



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2021 – 08:04 AM EDT

PDB ID : 3O0E
Title : Crystal structure of OmpF in complex with colicin peptide OBS1
Authors : Wojdyla, J.A.; Housden, N.G.; Korczynska, J.; Grishkovskaya, I.; Kirkpatrick, N.; Brzozowski, A.M.; Kleanthous, C.
Deposited on : 2010-07-19
Resolution : 3.01 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.18
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) : 2.18

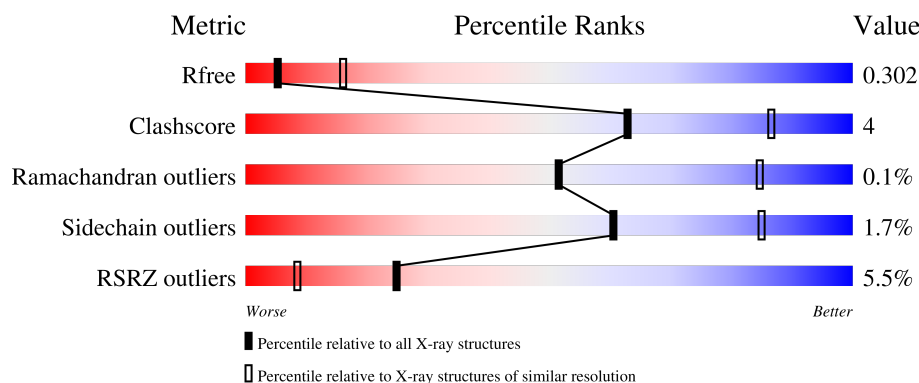
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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}	130704	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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	340	<div> <div style="width: 91%;"></div> <div style="width: 8%;"></div> </div> <div>91% 8%</div>
1	B	340	<div> <div style="width: 89%;"></div> <div style="width: 11%;"></div> </div> <div>89% 11%</div>
1	C	340	<div> <div style="width: 5%;"></div> <div style="width: 88%;"></div> <div style="width: 12%;"></div> </div> <div>5% 88% 12%</div>
1	D	340	<div> <div style="width: 9%;"></div> <div style="width: 86%;"></div> <div style="width: 14%;"></div> </div> <div>9% 86% 14%</div>
1	E	340	<div> <div style="width: 9%;"></div> <div style="width: 91%;"></div> <div style="width: 9%;"></div> </div> <div>9% 91% 9%</div>

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Mol	Chain	Length	Quality of chain
1	F	340	
2	L	17	
2	M	17	
2	N	17	
2	O	17	
2	P	17	
2	Q	17	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BOG	E	401	-	-	-	X
3	BOG	E	402	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31735 atoms, of which 15269 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.

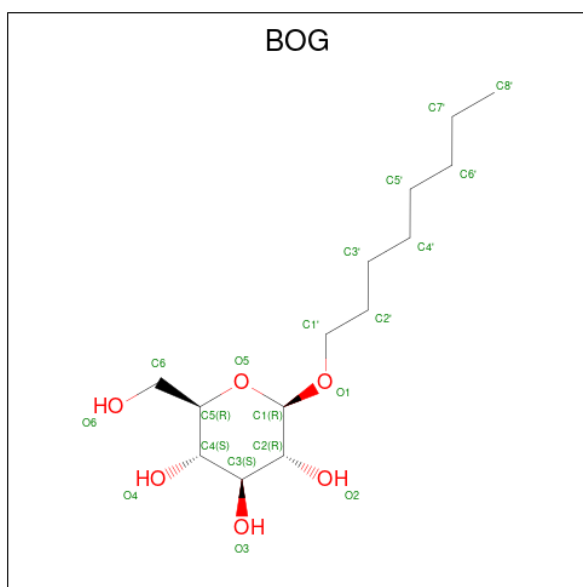
- Molecule 1 is a protein called Porin OmpF.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	340	Total	C	H	N	O	S	0	0	0
			5071	1654	2444	438	532	3			
1	B	340	Total	C	H	N	O	S	0	0	0
			5071	1654	2444	438	532	3			
1	C	340	Total	C	H	N	O	S	0	0	0
			5071	1654	2444	438	532	3			
1	D	340	Total	C	H	N	O	S	0	0	0
			5071	1654	2444	438	532	3			
1	E	340	Total	C	H	N	O	S	0	0	0
			5071	1654	2444	438	532	3			
1	F	340	Total	C	H	N	O	S	0	0	0
			5071	1654	2444	438	532	3			

- Molecule 2 is a protein called Colicin-E9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	14	Total	C	H	N	O	0	0	0
			164	49	73	22	20			
2	M	13	Total	C	H	N	O	0	0	0
			153	46	68	21	18			
2	N	13	Total	C	H	N	O	0	0	0
			153	46	68	21	18			
2	O	15	Total	C	H	N	O	0	0	0
			178	53	80	23	22			
2	P	13	Total	C	H	N	O	0	0	0
			153	46	68	21	18			
2	Q	15	Total	C	H	N	O	0	0	0
			178	53	80	23	22			

- Molecule 3 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: C₁₄H₂₈O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			48	14	28	6		
3	C	1	Total	C	H	O	0	0
			48	14	28	6		
3	D	1	Total	C	H	O	0	0
			48	14	28	6		
3	E	1	Total	C	H	O	0	0
			48	14	28	6		
3	E	1	Total	C	H	O	0	0
			48	14	28	6		
3	F	1	Total	C	H	O	0	0
			48	14	28	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total	O	0	0
			12	12		
4	B	11	Total	O	0	0
			11	11		
4	C	8	Total	O	0	0
			8	8		
4	D	6	Total	O	0	0
			6	6		
4	E	2	Total	O	0	0
			2	2		
4	F	2	Total	O	0	0
			2	2		

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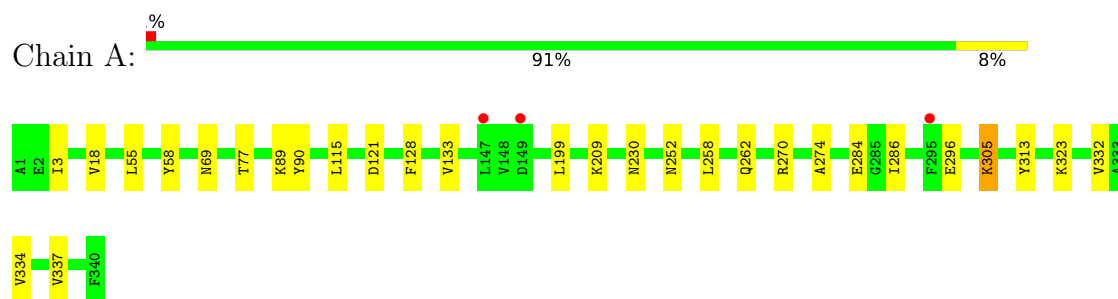
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	1	Total	O	0	0
			1	1		

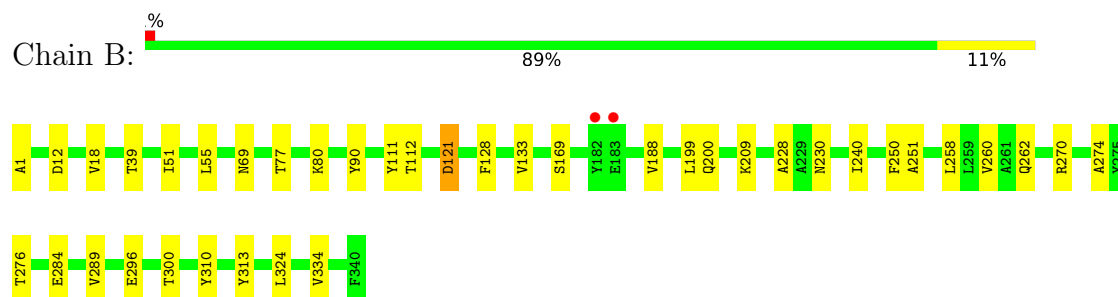
3 Residue-property plots [i](#)

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.

