



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:02 AM UTC

PDB ID : 6SSP / pdb_00006ssp
Title : Structure of the pentameric ligand-gated ion channel ELIC in complex with a NAM nanobody
Authors : Ulens, C.; Brams, M.; Evans, G.L.; Spurny, R.; Govaerts, C.; Pardon, E.; Steyaert, J.
Deposited on : 2019-09-09
Resolution : 3.25 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:

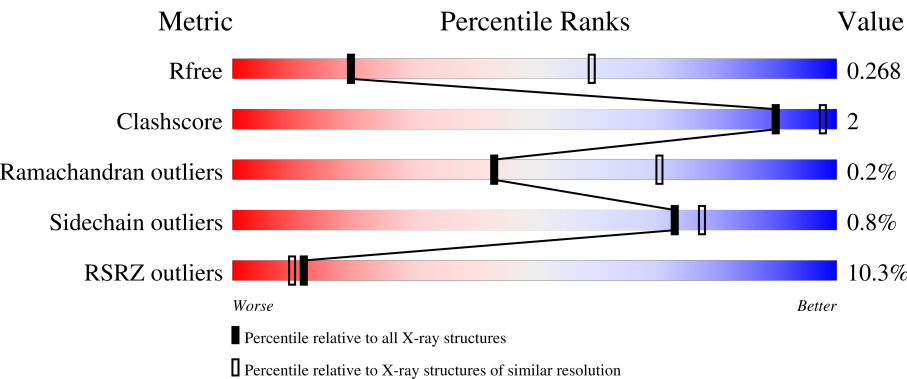
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 3.25 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	318	11% 87% 7% 6%
1	B	318	7% 89% 6% . .
1	C	318	9% 90% 5% . .
1	D	318	11% 89% 5% 6%

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Mol	Chain	Length	Quality of chain
1	E	318	8% 90% 5%5%
1	F	318	7% 89% •7%
1	G	318	10% 89% 6%5%
1	H	318	8% 91% •5%
1	I	318	3% 90% •6%
1	J	318	5% 86% 6%•7%
2	K	139	% 87% 6%7%
2	L	139	58% 88% •11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26239 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 Cys-loop ligand-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2387	1560	396	425	6			
1	B	304	Total	C	N	O	S	0	0	0
			2425	1579	400	440	6			
1	C	304	Total	C	N	O	S	0	1	0
			2444	1591	405	442	6			
1	D	299	Total	C	N	O	S	0	0	0
			2386	1564	395	421	6			
1	E	303	Total	C	N	O	S	0	0	0
			2371	1552	389	424	6			
1	F	296	Total	C	N	O	S	0	0	0
			2356	1538	392	420	6			
1	G	303	Total	C	N	O	S	0	0	0
			2407	1579	396	426	6			
1	H	302	Total	C	N	O	S	0	0	0
			2423	1585	397	435	6			
1	I	300	Total	C	N	O	S	0	0	0
			2415	1579	397	433	6			
1	J	297	Total	C	N	O	S	0	0	0
			2384	1562	390	426	6			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	GLY	-	expression tag	UNP P0C7B7
A	6	PRO	-	expression tag	UNP P0C7B7
A	7	VAL	-	expression tag	UNP P0C7B7
A	164	GLY	-	insertion	UNP P0C7B7
A	289	ASN	MET	conflict	UNP P0C7B7
A	322	GLY	-	expression tag	UNP P0C7B7
B	5	GLY	-	expression tag	UNP P0C7B7
B	6	PRO	-	expression tag	UNP P0C7B7
B	7	VAL	-	expression tag	UNP P0C7B7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	164	GLY	-	insertion	UNP P0C7B7
B	289	ASN	MET	conflict	UNP P0C7B7
B	322	GLY	-	expression tag	UNP P0C7B7
C	5	GLY	-	expression tag	UNP P0C7B7
C	6	PRO	-	expression tag	UNP P0C7B7
C	7	VAL	-	expression tag	UNP P0C7B7
C	164	GLY	-	insertion	UNP P0C7B7
C	289	ASN	MET	conflict	UNP P0C7B7
C	322	GLY	-	expression tag	UNP P0C7B7
D	5	GLY	-	expression tag	UNP P0C7B7
D	6	PRO	-	expression tag	UNP P0C7B7
D	7	VAL	-	expression tag	UNP P0C7B7
D	164	GLY	-	insertion	UNP P0C7B7
D	289	ASN	MET	conflict	UNP P0C7B7
D	322	GLY	-	expression tag	UNP P0C7B7
E	5	GLY	-	expression tag	UNP P0C7B7
E	6	PRO	-	expression tag	UNP P0C7B7
E	7	VAL	-	expression tag	UNP P0C7B7
E	164	GLY	-	insertion	UNP P0C7B7
E	289	ASN	MET	conflict	UNP P0C7B7
E	322	GLY	-	expression tag	UNP P0C7B7
F	5	GLY	-	expression tag	UNP P0C7B7
F	6	PRO	-	expression tag	UNP P0C7B7
F	7	VAL	-	expression tag	UNP P0C7B7
F	164	GLY	-	insertion	UNP P0C7B7
F	289	ASN	MET	conflict	UNP P0C7B7
F	322	GLY	-	expression tag	UNP P0C7B7
G	5	GLY	-	expression tag	UNP P0C7B7
G	6	PRO	-	expression tag	UNP P0C7B7
G	7	VAL	-	expression tag	UNP P0C7B7
G	164	GLY	-	insertion	UNP P0C7B7
G	289	ASN	MET	conflict	UNP P0C7B7
G	322	GLY	-	expression tag	UNP P0C7B7
H	5	GLY	-	expression tag	UNP P0C7B7
H	6	PRO	-	expression tag	UNP P0C7B7
H	7	VAL	-	expression tag	UNP P0C7B7
H	164	GLY	-	insertion	UNP P0C7B7
H	289	ASN	MET	conflict	UNP P0C7B7
H	322	GLY	-	expression tag	UNP P0C7B7
I	5	GLY	-	expression tag	UNP P0C7B7
I	6	PRO	-	expression tag	UNP P0C7B7
I	7	VAL	-	expression tag	UNP P0C7B7

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Chain	Residue	Modelled	Actual	Comment	Reference
I	164	GLY	-	insertion	UNP P0C7B7
I	289	ASN	MET	conflict	UNP P0C7B7
I	322	GLY	-	expression tag	UNP P0C7B7
J	5	GLY	-	expression tag	UNP P0C7B7
J	6	PRO	-	expression tag	UNP P0C7B7
J	7	VAL	-	expression tag	UNP P0C7B7
J	164	GLY	-	insertion	UNP P0C7B7
J	289	ASN	MET	conflict	UNP P0C7B7
J	322	GLY	-	expression tag	UNP P0C7B7

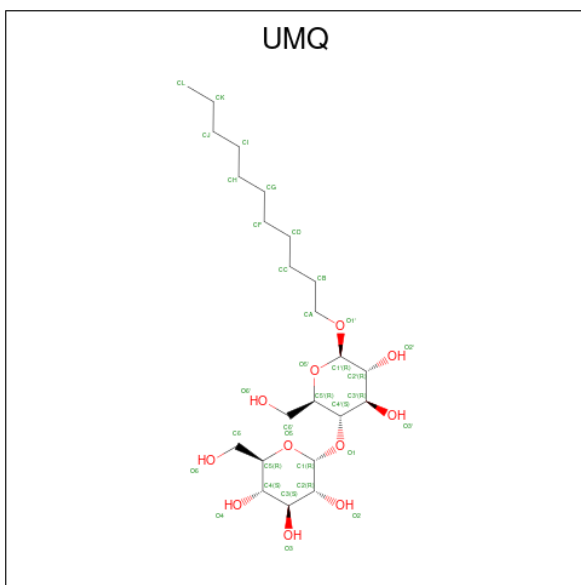
- Molecule 2 is a protein called NANOBODY 21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	129	Total	C	N	O	S	0	0	0
			972	609	163	197	3			
2	L	124	Total	C	N	O	S	0	0	0
			941	593	158	187	3			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	F	2	Total	Ca	0	0
			2	2		
3	G	1	Total	Ca	0	0
			1	1		
3	H	1	Total	Ca	0	0
			1	1		

- Molecule 4 is UNDECYL-MALTOSIDE (CCD ID: UMQ) (formula: C₂₃H₄₄O₁₁).

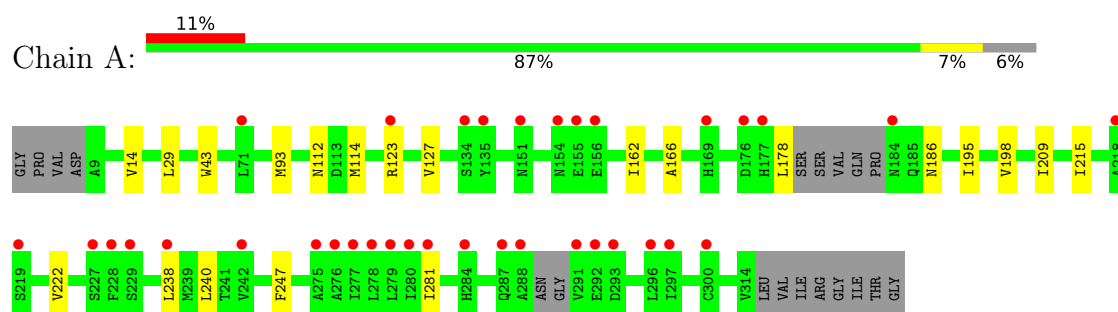


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 32	C 21	O 11	0	0
4	B	1	Total 32	C 21	O 11	0	0
4	B	1	Total 32	C 21	O 11	0	0
4	C	1	Total 32	C 21	O 11	0	0
4	E	1	Total 32	C 21	O 11	0	0
4	F	1	Total 32	C 21	O 11	0	0
4	G	1	Total 32	C 21	O 11	0	0
4	G	1	Total 32	C 21	O 11	0	0
4	I	1	Total 32	C 21	O 11	0	0
4	J	1	Total 32	C 21	O 11	0	0

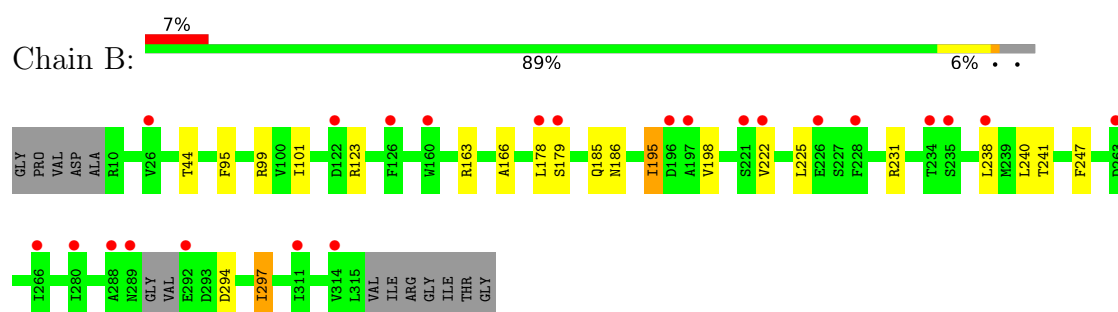
3 Residue-property plots [i](#)

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.

