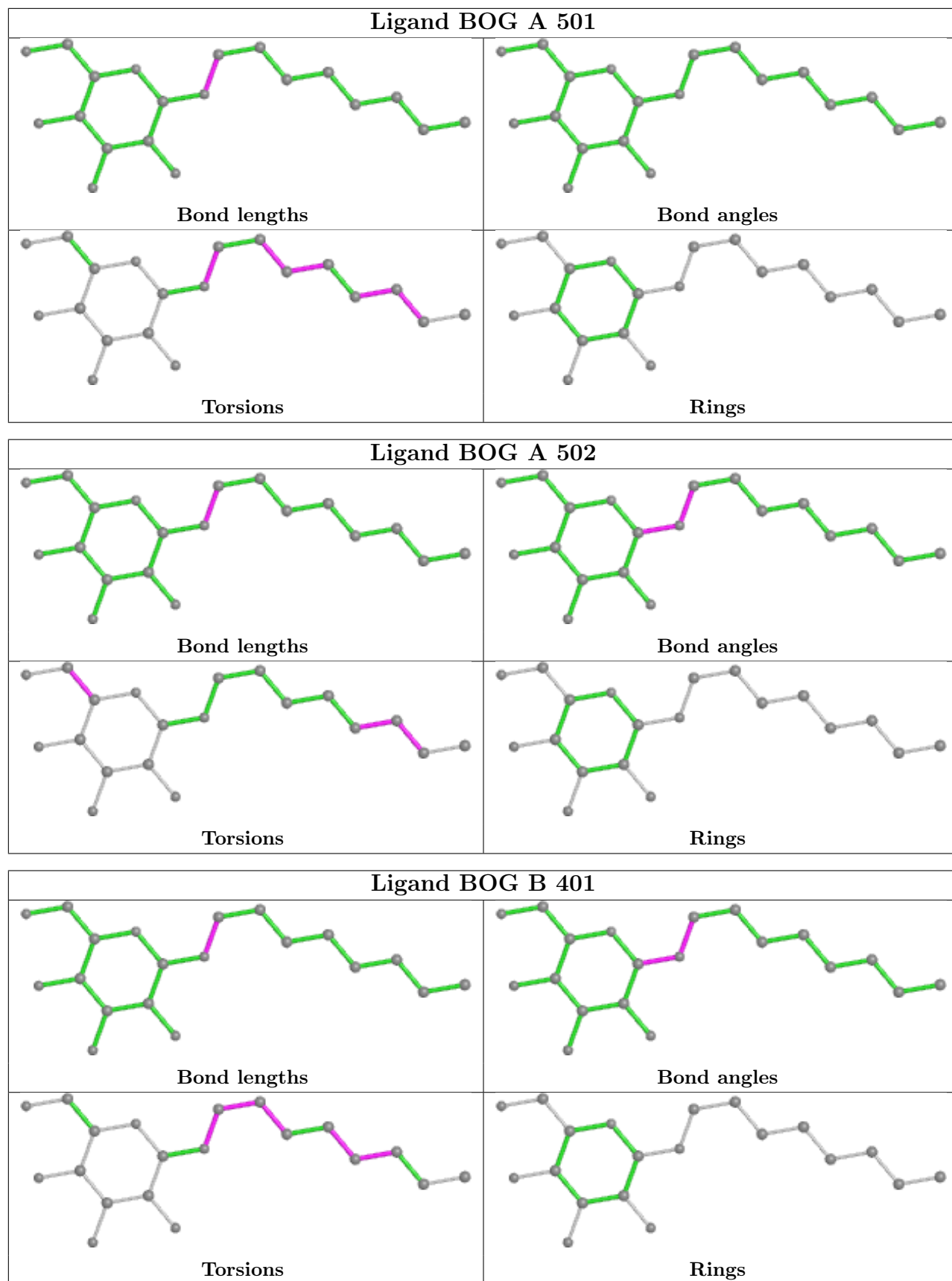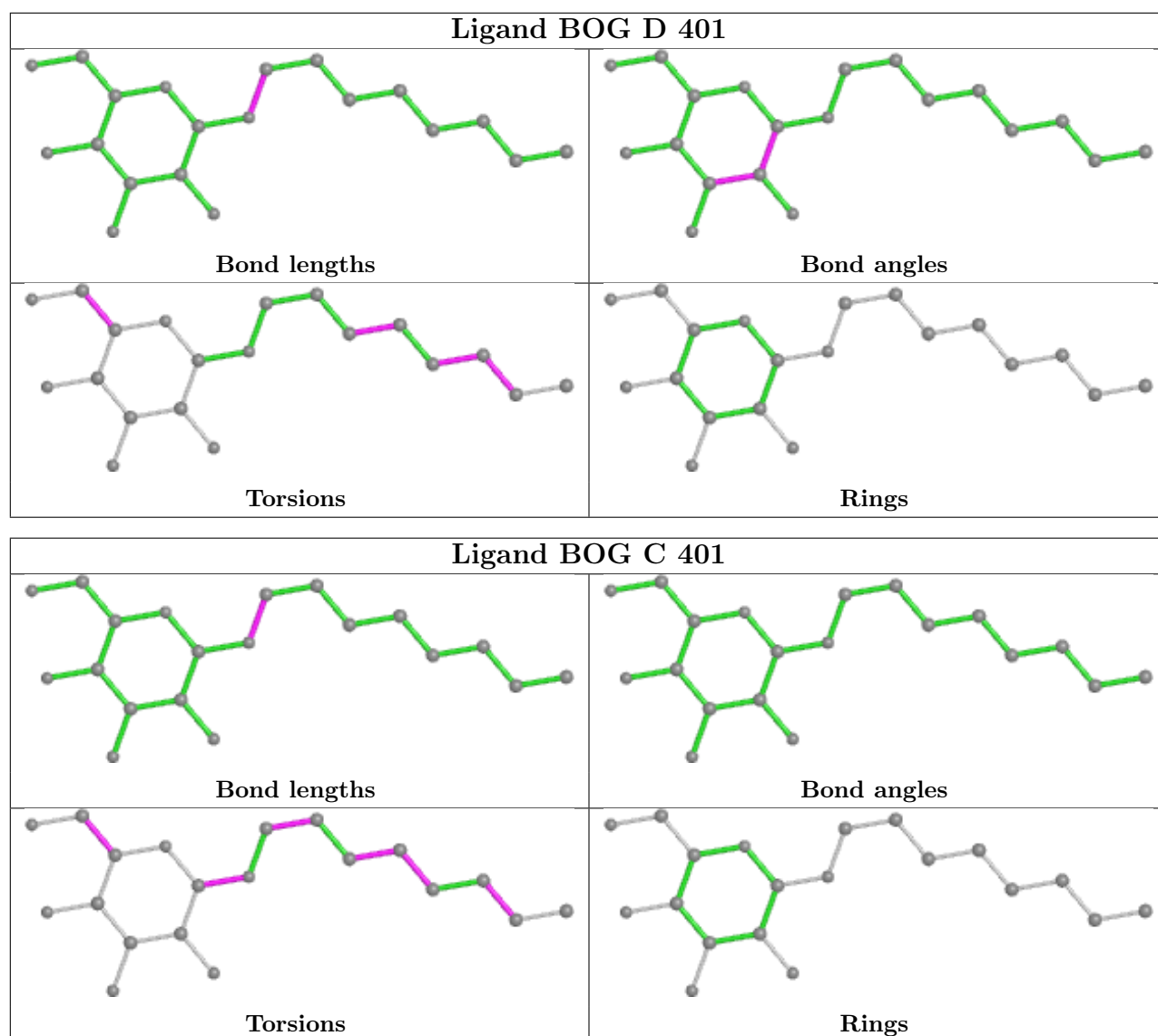
5.7 Other polymers (i)

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	266/343 (77%)	-0.15	14 (5%)	26	29	32, 43, 73, 103	0
1	B	332/343 (96%)	-0.04	22 (6%)	18	20	32, 47, 92, 100	0
1	C	262/343 (76%)	-0.33	2 (0%)	86	87	29, 44, 61, 85	0
1	D	333/343 (97%)	0.08	28 (8%)	11	12	30, 47, 116, 134	0
All	All	1193/1372 (86%)	-0.10	66 (5%)	25	27	29, 45, 94, 134	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	266	MET	8.0
1	D	264	GLY	6.5
1	D	265	ALA	5.8
1	D	305	LYS	5.6
1	B	261	ALA	5.3
1	B	194	GLY	5.2
1	B	264	GLY	5.1