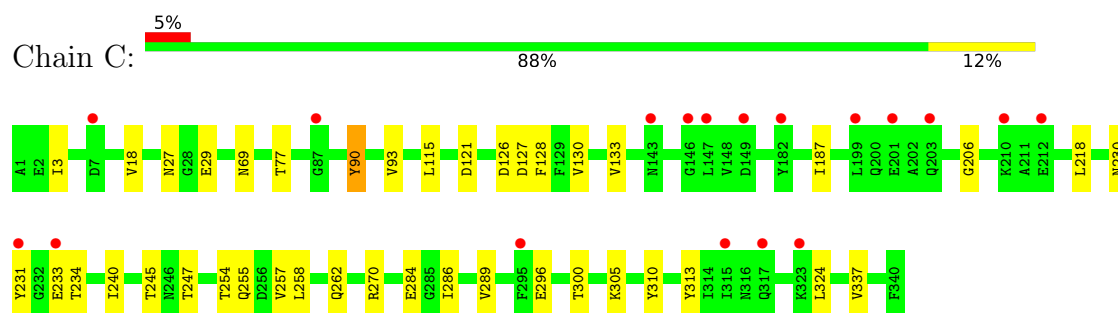
• Molecule 1: Porin OmpF



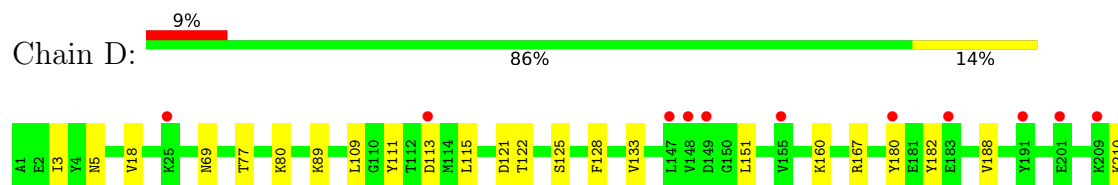
• Molecule 1: Porin OmpF

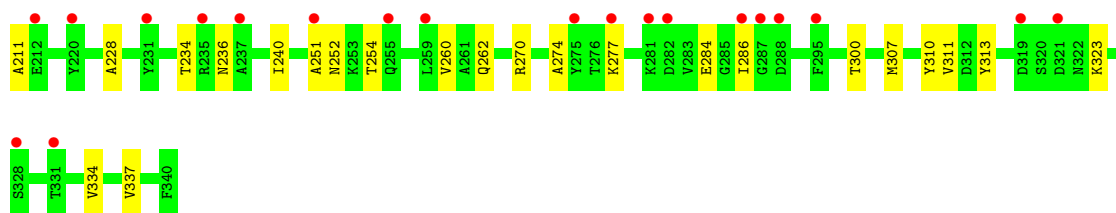


• Molecule 1: Porin OmpF

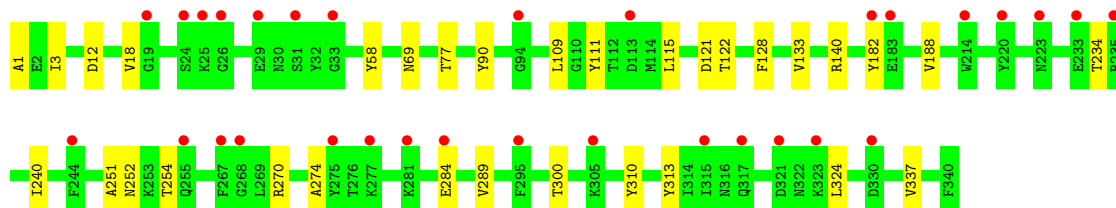
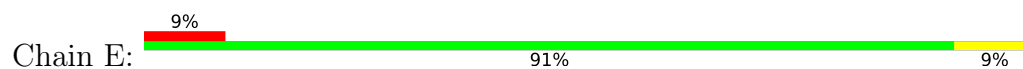


• Molecule 1: Porin OmpF





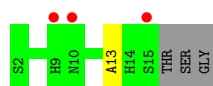
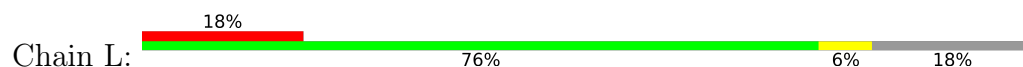
● Molecule 1: Porin OmpF



● Molecule 1: Porin OmpF



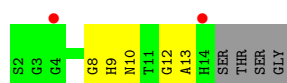
● Molecule 2: Colicin-E9



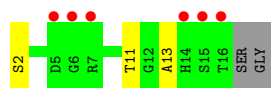
● Molecule 2: Colicin-E9



● Molecule 2: Colicin-E9



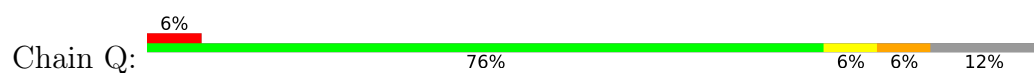
● Molecule 2: Colicin-E9



● Molecule 2: Colicin-E9



● Molecule 2: Colicin-E9



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.49Å 101.62Å 162.14Å 90.00° 94.46° 90.00°	Depositor
Resolution (Å)	20.00 – 3.01 20.12 – 3.01	Depositor EDS
% Data completeness (in resolution range)	73.1 (20.00-3.01) 73.2 (20.12-3.01)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.39 (at 3.04Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.265 , 0.302 0.268 , 0.302	Depositor DCC
R_{free} test set	2399 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	59.4	Xtriage
Anisotropy	0.774	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	31735	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.27	0/2683	0.50	0/3628
1	B	0.27	0/2683	0.50	0/3628
1	C	0.26	0/2683	0.50	0/3628
1	D	0.26	0/2683	0.50	0/3628
1	E	0.26	0/2683	0.50	0/3628
1	F	0.27	0/2683	0.49	0/3628
2	L	0.22	0/92	0.57	0/121
2	M	0.26	0/86	0.76	0/113
2	N	0.24	0/86	0.60	0/113
2	O	0.27	0/99	0.57	0/131
2	P	0.26	0/86	0.68	0/113
2	Q	0.25	0/99	0.59	0/131
All	All	0.26	0/16646	0.50	0/22490

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2627	2444	2444	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2627	2444	2444	23	0
1	C	2627	2444	2444	25	0
1	D	2627	2444	2444	31	0
1	E	2627	2444	2444	15	0
1	F	2627	2444	2444	20	0
2	L	91	73	73	1	0
2	M	85	68	68	6	0
2	N	85	68	68	2	0
2	O	98	80	80	5	0
2	P	85	68	68	4	0
2	Q	98	80	80	1	0
3	B	20	28	28	1	0
3	C	20	28	28	0	0
3	D	20	28	28	2	0
3	E	40	56	56	1	0
3	F	20	28	28	1	0
4	A	12	0	0	0	0
4	B	11	0	0	0	0
4	C	8	0	0	0	0
4	D	6	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	M	1	0	0	0	0
All	All	16466	15269	15269	135	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 4.

