



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:01 PM UTC

PDB ID : 6SSI / pdb_00006ssi
Title : Structure of the pentameric ligand-gated ion channel ELIC in complex with a PAM nanobody
Authors : Ulens, C.; Brams, M.; Evans, G.L.; Spurny, R.; Govaerts, C.; Pardon, E.; Steyaert, J.
Deposited on : 2019-09-07
Resolution : 2.59 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

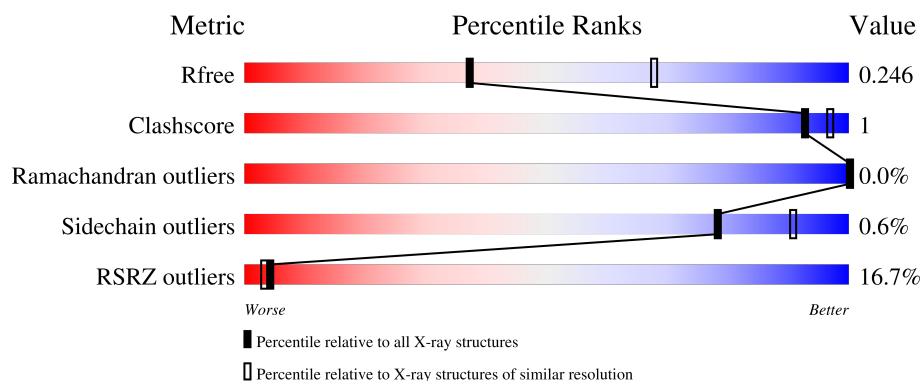
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	12% 89% 6% 5%
1	B	318	13% 92% 5% .
1	C	318	14% 93% . .
1	D	318	15% 90% 6% .

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Mol	Chain	Length	Quality of chain
1	E	318	14% 90% 6%
2	F	121	33% 91% 9%
2	G	121	11% 90% 8%
2	H	121	7% 88% 7%
2	I	121	20% 88% 8%
2	J	121	37% 89% 9%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 16941 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	303	Total	C	N	O	S	0	0	0
			2453	1600	410	437	6			
1	B	308	Total	C	N	O	S	0	1	0
			2477	1612	412	447	6			
1	C	307	Total	C	N	O	S	0	0	0
			2461	1608	406	441	6			
1	D	305	Total	C	N	O	S	0	1	0
			2424	1583	403	432	6			
1	E	304	Total	C	N	O	S	0	0	0
			2457	1606	406	439	6			

There are 30 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
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

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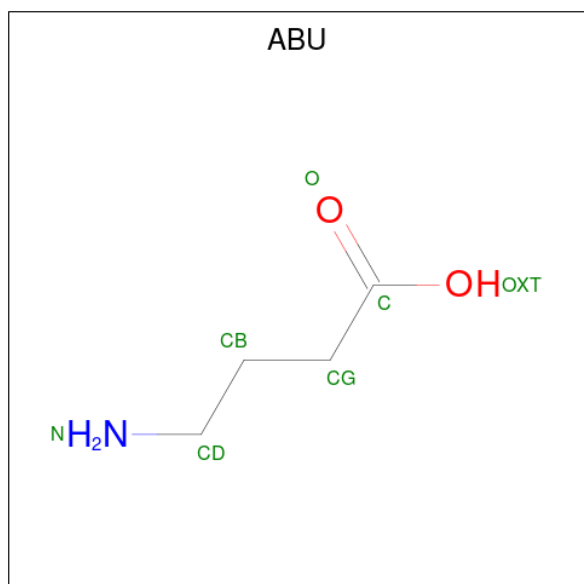
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Chain	Residue	Modelled	Actual	Comment	Reference
D	6	PRO	-	expression tag	UNP P0C7B7
D	7	VAL	-	expression tag	UNP P0C7B7
D	164	GLY	-	insertion	UNP P0C7B7
D	289	ASN	MET	conflict	UNP P0C7B7
D	322	GLY	-	expression tag	UNP P0C7B7
E	5	GLY	-	expression tag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

- Molecule 2 is a protein called NANOBODY 22.

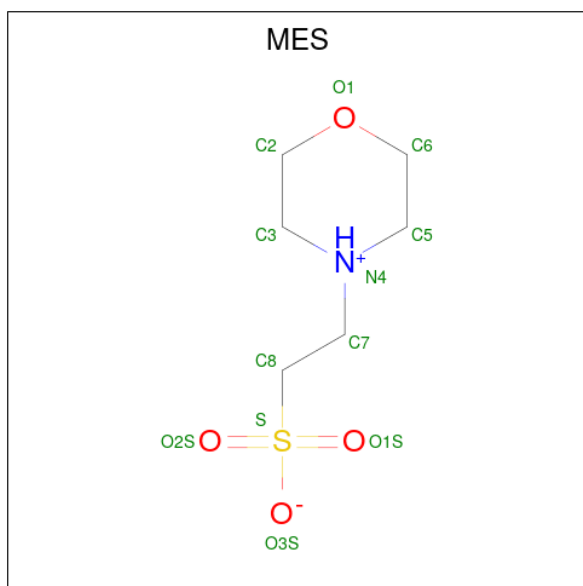
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	110	Total	C	N	O	S	0	0	0
			815	502	146	162	5			
2	G	111	Total	C	N	O	S	0	0	0
			838	516	151	166	5			
2	H	112	Total	C	N	O	S	0	0	0
			843	519	152	167	5			
2	I	111	Total	C	N	O	S	0	0	0
			841	516	154	166	5			
2	J	110	Total	C	N	O	S	0	0	0
			831	510	152	164	5			

- Molecule 3 is GAMMA-AMINO-BUTANOIC ACID (CCD ID: ABU) (formula: C₄H₉NO₂).



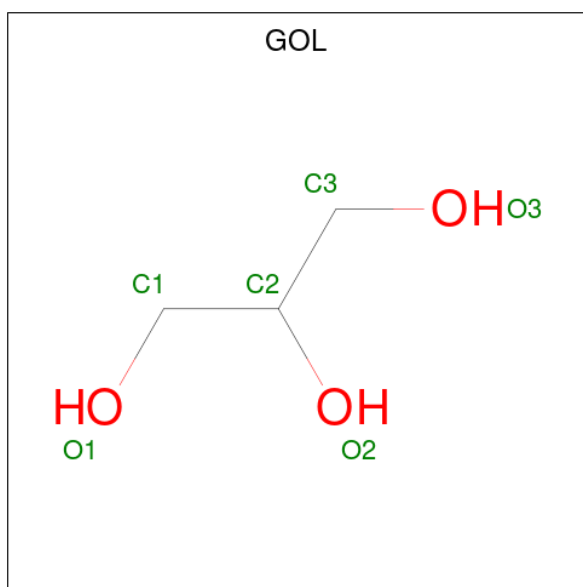
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			7	4	1	2		
3	B	1	Total	C	N	O	0	0
			7	4	1	2		
3	C	1	Total	C	N	O	0	0
			7	4	1	2		
3	D	1	Total	C	N	O	0	0
			7	4	1	2		
3	E	1	Total	C	N	O	0	0
			7	4	1	2		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

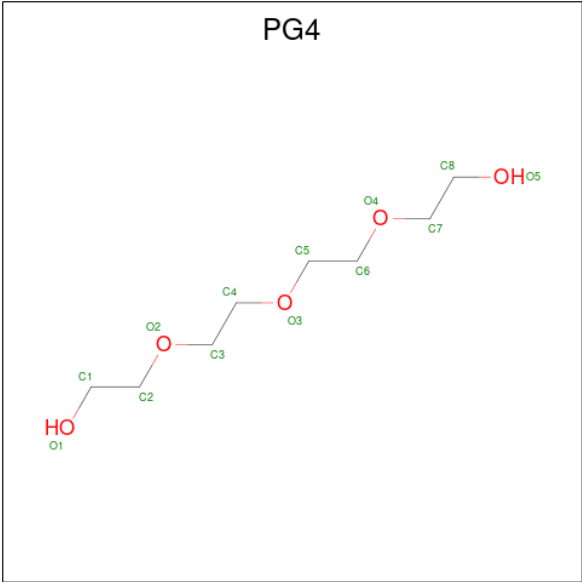


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

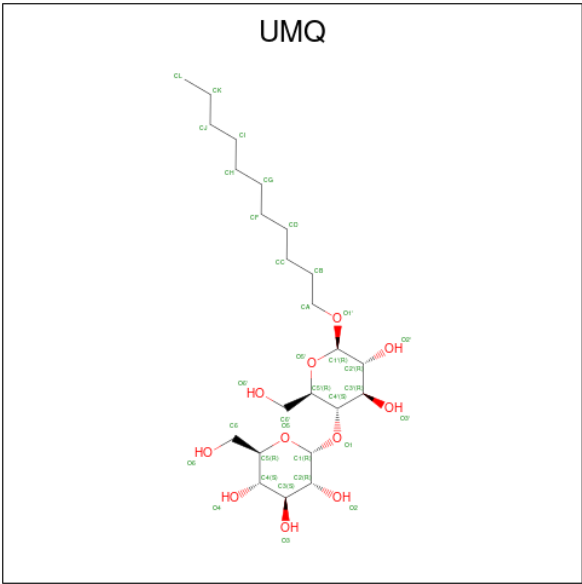
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		
6	B	1	Total	Ca	0	0
			1	1		
6	C	1	Total	Ca	0	0
			1	1		
6	D	1	Total	Ca	0	0
			1	1		
6	E	1	Total	Ca	0	0
			1	1		