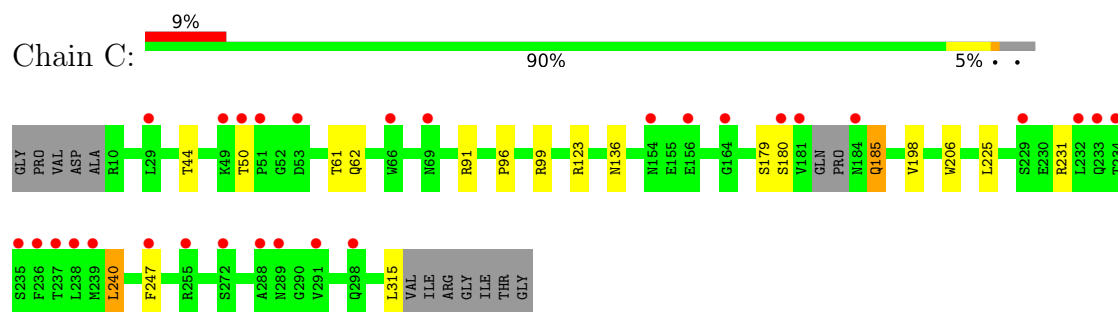
- Molecule 1: Cys-loop ligand-gated ion channel



- Molecule 1: Cys-loop ligand-gated ion channel

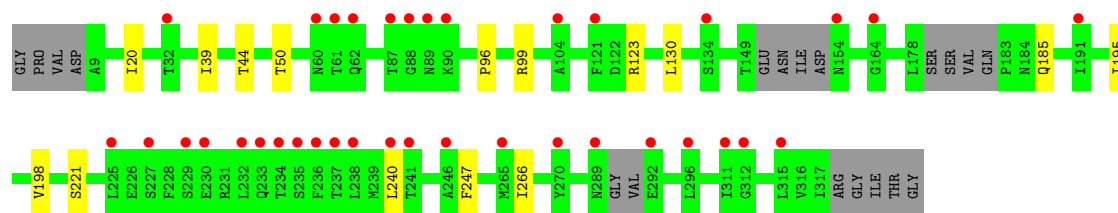


- Molecule 1: Cys-loop ligand-gated ion channel

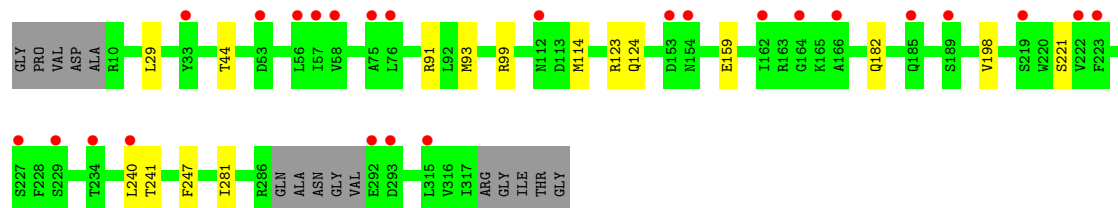
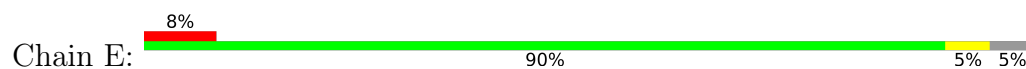


- Molecule 1: Cys-loop ligand-gated ion channel

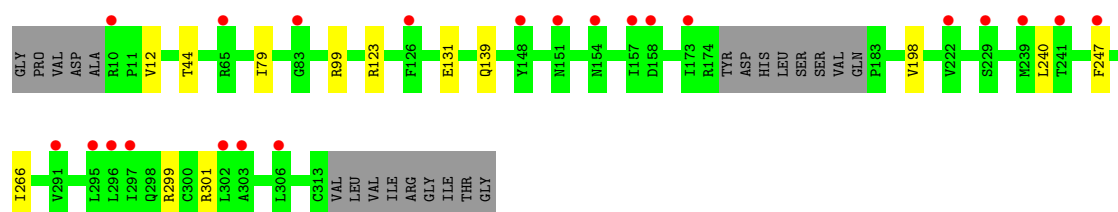
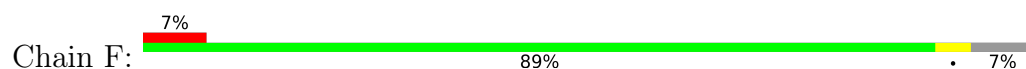




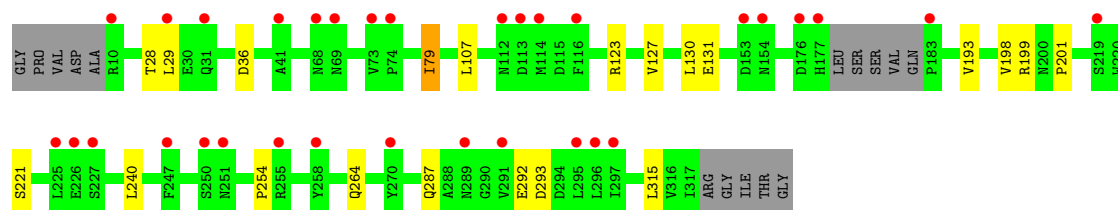
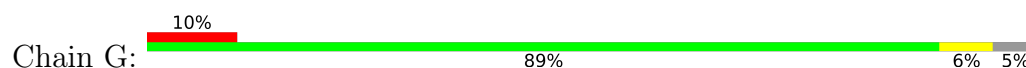
• Molecule 1: Cys-loop ligand-gated ion channel



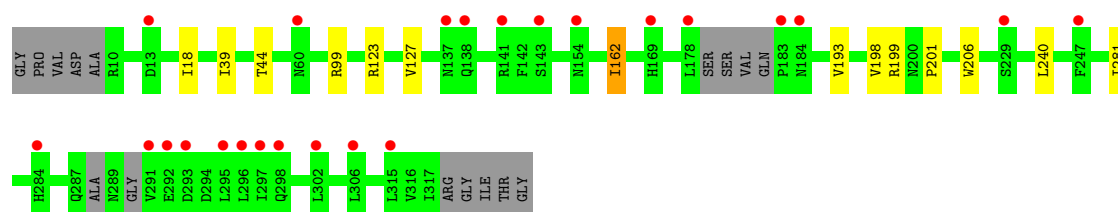
• Molecule 1: Cys-loop ligand-gated ion channel



• Molecule 1: Cys-loop ligand-gated ion channel



• Molecule 1: Cys-loop ligand-gated ion channel



- Chain I:
-
- 3% 90% 6%
- GLY PRO VAL ASP ALA R10 T23 T44 R69 R99 G108 S109 R123 E150 D153 I157 S179 SER VAL GLN PRO N184 V198 S221 L225 R231 L240 T241 F247 Q287 ALA ASN GLY V291 E292 D293 Q298 L306 L309

- Chain J: 
- GLY PRO VAL ASP ALA R10 I18 I39 T44 M69 I79 R99 S109 R117 R123 V127 L130 E131 Q138 Y148 I149 ASN ILE ASP ASN E155 A166 S167 T168 H169 H177 LEU SER SER SER VAL GLN PRO M184 V193 V198 R199 R200
- P201 L225 R231 F236 L240 A244 Y245 A246 F247 Y248 E255 Y270 Q287 A288 M289 G290 L295 C300 I317 ARG GLY ILE THR GLY

- Chain K: 
Chain K:

- Chain L:
-
- 58%
- 88%
- 11%
- GLN1 V2 Q3 L4 Q5 G9 G10 L11 L12 V12 Q13 A14 G15 G16 C22 A23 A24 S25 G26 F27 F28 T28 F29 D30 D31 V32 T33 T34 F37 R38 Q39 A40 A41 S112 P41 Q42 K43 E44 R45 D117 E46 Q47 V48 S49 L50 L51 S52 S53 S54 L55 S56 S57 D62 S63 V64 K65 G66 R67 T68 S71
- 0.00 0.05 0.10 0.15 0.20 0.25
- bits
- GLN1 V2 Q3 L4 Q5 G9 G10 L11 L12 V12 Q13 A14 G15 G16 C22 A23 A24 S25 G26 F27 F28 T28 F29 D30 D31 V32 T33 T34 F37 R38 Q39 A40 A41 S112 P41 Q42 K43 E44 R45 D117 E46 Q47 V48 S49 L50 L51 S52 S53 S54 L55 S56 S57 D62 S63 V64 K65 G66 R67 T68 S71

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	121.80Å 122.35Å 128.22Å 71.02° 64.19° 61.66°	Depositor
Resolution (Å)	48.32 – 3.25 48.32 – 3.25	Depositor EDS
% Data completeness (in resolution range)	89.9 (48.32-3.25) 89.9 (48.32-3.25)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.16-3549, BUSTER 2.10.3	Depositor
R, R_{free}	0.248 , 0.264 0.263 , 0.268	Depositor DCC
R_{free} test set	4097 reflections (4.48%)	wwPDB-VP
Wilson B-factor (Å ²)	97.6	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for h,h-k,h-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	26239	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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: CA, UMQ