All (135) 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:117:GLU:O	2:M:2:SER:N	2.05	0.89
1:D:89:LYS:HD3	2:O:13:ALA:HB3	1.62	0.82
1:C:262:GLN:OE1	1:C:270:ARG:NH1	2.15	0.79
1:A:252:ASN:ND2	1:A:284:GLU:OE2	2.16	0.79
1:F:252:ASN:ND2	1:F:284:GLU:OE2	2.16	0.78
1:A:262:GLN:OE1	1:A:270:ARG:NH1	2.16	0.78
1:C:128:PHE:O	1:C:133:VAL:HG11	1.85	0.76
1:B:262:GLN:OE1	1:B:270:ARG:NH1	2.20	0.74
1:C:233:GLU:OE2	1:C:255:GLN:NE2	2.25	0.70
1:A:313:TYR:CD1	1:A:332:VAL:HG22	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:ILE:HG21	1:F:3:ILE:HD12	1.77	0.67
1:C:206:GLY:N	1:C:284:GLU:OE2	2.29	0.66
1:D:128:PHE:O	1:D:133:VAL:HG11	1.97	0.65
1:C:231:TYR:OH	1:C:255:GLN:OE1	2.14	0.65
1:C:115:LEU:HD13	1:C:296:GLU:OE1	1.96	0.65
1:D:334:VAL:HG12	3:F:401:BOG:H8'3	1.79	0.64
1:E:18:VAL:HG22	1:E:337:VAL:HG22	1.79	0.63
1:F:262:GLN:OE1	1:F:270:ARG:NH1	2.31	0.62
1:D:252:ASN:ND2	1:D:284:GLU:OE2	2.32	0.61
1:C:187:ILE:HD13	1:C:218:LEU:HD12	1.83	0.61
1:E:128:PHE:O	1:E:133:VAL:HG11	1.99	0.61
1:A:89:LYS:HD2	2:L:13:ALA:HB3	1.83	0.61
1:C:240:ILE:HD11	1:C:324:LEU:HD11	1.83	0.60
1:C:3:ILE:HD12	1:E:3:ILE:HG21	1.84	0.59
1:F:32:TYR:CD2	1:F:314:ILE:HG21	2.37	0.59
1:A:128:PHE:O	1:A:133:VAL:HG11	2.03	0.58
1:F:140:ARG:HB2	2:M:11:THR:HG23	1.85	0.58
1:E:289:VAL:HG11	1:E:324:LEU:HD12	1.86	0.58
1:B:128:PHE:O	1:B:133:VAL:HG11	2.03	0.58
1:C:240:ILE:HD11	1:C:324:LEU:CD1	2.34	0.58
1:E:1:ALA:N	1:E:12:ASP:OD1	2.27	0.57
1:D:228:ALA:HB3	1:D:260:VAL:HG12	1.87	0.57
1:C:69:ASN:ND2	1:C:77:THR:O	2.34	0.56
1:B:209:LYS:O	1:B:209:LYS:HG3	2.06	0.56
1:F:240:ILE:CD1	1:F:251:ALA:HB2	2.37	0.55
1:E:109:LEU:HD22	1:E:122:THR:OG1	2.07	0.55
1:A:55:LEU:HD12	1:A:89:LYS:O	2.07	0.55
1:A:199:LEU:HD13	1:B:199:LEU:HD13	1.89	0.55
1:D:262:GLN:OE1	1:D:270:ARG:NH1	2.39	0.54
1:B:274:ALA:HB3	1:B:296:GLU:HB3	1.88	0.54
1:B:112:THR:HG21	1:B:258:LEU:HB3	1.88	0.54
1:D:151:LEU:HD13	1:D:180:TYR:CE2	2.43	0.53
1:B:284:GLU:N	1:B:284:GLU:OE1	2.40	0.53
1:F:128:PHE:O	1:F:133:VAL:HG11	2.08	0.53
1:A:334:VAL:HG12	3:E:401:BOG:H8'3	1.89	0.53
3:B:401:BOG:H8'3	1:F:334:VAL:HG12	1.90	0.53
1:E:252:ASN:ND2	1:E:284:GLU:OE2	2.42	0.52
1:B:300:THR:HG23	1:B:310:TYR:HB3	1.91	0.52
1:C:115:LEU:HD22	1:C:296:GLU:OE1	2.09	0.52
1:A:18:VAL:HG13	1:A:337:VAL:HG22	1.93	0.51
1:D:69:ASN:ND2	1:D:77:THR:O	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:LEU:CD2	1:B:276:THR:HG23	2.41	0.51
1:E:69:ASN:ND2	1:E:77:THR:O	2.42	0.51
1:B:69:ASN:ND2	1:B:77:THR:O	2.31	0.51
1:A:313:TYR:CE1	1:A:332:VAL:HG22	2.46	0.51
1:E:115:LEU:HD21	1:E:274:ALA:HB2	1.92	0.51
1:C:27:ASN:ND2	1:C:29:GLU:OE1	2.44	0.51
1:D:113:ASP:OD1	2:O:2:SER:O	2.28	0.50
1:D:240:ILE:HD12	1:D:251:ALA:HB2	1.93	0.50
1:F:56:THR:HB	1:F:89:LYS:HG2	1.93	0.50
1:D:89:LYS:CD	2:O:13:ALA:HB3	2.38	0.50
2:M:7:ARG:HG3	2:M:7:ARG:HH11	1.77	0.50
1:B:334:VAL:HG12	3:D:401:BOG:H8'3	1.94	0.49
1:D:151:LEU:HD13	1:D:180:TYR:CD2	2.46	0.49
1:B:228:ALA:HB3	1:B:260:VAL:HG12	1.95	0.49
1:B:289:VAL:HG21	1:B:324:LEU:HD12	1.93	0.49
1:D:211:ALA:HA	1:D:236:ASN:OD1	2.13	0.48
1:E:234:THR:OG1	1:E:254:THR:OG1	2.30	0.48
1:D:109:LEU:HD21	1:D:122:THR:OG1	2.13	0.48
1:D:125:SER:O	1:D:167:ARG:NH2	2.42	0.48
1:D:18:VAL:HG13	1:D:337:VAL:HG22	1.96	0.48
1:C:18:VAL:HG22	1:C:337:VAL:HG22	1.95	0.47
1:F:69:ASN:ND2	1:F:77:THR:O	2.38	0.47
1:D:160:LYS:HG2	3:D:401:BOG:H62	1.96	0.47
1:F:257:VAL:O	1:F:258:LEU:HD22	2.14	0.47
2:N:12:GLY:O	2:N:13:ALA:HB3	2.15	0.47
1:A:274:ALA:HB3	1:A:296:GLU:HB3	1.96	0.47
1:D:180:TYR:HB3	1:D:182:TYR:CE1	2.50	0.46
1:D:210:LYS:O	1:D:236:ASN:ND2	2.45	0.46
2:M:11:THR:HG22	2:M:12:GLY:N	2.30	0.46
1:A:69:ASN:ND2	1:A:77:THR:O	2.40	0.46
1:A:115:LEU:HD21	1:A:274:ALA:HB2	1.96	0.46
1:A:313:TYR:HD1	1:A:332:VAL:HG22	1.76	0.45
1:D:300:THR:HG23	1:D:310:TYR:HB3	1.98	0.45
1:A:305:LYS:HD2	1:A:305:LYS:H	1.81	0.45
1:E:111:TYR:OH	1:E:188:VAL:HG23	2.16	0.45
1:D:234:THR:OG1	1:D:254:THR:OG1	2.31	0.45
1:C:234:THR:OG1	1:C:254:THR:OG1	2.34	0.45
1:D:115:LEU:HD21	1:D:274:ALA:HB2	1.98	0.45
1:B:169:SER:O	1:B:200:GLN:NE2	2.50	0.45
1:C:245:THR:HG23	1:C:247:THR:OG1	2.17	0.45
1:F:90:TYR:HB3	1:F:93:VAL:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:ASP:HA	1:C:133:VAL:HG12	1.99	0.45
1:A:230:ASN:HB2	1:A:258:LEU:HB2	2.00	0.45
1:C:18:VAL:HG13	1:C:337:VAL:HG22	1.99	0.45
2:Q:13:ALA:O	2:Q:14:HIS:O	2.35	0.45
1:D:111:TYR:OH	1:D:188:VAL:HG23	2.17	0.44
1:B:111:TYR:OH	1:B:188:VAL:HG23	2.16	0.44
1:B:51:ILE:HG21	1:B:55:LEU:HD23	1.99	0.44
1:C:286:ILE:HG21	1:C:289:VAL:HG11	2.00	0.43
1:D:307:MET:SD	1:F:57:GLY:HA3	2.58	0.43
1:F:115:LEU:O	2:M:3:GLY:HA3	2.18	0.43
1:E:300:THR:HG23	1:E:310:TYR:HB3	1.99	0.43
1:C:300:THR:HG23	1:C:310:TYR:HB3	2.00	0.43
1:F:1:ALA:N	1:F:12:ASP:OD1	2.36	0.43
1:B:240:ILE:CD1	1:B:251:ALA:HB2	2.48	0.43
1:E:240:ILE:CD1	1:E:251:ALA:HB2	2.49	0.43
2:P:2:SER:O	2:P:2:SER:OG	2.31	0.43
1:F:115:LEU:HD21	1:F:274:ALA:HB2	2.01	0.43
1:A:3:ILE:HD12	1:C:3:ILE:HG21	2.00	0.42
1:B:289:VAL:HG21	1:B:324:LEU:CD1	2.48	0.42
1:F:140:ARG:HB3	2:M:11:THR:OG1	2.19	0.42
2:O:11:THR:O	2:O:11:THR:HG22	2.20	0.42
1:C:90:TYR:HB3	1:C:93:VAL:HB	2.01	0.42
1:B:121:ASP:N	1:B:121:ASP:OD1	2.53	0.42
1:D:311:VAL:HG22	1:D:334:VAL:HG13	2.02	0.42
1:D:236:ASN:OD1	1:D:236:ASN:O	2.38	0.41
1:B:200:GLN:HG2	1:B:250:PHE:CE1	2.55	0.41
1:C:127:ASP:O	1:C:130:VAL:HG22	2.21	0.41
1:C:257:VAL:O	1:C:258:LEU:HD22	2.20	0.41
1:D:286:ILE:HG23	1:D:323:LYS:HD2	2.02	0.41
2:P:8:GLY:O	2:P:10:ASN:N	2.53	0.41
1:B:112:THR:OG1	1:B:230:ASN:OD1	2.24	0.41
1:D:240:ILE:CD1	1:D:251:ALA:HB2	2.51	0.41
1:E:140:ARG:HH11	2:P:11:THR:HA	1.84	0.41
1:C:230:ASN:HB2	1:C:258:LEU:HB2	2.01	0.41
1:E:140:ARG:NH1	2:P:11:THR:HA	2.36	0.41
1:F:240:ILE:HD11	1:F:251:ALA:HB2	2.01	0.41
2:N:8:GLY:O	2:N:10:ASN:N	2.54	0.41
1:B:1:ALA:N	1:B:12:ASP:OD1	2.43	0.40
1:D:89:LYS:HE2	2:O:13:ALA:O	2.21	0.40
1:F:127:ASP:O	1:F:130:VAL:HG22	2.21	0.40
1:A:286:ILE:HG23	1:A:323:LYS:HD2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:ASN:HA	1:D:251:ALA:O	2.21	0.40
1:B:18:VAL:O	1:B:39:THR:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	338/340 (99%)	320 (95%)	18 (5%)	0	100	100
1	B	338/340 (99%)	321 (95%)	17 (5%)	0	100	100
1	C	338/340 (99%)	321 (95%)	17 (5%)	0	100	100
1	D	338/340 (99%)	323 (96%)	15 (4%)	0	100	100
1	E	338/340 (99%)	321 (95%)	17 (5%)	0	100	100
1	F	338/340 (99%)	321 (95%)	17 (5%)	0	100	100
2	L	12/17 (71%)	12 (100%)	0	0	100	100
2	M	11/17 (65%)	9 (82%)	1 (9%)	1 (9%)	1	3
2	N	11/17 (65%)	8 (73%)	2 (18%)	1 (9%)	1	3
2	O	13/17 (76%)	10 (77%)	3 (23%)	0	100	100
2	P	11/17 (65%)	9 (82%)	2 (18%)	0	100	100
2	Q	13/17 (76%)	11 (85%)	1 (8%)	1 (8%)	1	4
All	All	2099/2142 (98%)	1986 (95%)	110 (5%)	3 (0%)	51	85