- Molecule 7 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



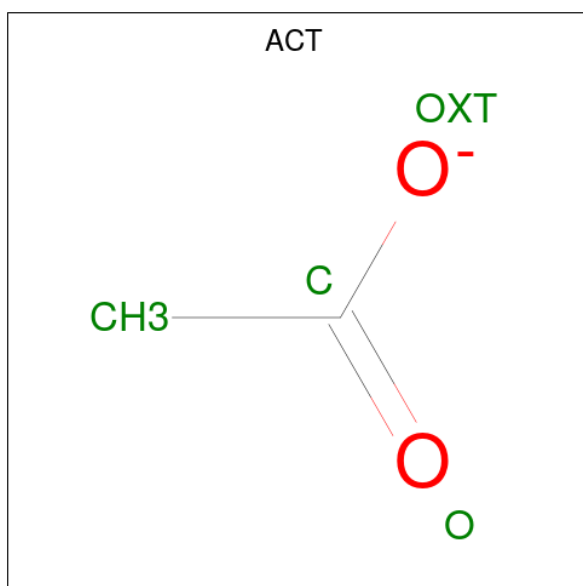
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			13	8	5		
7	C	1	Total	C	O	0	0
			13	8	5		
7	D	1	Total	C	O	0	0
			13	8	5		
7	E	1	Total	C	O	0	0
			13	8	5		

- Molecule 8 is UNDECYL-MALTOSIDE (CCD ID: UMQ) (formula: C₂₃H₄₄O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			32	21	11		
8	B	1	Total	C	O	0	0
			32	21	11		
8	C	1	Total	C	O	0	0
			32	21	11		
8	E	1	Total	C	O	0	0
			32	21	11		
8	E	1	Total	C	O	0	0
			32	21	11		

- Molecule 9 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	C	O	0	0
			4	2	2		
9	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	18	Total	O	0	0
			18	18		
10	B	22	Total	O	0	0
			22	22		
10	C	31	Total	O	0	0
			31	31		

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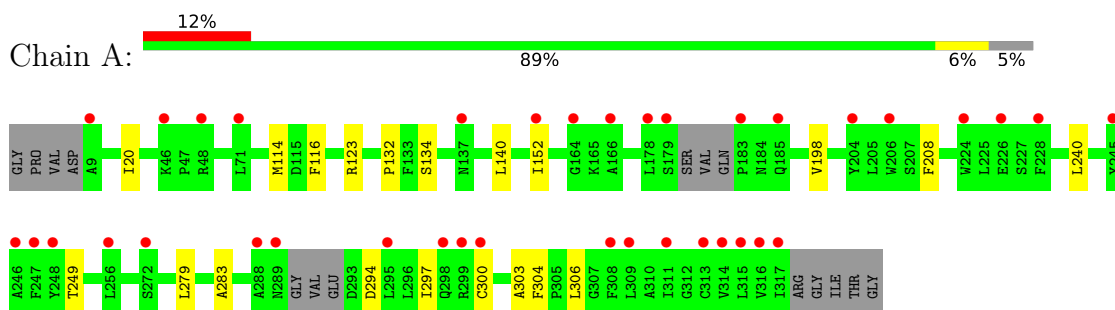
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	18	Total 18	O 18	0	0
10	E	16	Total 16	O 16	0	0
10	G	14	Total 14	O 14	0	0
10	H	18	Total 18	O 18	0	0
10	I	6	Total 6	O 6	0	0
10	J	2	Total 2	O 2	0	0

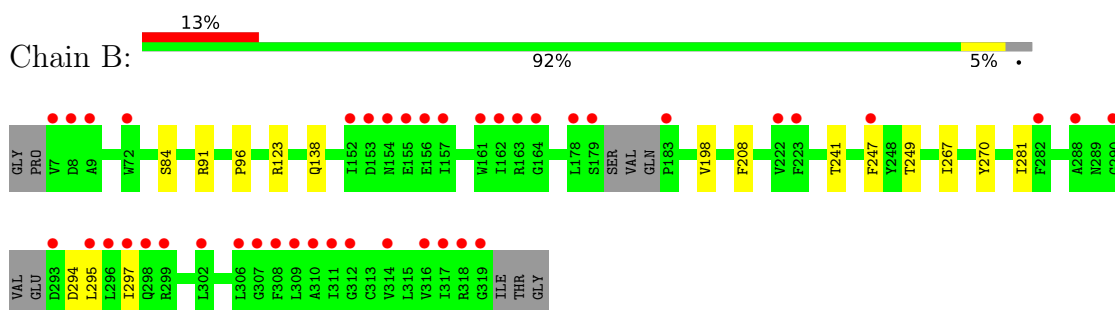
3 Residue-property plots [i](#)

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.

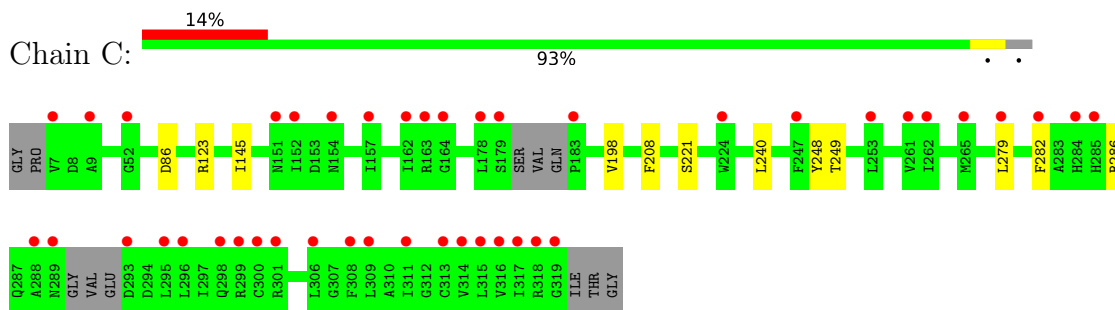
• Molecule 1: Cys-loop ligand-gated ion channel



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

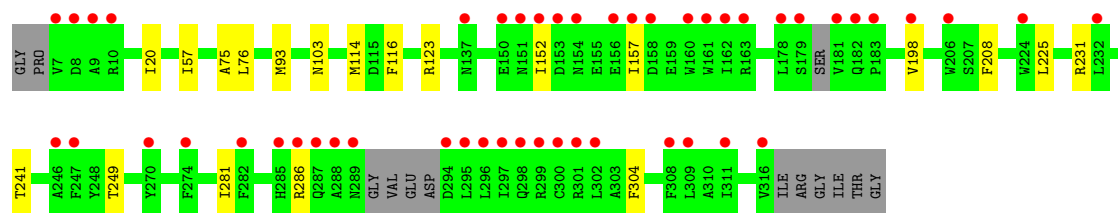


• Molecule 1: Cys-loop ligand-gated ion channel

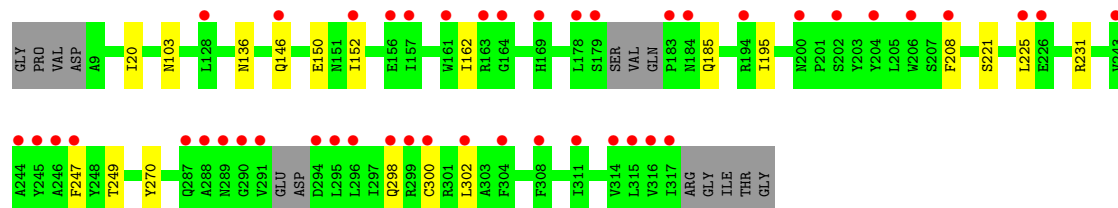
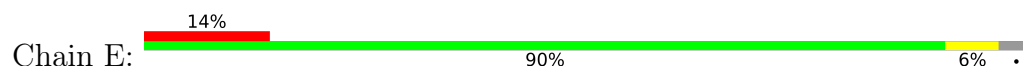