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	0.69	4/2452 (0.2%)	1.08	4/3348 (0.1%)
1	B	0.66	1/2492 (0.0%)	1.07	2/3406 (0.1%)
1	C	0.62	0/2513	1.03	0/3431
1	D	0.64	1/2451 (0.0%)	1.03	0/3347
1	E	0.66	1/2436 (0.0%)	1.06	0/3334
1	F	0.66	1/2421 (0.0%)	1.07	0/3306
1	G	0.67	1/2474 (0.0%)	1.08	0/3381
1	H	0.65	0/2488	1.08	1/3397 (0.0%)
1	I	0.65	0/2480	1.10	3/3385 (0.1%)
1	J	0.66	1/2449 (0.0%)	1.07	3/3344 (0.1%)
2	K	0.62	0/992	0.99	0/1346
2	L	0.67	1/961 (0.1%)	0.97	0/1303
All	All	0.66	11/26609 (0.0%)	1.06	13/36328 (0.0%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	83	MET	SD-CE	-10.50	1.53	1.79
1	J	79	ILE	CG1-CD1	-7.06	1.24	1.51
1	B	195	ILE	CG1-CD1	-6.80	1.25	1.51
1	A	215	ILE	CG1-CD1	-5.71	1.29	1.51
1	E	114	MET	SD-CE	-5.45	1.66	1.79
1	D	266	ILE	CG1-CD1	-5.25	1.31	1.51
1	A	93	MET	SD-CE	-5.24	1.66	1.79
1	G	79	ILE	CG1-CD1	-5.21	1.31	1.51
1	F	266	ILE	CG1-CD1	-5.12	1.31	1.51
1	A	114	MET	SD-CE	-5.07	1.66	1.79
1	A	209	ILE	CG1-CD1	-5.05	1.32	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	293	ASP	N-CA-C	-6.75	96.42	110.80
1	B	163	ARG	NE-CZ-NH2	6.57	125.11	119.20
1	H	162	ILE	CB-CG1-CD1	6.29	127.00	113.80
1	B	163	ARG	NE-CZ-NH1	-6.24	115.26	121.50
1	I	23	ILE	CB-CA-C	6.05	117.81	111.09
1	J	270	TYR	CA-C-N	5.90	126.49	119.94
1	J	270	TYR	C-N-CA	5.90	126.49	119.94
1	I	23	ILE	N-CA-CB	-5.69	105.58	112.35
1	A	209	ILE	CB-CG1-CD1	5.69	125.75	113.80
1	A	162	ILE	CB-CA-C	5.45	117.28	111.35
1	A	162	ILE	CB-CG1-CD1	5.28	124.88	113.80
1	J	79	ILE	CB-CG1-CD1	5.22	124.75	113.80
1	A	215	ILE	CB-CG1-CD1	5.18	124.67	113.80

There are no chirality outliers.

There are no planarity outliers.

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	2387	0	2298	13	0
1	B	2425	0	2320	15	0
1	C	2444	0	2359	14	0
1	D	2386	0	2315	9	0
1	E	2371	0	2262	11	0
1	F	2356	0	2271	7	0
1	G	2407	0	2332	10	0
1	H	2423	0	2342	7	0
1	I	2415	0	2345	7	0
1	J	2384	0	2315	13	0
2	K	972	0	917	4	0
2	L	941	0	893	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	F	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	32	0	37	0	0
4	B	64	0	74	2	0
4	C	32	0	37	1	0
4	E	32	0	37	0	0
4	F	32	0	37	0	0
4	G	64	0	74	0	0
4	I	32	0	37	1	0
4	J	32	0	37	0	0
All	All	26239	0	25339	92	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 2.

All (92) 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:G:79:ILE:HD11	1:G:131:GLU:HB2	1.66	0.76
1:A:123:ARG:HG2	1:A:198:VAL:HG12	1.74	0.69
1:I:123:ARG:HG2	1:I:198:VAL:HG22	1.75	0.68
1:B:294:ASP:HB2	1:B:297:ILE:HG22	1.77	0.67
4:B:403:UMQ:HC1	1:C:315:LEU:HD13	1.78	0.63
1:H:18:ILE:HG12	1:H:39:ILE:HD12	1.82	0.61
1:B:95:PHE:HE1	1:B:101:ILE:HD12	1.65	0.61
1:D:20:ILE:CD1	1:D:195:ILE:HD11	2.32	0.59
1:B:178:LEU:HD22	1:B:186:ASN:HA	1.87	0.56
1:B:95:PHE:CE1	1:B:101:ILE:HD12	2.41	0.55
1:G:221:SER:HB2	1:H:281:ILE:HD11	1.90	0.54
1:D:20:ILE:HD12	1:D:195:ILE:HD11	1.90	0.54
1:A:29:LEU:HD11	1:E:159:GLU:CD	2.33	0.53
1:B:166:ALA:HB2	1:B:195:ILE:CD1	2.39	0.53
1:C:206:TRP:CZ2	4:C:402:UMQ:H5'1	2.45	0.51
2:K:64:VAL:HB	2:K:68:ILE:HD12	1.92	0.50
1:A:281:ILE:HD11	1:E:221:SER:HB2	1.94	0.50
1:C:61:THR:HG23	1:C:62:GLN:HE21	1.77	0.49
1:C:123:ARG:HG2	1:C:198:VAL:HG22	1.95	0.49
1:G:28:THR:HG21	1:G:254:PRO:HB2	1.93	0.49
1:B:101:ILE:HD13	1:C:179:SER:HB3	1.95	0.49
1:A:178:LEU:HD11	1:A:186:ASN:HB3	1.94	0.49
4:B:403:UMQ:HC1	1:C:315:LEU:CD1	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:123:ARG:HG2	1:F:198:VAL:HG22	1.96	0.48
1:B:101:ILE:HD13	1:C:179:SER:CB	2.43	0.48
1:J:123:ARG:HG2	1:J:198:VAL:HG22	1.95	0.48
1:C:136:ASN:ND2	1:C:185:GLN:HG3	2.29	0.48
1:F:79:ILE:HD11	1:F:131:GLU:HB3	1.94	0.48
1:A:166:ALA:HB2	1:A:195:ILE:HD13	1.96	0.47
1:J:79:ILE:HD11	1:J:131:GLU:HB3	1.95	0.47
1:A:240:LEU:HD21	1:E:240:LEU:HD22	1.95	0.47
1:A:166:ALA:HB2	1:A:195:ILE:CD1	2.44	0.47
1:I:157:ILE:HD11	1:J:117:ARG:NE	2.29	0.47
1:G:123:ARG:HG2	1:G:198:VAL:HG22	1.96	0.46
2:K:11:LEU:HD23	2:K:126:THR:HB	1.96	0.46
1:B:123:ARG:HG2	1:B:198:VAL:HG22	1.97	0.46
1:G:264:GLN:HB3	1:G:315:LEU:HD11	1.98	0.46
1:D:44:THR:HA	1:D:99:ARG:HA	1.98	0.45
1:A:247:PHE:HE2	1:E:247:PHE:CG	2.35	0.45
1:B:247:PHE:CD2	1:C:247:PHE:HE2	2.34	0.45
1:D:39:ILE:HD11	1:D:130:LEU:HD11	1.98	0.45
1:E:123:ARG:HG2	1:E:198:VAL:HG22	1.98	0.45
1:J:18:ILE:HG12	1:J:39:ILE:HD12	1.98	0.45
1:F:44:THR:HA	1:F:99:ARG:HA	1.99	0.45
1:G:287:GLN:OE1	1:G:292:GLU:CB	2.65	0.45
1:B:241:THR:OG1	1:C:240:LEU:HD12	2.17	0.44
1:D:50:THR:HG22	1:D:96:PRO:HB3	1.99	0.44
1:G:36:ASP:HB2	1:G:107:LEU:HD13	1.99	0.44
1:H:206:TRP:CZ2	4:I:401:UMQ:H5'1	2.51	0.44
2:K:50:LEU:HD12	2:K:59:TYR:HD1	1.83	0.44
1:C:50:THR:OG1	1:C:96:PRO:HG3	2.17	0.44
1:F:299:ARG:C	1:F:301:ARG:H	2.26	0.44
1:J:79:ILE:CD1	1:J:131:GLU:HB3	2.48	0.44
1:J:44:THR:HA	1:J:99:ARG:HA	2.00	0.43
1:G:199:ARG:O	1:G:201:PRO:HD3	2.19	0.43
1:J:199:ARG:O	1:J:201:PRO:HD3	2.18	0.43
1:D:20:ILE:CD1	1:D:195:ILE:CD1	2.97	0.43
1:A:240:LEU:HD13	1:E:241:THR:HA	2.01	0.43
1:H:123:ARG:HG2	1:H:198:VAL:HG22	2.00	0.43
1:E:44:THR:HA	1:E:99:ARG:HA	2.00	0.42
1:B:294:ASP:HB2	1:B:297:ILE:CG2	2.46	0.42
1:B:222:VAL:HG13	1:B:238:LEU:HD21	2.00	0.42
1:C:247:PHE:CD2	1:D:247:PHE:HE2	2.37	0.42
1:E:91:ARG:NH1	1:E:93:MET:HB2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:199:ARG:O	1:H:201:PRO:HD3	2.20	0.42
1:A:14:VAL:HG22	1:A:43:TRP:HB3	2.02	0.42
1:A:247:PHE:HE2	1:E:247:PHE:CD2	2.37	0.42
1:B:44:THR:HA	1:B:99:ARG:HA	2.02	0.42
1:B:222:VAL:HG13	1:B:238:LEU:CD2	2.50	0.42
1:D:123:ARG:HG2	1:D:198:VAL:HG22	2.01	0.42
1:H:44:THR:HA	1:H:99:ARG:HA	2.01	0.42
1:J:127:VAL:HA	1:J:193:VAL:O	2.20	0.41
1:D:221:SER:HB2	1:E:281:ILE:HD11	2.02	0.41
1:E:29:LEU:HD12	1:E:29:LEU:HA	1.94	0.41
1:G:29:LEU:HD12	1:G:29:LEU:HA	1.92	0.41
1:F:247:PHE:HA	1:J:248:TYR:HD1	1.85	0.41
1:F:247:PHE:HE2	1:J:247:PHE:CD2	2.38	0.41
1:C:44:THR:HA	1:C:99:ARG:HA	2.03	0.41
1:C:225:LEU:HB2	1:C:231:ARG:HG3	2.03	0.41
1:I:44:THR:HA	1:I:99:ARG:HA	2.02	0.41
1:I:221:SER:OG	1:J:236:PHE:HZ	2.04	0.41
1:I:225:LEU:HB2	1:I:231:ARG:HG3	2.03	0.41
1:J:225:LEU:HB2	1:J:231:ARG:HG3	2.03	0.41
2:K:28:THR:HB	2:K:31:ASP:OD1	2.20	0.41
1:I:241:THR:OG1	1:J:240:LEU:HD12	2.21	0.41
1:B:225:LEU:HB2	1:B:231:ARG:HG3	2.02	0.40
1:A:112:ASN:HB2	1:A:127:VAL:HG22	2.02	0.40
1:G:127:VAL:HA	1:G:193:VAL:O	2.21	0.40
1:A:222:VAL:HG13	1:A:238:LEU:HD21	2.03	0.40
1:F:12:VAL:HG12	1:F:139:GLN:O	2.22	0.40
1:H:127:VAL:HA	1:H:193:VAL:O	2.21	0.40
1:I:293:ASP:O	1:I:298:GLN:NE2	2.51	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	293/318 (92%)	287 (98%)	6 (2%)	0	100	100
1	B	300/318 (94%)	291 (97%)	8 (3%)	1 (0%)	36	66
1	C	301/318 (95%)	289 (96%)	10 (3%)	2 (1%)	18	48
1	D	291/318 (92%)	284 (98%)	7 (2%)	0	100	100
1	E	299/318 (94%)	288 (96%)	10 (3%)	1 (0%)	36	66
1	F	292/318 (92%)	279 (96%)	13 (4%)	0	100	100
1	G	299/318 (94%)	284 (95%)	14 (5%)	1 (0%)	36	66
1	H	295/318 (93%)	288 (98%)	7 (2%)	0	100	100
1	I	294/318 (92%)	282 (96%)	12 (4%)	0	100	100
1	J	291/318 (92%)	285 (98%)	6 (2%)	0	100	100
2	K	127/139 (91%)	119 (94%)	8 (6%)	0	100	100
2	L	122/139 (88%)	115 (94%)	7 (6%)	0	100	100
All	All	3204/3458 (93%)	3091 (96%)	108 (3%)	5 (0%)	43	70