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Q	14	HIS
2	N	9	HIS

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Mol	Chain	Res	Type
2	M	10	ASN

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	263/263 (100%)	258 (98%)	5 (2%)	57	83
1	B	263/263 (100%)	259 (98%)	4 (2%)	65	86
1	C	263/263 (100%)	259 (98%)	4 (2%)	65	86
1	D	263/263 (100%)	258 (98%)	5 (2%)	57	83
1	E	263/263 (100%)	257 (98%)	6 (2%)	50	79
1	F	263/263 (100%)	259 (98%)	4 (2%)	65	86
2	L	8/10 (80%)	8 (100%)	0	100	100
2	M	7/10 (70%)	7 (100%)	0	100	100
2	N	7/10 (70%)	7 (100%)	0	100	100
2	O	9/10 (90%)	9 (100%)	0	100	100
2	P	7/10 (70%)	7 (100%)	0	100	100
2	Q	9/10 (90%)	9 (100%)	0	100	100
All	All	1625/1638 (99%)	1597 (98%)	28 (2%)	60	85

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	TYR
1	A	90	TYR
1	A	121	ASP
1	A	209	LYS
1	A	305	LYS
1	B	80	LYS
1	B	90	TYR
1	B	121	ASP
1	B	313	TYR

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Mol	Chain	Res	Type
1	C	90	TYR
1	C	121	ASP
1	C	305	LYS
1	C	313	TYR
1	D	5	ASN
1	D	80	LYS
1	D	121	ASP
1	D	277	LYS
1	D	313	TYR
1	E	58	TYR
1	E	90	TYR
1	E	121	ASP
1	E	182	TYR
1	E	270	ARG
1	E	313	TYR
1	F	90	TYR
1	F	121	ASP
1	F	196	ARG
1	F	313	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	252	ASN
2	M	9	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

6 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
3	BOG	F	401	-	20,20,20	1.27	2 (10%)	25,25,25	1.40	3 (12%)
3	BOG	E	401	-	20,20,20	1.27	2 (10%)	25,25,25	1.11	2 (8%)
3	BOG	B	401	-	20,20,20	1.28	2 (10%)	25,25,25	0.83	0
3	BOG	C	401	-	20,20,20	1.27	2 (10%)	25,25,25	0.92	0
3	BOG	D	401	-	20,20,20	1.29	2 (10%)	25,25,25	0.79	0
3	BOG	E	402	-	20,20,20	1.27	2 (10%)	25,25,25	1.06	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	BOG	F	401	-	-	5/11/31/31	0/1/1/1
3	BOG	E	401	-	-	7/11/31/31	0/1/1/1
3	BOG	B	401	-	-	7/11/31/31	0/1/1/1
3	BOG	C	401	-	-	9/11/31/31	0/1/1/1
3	BOG	D	401	-	-	7/11/31/31	0/1/1/1
3	BOG	E	402	-	-	7/11/31/31	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	BOG	O5-C1	4.14	1.52	1.41
3	B	401	BOG	O5-C1	4.13	1.52	1.41
3	E	401	BOG	O5-C1	4.12	1.52	1.41
3	C	401	BOG	O5-C1	4.10	1.52	1.41
3	E	402	BOG	O5-C1	4.08	1.52	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	401	BOG	O5-C1	3.97	1.51	1.41
3	D	401	BOG	O1-C1	-2.38	1.36	1.40
3	E	402	BOG	O1-C1	-2.26	1.36	1.40
3	B	401	BOG	O1-C1	-2.26	1.36	1.40
3	C	401	BOG	O1-C1	-2.23	1.36	1.40
3	F	401	BOG	O1-C1	-2.18	1.36	1.40
3	E	401	BOG	O1-C1	-2.08	1.36	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	401	BOG	C4-C3-C2	3.55	117.02	110.82
3	F	401	BOG	C1-C2-C3	2.70	115.63	110.00
3	F	401	BOG	C3-C4-C5	2.58	114.84	110.24
3	E	401	BOG	C1'-O1-C1	2.31	117.67	113.84
3	E	401	BOG	O5-C5-C4	2.14	113.58	109.69

