Full wwPDB X-ray Structure Validation Report (i)

Nov 11, 2023 – 07:26 pm GMT

PDB ID	:	6SSI
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 (i) 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 (i)) were used in the production of this report:

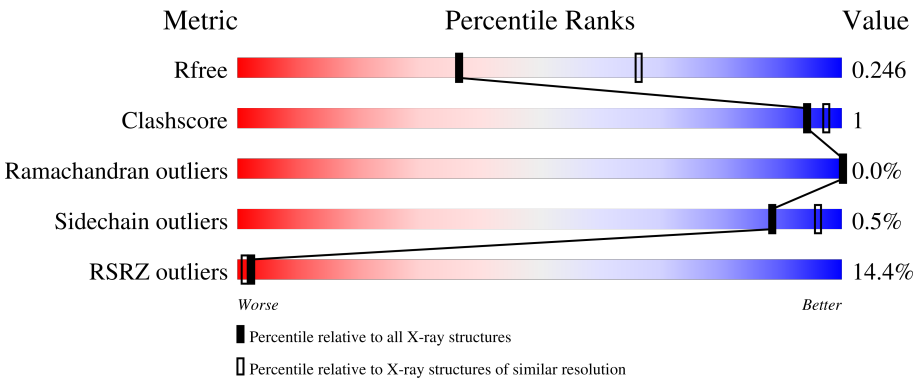
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 <=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	9% 90% 5% 5%
1	B	318	15% 92% . .
1	C	318	14% 93% . .
1	D	318	13% 92% . .

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Mol	Chain	Length	Quality of chain
1	E	318	12% 92%
2	F	121	35% 91% 9%
2	G	121	4% 90% 8%
2	H	121	90% 7%
2	I	121	19% 88% 8%
2	J	121	23% 89% 9%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	303	2453	1600	410	437	6	0	0	0
1	B	308	2477	1612	412	447	6	0	1	0
1	C	307	2461	1608	406	441	6	0	0	0
1	D	305	2424	1583	403	432	6	0	1	0
1	E	304	2457	1606	406	439	6	0	0	0

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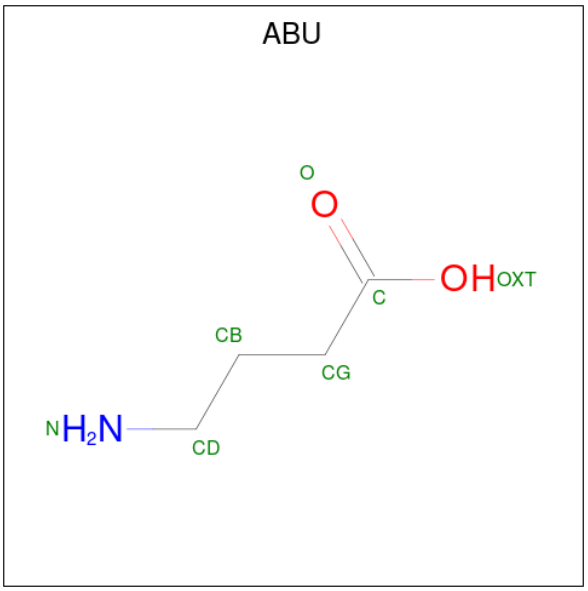
Chain	Residue	Modelled	Actual	Comment	Reference
D	6	PRO	-	expression tag	UNP P0C7B7
D	7	VAL	-	expression tag	UNP P0C7B7
D	164	GLY	-	insertion	UNP P0C7B7
D	289	ASN	MET	conflict	UNP P0C7B7
D	322	GLY	-	expression tag	UNP P0C7B7
E	5	GLY	-	expression tag	UNP P0C7B7
E	6	PRO	-	expression tag	UNP P0C7B7
E	7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