• Molecule 1: Cys-loop ligand-gated ion channel

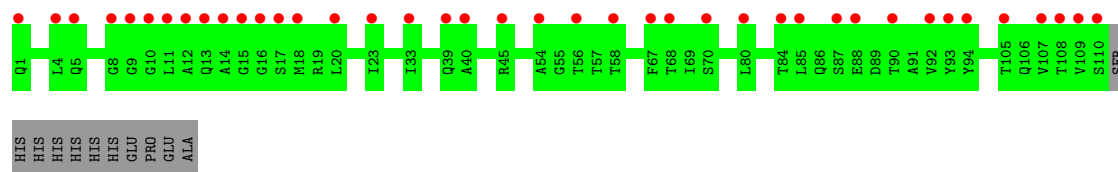




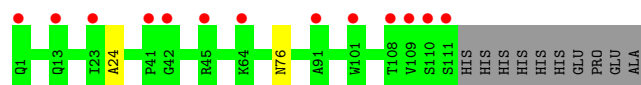
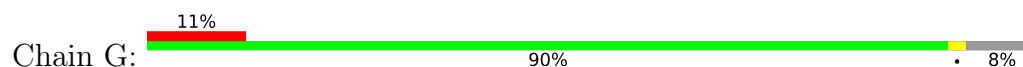
- Molecule 1: Cys-loop ligand-gated ion channel



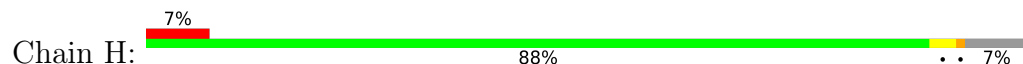
- Molecule 2: NANOBODY 22



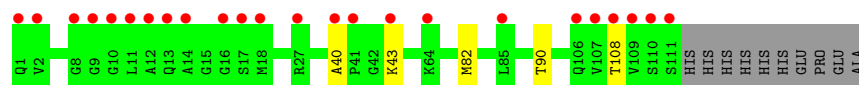
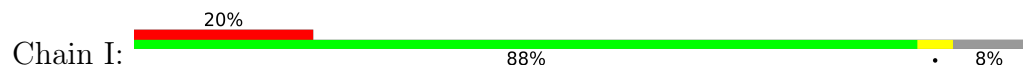
- Molecule 2: NANOBODY 22



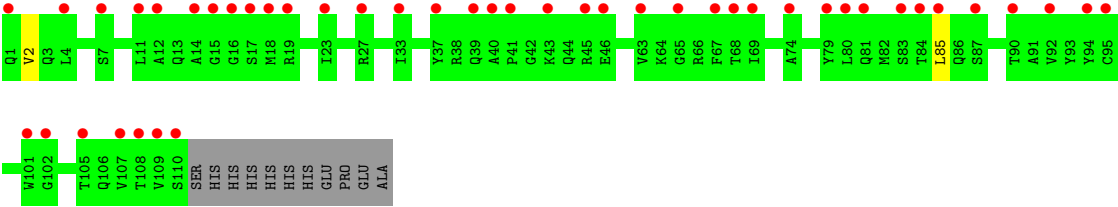
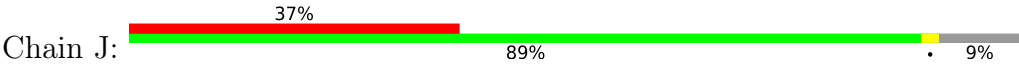
- Molecule 2: NANOBODY 22



- Molecule 2: NANOBODY 22



- Molecule 2: NANOBODY 22



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.60Å 146.56Å 140.24Å 90.00° 111.39° 90.00°	Depositor
Resolution (Å)	47.06 – 2.59 47.06 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.06-2.59) 99.9 (47.06-2.59)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.58Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.230 , 0.246 0.231 , 0.246	Depositor DCC
R_{free} test set	6188 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	68.3	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16941	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, ABU, PG4, GOL, UMQ, CA, MES

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	0.66	0/2519	1.07	2/3432 (0.1%)
1	B	0.66	0/2543	1.06	3/3467 (0.1%)
1	C	0.66	0/2527	1.06	1/3448 (0.0%)
1	D	0.67	0/2490	1.05	1/3401 (0.0%)
1	E	0.66	0/2523	1.06	6/3439 (0.2%)
2	F	0.60	0/827	0.93	0/1121
2	G	0.64	0/850	0.92	0/1149
2	H	0.71	1/855 (0.1%)	0.99	0/1156
2	I	0.63	1/853 (0.1%)	0.93	0/1152
2	J	0.64	0/843	0.96	0/1140
All	All	0.66	2/16830 (0.0%)	1.03	13/22905 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	82	MET	SD-CE	-6.24	1.64	1.79
2	I	82	MET	SD-CE	-5.19	1.66	1.79

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	136	ASN	CA-C-N	5.73	128.24	120.38
1	E	136	ASN	C-N-CA	5.73	128.24	120.38
1	B	138	GLN	N-CA-C	-5.32	106.84	113.38
1	D	286	ARG	N-CA-C	-5.26	106.71	113.23
1	A	306	LEU	CA-C-N	5.24	125.79	119.98
1	A	306	LEU	C-N-CA	5.24	125.79	119.98
1	E	300	CYS	N-CA-C	-5.16	107.15	112.93
1	B	270	TYR	CA-C-N	5.16	125.66	119.94
1	B	270	TYR	C-N-CA	5.16	125.66	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	270	TYR	CA-C-N	5.14	125.65	119.94
1	E	270	TYR	C-N-CA	5.14	125.65	119.94
1	C	86	ASP	CA-CB-CG	5.12	117.72	112.60
1	E	185	GLN	N-CA-C	-5.02	106.47	112.59

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	2453	0	2404	13	0
1	B	2477	0	2399	9	0
1	C	2461	0	2396	7	0
1	D	2424	0	2330	11	0
1	E	2457	0	2416	8	0
2	F	815	0	773	0	0
2	G	838	0	813	1	0
2	H	843	0	815	3	0
2	I	841	0	815	2	0
2	J	831	0	799	2	0
3	A	7	0	0	0	0
3	B	7	0	0	0	0
3	C	7	0	0	0	0
3	D	7	0	0	0	0
3	E	7	0	0	1	0
4	A	12	0	13	0	0
4	B	12	0	13	0	0
4	C	12	0	13	0	0
4	D	12	0	13	0	0
4	E	12	0	13	0	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0
5	D	6	0	8	0	0
5	E	12	0	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
7	B	13	0	18	0	0
7	C	13	0	18	0	0
7	D	13	0	18	2	0
7	E	13	0	18	0	0
8	B	64	0	74	0	0
8	C	32	0	37	0	0
8	E	64	0	74	0	0
9	D	4	0	3	0	0
9	E	4	0	3	0	0
10	A	18	0	0	0	0
10	B	22	0	0	1	0
10	C	31	0	0	0	0
10	D	18	0	0	0	0
10	E	16	0	0	0	0
10	G	14	0	0	0	0
10	H	18	0	0	0	0
10	I	6	0	0	0	0
10	J	2	0	0	0	0
All	All	16941	0	16336	49	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 1.