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	BOG	C2'-C1'-O1-C1
3	C	401	BOG	C2-C1-O1-C1'
3	C	401	BOG	C2'-C1'-O1-C1
3	D	401	BOG	C2'-C1'-O1-C1
3	E	401	BOG	C2'-C1'-O1-C1
3	E	402	BOG	C2-C1-O1-C1'
3	E	402	BOG	O5-C1-O1-C1'
3	E	402	BOG	C2'-C1'-O1-C1
3	F	401	BOG	C2'-C1'-O1-C1
3	C	401	BOG	O5-C5-C6-O6
3	D	401	BOG	O5-C5-C6-O6
3	C	401	BOG	C4-C5-C6-O6
3	D	401	BOG	C4-C5-C6-O6
3	C	401	BOG	O5-C1-O1-C1'
3	D	401	BOG	O1-C1'-C2'-C3'
3	E	402	BOG	O1-C1'-C2'-C3'
3	E	401	BOG	C2-C1-O1-C1'
3	C	401	BOG	O1-C1'-C2'-C3'
3	E	401	BOG	O1-C1'-C2'-C3'
3	F	401	BOG	O1-C1'-C2'-C3'
3	B	401	BOG	O1-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
3	D	401	BOG	C4'-C5'-C6'-C7'
3	E	402	BOG	C4'-C5'-C6'-C7'
3	F	401	BOG	C4'-C5'-C6'-C7'
3	C	401	BOG	C4'-C5'-C6'-C7'
3	B	401	BOG	C4'-C5'-C6'-C7'
3	E	401	BOG	C4'-C5'-C6'-C7'
3	E	401	BOG	O5-C1-O1-C1'
3	B	401	BOG	C3'-C4'-C5'-C6'
3	F	401	BOG	C3'-C4'-C5'-C6'
3	C	401	BOG	C3'-C4'-C5'-C6'
3	E	402	BOG	C3'-C4'-C5'-C6'
3	E	401	BOG	C3'-C4'-C5'-C6'
3	D	401	BOG	C3'-C4'-C5'-C6'
3	B	401	BOG	C1'-C2'-C3'-C4'
3	C	401	BOG	C1'-C2'-C3'-C4'
3	E	402	BOG	C1'-C2'-C3'-C4'
3	F	401	BOG	C1'-C2'-C3'-C4'
3	D	401	BOG	C1'-C2'-C3'-C4'
3	E	401	BOG	C1'-C2'-C3'-C4'
3	B	401	BOG	C2-C1-O1-C1'
3	B	401	BOG	O5-C1-O1-C1'

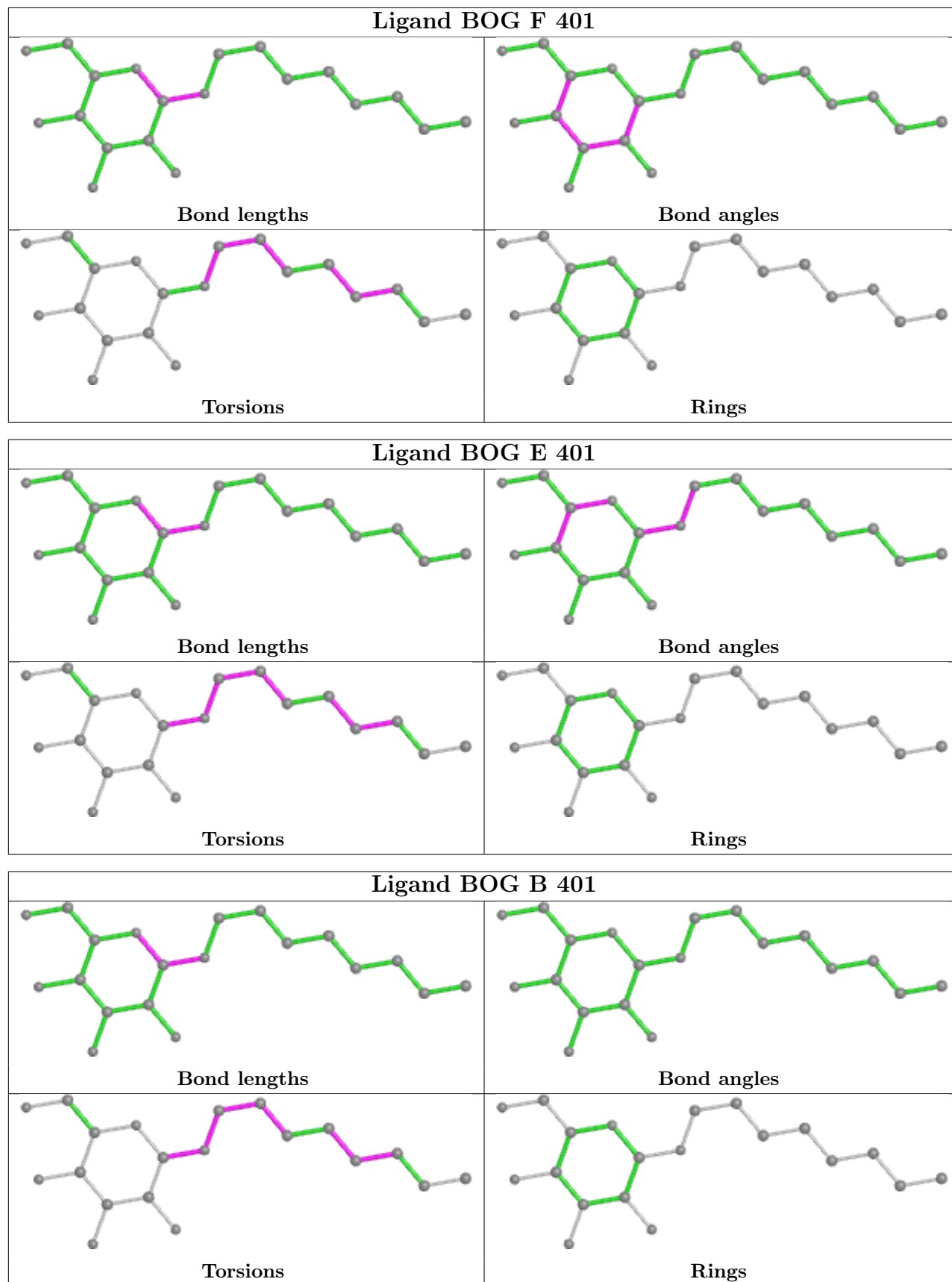
There are no ring outliers.