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	182	GLN
1	C	185	GLN
1	G	293	ASP
1	B	179	SER
1	C	180	SER

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	250/282 (89%)	250 (100%)	0	100	100
1	B	257/282 (91%)	254 (99%)	3 (1%)	63	74
1	C	261/282 (93%)	259 (99%)	2 (1%)	73	78
1	D	252/282 (89%)	250 (99%)	2 (1%)	73	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	246/282 (87%)	245 (100%)	1 (0%)	84	84
1	F	247/282 (88%)	246 (100%)	1 (0%)	84	84
1	G	253/282 (90%)	251 (99%)	2 (1%)	73	78
1	H	259/282 (92%)	257 (99%)	2 (1%)	73	78
1	I	259/282 (92%)	256 (99%)	3 (1%)	63	74
1	J	254/282 (90%)	249 (98%)	5 (2%)	48	66
2	K	101/113 (89%)	101 (100%)	0	100	100
2	L	97/113 (86%)	96 (99%)	1 (1%)	68	75
All	All	2736/3046 (90%)	2714 (99%)	22 (1%)	73	78

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	185	GLN
1	B	240	LEU
1	B	297	ILE
1	C	91	ARG
1	C	240	LEU
1	D	185	GLN
1	D	240	LEU
1	E	124	GLN
1	F	240	LEU
1	G	130	LEU
1	G	240	LEU
1	H	162	ILE
1	H	240	LEU
1	I	109	SER
1	I	150	GLU
1	I	240	LEU
1	J	39	ILE
1	J	109	SER
1	J	130	LEU
1	J	138	GLN
1	J	240	LEU
2	L	83	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	89	ASN
1	A	177	HIS
1	A	184	ASN
1	A	251	ASN
1	B	124	GLN
1	B	251	ASN
1	B	285	HIS
1	C	62	GLN
1	C	103	ASN
1	C	124	GLN
1	C	151	ASN
1	C	251	ASN
1	C	285	HIS
1	D	124	GLN
1	D	138	GLN
1	D	251	ASN
1	E	151	ASN
1	E	169	HIS
1	E	251	ASN
1	F	124	GLN
1	F	138	GLN
1	F	251	ASN
1	F	264	GLN
1	G	154	ASN
1	G	251	ASN
1	G	285	HIS
1	H	62	GLN
1	H	124	GLN
1	H	251	ASN
1	H	264	GLN
1	H	285	HIS
1	H	298	GLN
1	I	69	ASN
1	I	124	GLN
1	I	185	GLN
1	I	251	ASN
1	J	124	GLN
1	J	185	GLN
1	J	251	ASN
1	J	298	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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	$\# Z > 2$
4	UMQ	A	402	-	33,33,35	0.21	0	44,44,46	0.52	0
4	UMQ	G	403	-	33,33,35	0.21	0	44,44,46	0.48	0
4	UMQ	B	403	-	33,33,35	0.22	0	44,44,46	0.53	0
4	UMQ	B	402	-	33,33,35	0.24	0	44,44,46	0.78	1 (2%)
4	UMQ	F	403	-	33,33,35	0.21	0	44,44,46	0.50	0
4	UMQ	J	401	-	33,33,35	0.22	0	44,44,46	0.50	0
4	UMQ	C	402	-	33,33,35	0.25	0	44,44,46	0.46	0
4	UMQ	E	401	-	33,33,35	0.24	0	44,44,46	0.54	0
4	UMQ	I	401	-	33,33,35	0.25	0	44,44,46	0.48	0
4	UMQ	G	402	-	33,33,35	0.23	0	44,44,46	0.70	1 (2%)

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
4	UMQ	A	402	-	-	6/18/58/60	0/2/2/2
4	UMQ	G	403	-	-	5/18/58/60	0/2/2/2
4	UMQ	B	403	-	-	6/18/58/60	0/2/2/2
4	UMQ	B	402	-	-	9/18/58/60	0/2/2/2
4	UMQ	F	403	-	-	5/18/58/60	0/2/2/2
4	UMQ	J	401	-	-	6/18/58/60	0/2/2/2
4	UMQ	C	402	-	-	8/18/58/60	0/2/2/2
4	UMQ	E	401	-	-	6/18/58/60	0/2/2/2
4	UMQ	I	401	-	-	6/18/58/60	0/2/2/2
4	UMQ	G	402	-	-	9/18/58/60	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	402	UMQ	C3'-C4'-C5'	2.20	115.80	110.93
4	G	402	UMQ	C3'-C4'-C5'	2.01	115.39	110.93

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	403	UMQ	C2'-C1'-O1'-CA
4	E	401	UMQ	O5-C1-O1-C4'
4	J	401	UMQ	O5-C1-O1-C4'
4	G	402	UMQ	C3'-C4'-O1-C1
4	B	402	UMQ	C3'-C4'-O1-C1
4	G	402	UMQ	O5'-C5'-C6'-O6'
4	A	402	UMQ	O5'-C1'-O1'-CA
4	B	403	UMQ	O5'-C1'-O1'-CA
4	F	403	UMQ	O5'-C1'-O1'-CA
4	G	403	UMQ	O5'-C1'-O1'-CA
4	A	402	UMQ	C2'-C1'-O1'-CA
4	B	403	UMQ	C2'-C1'-O1'-CA
4	G	403	UMQ	C2'-C1'-O1'-CA
4	B	402	UMQ	C5'-C4'-O1-C1
4	B	402	UMQ	O5'-C5'-C6'-O6'
4	C	402	UMQ	O5-C1-O1-C4'
4	G	402	UMQ	C5'-C4'-O1-C1
4	I	401	UMQ	O5-C1-O1-C4'

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Mol	Chain	Res	Type	Atoms
4	I	401	UMQ	C2'-C1'-O1'-CA
4	E	401	UMQ	O1'-CA-CB-CC
4	J	401	UMQ	O1'-CA-CB-CC
4	J	401	UMQ	CA-CB-CC-CD
4	G	402	UMQ	C4'-C5'-C6'-O6'
4	E	401	UMQ	CA-CB-CC-CD
4	C	402	UMQ	O5'-C1'-O1'-CA
4	I	401	UMQ	O5'-C1'-O1'-CA
4	C	402	UMQ	C2'-C1'-O1'-CA
4	B	402	UMQ	O5-C5-C6-O6
4	B	402	UMQ	CA-CB-CC-CD
4	C	402	UMQ	C4-C5-C6-O6
4	B	402	UMQ	O5-C1-O1-C4'
4	G	402	UMQ	CA-CB-CC-CD
4	B	403	UMQ	C4-C5-C6-O6
4	J	401	UMQ	C3'-C4'-O1-C1
4	J	401	UMQ	C5'-C4'-O1-C1
4	B	403	UMQ	O5'-C5'-C6'-O6'
4	E	401	UMQ	C3'-C4'-O1-C1
4	G	403	UMQ	O5'-C5'-C6'-O6'
4	J	401	UMQ	O5'-C5'-C6'-O6'
4	E	401	UMQ	O5'-C5'-C6'-O6'
4	G	402	UMQ	O5-C1-O1-C4'
4	B	403	UMQ	CB-CC-CD-CF
4	E	401	UMQ	C5'-C4'-O1-C1
4	G	402	UMQ	O5-C5-C6-O6
4	A	402	UMQ	CF-CG-CH-CI
4	B	402	UMQ	C4'-C5'-C6'-O6'
4	F	403	UMQ	CF-CG-CH-CI
4	G	402	UMQ	O1'-CA-CB-CC
4	B	403	UMQ	O5-C5-C6-O6
4	B	402	UMQ	O1'-CA-CB-CC
4	C	402	UMQ	O5-C5-C6-O6
4	G	403	UMQ	CB-CC-CD-CF
4	B	402	UMQ	C2-C1-O1-C4'
4	G	402	UMQ	C2-C1-O1-C4'
4	A	402	UMQ	C3'-C4'-O1-C1
4	F	403	UMQ	C3'-C4'-O1-C1
4	I	401	UMQ	C3'-C4'-O1-C1
4	I	401	UMQ	C2-C1-O1-C4'
4	C	402	UMQ	C3'-C4'-O1-C1
4	F	403	UMQ	C5'-C4'-O1-C1