All (49) 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:A:283:ALA:HB2	1:A:297:ILE:HG21	1.85	0.59
2:I:40:ALA:HB3	2:I:43:LYS:HB2	1.85	0.58
1:E:152:ILE:HG21	1:E:162:ILE:HG13	1.85	0.57
1:D:123:ARG:HG2	1:D:198:VAL:HG22	1.86	0.57
1:D:76:LEU:H	7:D:404:PG4:H52	1.69	0.56
1:E:208:PHE:HD1	1:E:249:THR:HG22	1.73	0.53
1:B:208:PHE:HD1	1:B:249:THR:HG22	1.74	0.53
1:C:123:ARG:HG2	1:C:198:VAL:HG22	1.92	0.52
1:E:146:GLN:OE1	2:J:2:VAL:HG23	2.10	0.51
1:A:208:PHE:HD1	1:A:249:THR:HG22	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:ILE:HG22	1:E:152:ILE:HD11	1.96	0.48
1:A:114:MET:HE3	1:A:116:PHE:HZ	1.78	0.48
1:D:208:PHE:HD1	1:D:249:THR:HG22	1.79	0.48
2:G:24:ALA:HB3	2:G:76:ASN:HB3	1.95	0.48
2:H:40:ALA:HB3	2:H:43:LYS:HB2	1.96	0.48
1:C:208:PHE:HD1	1:C:249:THR:HG22	1.79	0.48
1:B:123:ARG:HG2	1:B:198:VAL:HG22	1.97	0.47
1:A:283:ALA:HB2	1:A:297:ILE:CG2	2.44	0.47
1:D:75:ALA:HA	7:D:404:PG4:H41	1.95	0.47
1:A:134:SER:OG	1:B:91:ARG:HD3	2.15	0.47
1:A:123:ARG:HG2	1:A:198:VAL:HG22	1.96	0.46
1:E:208:PHE:CD1	1:E:249:THR:HG22	2.50	0.46
1:B:294:ASP:O	1:B:297:ILE:HG22	2.15	0.46
1:A:20:ILE:HG22	1:A:152:ILE:HD11	1.99	0.45
1:A:240:LEU:HD13	1:B:241:THR:HA	1.99	0.45
1:E:162:ILE:HG23	1:E:195:ILE:HG23	1.98	0.45
1:B:96:PRO:HD2	10:B:502:HOH:O	2.18	0.44
1:C:282:PHE:O	1:C:286:ARG:HB2	2.17	0.44
3:E:401:ABU:OXT	5:E:404:GOL:H12	2.18	0.44
1:C:240:LEU:HD13	1:D:241:THR:HA	2.00	0.44
1:B:208:PHE:CD1	1:B:249:THR:HG22	2.52	0.43
1:D:281:ILE:HD11	1:E:221:SER:HB2	2.00	0.43
2:H:82:MET:HE1	2:H:107:VAL:HG21	2.01	0.43
1:D:20:ILE:HG22	1:D:152:ILE:HD11	2.02	0.42
1:B:281:ILE:HD11	1:C:221:SER:HB2	2.02	0.42
2:I:90:THR:HG23	2:I:108:THR:HA	2.01	0.41
1:A:279:LEU:HD22	1:A:304:PHE:HE1	1.85	0.41
1:B:247:PHE:HB2	1:C:248:TYR:HB2	2.02	0.41
1:A:132:PRO:HG3	1:A:140:LEU:HD22	2.02	0.41
1:A:114:MET:HE3	1:A:116:PHE:CZ	2.55	0.41
1:D:208:PHE:CD1	1:D:249:THR:HG22	2.56	0.41
1:D:57:ILE:HD11	1:D:93:MET:HE2	2.02	0.41
2:J:85:LEU:HD12	2:J:85:LEU:H	1.85	0.41
1:D:225:LEU:HB2	1:D:231:ARG:HG2	2.03	0.41
1:E:225:LEU:HB2	1:E:231:ARG:HG2	2.02	0.41
1:A:300:CYS:HB2	1:A:303:ALA:HB3	2.02	0.40
1:A:294:ASP:O	1:A:297:ILE:HG22	2.21	0.40
1:D:114:MET:HE3	1:D:116:PHE:HZ	1.87	0.40
1:C:145:ILE:O	2:H:29:PHE:HA	2.21	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	297/318 (93%)	289 (97%)	8 (3%)	0	100	100
1	B	303/318 (95%)	292 (96%)	10 (3%)	1 (0%)	36	58
1	C	301/318 (95%)	292 (97%)	9 (3%)	0	100	100
1	D	300/318 (94%)	293 (98%)	7 (2%)	0	100	100
1	E	298/318 (94%)	293 (98%)	5 (2%)	0	100	100
2	F	108/121 (89%)	106 (98%)	2 (2%)	0	100	100
2	G	109/121 (90%)	109 (100%)	0	0	100	100
2	H	110/121 (91%)	107 (97%)	3 (3%)	0	100	100
2	I	109/121 (90%)	104 (95%)	5 (5%)	0	100	100
2	J	108/121 (89%)	100 (93%)	8 (7%)	0	100	100
All	All	2043/2195 (93%)	1985 (97%)	57 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	295	LEU

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	264/282 (94%)	264 (100%)	0	100	100
1	B	264/282 (94%)	262 (99%)	2 (1%)	73	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	263/282 (93%)	262 (100%)	1 (0%)	84	93
1	D	254/282 (90%)	251 (99%)	3 (1%)	63	83
1	E	266/282 (94%)	261 (98%)	5 (2%)	50	75
2	F	83/98 (85%)	83 (100%)	0	100	100
2	G	88/98 (90%)	88 (100%)	0	100	100
2	H	88/98 (90%)	88 (100%)	0	100	100
2	I	88/98 (90%)	88 (100%)	0	100	100
2	J	86/98 (88%)	86 (100%)	0	100	100
All	All	1744/1900 (92%)	1733 (99%)	11 (1%)	78	91

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	84	SER
1	B	267	ILE
1	C	279	LEU
1	D	103	ASN
1	D	157	ILE
1	D	304	PHE
1	E	103	ASN
1	E	150	GLU
1	E	247	PHE
1	E	298	GLN
1	E	302	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	124	GLN
1	A	151	ASN
1	B	124	GLN
1	B	285	HIS
1	C	125	GLN
1	C	169	HIS
1	C	200	ASN
1	C	285	HIS
1	D	124	GLN

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Mol	Chain	Res	Type
1	D	136	ASN
1	D	137	ASN
1	D	154	ASN
1	D	200	ASN
1	D	264	GLN
1	D	285	HIS
1	E	137	ASN
1	E	138	GLN
1	E	184	ASN
2	F	32	ASN
2	F	81	GLN
2	G	32	ASN
2	H	28	ASN
2	H	32	ASN
2	H	106	GLN
2	I	1	GLN
2	I	32	ASN
2	J	13	GLN
2	J	32	ASN

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 32 ligands modelled in this entry, 5 are monoatomic - leaving 27 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	$\# Z > 2$
8	UMQ	B	407	-	33,33,35	0.22	0	44,44,46	0.65	1 (2%)
5	GOL	C	403	-	5,5,5	0.12	0	5,5,5	0.45	0
4	MES	E	402	-	12,12,12	1.19	1 (8%)	15,16,16	0.48	0
8	UMQ	E	409	-	33,33,35	0.21	0	44,44,46	0.54	0
3	ABU	C	401	-	6,6,6	1.63	2 (33%)	6,6,6	1.59	2 (33%)
3	ABU	B	401	-	6,6,6	0.11	0	6,6,6	0.21	0
7	PG4	E	405	-	12,12,12	0.19	0	11,11,11	0.20	0
4	MES	B	402	-	12,12,12	1.24	2 (16%)	15,16,16	0.47	0
5	GOL	E	404	-	5,5,5	0.11	0	5,5,5	0.40	0
8	UMQ	B	406	-	33,33,35	0.21	0	44,44,46	0.53	0
7	PG4	C	404	-	12,12,12	0.22	0	11,11,11	0.17	0
3	ABU	D	401	-	6,6,6	1.59	2 (33%)	6,6,6	1.80	2 (33%)
9	ACT	D	406	-	3,3,3	1.20	0	3,3,3	1.01	0
4	MES	A	402	-	12,12,12	0.83	0	15,16,16	0.41	0
4	MES	C	402	-	12,12,12	1.08	1 (8%)	15,16,16	0.43	0
5	GOL	E	403	-	5,5,5	0.16	0	5,5,5	0.26	0
9	ACT	E	407	-	3,3,3	1.27	0	3,3,3	0.92	0
5	GOL	B	403	-	5,5,5	0.05	0	5,5,5	0.46	0
5	GOL	A	403	-	5,5,5	0.10	0	5,5,5	0.26	0
4	MES	D	402	-	12,12,12	0.83	0	15,16,16	0.26	0
5	GOL	D	403	-	5,5,5	0.20	0	5,5,5	0.14	0
8	UMQ	E	408	-	33,33,35	0.24	0	44,44,46	0.81	2 (4%)
7	PG4	D	404	-	12,12,12	0.29	0	11,11,11	0.33	0
3	ABU	A	401	-	6,6,6	1.53	2 (33%)	6,6,6	2.03	2 (33%)
3	ABU	E	401	-	6,6,6	1.67	2 (33%)	6,6,6	1.65	2 (33%)
7	PG4	B	404	-	12,12,12	0.23	0	11,11,11	0.11	0
8	UMQ	C	406	-	33,33,35	0.23	0	44,44,46	0.48	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
8	UMQ	B	407	-	-	6/18/58/60	0/2/2/2
5	GOL	C	403	-	-	0/4/4/4	-
4	MES	E	402	-	-	0/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	UMQ	E	409	-	-	6/18/58/60	0/2/2/2
3	ABU	C	401	-	-	0/4/4/4	-
3	ABU	B	401	-	-	2/4/4/4	-
7	PG4	E	405	-	-	6/10/10/10	-
4	MES	B	402	-	-	0/6/14/14	0/1/1/1
5	GOL	E	404	-	-	3/4/4/4	-
8	UMQ	B	406	-	-	6/18/58/60	0/2/2/2
7	PG4	C	404	-	-	6/10/10/10	-
3	ABU	D	401	-	-	2/4/4/4	-
4	MES	A	402	-	-	3/6/14/14	0/1/1/1
4	MES	C	402	-	-	1/6/14/14	0/1/1/1
5	GOL	E	403	-	-	0/4/4/4	-
5	GOL	B	403	-	-	2/4/4/4	-
5	GOL	A	403	-	-	0/4/4/4	-
4	MES	D	402	-	-	2/6/14/14	0/1/1/1
5	GOL	D	403	-	-	0/4/4/4	-
8	UMQ	E	408	-	-	9/18/58/60	0/2/2/2
7	PG4	D	404	-	-	5/10/10/10	-
3	ABU	A	401	-	-	0/4/4/4	-
3	ABU	E	401	-	-	2/4/4/4	-
7	PG4	B	404	-	-	4/10/10/10	-
8	UMQ	C	406	-	-	8/18/58/60	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	ABU	O-C	2.96	1.31	1.22
3	E	401	ABU	O-C	2.95	1.31	1.22
3	D	401	ABU	O-C	2.88	1.31	1.22
3	E	401	ABU	OXT-C	-2.84	1.21	1.30
3	A	401	ABU	O-C	2.70	1.30	1.22
4	E	402	MES	C8-S	-2.69	1.73	1.77
3	C	401	ABU	OXT-C	-2.64	1.22	1.30
3	D	401	ABU	OXT-C	-2.62	1.22	1.30
3	A	401	ABU	OXT-C	-2.59	1.22	1.30
4	B	402	MES	C8-S	2.44	1.81	1.77
4	C	402	MES	C8-S	2.40	1.81	1.77
4	B	402	MES	C7-N4	2.22	1.52	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	ABU	OXT-C-CG	3.48	125.01	114.00
3	A	401	ABU	O-C-CG	-3.45	112.14	123.09
3	D	401	ABU	O-C-CG	-3.12	113.20	123.09
3	D	401	ABU	OXT-C-CG	3.09	123.78	114.00
3	E	401	ABU	OXT-C-CG	2.83	122.95	114.00
3	E	401	ABU	O-C-CG	-2.81	114.19	123.09
3	C	401	ABU	OXT-C-CG	2.60	122.21	114.00
3	C	401	ABU	O-C-CG	-2.36	115.59	123.09
8	E	408	UMQ	C3'-C4'-C5'	2.23	115.88	110.93
8	E	408	UMQ	O5'-C5'-C4'	2.19	114.25	109.72
8	B	407	UMQ	O2'-C2'-C1'	-2.07	105.15	110.08