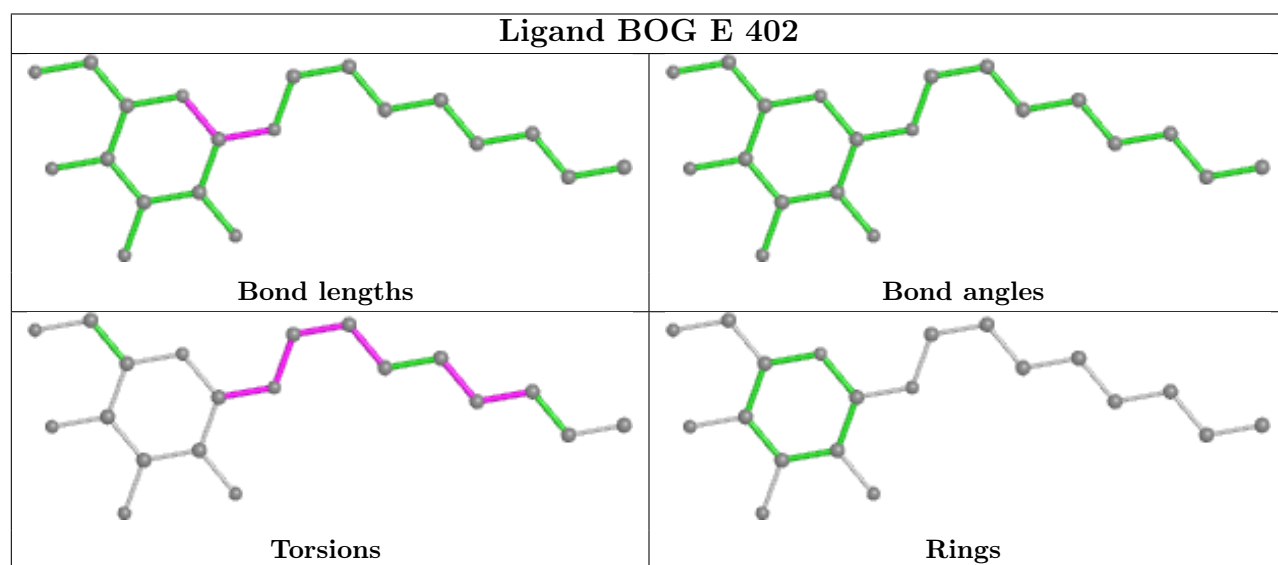
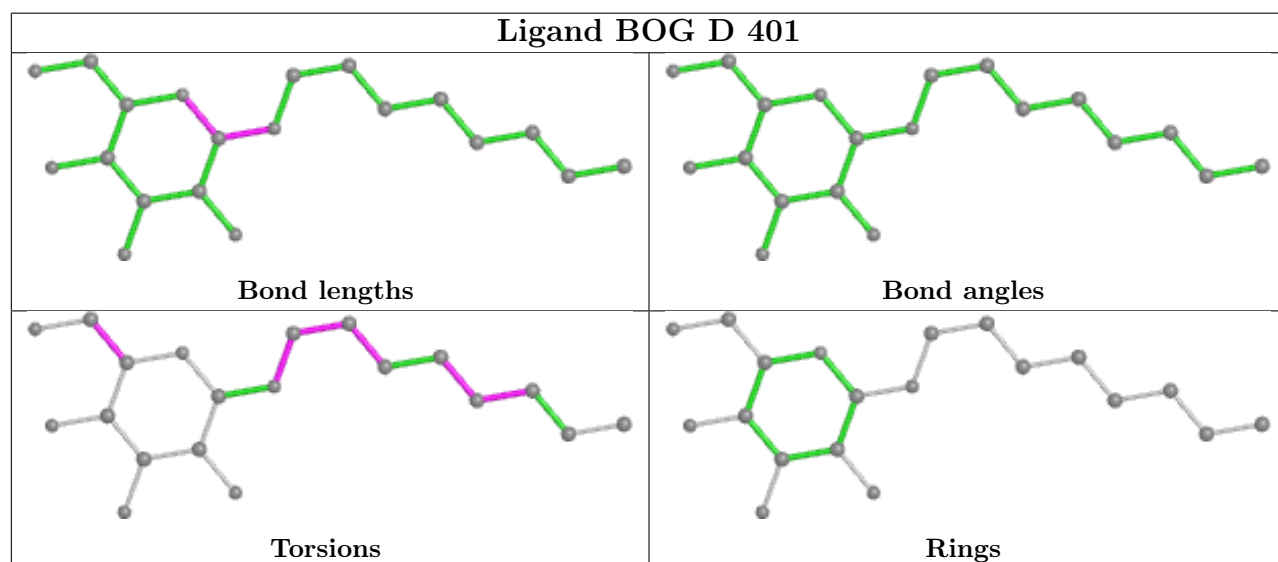
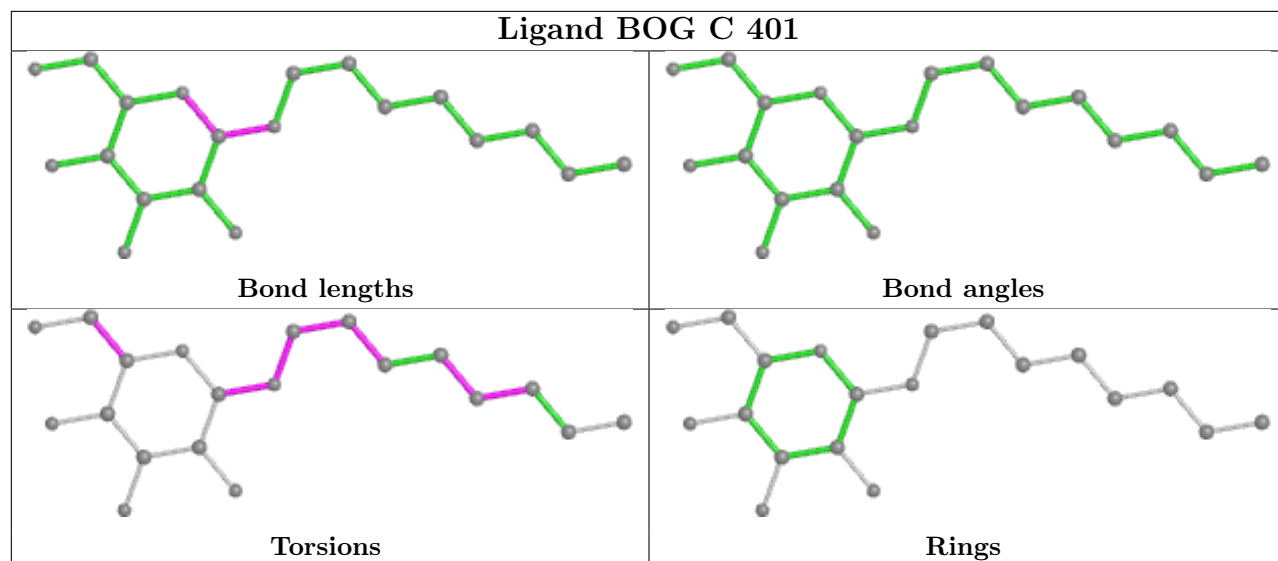
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	401	BOG	1	0
3	E	401	BOG	1	0
3	B	401	BOG	1	0
3	D	401	BOG	2	0

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

equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	340/340 (100%)	-0.13	3 (0%) 84 62	37, 70, 95, 110	0
1	B	340/340 (100%)	-0.24	2 (0%) 89 72	35, 66, 89, 106	0
1	C	340/340 (100%)	0.27	18 (5%) 26 9	39, 95, 120, 139	0
1	D	340/340 (100%)	0.40	31 (9%) 9 3	40, 96, 126, 138	0
1	E	340/340 (100%)	0.45	31 (9%) 9 3	48, 108, 137, 145	0
1	F	340/340 (100%)	0.24	17 (5%) 28 10	40, 93, 118, 130	0
2	L	14/17 (82%)	0.91	3 (21%) 0 0	73, 87, 108, 111	0
2	M	13/17 (76%)	0.81	0 100 100	75, 104, 121, 129	0
2	N	13/17 (76%)	1.18	2 (15%) 2 0	81, 96, 130, 131	0
2	O	15/17 (88%)	1.99	6 (40%) 0 0	99, 111, 138, 141	0
2	P	13/17 (76%)	1.56	3 (23%) 0 0	104, 117, 127, 136	0
2	Q	15/17 (88%)	0.56	1 (6%) 17 5	60, 73, 101, 102	0
All	All	2123/2142 (99%)	0.20	117 (5%) 25 8	35, 87, 126, 145	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	25	LYS	8.7
2	P	14	HIS	6.7
2	O	16	THR	5.8
1	D	113	ASP	5.2
1	E	323	LYS	4.8
1	E	255	GLN	4.7
1	F	223	ASN	4.5
1	E	33	GLY	4.0
2	O	5	ASP	4.0
2	O	14	HIS	4.0
2	P	12	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	295	PHE	3.6
1	D	147	LEU	3.5
1	B	183	GLU	3.5
1	E	244	PHE	3.3
2	N	14	HIS	3.3
1	D	255	GLN	3.3
1	C	201	GLU	3.3
2	L	10	ASN	3.2
1	D	287	GLY	3.2
1	E	29	GLU	3.1
1	C	295	PHE	3.1
1	E	220	TYR	3.1
1	C	87	GLY	3.0
1	D	209	LYS	3.0
1	E	277	LYS	3.0
1	E	24	SER	3.0
1	D	148	VAL	2.9
1	F	233	GLU	2.9
1	E	330	ASP	2.9
1	E	26	GLY	2.9
1	E	295	PHE	2.9
1	E	267	PHE	2.9
1	E	31	SER	2.9
1	D	288	ASP	2.8
2	L	15	SER	2.8
1	F	57	GLY	2.7
1	F	145	PHE	2.7
1	C	233	GLU	2.7
1	F	146	GLY	2.7
1	E	183	GLU	2.7
1	F	26	GLY	2.6
1	A	149	ASP	2.6
1	E	315	ILE	2.6
1	F	147	LEU	2.6
1	E	113	ASP	2.6
1	D	231	TYR	2.6
1	D	282	ASP	2.6
1	C	323	LYS	2.6
1	C	210	LYS	2.6
1	D	220	TYR	2.5
1	F	142	SER	2.5
1	D	212	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
2	O	15	SER	2.5
1	C	231	TYR	2.5
1	D	25	LYS	2.5
1	E	233	GLU	2.5
1	F	25	LYS	2.5
1	D	180	TYR	2.4
2	O	7	ARG	2.4
1	C	146	GLY	2.4
2	Q	8	GLY	2.4
1	F	182	TYR	2.4
1	C	315	ILE	2.4
1	F	160	LYS	2.4
1	E	275	TYR	2.4
1	C	147	LEU	2.4
1	E	321	ASP	2.3
1	D	275	TYR	2.3
1	F	106	TYR	2.3
1	C	149	ASP	2.3
1	F	235	ARG	2.3
2	N	4	GLY	2.3
1	D	183	GLU	2.3
1	D	237	ALA	2.3
1	E	305	LYS	2.3
1	C	317	GLN	2.3
1	D	319	ASP	2.3
1	D	251	ALA	2.3
1	E	94	GLY	2.2
1	C	199	LEU	2.2
1	C	143	ASN	2.2
1	F	151	LEU	2.2
1	D	321	ASP	2.2
1	A	147	LEU	2.2
2	P	11	THR	2.2
1	E	235	ARG	2.2
1	E	281	LYS	2.2
1	C	212	GLU	2.2
1	D	155	VAL	2.2
1	E	317	GLN	2.2
1	E	214	TRP	2.2
1	C	182	TYR	2.2
1	D	191	TYR	2.2
1	E	19	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	286	ILE	2.1
1	B	182	TYR	2.1
1	F	263	TYR	2.1
2	O	6	GLY	2.1
1	E	223	ASN	2.1
1	C	7	ASP	2.1
1	D	281	LYS	2.1
1	E	268	GLY	2.1
1	F	285	GLY	2.1
1	D	235	ARG	2.1
1	F	210	LYS	2.1
1	D	331	THR	2.1
1	D	149	ASP	2.1
1	D	259	LEU	2.0
1	D	277	LYS	2.0
1	D	201	GLU	2.0
1	E	284	GLU	2.0
1	D	328	SER	2.0
2	L	9	HIS	2.0
1	A	295	PHE	2.0
1	E	182	TYR	2.0
1	C	203	GLN	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 monosaccharides in this entry.