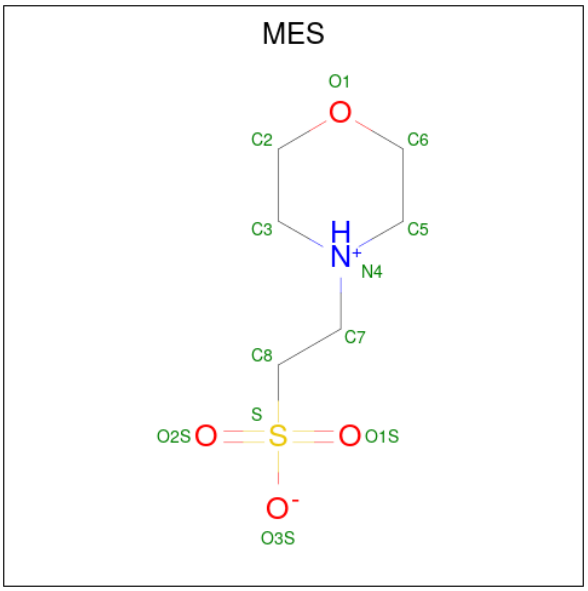
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	F	110	815	502	146	162	5	0	0	0
2	G	111	838	516	151	166	5	0	0	0
2	H	112	843	519	152	167	5	0	0	0
2	I	111	841	516	154	166	5	0	0	0
2	J	110	831	510	152	164	5	0	0	0

- Molecule 3 is GAMMA-AMINO-BUTANOIC ACID (three-letter code: ABU) (formula: $C_4H_9NO_2$).



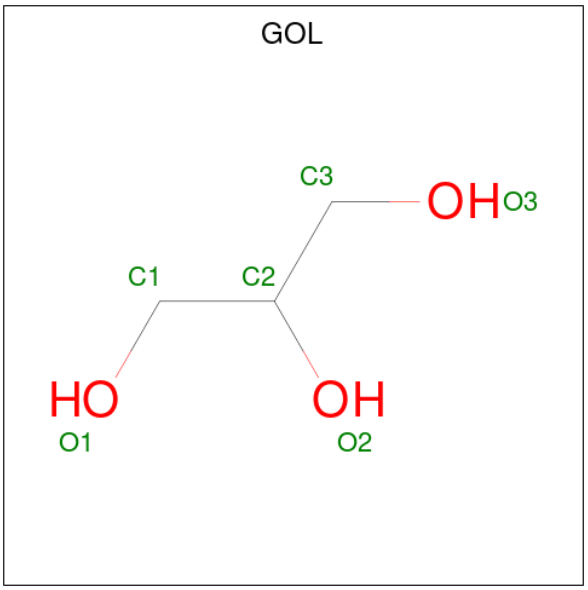
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	7	4	1	2	0	0
3	B	1	7	4	1	2	0	0
3	C	1	7	4	1	2	0	0
3	D	1	7	4	1	2	0	0
3	E	1	7	4	1	2	0	0

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



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

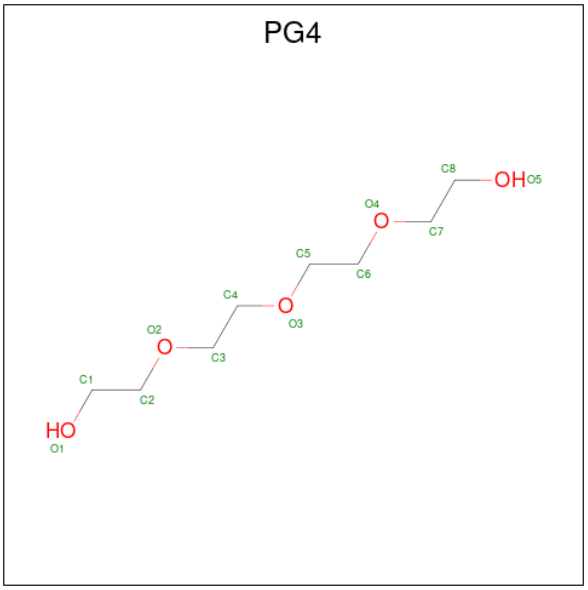


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	6	3	3	0	0
5	B	1	6	3	3	0	0
5	C	1	6	3	3	0	0
5	D	1	6	3	3	0	0
5	E	1	6	3	3	0	0
5	E	1	6	3	3	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