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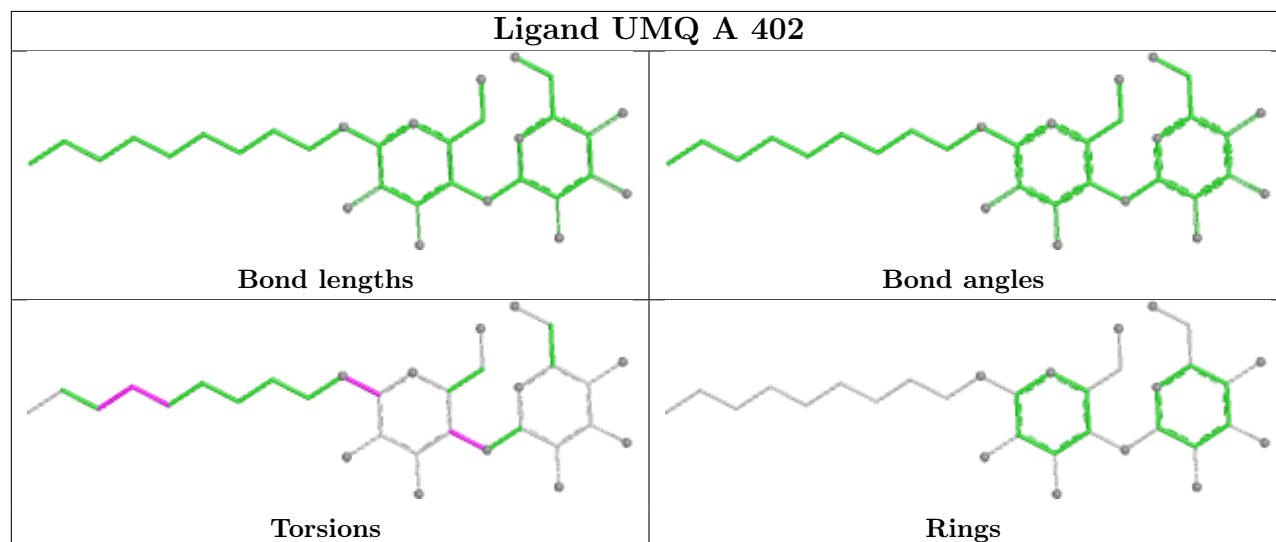
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4	C	402	UMQ	C2-C1-O1-C4'
4	I	401	UMQ	C5'-C4'-O1-C1
4	C	402	UMQ	C5'-C4'-O1-C1
4	A	402	UMQ	CD-CF-CG-CH
4	G	403	UMQ	C4-C5-C6-O6

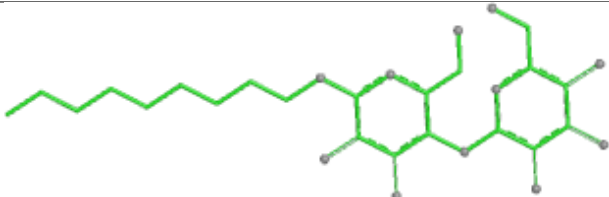
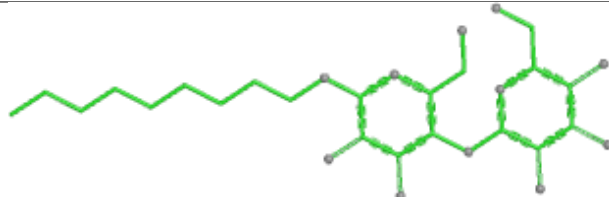
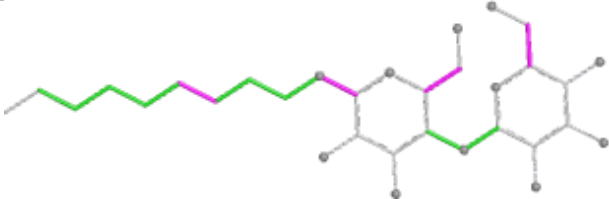
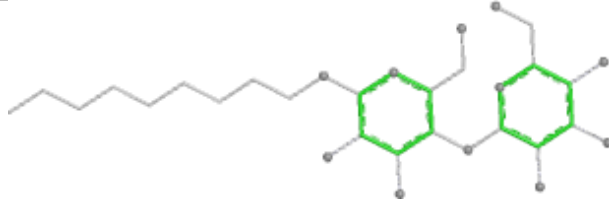
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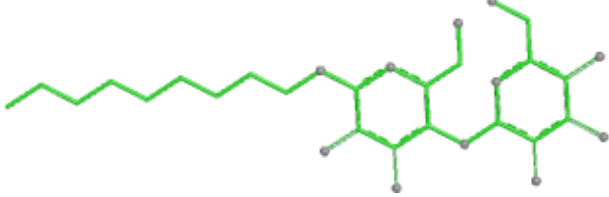
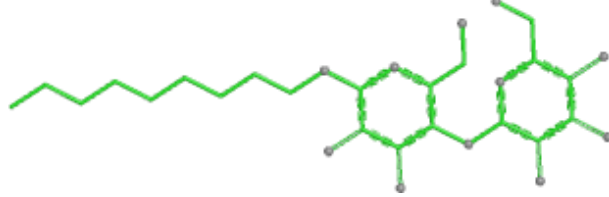
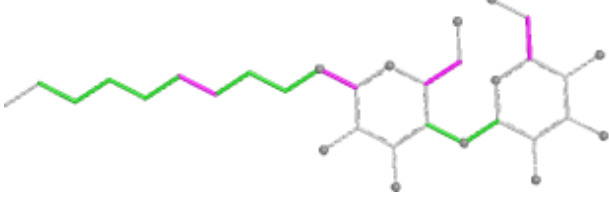
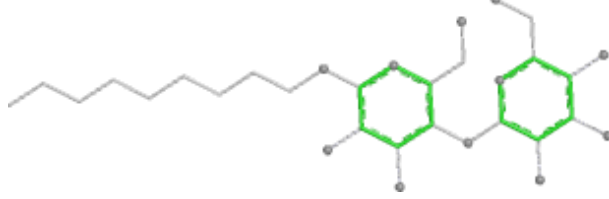
3 monomers are involved in 4 short contacts:

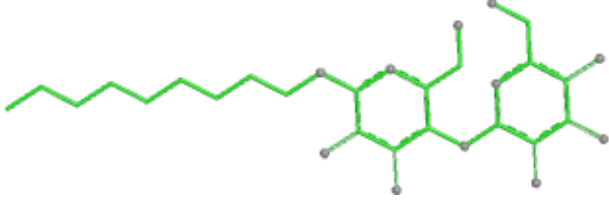
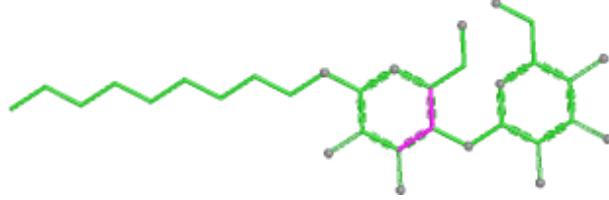
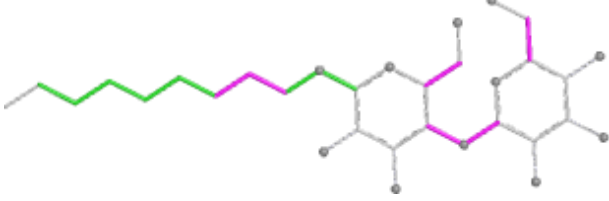
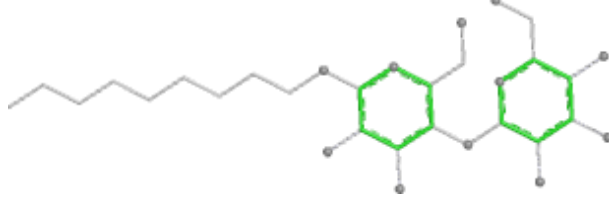
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	403	UMQ	2	0
4	C	402	UMQ	1	0
4	I	401	UMQ	1	0

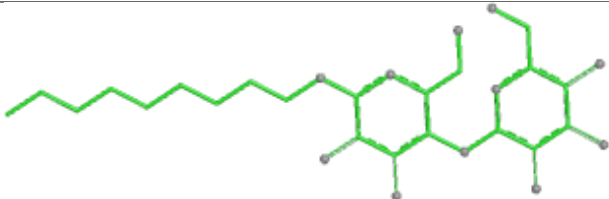
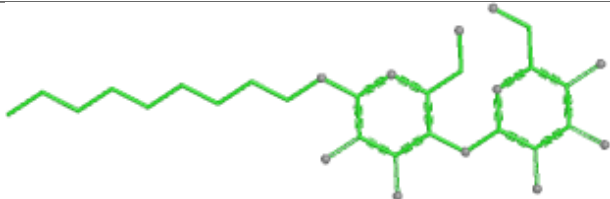
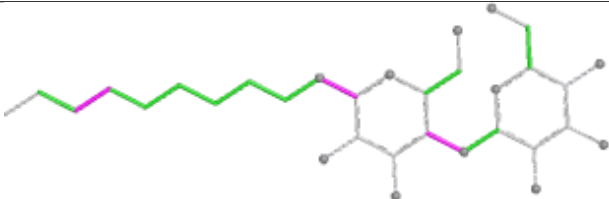
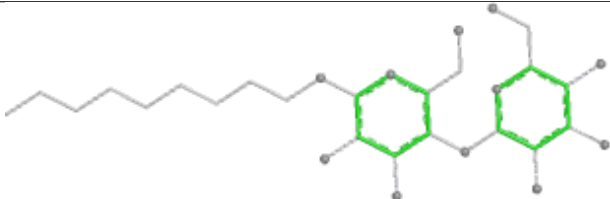
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

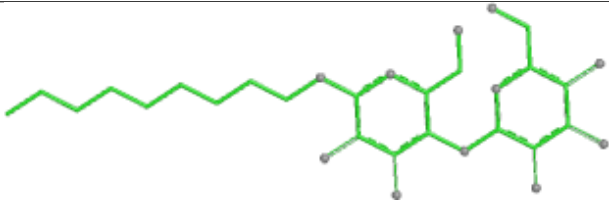
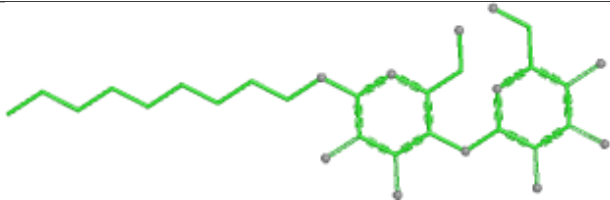
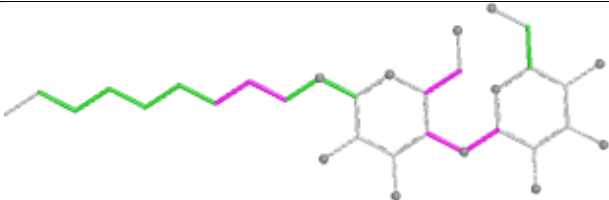
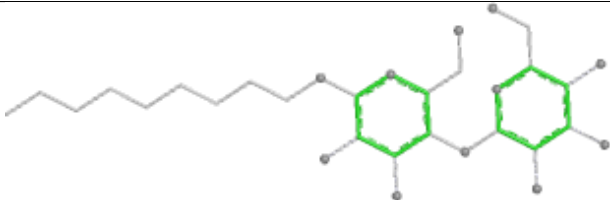