6.4 Ligands [i](#)

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

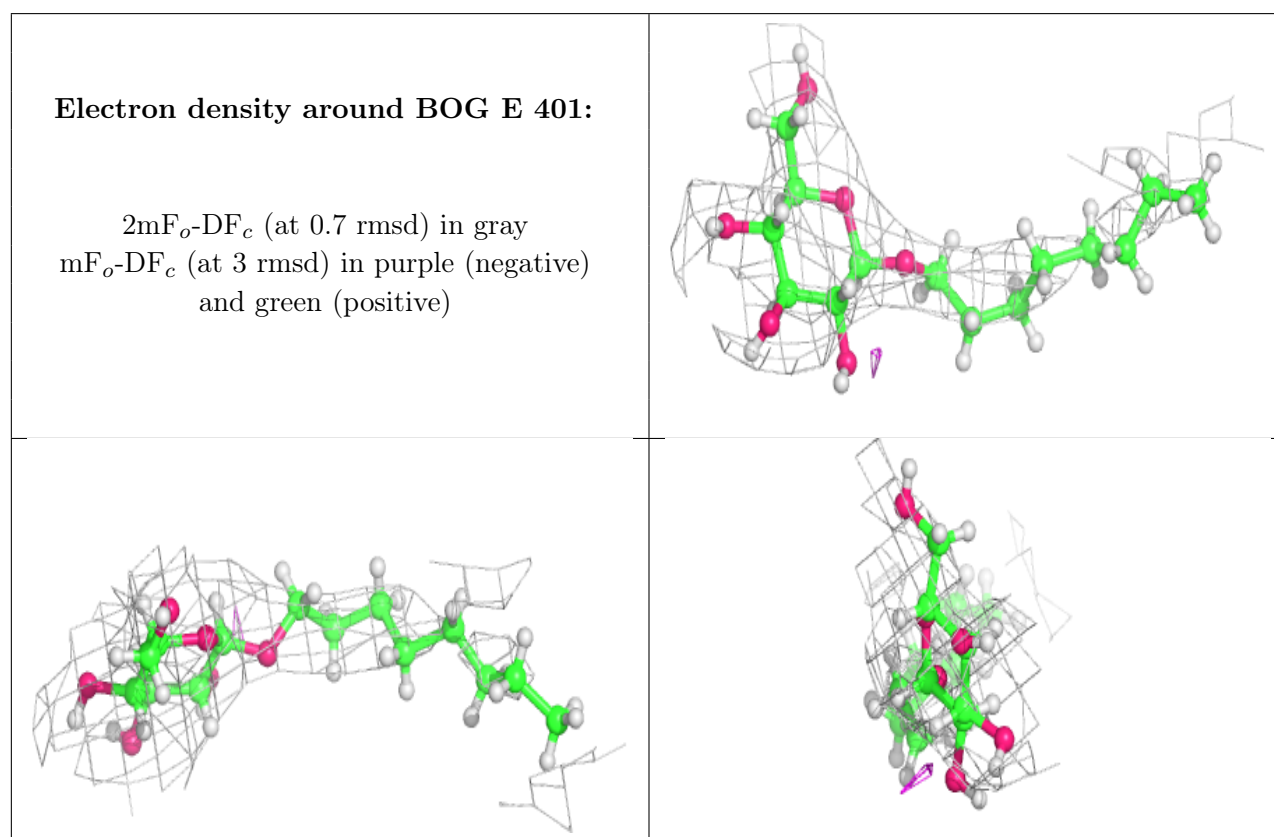
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BOG	E	401	20/20	0.69	0.50	76,110,137,144	0

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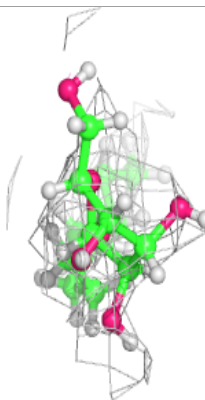
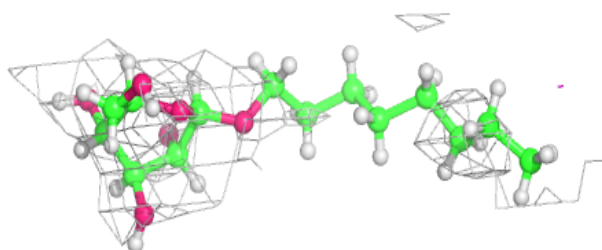
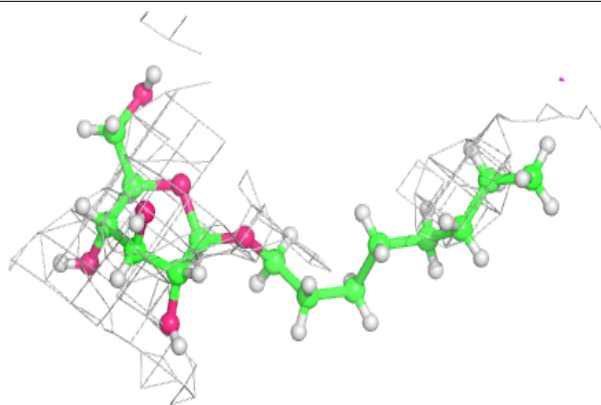
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	BOG	E	402	20/20	0.74	0.57	86,132,166,173	0
3	BOG	D	401	20/20	0.76	0.37	62,95,116,125	0
3	BOG	F	401	20/20	0.78	0.38	81,117,146,151	0
3	BOG	C	401	20/20	0.90	0.41	51,79,103,112	0
3	BOG	B	401	20/20	0.92	0.21	52,79,108,113	0

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.