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	402	MES	C7-C8-S-O1S
4	A	402	MES	C7-C8-S-O3S
5	B	403	GOL	C1-C2-C3-O3
8	B	406	UMQ	C2'-C1'-O1'-CA
8	B	407	UMQ	O5-C1-O1-C4'
8	E	408	UMQ	C3'-C4'-O1-C1
8	B	406	UMQ	O5'-C1'-O1'-CA
8	E	409	UMQ	O5'-C1'-O1'-CA
7	D	404	PG4	O3-C5-C6-O4
8	E	409	UMQ	C2'-C1'-O1'-CA
8	E	408	UMQ	C5'-C4'-O1-C1
8	E	408	UMQ	O5'-C5'-C6'-O6'
8	C	406	UMQ	O5-C1-O1-C4'
7	C	404	PG4	O3-C5-C6-O4
7	B	404	PG4	O2-C3-C4-O3
7	D	404	PG4	C6-C5-O3-C4
5	E	404	GOL	O1-C1-C2-C3
5	E	404	GOL	C1-C2-C3-O3
7	C	404	PG4	O4-C7-C8-O5
8	B	407	UMQ	O1'-CA-CB-CC
5	B	403	GOL	O2-C2-C3-O3
5	E	404	GOL	O1-C1-C2-O2
8	B	407	UMQ	CA-CB-CC-CD
8	E	408	UMQ	O5-C5-C6-O6
8	E	408	UMQ	O5-C1-O1-C4'

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Mol	Chain	Res	Type	Atoms
8	E	408	UMQ	CA-CB-CC-CD
7	D	404	PG4	O1-C1-C2-O2
8	E	409	UMQ	C4-C5-C6-O6
8	E	409	UMQ	O5'-C5'-C6'-O6'
7	D	404	PG4	O2-C3-C4-O3
8	B	407	UMQ	O5'-C5'-C6'-O6'
8	B	407	UMQ	C3'-C4'-O1-C1
7	E	405	PG4	O2-C3-C4-O3
8	B	407	UMQ	C5'-C4'-O1-C1
8	B	406	UMQ	CF-CG-CH-CI
8	E	408	UMQ	C4'-C5'-C6'-O6'
8	E	409	UMQ	CB-CC-CD-CF
8	E	408	UMQ	O1'-CA-CB-CC
4	A	402	MES	C7-C8-S-O2S
8	E	409	UMQ	O5-C5-C6-O6
7	C	404	PG4	C5-C6-O4-C7
7	E	405	PG4	C5-C6-O4-C7
7	E	405	PG4	C8-C7-O4-C6
8	C	406	UMQ	O5'-C1'-O1'-CA
7	C	404	PG4	C4-C3-O2-C2
8	C	406	UMQ	C4-C5-C6-O6
8	E	408	UMQ	C2-C1-O1-C4'
7	E	405	PG4	O1-C1-C2-O2
8	C	406	UMQ	C2'-C1'-O1'-CA
7	B	404	PG4	C6-C5-O3-C4
8	C	406	UMQ	C3'-C4'-O1-C1
7	E	405	PG4	O4-C7-C8-O5
3	B	401	ABU	OXT-C-CG-CB
4	D	402	MES	C7-C8-S-O3S
4	D	402	MES	C7-C8-S-O1S
7	B	404	PG4	C5-C6-O4-C7
8	C	406	UMQ	C2-C1-O1-C4'
8	B	406	UMQ	C3'-C4'-O1-C1
4	C	402	MES	C8-C7-N4-C3
3	B	401	ABU	O-C-CG-CB
7	D	404	PG4	O4-C7-C8-O5
8	C	406	UMQ	O5-C5-C6-O6
8	B	406	UMQ	CD-CF-CG-CH
7	C	404	PG4	C1-C2-O2-C3
8	C	406	UMQ	C5'-C4'-O1-C1
3	E	401	ABU	O-C-CG-CB
7	E	405	PG4	O3-C5-C6-O4

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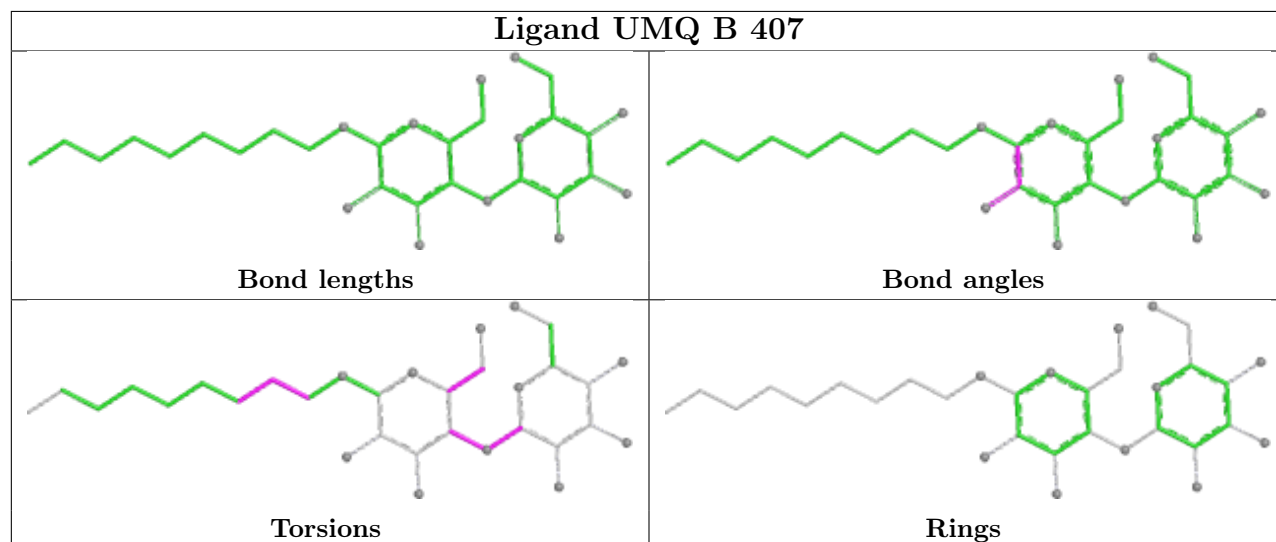
Mol	Chain	Res	Type	Atoms
3	D	401	ABU	O-C-CG-CB
8	B	406	UMQ	C5'-C4'-O1-C1
7	B	404	PG4	O3-C5-C6-O4
7	C	404	PG4	O2-C3-C4-O3
3	E	401	ABU	OXT-C-CG-CB
3	D	401	ABU	OXT-C-CG-CB