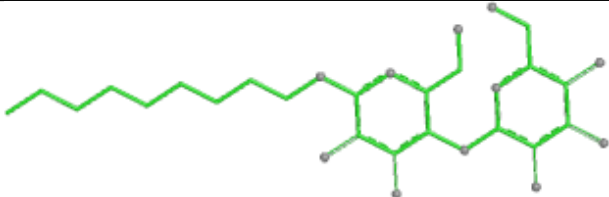
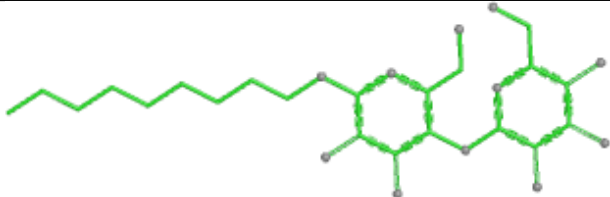
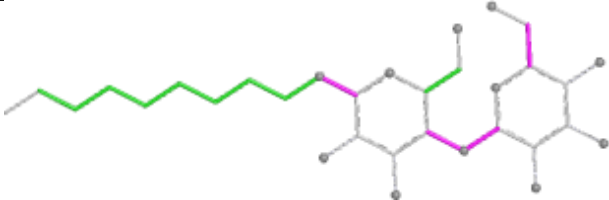
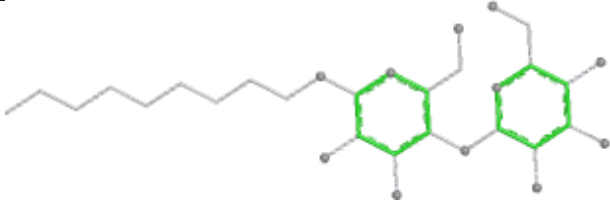
Ligand UMQ G 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

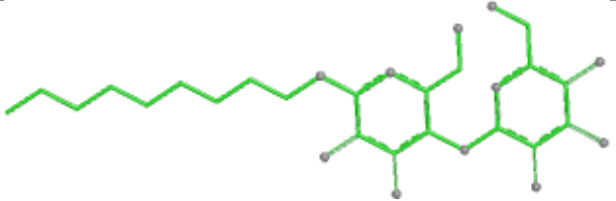
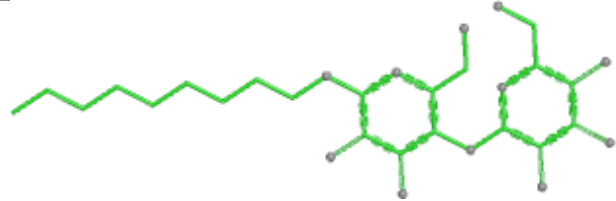
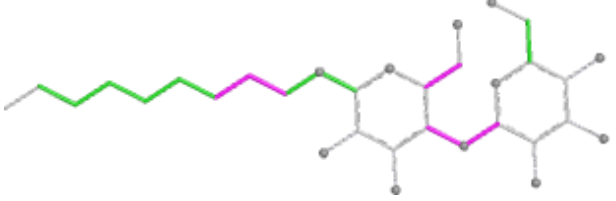
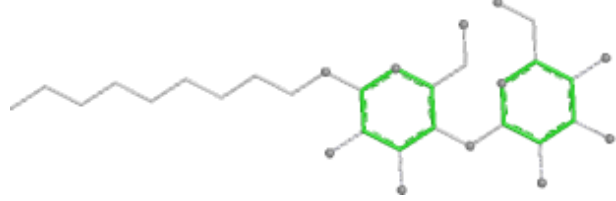
Ligand UMQ B 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

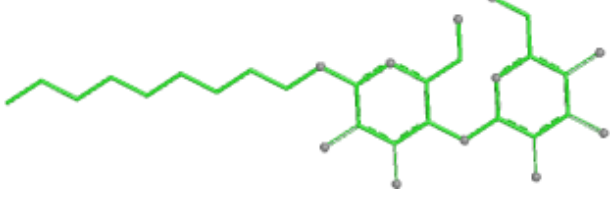
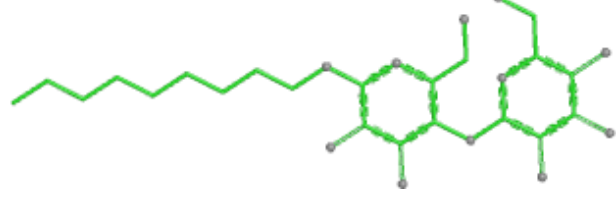
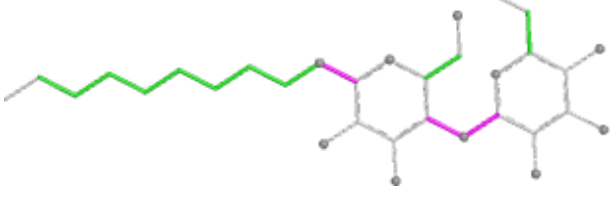
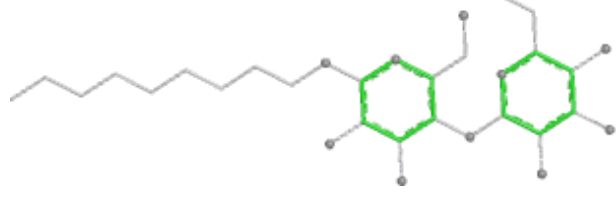
Ligand UMQ B 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

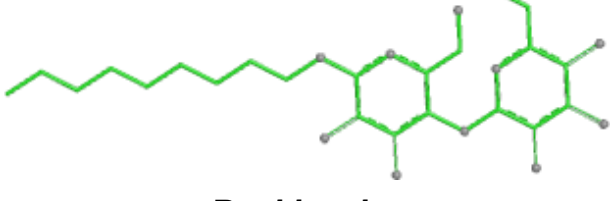
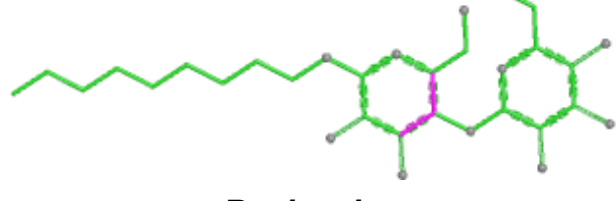
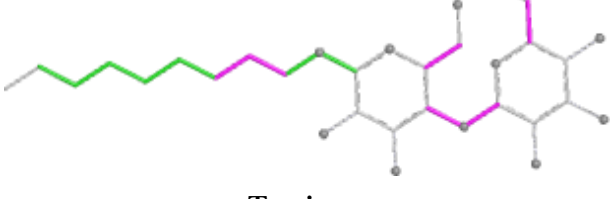
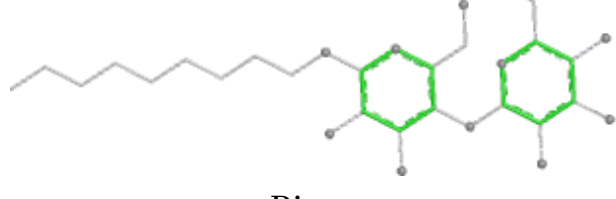
Ligand UMQ F 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand UMQ J 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand UMQ C 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand UMQ E 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand UMQ I 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand UMQ G 402	
	
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	299/318 (94%)	0.62	35 (11%) 9 8	56, 96, 170, 196	0
1	B	304/318 (95%)	0.49	23 (7%) 20 15	53, 91, 164, 188	0
1	C	304/318 (95%)	0.61	29 (9%) 14 11	73, 105, 160, 183	1 (0%)
1	D	299/318 (94%)	0.79	36 (12%) 9 7	77, 112, 168, 185	0
1	E	303/318 (95%)	0.64	25 (8%) 17 13	63, 103, 155, 184	0
1	F	296/318 (93%)	0.62	22 (7%) 20 15	75, 109, 169, 184	0
1	G	303/318 (95%)	0.71	32 (10%) 11 9	74, 108, 173, 201	0
1	H	302/318 (94%)	0.59	24 (7%) 18 14	65, 100, 178, 208	0
1	I	300/318 (94%)	0.35	10 (3%) 49 33	55, 90, 168, 190	0
1	J	297/318 (93%)	0.42	17 (5%) 29 20	63, 95, 155, 188	0
2	K	129/139 (92%)	-0.01	1 (0%) 82 68	63, 81, 110, 113	0
2	L	124/139 (89%)	3.26	81 (65%) 0 0	21, 29, 33, 34	124 (100%)
All	All	3260/3458 (94%)	0.66	335 (10%) 12 10	21, 100, 166, 208	125 (3%)

All (335) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	31	ASP	11.8
2	L	118	TYR	10.7
2	L	54	SER	9.8
1	A	291	VAL	9.4
1	D	88	GLY	9.4
2	L	3	GLN	8.5
2	L	100	ARG	8.1
2	L	114	TYR	8.1
1	D	233	GLN	8.1
1	C	234	THR	7.4
1	D	60	ASN	6.8