1	D	259	GLY	4.9
1	D	267	ALA	4.9
1	D	329	LYS	4.9
1	A	193	ASN	4.8
1	D	325	GLU	4.6
1	D	303	GLY	4.6
1	D	268	THR	4.5
1	D	328	LYS	4.3
1	D	275	GLY	4.2
1	B	304	GLY	3.9
1	B	325	GLU	3.9
1	D	276	GLU	3.8
1	B	262	GLY	3.8
1	D	284	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	300	ASP	3.6
1	B	327	GLN	3.6
1	A	197	ASP	3.6
1	A	195	GLU	3.5
1	B	326	LYS	3.5
1	D	326	LYS	3.5
1	D	304	GLY	3.5
1	B	263	ALA	3.3
1	A	190	TYR	3.1
1	B	195	GLU	3.1
1	D	327	GLN	3.0
1	B	305	LYS	3.0
1	B	303	GLY	2.9
1	B	302	GLY	2.9
1	A	259	GLY	2.9
1	C	-3	ASP	2.8
1	D	102	LEU	2.8
1	D	283	SER	2.8
1	D	256	ARG	2.8
1	A	196	ARG	2.7
1	C	256	ARG	2.6
1	B	197	ASP	2.6
1	B	310	ALA	2.6
1	D	301	GLU	2.6
1	A	163	GLU	2.6
1	A	191	ASP	2.5
1	B	275	GLY	2.5
1	B	276	GLU	2.4
1	D	272	LYS	2.4
1	D	277	GLU	2.4
1	D	-3	ASP	2.4
1	B	309	GLY	2.4
1	A	194	GLY	2.3
1	B	193	ASN	2.3
1	A	260	GLU	2.3
1	B	192	ARG	2.2
1	D	273	TYR	2.2
1	A	88	CYS	2.2
1	D	-2	ASP	2.2
1	B	190	TYR	2.1
1	B	-4	ASP	2.1
1	A	89	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	306	THR	2.1
1	A	189	ASP	2.0
1	A	180	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides 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
2	BOG	A	501	20/20	0.73	0.31	88,95,98,98	0
2	BOG	C	401	20/20	0.75	0.29	81,108,113,113	0