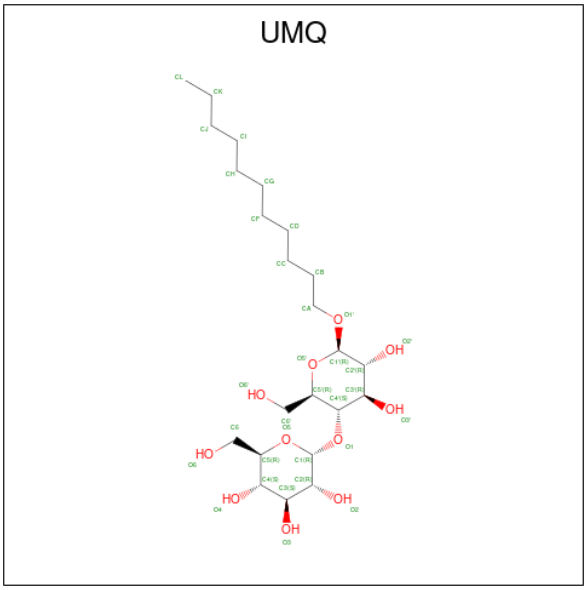
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
6	A	1	1	1	0	0
6	B	1	1	1	0	0
6	C	1	1	1	0	0
6	D	1	1	1	0	0
6	E	1	1	1	0	0

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



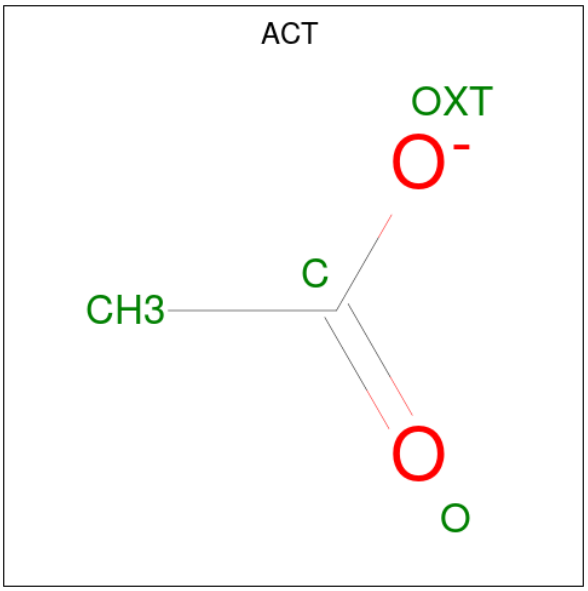
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	B	1	13	8	5	0	0
7	C	1	13	8	5	0	0
7	D	1	13	8	5	0	0
7	E	1	13	8	5	0	0

- Molecule 8 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: $C_{23}H_{44}O_{11}$).



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

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 10 is water.

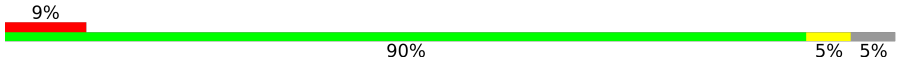
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	18	18	18	0	0
10	B	22	22	22	0	0
10	C	31	31	31	0	0
10	D	18	18	18	0	0
10	E	16	16	16	0	0
10	G	14	14	14	0	0
10	H	18	18	18	0	0
10	I	6	6	6	0	0
10	J	2	2	2	0	0

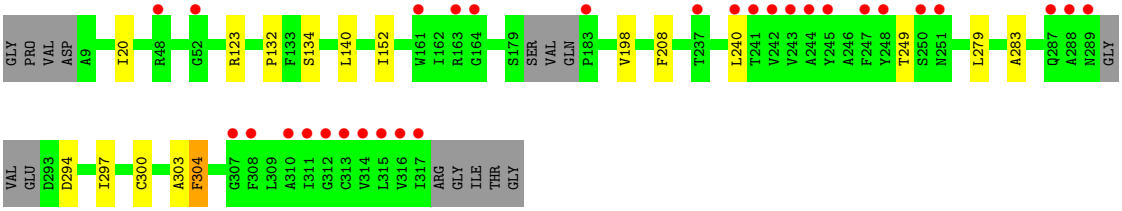
3 Residue-property plots (i)

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

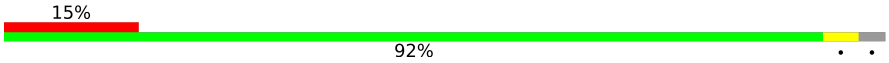
Chain A:

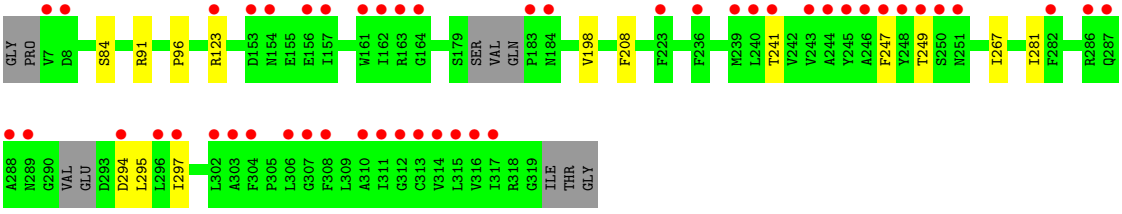




• Molecule 1: Cys-loop ligand-gated ion channel

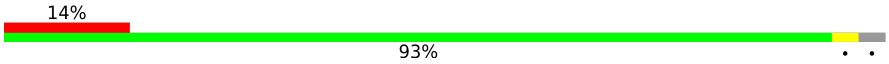
Chain B:

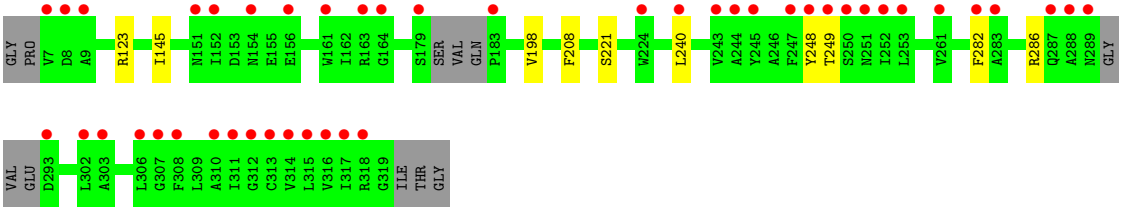




• Molecule 1: Cys-loop ligand-gated ion channel

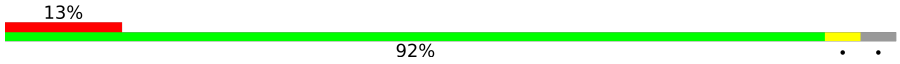
Chain C:

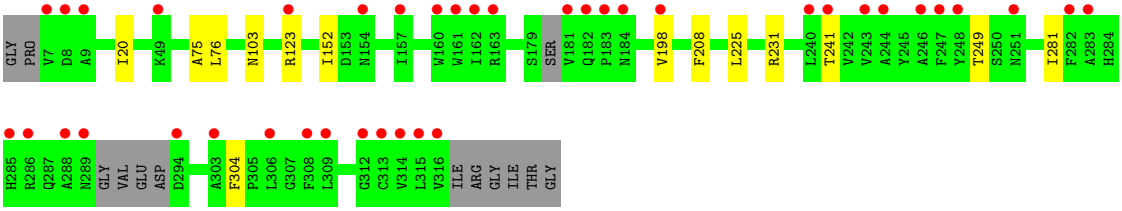




• Molecule 1: Cys-loop ligand-gated ion channel

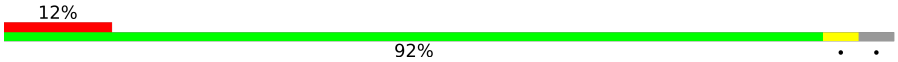
Chain D:

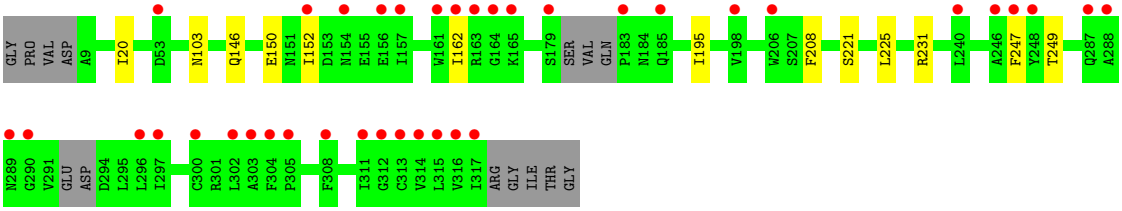




- Molecule 1: Cys-loop ligand-gated ion channel

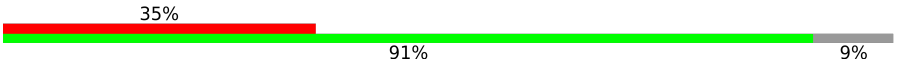
Chain E:

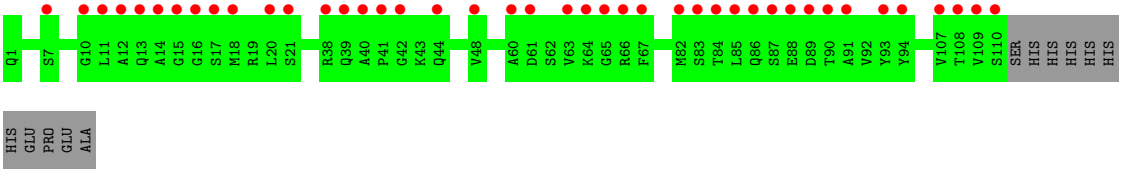




- Molecule 2: NANOBODY 22

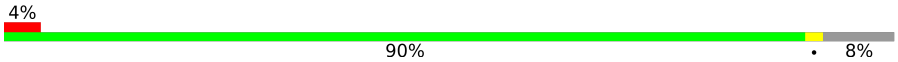
Chain F:

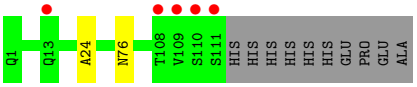




- Molecule 2: NANOBODY 22

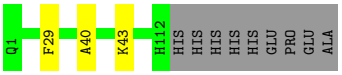
Chain G:





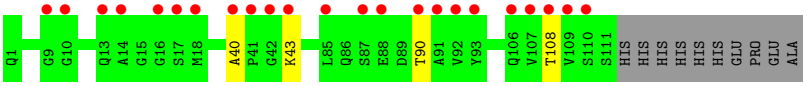
- Molecule 2: NANOBODY 22

Chain H:



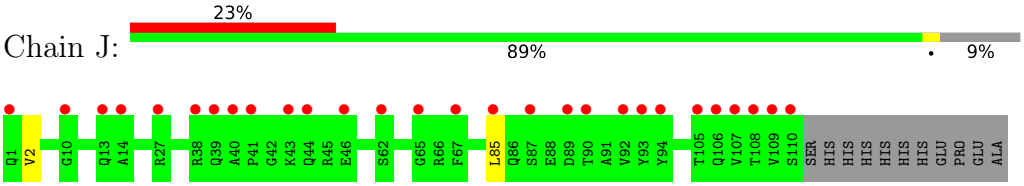
- Molecule 2: NANOBODY 22

Chain I:



- Molecule 2: NANOBODY 22

Chain J:


23%
89%
9%
Q1
V2
G10
Q13
A14
R27
R38
Q39
A40
P41
G42
K43
Q44
R45
E46
S62
G65
R66
F67
L85
Q86
S87
E88
D89
T90
A91
V92
Y93
Y94
T105
Q106
V107
T108
V109
S110
SER
HIS
HIS
HIS
HIS
HIS
HIS
GLU
PRO
GLU
ALA

4 Data and refinement statistics (i)

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) 99.7 (47.06-2.59)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.00%)	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 , 49.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MES, ACT, PG4, GOL, ABU, 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	0.40	0/2519	0.58	0/3432
1	B	0.40	0/2543	0.59	0/3467
1	C	0.40	0/2527	0.59	0/3448
1	D	0.41	0/2490	0.58	0/3401
1	E	0.40	0/2523	0.59	0/3439
2	F	0.35	0/827	0.57	0/1121
2	G	0.38	0/850	0.59	0/1149
2	H	0.41	0/855	0.62	0/1156
2	I	0.38	0/853	0.59	0/1152
2	J	0.36	0/843	0.60	0/1140
All	All	0.40	0/16830	0.59	0/22905