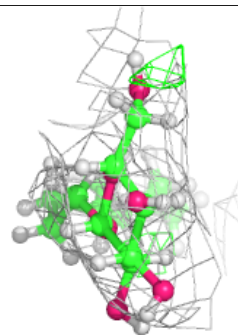
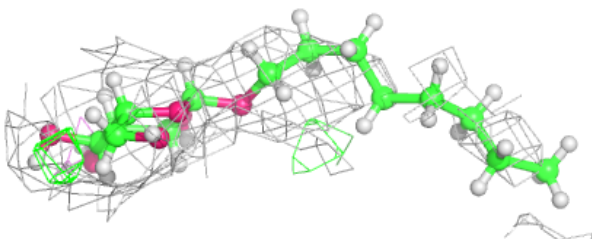
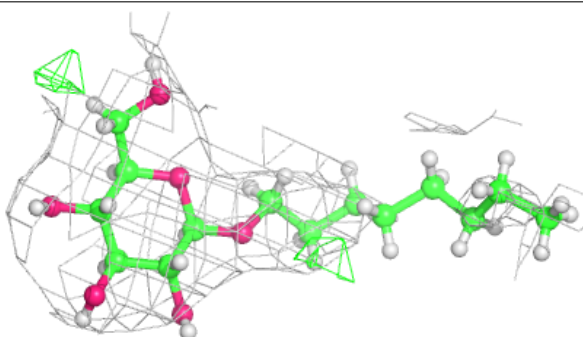


Electron density around BOG E 402:

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

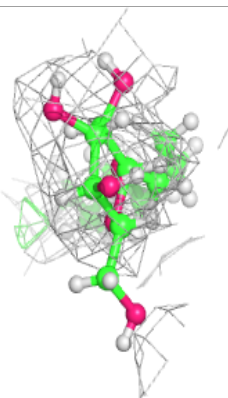
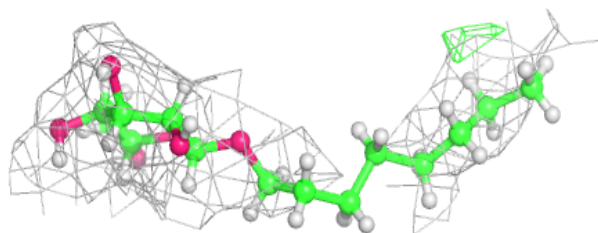
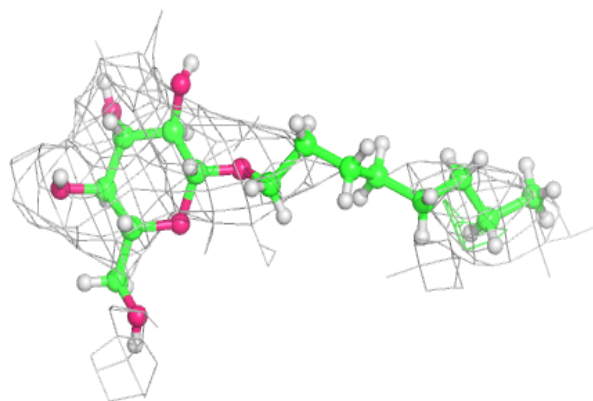
**Electron density around BOG D 401:**

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

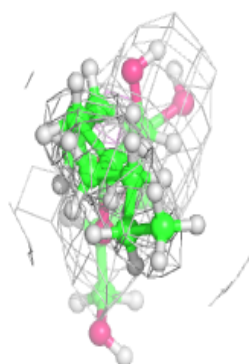
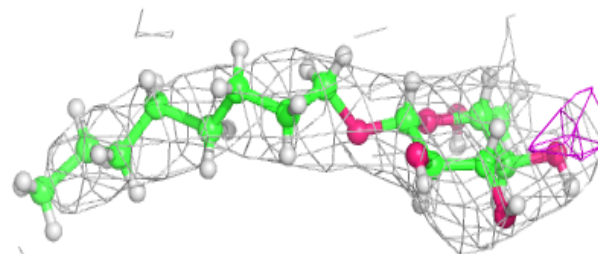
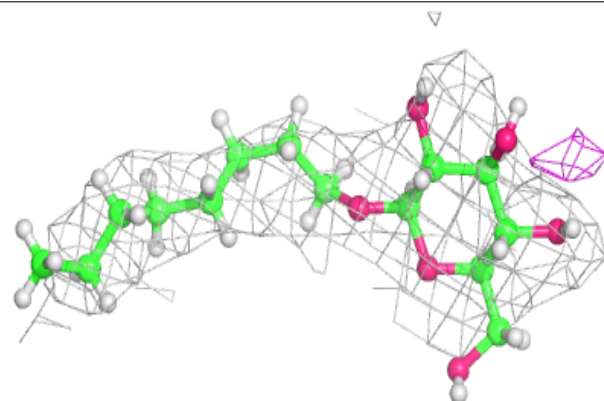


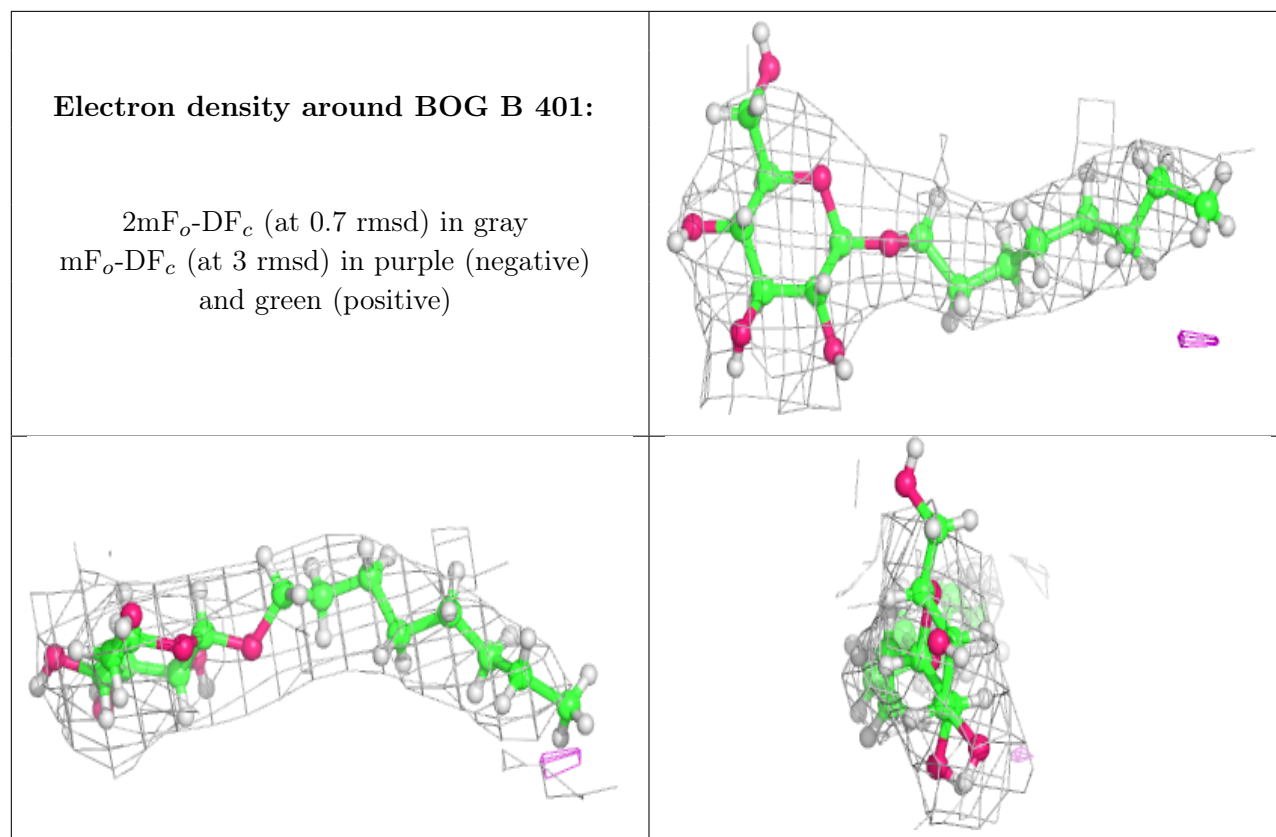
Electron density around BOG F 401:

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

**Electron density around BOG 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.