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Mol	Chain	Res	Type	RSRZ
2	L	121	GLN	6.7
2	L	117	ASP	6.7
2	L	109	ILE	6.6
2	L	30	ASP	6.4
1	C	164	GLY	6.4
2	L	115	PRO	5.9
2	L	106	ILE	5.9
1	C	235	SER	5.7
2	L	37	PHE	5.6
2	L	112	SER	5.6
1	G	177	HIS	5.5
2	L	110	LEU	5.5
2	L	99	GLY	5.4
2	L	113	GLU	5.4
2	L	4	LEU	5.4
2	L	32	TYR	5.3
1	C	49	LYS	5.3
1	D	90	LYS	5.3
2	L	28	THR	5.3
2	L	105	THR	5.3
1	B	179	SER	5.2
2	L	86	LEU	5.2
2	L	90	ASP	5.2
1	D	227	SER	5.1
1	H	169	HIS	5.1
1	F	303	ALA	4.9
1	C	181	VAL	4.8
2	L	101	ASP	4.8
1	A	296	LEU	4.7
1	C	51	PRO	4.6
1	C	237	THR	4.6
2	L	120	GLY	4.6
1	H	292	GLU	4.5
2	L	43	LYS	4.5
2	L	34	ILE	4.5
1	D	61	THR	4.5
1	A	284	HIS	4.4
1	C	255	ARG	4.4
2	L	83	MET	4.4
2	L	107	PHE	4.3
1	G	183	PRO	4.3
2	L	25	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	280	ILE	4.3
2	L	66	GLY	4.3
2	L	55	LEU	4.3
2	L	74	ASN	4.3
1	A	176	ASP	4.2
1	G	291	VAL	4.2
2	L	44	GLU	4.1
1	E	229	SER	4.1
1	G	176	ASP	4.1
1	H	137	ASN	4.1
2	L	2	VAL	4.1
2	L	91	THR	4.1
1	F	157	ILE	4.1
1	E	240	LEU	4.1
1	F	291	VAL	4.1
1	J	289	ASN	4.0
1	G	297	ILE	4.0
2	L	111	ARG	4.0
1	G	295	LEU	4.0
1	D	89	ASN	4.0
1	H	184	ASN	4.0
1	E	292	GLU	4.0
1	A	288	ALA	3.9
1	C	180	SER	3.9
1	B	289	ASN	3.9
1	H	229	SER	3.9
1	F	239	MET	3.8
1	A	277	ILE	3.8
1	F	173	ILE	3.8
1	A	278	LEU	3.8
1	H	295	LEU	3.8
1	E	164	GLY	3.8
1	D	87	THR	3.8
2	L	5	GLN	3.8
2	L	48	VAL	3.7
2	L	63	SER	3.7
2	L	14	ALA	3.7
1	C	233	GLN	3.7
1	D	315	LEU	3.7
1	C	154	ASN	3.7
1	G	74	PRO	3.6
2	L	108	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	238	LEU	3.6
1	D	236	PHE	3.6
1	G	69	ASN	3.6
2	L	92	ALA	3.6
2	L	53	SER	3.6
1	H	315	LEU	3.6
2	L	75	ALA	3.5
2	L	11	LEU	3.5
2	L	94	TYR	3.5
2	L	78	THR	3.5
1	D	237	THR	3.5
1	A	287	GLN	3.5
1	A	134	SER	3.5
1	G	10	ARG	3.4
2	L	104	PRO	3.4
2	L	73	ASP	3.4
1	D	230	GLU	3.4
2	L	102	ALA	3.4
2	L	29	PHE	3.3
1	G	296	LEU	3.3
2	L	38	ARG	3.3
2	L	103	ASP	3.3
1	A	292	GLU	3.3
1	A	229	SER	3.3
1	C	236	PHE	3.3
2	L	9	GLY	3.3
1	D	296	LEU	3.3
1	A	227	SER	3.2
2	L	27	PHE	3.2
2	L	13	GLN	3.2
1	A	276	ALA	3.2
1	A	154	ASN	3.2
1	C	232	LEU	3.2
2	L	45	ARG	3.2
2	L	119	TRP	3.2
1	C	289	ASN	3.2
1	A	135	TYR	3.2
1	A	228	PHE	3.1
2	L	24	ALA	3.1
1	I	179	SER	3.1
2	K	11	LEU	3.1
1	E	153	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	126	PHE	3.1
1	E	33	TYR	3.1
2	L	125	VAL	3.1
1	J	288	ALA	3.1
1	C	29	LEU	3.1
1	E	222	VAL	3.0
1	D	134	SER	3.0
2	L	57	SER	3.0
1	H	293	ASP	3.0
1	J	177	HIS	3.0
1	B	234	THR	3.0
1	B	178	LEU	3.0
1	D	238	LEU	3.0
1	B	197	ALA	3.0
1	G	113	ASP	3.0
1	C	50	THR	3.0
1	G	114	MET	3.0
2	L	41	PRO	3.0
1	B	122	ASP	3.0
1	J	169	HIS	3.0
1	I	69	ASN	3.0
1	A	156	GLU	2.9
1	I	291	VAL	2.9
1	D	265	MET	2.9
1	A	279	LEU	2.9
1	G	73	VAL	2.9
1	F	158	ASP	2.9
1	C	184	ASN	2.9
1	B	160	TRP	2.9
1	A	169	HIS	2.9
1	G	153	ASP	2.8
1	F	297	ILE	2.8
1	H	302	LEU	2.8
1	G	219	SER	2.8
1	A	293	ASP	2.8
2	L	87	LYS	2.8
2	L	40	ALA	2.8
1	H	247	PHE	2.8
1	H	284	HIS	2.8
1	G	227	SER	2.8
1	H	297	ILE	2.8
1	H	141	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	315	LEU	2.8
1	D	164	GLY	2.7
1	D	235	SER	2.7
2	L	116	PHE	2.7
1	D	270	TYR	2.7
1	G	68	ASN	2.7
2	L	64	VAL	2.7
1	H	296	LEU	2.7
1	I	309	LEU	2.7
1	A	297	ILE	2.7
1	E	154	ASN	2.7
2	L	98	ALA	2.7
1	F	241	THR	2.7
1	C	288	ALA	2.7
1	G	251	ASN	2.7
1	E	57	ILE	2.7
1	F	126	PHE	2.7
1	G	116	PHE	2.7
1	A	300	CYS	2.7
1	A	281	ILE	2.6
1	G	226	GLU	2.6
2	L	26	GLY	2.6
1	A	238	LEU	2.6
1	D	225	LEU	2.6
1	D	246	ALA	2.6
1	E	162	ILE	2.6
1	I	316	VAL	2.6
1	E	219	SER	2.6
1	B	311	ILE	2.6
1	A	184	ASN	2.6
2	L	47	GLY	2.6
1	D	240	LEU	2.6
1	H	291	VAL	2.6
1	A	177	HIS	2.6
1	J	245	TYR	2.6
1	F	247	PHE	2.6
2	L	22	CYS	2.6
1	J	167	SER	2.6
1	F	151	ASN	2.6
1	H	13	ASP	2.6
1	C	238	LEU	2.6
1	B	288	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	J	244	ALA	2.6
1	D	241	THR	2.6
1	E	166	ALA	2.5
1	J	69	ASN	2.5
1	B	280	ILE	2.5
1	D	229	SER	2.5
1	C	69	ASN	2.5
1	G	258	TYR	2.5
2	L	77	ASN	2.5
1	A	275	ALA	2.4
1	A	151	ASN	2.4
1	B	26	VAL	2.4
1	J	290	GLY	2.4
2	L	42	GLY	2.4
1	A	219	SER	2.4
1	J	184	ASN	2.4
1	B	266	ILE	2.4
1	D	311	ILE	2.4
1	B	221	SER	2.4
1	D	104	ALA	2.4
1	G	247	PHE	2.4
1	B	226	GLU	2.4
1	H	183	PRO	2.4
1	D	292	GLU	2.4
1	B	235	SER	2.4
1	G	31	GLN	2.3
1	F	229	SER	2.3
1	D	154	ASN	2.3
1	D	121	PHE	2.3
1	F	302	LEU	2.3
1	J	247	PHE	2.3
1	D	234	THR	2.3
1	D	232	LEU	2.3
2	L	62	ASP	2.3
1	H	298	GLN	2.3
1	B	292	GLU	2.3
1	J	255	ARG	2.3
2	L	56	GLY	2.3
1	F	295	LEU	2.3
1	G	270	TYR	2.3
1	J	148	TYR	2.3
1	A	242	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	156	GLU	2.3
1	G	41	ALA	2.3
1	C	66	TRP	2.3
1	C	247	PHE	2.3
2	L	71	SER	2.3
1	B	263	ASP	2.3
1	E	58	VAL	2.3
1	F	296	LEU	2.2
1	H	306	LEU	2.2
1	G	112	ASN	2.2
2	L	124	GLN	2.2
1	J	300	CYS	2.2
1	C	53	ASP	2.2
1	G	29	LEU	2.2
1	I	247	PHE	2.2
1	G	255	ARG	2.2
1	E	189	SER	2.2
1	C	291	VAL	2.2
1	I	108	GLY	2.2
1	F	148	TYR	2.2
1	E	227	SER	2.2
1	F	154	ASN	2.2
1	C	272	SER	2.2
2	L	50	LEU	2.2
1	G	154	ASN	2.2
1	B	228	PHE	2.2
1	E	53	ASP	2.2
1	I	153	ASP	2.2
2	L	68	ILE	2.1
1	J	295	LEU	2.1
1	H	143	SER	2.1
1	F	83	GLY	2.1
1	E	234	THR	2.1
1	F	306	LEU	2.1
1	A	218	ALA	2.1
1	D	312	GLY	2.1
1	H	60	ASN	2.1
1	D	191	ILE	2.1
1	G	225	LEU	2.1
2	L	51	ILE	2.1
1	C	229	SER	2.1
1	E	223	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	250	SER	2.1
1	D	289	ASN	2.1
1	B	222	VAL	2.1
1	E	315	LEU	2.1
1	I	306	LEU	2.1
1	F	10	ARG	2.1
1	B	314	VAL	2.1
1	H	154	ASN	2.1
1	A	71	LEU	2.1
1	A	123	ARG	2.1
1	E	76	LEU	2.1
1	C	239	MET	2.1
1	E	293	ASP	2.1
1	D	32	THR	2.1
2	L	16	GLY	2.1
1	F	222	VAL	2.0
1	H	178	LEU	2.0
1	E	75	ALA	2.0
1	J	166	ALA	2.0
1	D	62	GLN	2.0
1	H	138	GLN	2.0
1	J	287	GLN	2.0
1	E	112	ASN	2.0
1	G	289	ASN	2.0
1	B	196	ASP	2.0
1	C	298	GLN	2.0
1	E	185	GLN	2.0
1	A	155	GLU	2.0
1	F	65	ARG	2.0
1	E	56	LEU	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

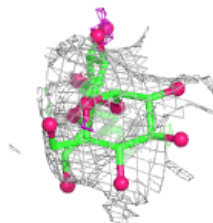
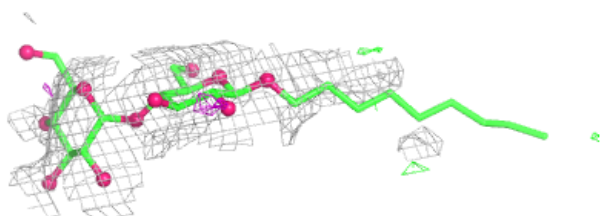
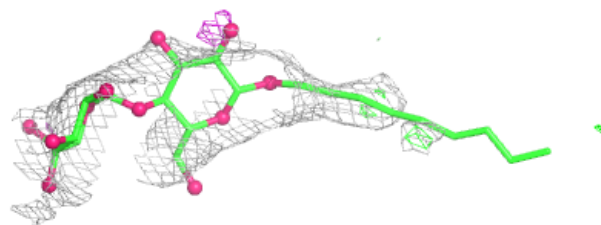
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	UMQ	A	402	32/34	0.58	0.17	117,139,146,147	0
3	CA	F	402	1/1	0.61	0.17	148,148,148,148	0
4	UMQ	G	402	32/34	0.64	0.16	130,148,156,157	0
4	UMQ	E	401	32/34	0.65	0.13	120,147,150,150	0
4	UMQ	B	403	32/34	0.66	0.17	119,143,145,147	0
4	UMQ	C	402	32/34	0.69	0.17	122,135,147,149	0
4	UMQ	I	401	32/34	0.72	0.17	121,135,145,146	0
4	UMQ	B	402	32/34	0.73	0.15	119,137,153,155	0
4	UMQ	F	403	32/34	0.73	0.17	122,142,149,150	0
4	UMQ	G	403	32/34	0.76	0.16	121,143,151,153	0
4	UMQ	J	401	32/34	0.79	0.16	121,142,145,147	0
3	CA	D	401	1/1	0.83	0.10	124,124,124,124	0
3	CA	B	401	1/1	0.85	0.10	115,115,115,115	0
3	CA	C	401	1/1	0.85	0.14	95,95,95,95	0
3	CA	F	401	1/1	0.86	0.14	112,112,112,112	0
3	CA	G	401	1/1	0.88	0.07	117,117,117,117	0
3	CA	A	401	1/1	0.92	0.09	111,111,111,111	0
3	CA	H	401	1/1	0.95	0.05	102,102,102,102	0