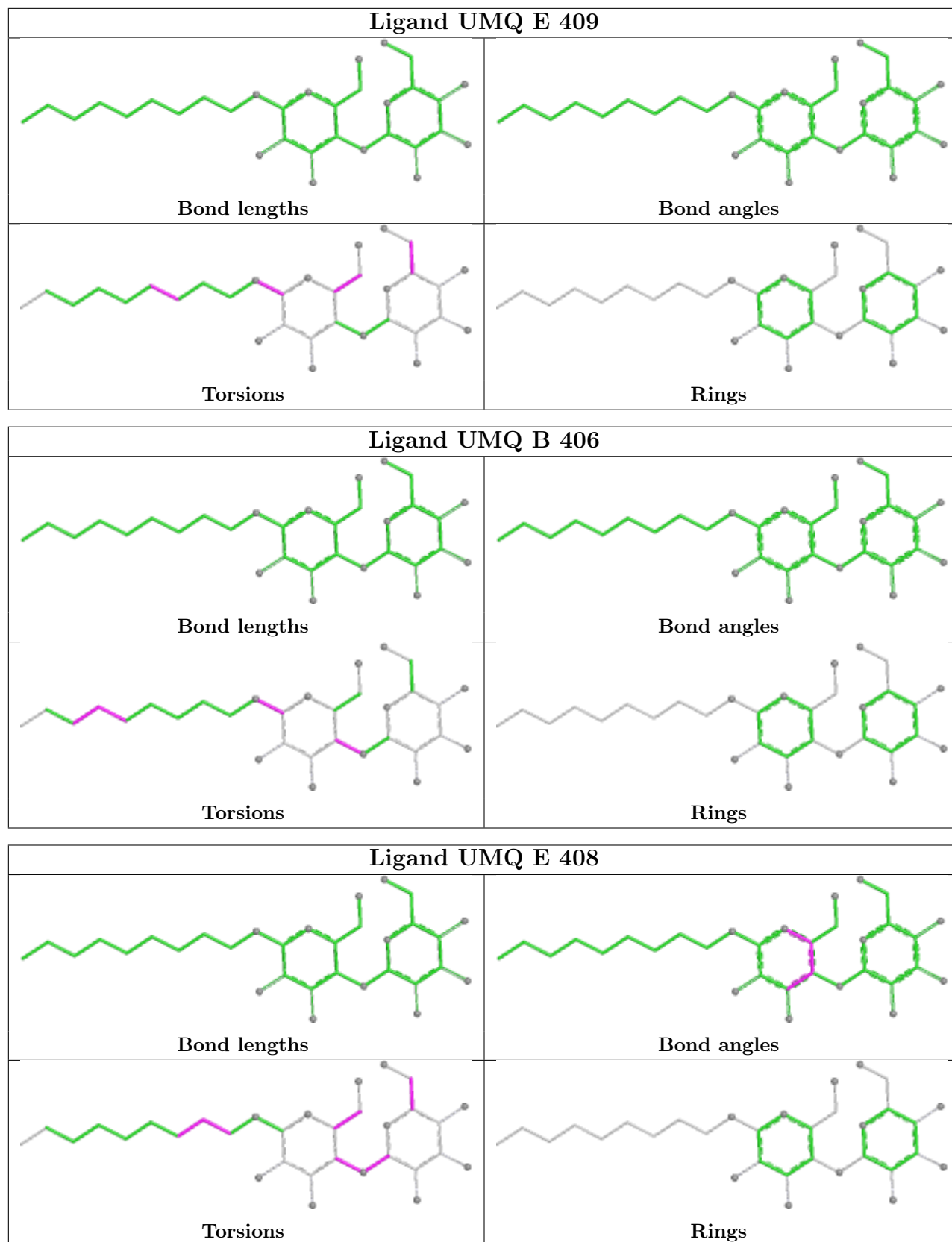
There are no ring outliers.

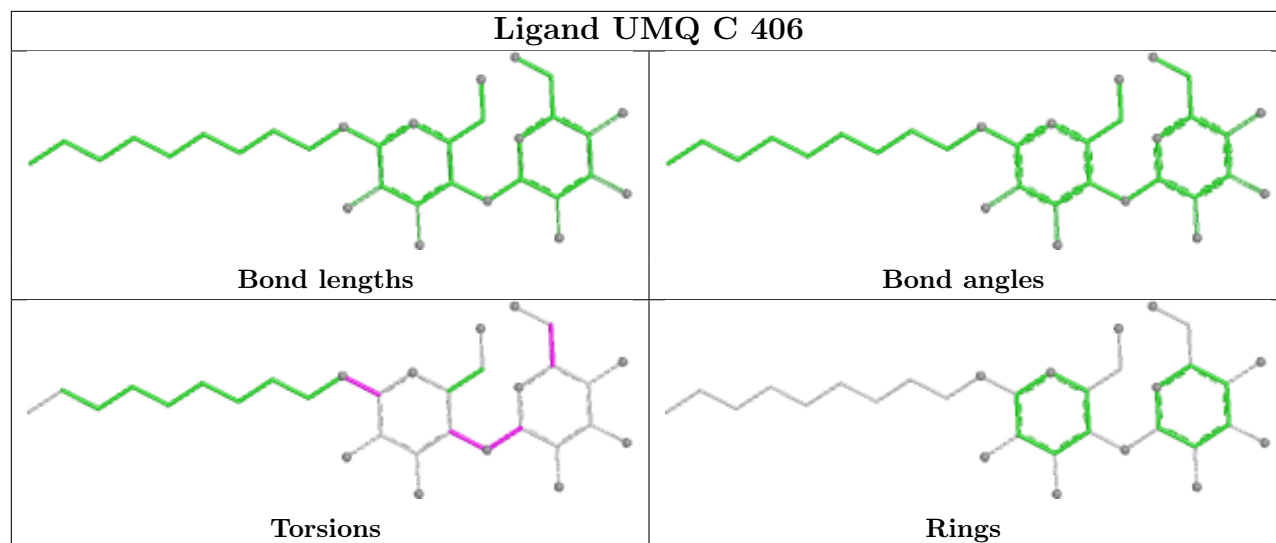
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	404	GOL	1	0
7	D	404	PG4	2	0
3	E	401	ABU	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.







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	303/318 (95%)	0.89	37 (12%) 8 6	48, 74, 113, 155	0
1	B	308/318 (96%)	0.95	42 (13%) 7 5	38, 71, 127, 158	1 (0%)
1	C	307/318 (96%)	0.88	43 (14%) 6 5	46, 71, 119, 143	0
1	D	305/318 (95%)	1.00	49 (16%) 4 3	27, 74, 124, 149	1 (0%)
1	E	304/318 (95%)	0.96	45 (14%) 5 4	48, 74, 112, 155	0
2	F	110/121 (90%)	1.63	40 (36%) 1 0	64, 97, 130, 138	0
2	G	111/121 (91%)	0.89	13 (11%) 9 7	50, 64, 87, 117	0
2	H	112/121 (92%)	0.55	9 (8%) 18 14	47, 62, 91, 105	0
2	I	111/121 (91%)	1.20	24 (21%) 2 2	54, 75, 116, 134	0
2	J	110/121 (90%)	1.86	45 (40%) 0 0	61, 99, 129, 138	0
All	All	2081/2195 (94%)	1.01	347 (16%) 4 3	27, 74, 123, 158	2 (0%)