2	BOG	B	401	20/20	0.84	0.20	73,93,95,95	0
2	BOG	D	401	20/20	0.85	0.18	61,90,95,96	0
2	BOG	A	502	20/20	0.87	0.20	67,94,100,102	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 BOG A 501:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
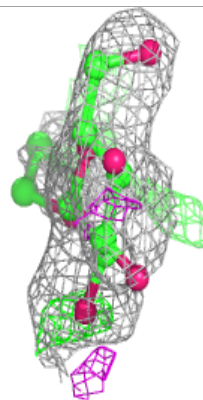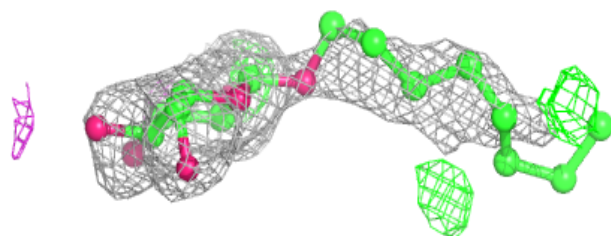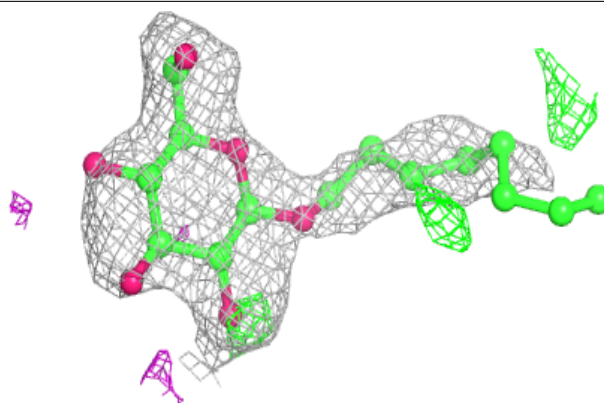
Electron density around BOG C 401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
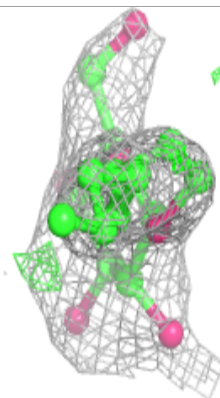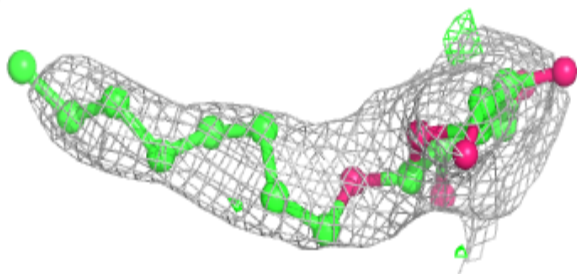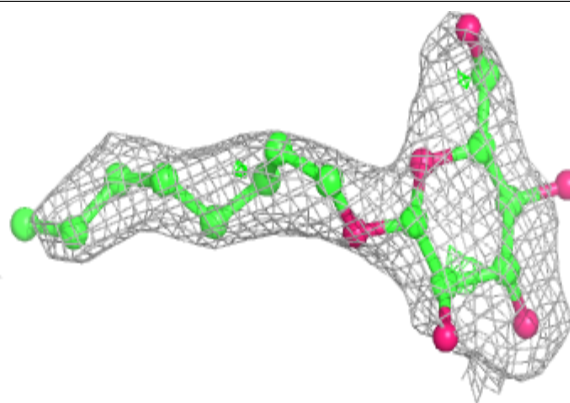