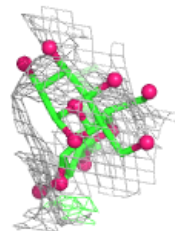
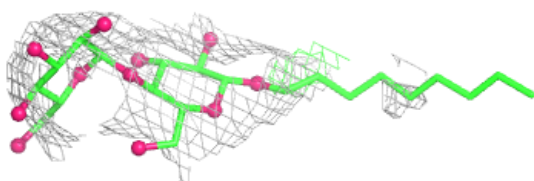
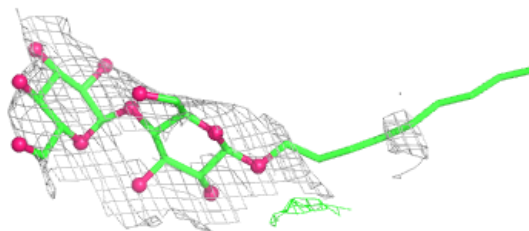
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UMQ 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)

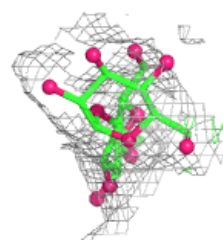
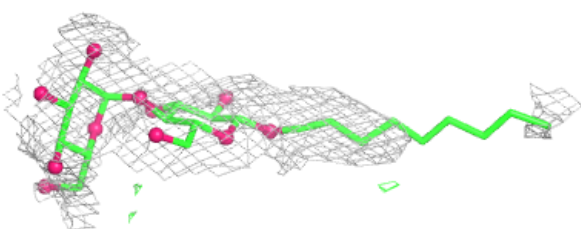
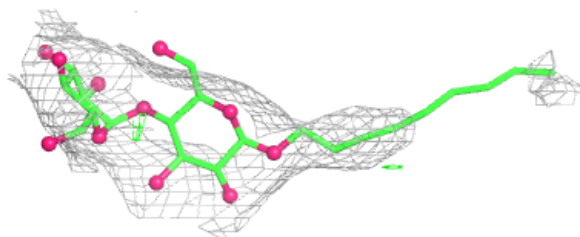
**Electron density around UMQ G 402:**

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

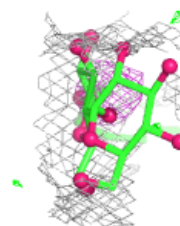
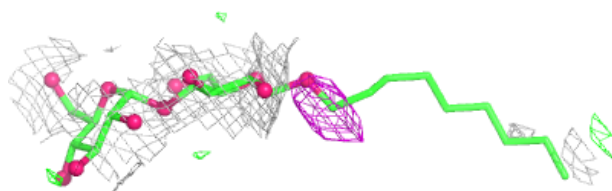
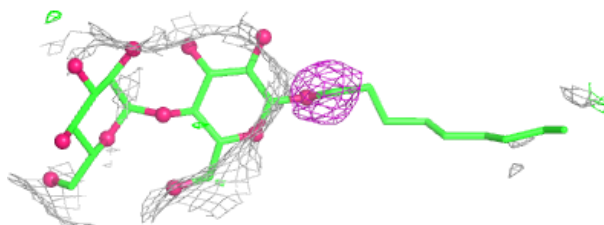


Electron density around UMQ E 401:

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

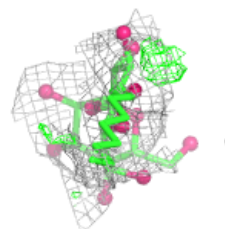
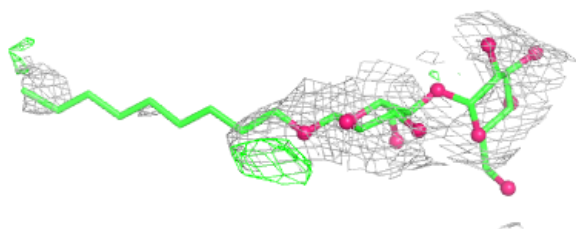
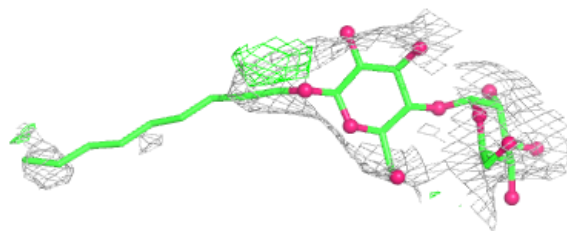
**Electron density around UMQ B 403:**

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

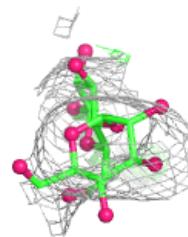
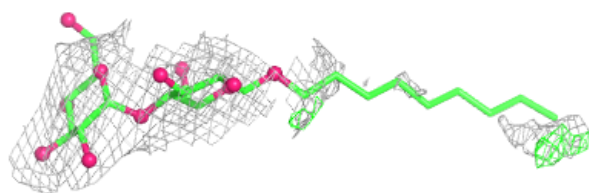
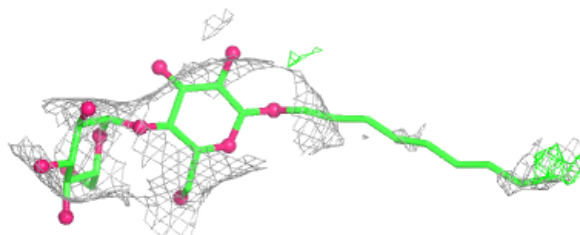


Electron density around UMQ C 402:

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

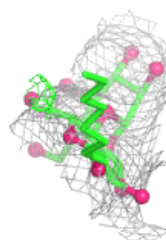
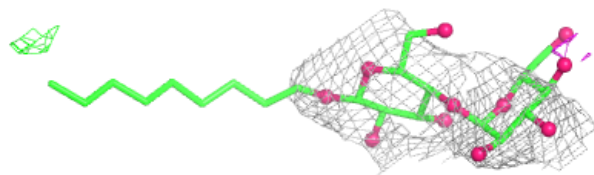
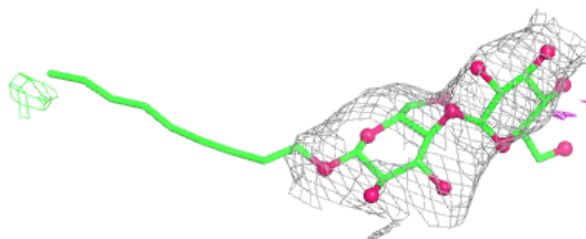
**Electron density around UMQ I 401:**

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

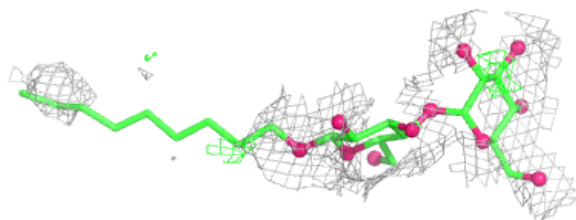
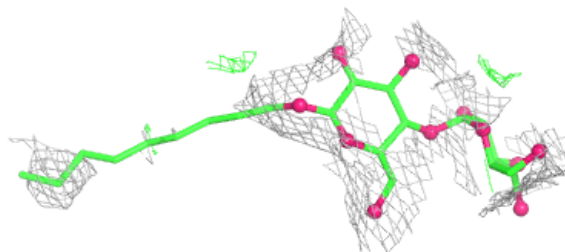


Electron density around UMQ B 402:

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

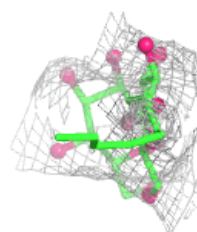
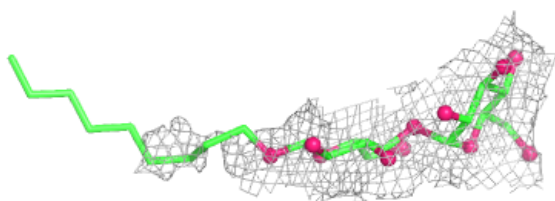
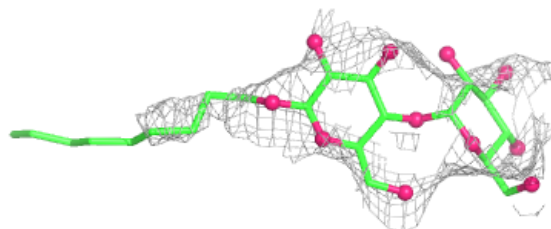
**Electron density around UMQ F 403:**

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

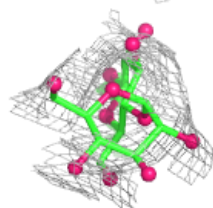
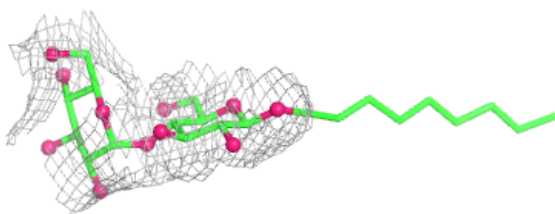
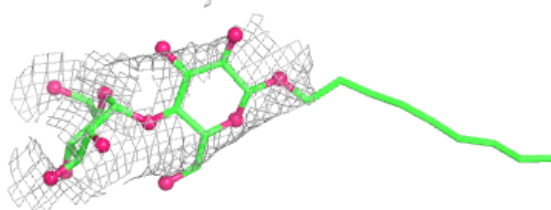


Electron density around UMQ G 403:

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

**Electron density around UMQ J 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.