All (347) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	181	VAL	8.8
2	H	112	HIS	6.2
1	B	319	GLY	6.1
1	D	7	VAL	5.6
1	C	7	VAL	5.6
1	E	183	PRO	5.5
1	A	288	ALA	5.3
1	B	179	SER	5.2
1	E	246	ALA	5.2
1	D	157	ILE	5.2
1	B	183	PRO	5.1
1	D	8	ASP	5.1
1	E	295	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	293	ASP	4.9
1	E	179	SER	4.9
2	I	9	GLY	4.9
2	J	110	SER	4.8
1	D	154	ASN	4.8
2	F	109	VAL	4.8
1	A	183	PRO	4.7
1	D	156	GLU	4.6
1	A	295	LEU	4.6
1	E	316	VAL	4.6
1	B	298	GLN	4.6
1	D	182	GLN	4.6
1	D	316	VAL	4.6
1	E	317	ILE	4.5
1	B	8	ASP	4.5
1	B	290	GLY	4.4
1	B	314	VAL	4.4
1	C	314	VAL	4.4
1	A	289	ASN	4.3
2	I	17	SER	4.3
1	A	247	PHE	4.3
1	C	288	ALA	4.3
1	C	183	PRO	4.3
1	E	291	VAL	4.3
1	B	312	GLY	4.2
2	F	90	THR	4.2
1	C	9	ALA	4.2
1	B	317	ILE	4.2
1	A	314	VAL	4.2
1	D	247	PHE	4.2
1	C	289	ASN	4.2
1	D	162	ILE	4.2
1	D	297	ILE	4.2
1	B	7	VAL	4.2
1	A	179	SER	4.2
1	A	298	GLN	4.2
1	B	153	ASP	4.1
1	E	290	GLY	4.1
2	F	15	GLY	4.1
1	B	296	LEU	4.0
1	B	154	ASN	4.0
2	J	107	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	246	ALA	4.0
2	J	65	GLY	4.0
2	I	18	MET	4.0
1	C	315	LEU	4.0
2	I	14	ALA	3.9
1	C	316	VAL	3.9
1	C	295	LEU	3.9
1	B	316	VAL	3.9
1	D	288	ALA	3.9
1	C	154	ASN	3.9
1	C	163	ARG	3.8
1	D	150	GLU	3.8
1	D	183	PRO	3.8
1	B	163	ARG	3.8
2	F	23	ILE	3.8
2	I	11	LEU	3.8
2	F	88	GLU	3.7
1	D	287	GLN	3.7
1	D	298	GLN	3.7
1	A	137	ASN	3.7
1	E	314	VAL	3.7
2	H	1	GLN	3.6
2	J	68	THR	3.6
2	J	108	THR	3.6
2	F	12	ALA	3.6
1	C	317	ILE	3.6
1	D	179	SER	3.5
2	F	45	ARG	3.5
2	G	111	SER	3.5
2	F	14	ALA	3.5
2	J	105	THR	3.5
1	C	179	SER	3.5
2	H	46	GLU	3.4
1	D	301	ARG	3.4
2	I	111	SER	3.4
1	B	302	LEU	3.4
2	J	11	LEU	3.4
1	B	9	ALA	3.4
1	E	157	ILE	3.4
2	G	1	GLN	3.4
1	B	311	ILE	3.4
1	B	318	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	178	LEU	3.3
2	F	54	ALA	3.3
2	F	13	GLN	3.3
2	G	42	GLY	3.3
1	B	310	ALA	3.3
1	D	294	ASP	3.2
2	G	109	VAL	3.2
2	F	108	THR	3.2
1	D	161	TRP	3.2
1	A	317	ILE	3.2
1	E	206	TRP	3.2
1	D	286	ARG	3.2
1	E	163	ARG	3.2
1	A	316	VAL	3.2
2	G	13	GLN	3.2
1	C	224	TRP	3.2
1	E	202	SER	3.2
2	J	41	PRO	3.2
2	I	10	GLY	3.2
1	B	157	ILE	3.2
2	F	1	GLN	3.1
1	C	261	VAL	3.1
1	E	152	ILE	3.1
1	E	311	ILE	3.1
1	D	163	ARG	3.1
1	B	247	PHE	3.1
2	J	40	ALA	3.1
1	C	313	CYS	3.1
1	B	295	LEU	3.1
1	B	152	ILE	3.1
1	A	226	GLU	3.0
1	C	308	PHE	3.0
1	C	319	GLY	3.0
2	G	23	ILE	3.0
1	B	288	ALA	3.0
1	D	295	LEU	3.0
2	F	10	GLY	3.0
1	D	9	ALA	3.0
1	C	279	LEU	3.0
1	E	315	LEU	3.0
1	E	299	ARG	3.0
1	C	164	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	208	PHE	3.0
2	F	110	SER	3.0
1	E	298	GLN	3.0
2	F	92	VAL	2.9
2	J	84	THR	2.9
1	C	298	GLN	2.9
1	E	289	ASN	2.9
1	A	224	TRP	2.9
1	C	309	LEU	2.9
2	J	94	TYR	2.9
2	H	110	SER	2.9
2	H	111	SER	2.9
1	B	162	ILE	2.9
1	D	152	ILE	2.9
2	I	41	PRO	2.9
2	J	4	LEU	2.9
1	B	72	TRP	2.9
1	B	308	PHE	2.9
2	I	13	GLN	2.9
1	E	156	GLU	2.9
2	J	15	GLY	2.9
1	C	318	ARG	2.9
2	J	102	GLY	2.9
2	G	110	SER	2.8
1	A	9	ALA	2.8
2	J	14	ALA	2.8
1	A	71	LEU	2.8
1	E	296	LEU	2.8
1	B	299	ARG	2.8
2	F	8	GLY	2.8
2	F	16	GLY	2.8
2	I	16	GLY	2.8
2	I	110	SER	2.8
2	J	95	CYS	2.8
2	J	18	MET	2.8
2	F	39	GLN	2.8
1	A	152	ILE	2.8
1	E	128	LEU	2.8
2	F	18	MET	2.8
2	J	46	GLU	2.8
1	D	160	TRP	2.8
1	A	311	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
2	J	83	SER	2.8
2	J	92	VAL	2.8
1	E	184	ASN	2.7
2	I	1	GLN	2.7
1	A	248	TYR	2.7
1	D	282	PHE	2.7
1	C	157	ILE	2.7
1	A	309	LEU	2.7
1	C	296	LEU	2.7
2	F	105	THR	2.7
1	E	164	GLY	2.7
1	B	223	PHE	2.7
2	J	90	THR	2.7
2	I	106	GLN	2.7
1	B	178	LEU	2.6
1	D	309	LEU	2.6
2	F	11	LEU	2.6
1	E	287	GLN	2.6
1	D	285	HIS	2.6
1	C	282	PHE	2.6
1	D	151	ASN	2.6
2	I	85	LEU	2.6
2	J	85	LEU	2.6
1	E	204	TYR	2.6
2	G	101	TRP	2.6
1	B	222	VAL	2.6
2	F	17	SER	2.6
1	E	288	ALA	2.6
2	G	108	THR	2.6
1	D	153	ASP	2.6
1	A	315	LEU	2.6
1	E	302	LEU	2.6
1	D	300	CYS	2.6
2	J	1	GLN	2.5
2	J	39	GLN	2.5
2	H	64	LYS	2.5
2	I	12	ALA	2.5
1	A	48	ARG	2.5
2	J	80	LEU	2.5
1	B	293	ASP	2.5
1	D	206	TRP	2.5
1	B	309	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	G	64	LYS	2.5
1	A	246	ALA	2.5
1	A	299	ARG	2.5
2	I	40	ALA	2.5
2	J	17	SER	2.5
2	G	41	PRO	2.5
1	B	164	GLY	2.5
2	F	85	LEU	2.5
1	E	247	PHE	2.5
2	J	7	SER	2.5
1	E	300	CYS	2.4
1	C	311	ILE	2.4
1	D	299	ARG	2.4
1	D	289	ASN	2.4
2	F	107	VAL	2.4
2	F	94	TYR	2.4
2	H	68	THR	2.4
2	I	108	THR	2.4
1	C	162	ILE	2.4
1	E	169	HIS	2.4
2	I	27	ARG	2.4
2	J	67	PHE	2.4
2	J	109	VAL	2.4
1	D	311	ILE	2.4
1	C	299	ARG	2.4
2	J	79	TYR	2.4
1	D	198	VAL	2.4
1	A	272	SER	2.3
2	J	23	ILE	2.3
1	C	284	HIS	2.3
2	I	43	LYS	2.3
2	F	56	THR	2.3
1	A	164	GLY	2.3
1	B	306	LEU	2.3
1	D	296	LEU	2.3
1	E	294	ASP	2.3
1	E	243	VAL	2.3
2	I	107	VAL	2.3
2	J	37	TYR	2.3
1	E	146	GLN	2.3
2	J	81	GLN	2.3
1	C	265	MET	2.3