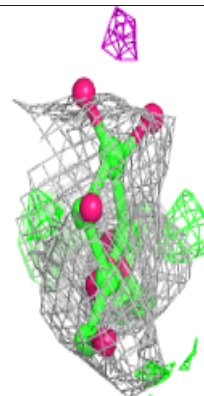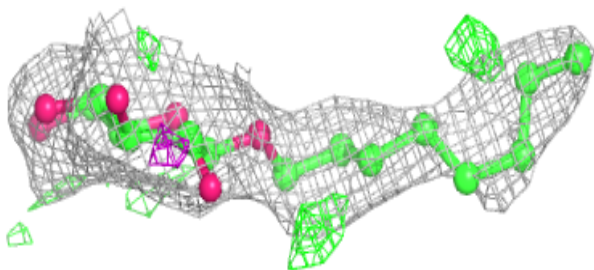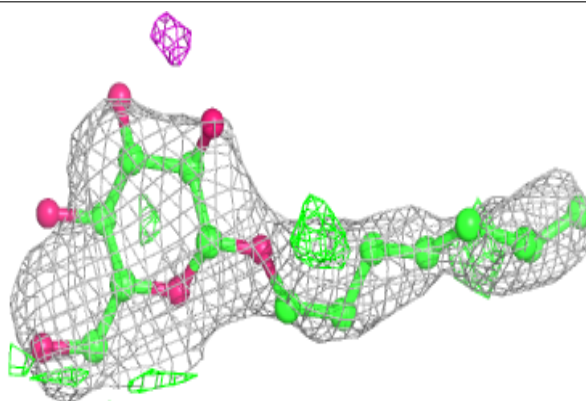$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
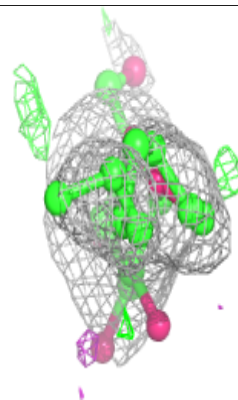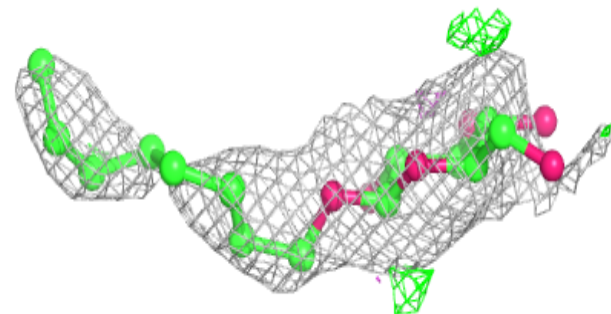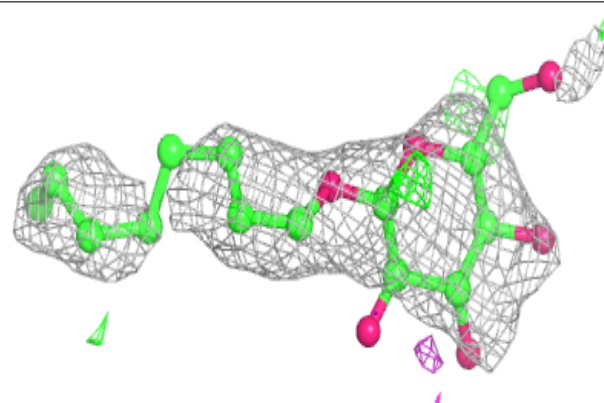
Electron density around BOG B 401:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
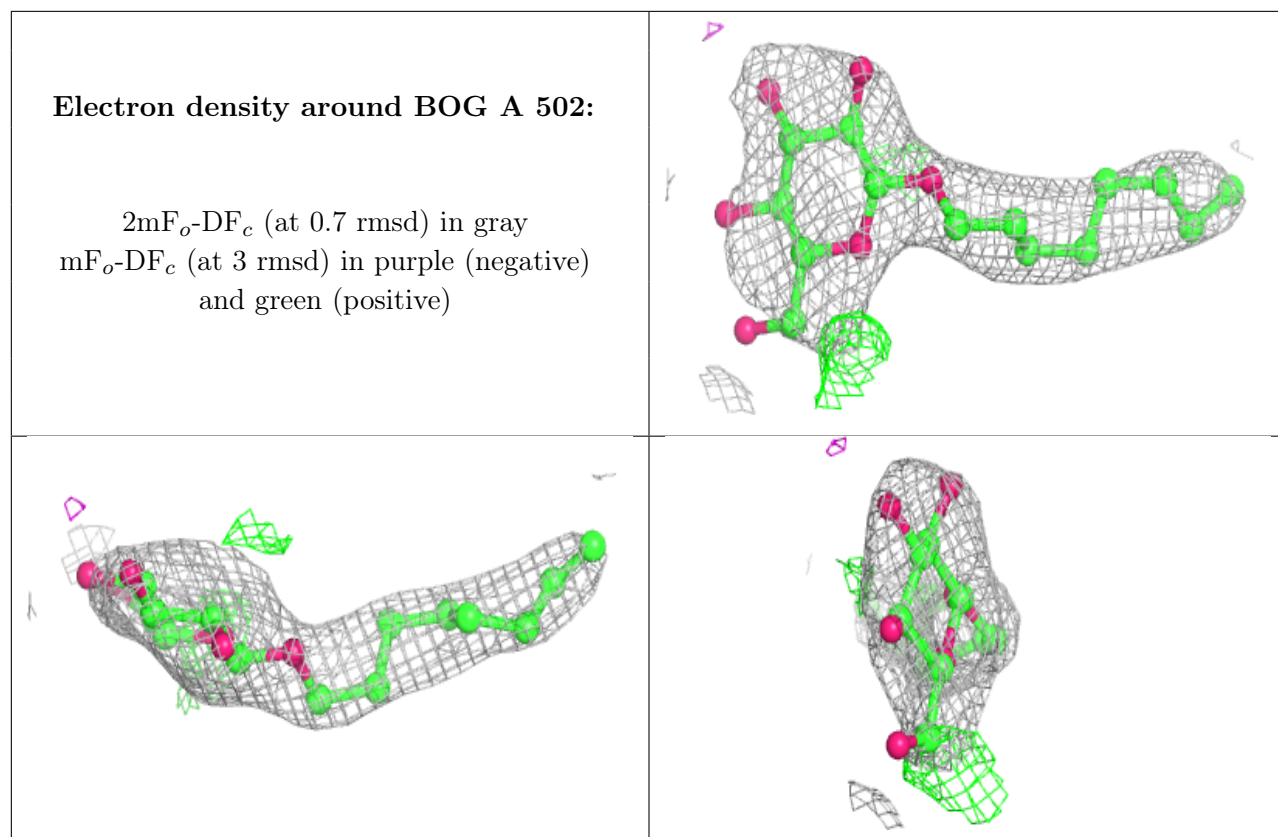mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around BOG D 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 BOG A 502:

$2mF_o$-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.