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Mol	Chain	Res	Type	RSRZ
2	J	87	SER	2.3
1	A	46	LYS	2.3
2	F	67	PHE	2.3
1	A	300	CYS	2.3
1	D	137	ASN	2.2
2	F	40	ALA	2.2
2	G	91	ALA	2.2
2	F	5	GLN	2.2
1	A	178	LEU	2.2
1	B	297	ILE	2.2
1	C	178	LEU	2.2
2	J	101	TRP	2.2
1	A	228	PHE	2.2
2	J	74	ALA	2.2
1	B	161	TRP	2.2
1	E	194	ARG	2.2
2	I	109	VAL	2.2
2	J	63	VAL	2.2
1	A	245	TYR	2.2
1	E	245	TYR	2.2
2	J	43	LYS	2.2
1	C	253	LEU	2.2
1	C	306	LEU	2.2
2	F	9	GLY	2.2
2	J	33	ILE	2.2
2	F	70	SER	2.2
2	F	87	SER	2.2
1	D	158	ASP	2.2
1	A	308	PHE	2.2
2	I	2	VAL	2.2
1	C	285	HIS	2.2
2	J	12	ALA	2.2
1	C	300	CYS	2.2
2	F	4	LEU	2.2
2	I	8	GLY	2.2
2	J	45	ARG	2.2
1	C	247	PHE	2.2
1	E	308	PHE	2.2
1	A	185	GLN	2.1
1	B	307	GLY	2.1
1	C	52	GLY	2.1
2	F	80	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	204	TYR	2.1
1	A	313	CYS	2.1
1	D	10	ARG	2.1
2	J	19	ARG	2.1
1	C	152	ILE	2.1
1	D	308	PHE	2.1
1	E	304	PHE	2.1
1	E	200	ASN	2.1
1	E	225	LEU	2.1
2	F	68	THR	2.1
2	G	45	ARG	2.1
1	C	262	ILE	2.1
2	H	61	ASP	2.1
2	I	64	LYS	2.1
1	A	256	LEU	2.1
1	C	151	ASN	2.1
1	D	224	TRP	2.1
1	C	301	ARG	2.1
2	J	16	GLY	2.1
2	F	58	THR	2.1
2	J	69	ILE	2.1
2	F	93	TYR	2.1
1	B	282	PHE	2.0
1	E	244	ALA	2.0
2	J	27	ARG	2.0
1	E	226	GLU	2.0
1	A	206	TRP	2.0
1	E	161	TRP	2.0
2	F	84	THR	2.0
1	D	274	PHE	2.0
1	A	166	ALA	2.0
1	B	155	GLU	2.0
1	B	156	GLU	2.0
1	D	232	LEU	2.0
1	D	302	LEU	2.0
1	E	178	LEU	2.0
2	F	20	LEU	2.0
2	H	42	GLY	2.0
2	F	33	ILE	2.0
1	D	270	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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
9	ACT	E	407	4/4	0.50	0.24	81,81,81,81	0
9	ACT	D	406	4/4	0.57	0.24	75,76,76,77	0
8	UMQ	E	409	32/34	0.75	0.21	99,131,137,138	0
4	MES	C	402	12/12	0.76	0.26	88,92,111,112	0
8	UMQ	B	406	32/34	0.77	0.19	98,121,137,140	0
5	GOL	C	403	6/6	0.77	0.27	68,69,71,71	0
8	UMQ	E	408	32/34	0.78	0.18	95,120,134,135	0
8	UMQ	C	406	32/34	0.79	0.19	106,122,131,134	0
6	CA	C	405	1/1	0.80	0.13	110,110,110,110	0
7	PG4	E	405	13/13	0.80	0.27	82,83,86,86	0
4	MES	A	402	12/12	0.80	0.23	87,92,116,116	0
6	CA	A	404	1/1	0.80	0.10	107,107,107,107	0
5	GOL	E	404	6/6	0.81	0.24	89,91,91,92	0
6	CA	E	406	1/1	0.81	0.13	126,126,126,126	0
8	UMQ	B	407	32/34	0.81	0.19	100,114,130,135	0
7	PG4	D	404	13/13	0.81	0.27	81,83,86,86	0
5	GOL	B	403	6/6	0.83	0.23	73,77,78,78	0
6	CA	B	405	1/1	0.83	0.12	118,118,118,118	0
7	PG4	C	404	13/13	0.83	0.25	97,101,103,103	0
4	MES	B	402	12/12	0.84	0.20	89,92,105,106	0
7	PG4	B	404	13/13	0.84	0.23	82,84,86,87	0
3	ABU	A	401	7/7	0.86	0.17	68,74,83,84	0
4	MES	D	402	12/12	0.86	0.19	82,86,106,107	0
5	GOL	A	403	6/6	0.86	0.17	72,73,75,75	0
4	MES	E	402	12/12	0.87	0.18	79,83,104,104	0
5	GOL	D	403	6/6	0.89	0.18	74,76,79,81	0
5	GOL	E	403	6/6	0.89	0.18	73,74,74,75	0

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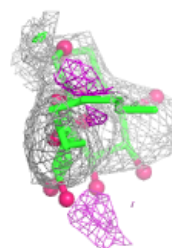
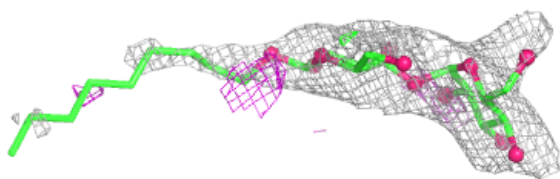
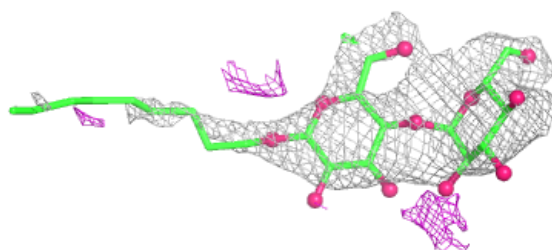
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ABU	B	401	7/7	0.89	0.15	64,69,77,77	0
3	ABU	E	401	7/7	0.90	0.17	63,68,76,78	0
3	ABU	C	401	7/7	0.91	0.12	58,62,71,72	0
3	ABU	D	401	7/7	0.93	0.14	68,70,77,77	0
6	CA	D	405	1/1	0.95	0.08	117,117,117,117	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.

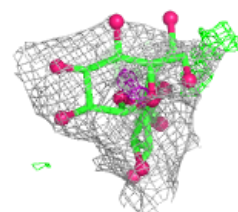
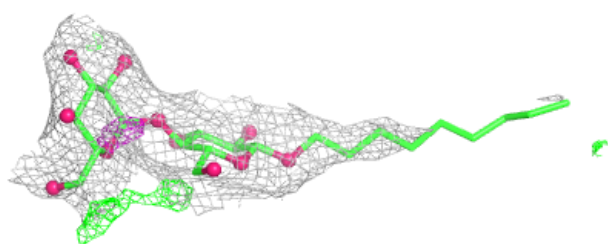
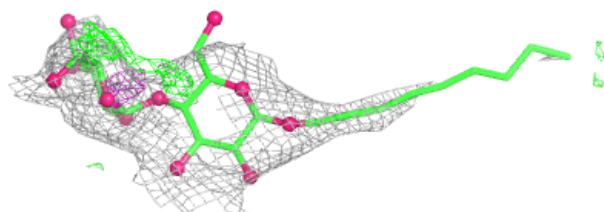
Electron density around UMQ E 409:

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

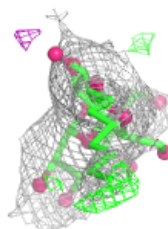
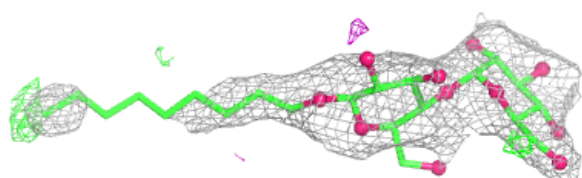
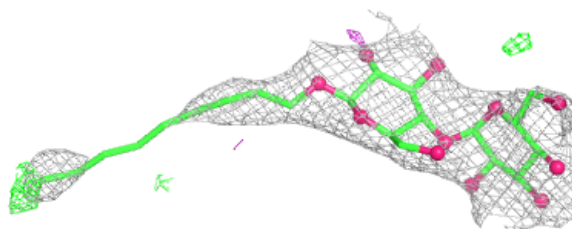


Electron density around UMQ B 406:

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

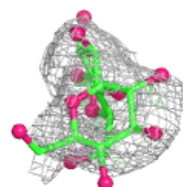
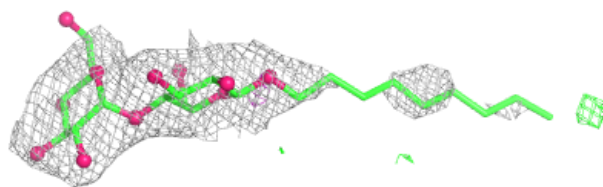
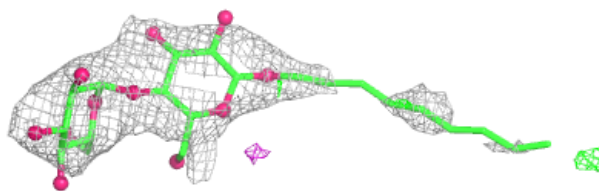
**Electron density around UMQ E 408:**

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

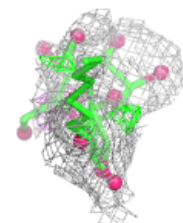
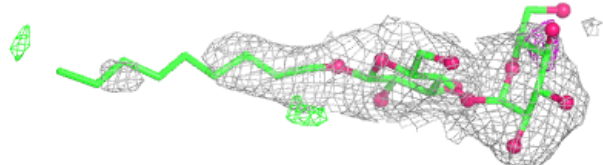
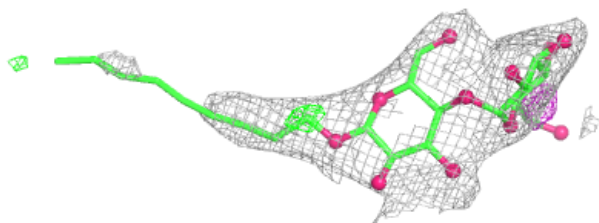


Electron density around UMQ C 406:

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

**Electron density around UMQ B 407:**

$2mF_o-DF_c$ (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.