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2453	0	2404	11	0
1	B	2477	0	2399	9	0
1	C	2461	0	2396	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2424	0	2330	9	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	2	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	44	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 (44) 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
1:E:20:ILE:HG22	1:E:152:ILE:HD11	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:ILE:HD11	1:E:221:SER:HB2	2.00	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:D:208:PHE:CD1	1:D:249:THR:HG22	2.56	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:C:145:ILE:O	2:H:29:PHE:HA	2.21	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	297/318 (93%)	289 (97%)	8 (3%)	0	100	100
1	B	303/318 (95%)	292 (96%)	10 (3%)	1 (0%)	41	64
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	264/282 (94%)	263 (100%)	1 (0%)	91	97
1	B	264/282 (94%)	262 (99%)	2 (1%)	81	92
1	C	263/282 (93%)	263 (100%)	0	100	100
1	D	254/282 (90%)	252 (99%)	2 (1%)	81	92
1	E	266/282 (94%)	263 (99%)	3 (1%)	73	88
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%)	1736 (100%)	8 (0%)	88	96

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	304	PHE
1	B	84	SER
1	B	267	ILE
1	D	103	ASN
1	D	304	PHE

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Mol	Chain	Res	Type
1	E	103	ASN
1	E	150	GLU
1	E	247	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	C	406	-	33,33,35	0.23	0	44,44,46	0.48	0
8	UMQ	B	407	-	33,33,35	0.23	0	44,44,46	0.65	1 (2%)
3	ABU	D	401	-	6,6,6	1.56	2 (33%)	6,6,6	1.77	2 (33%)
4	MES	B	402	-	12,12,12	1.24	2 (16%)	14,16,16	0.55	0
4	MES	D	402	-	12,12,12	0.82	0	14,16,16	0.30	0
8	UMQ	B	406	-	33,33,35	0.22	0	44,44,46	0.53	0
4	MES	E	402	-	12,12,12	1.15	1 (8%)	14,16,16	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GOL	D	403	-	5,5,5	0.19	0	5,5,5	0.15	0
7	PG4	D	404	-	12,12,12	0.30	0	11,11,11	0.33	0
4	MES	C	402	-	12,12,12	1.08	1 (8%)	14,16,16	0.56	0
5	GOL	B	403	-	5,5,5	0.05	0	5,5,5	0.44	0
3	ABU	E	401	-	6,6,6	1.64	2 (33%)	6,6,6	1.62	2 (33%)
7	PG4	E	405	-	12,12,12	0.19	0	11,11,11	0.20	0
3	ABU	B	401	-	6,6,6	0.12	0	6,6,6	0.21	0
5	GOL	A	403	-	5,5,5	0.09	0	5,5,5	0.23	0
3	ABU	A	401	-	6,6,6	1.49	2 (33%)	6,6,6	2.00	2 (33%)
7	PG4	B	404	-	12,12,12	0.23	0	11,11,11	0.11	0
9	ACT	D	406	-	3,3,3	1.13	0	3,3,3	1.02	0
7	PG4	C	404	-	12,12,12	0.22	0	11,11,11	0.17	0
3	ABU	C	401	-	6,6,6	1.60	2 (33%)	6,6,6	1.58	2 (33%)
4	MES	A	402	-	12,12,12	0.83	0	14,16,16	0.46	0
5	GOL	E	404	-	5,5,5	0.11	0	5,5,5	0.40	0
8	UMQ	E	408	-	33,33,35	0.24	0	44,44,46	0.80	2 (4%)
8	UMQ	E	409	-	33,33,35	0.21	0	44,44,46	0.54	0
5	GOL	E	403	-	5,5,5	0.16	0	5,5,5	0.26	0
9	ACT	E	407	-	3,3,3	1.20	0	3,3,3	0.92	0
5	GOL	C	403	-	5,5,5	0.13	0	5,5,5	0.44	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	C	406	-	-	8/18/58/60	0/2/2/2
8	UMQ	B	407	-	-	7/18/58/60	0/2/2/2
3	ABU	D	401	-	-	2/4/4/4	-
4	MES	B	402	-	-	0/6/14/14	0/1/1/1
4	MES	D	402	-	-	2/6/14/14	0/1/1/1
8	UMQ	B	406	-	-	5/18/58/60	0/2/2/2
4	MES	E	402	-	-	0/6/14/14	0/1/1/1
5	GOL	D	403	-	-	0/4/4/4	-
7	PG4	D	404	-	-	5/10/10/10	-
4	MES	C	402	-	-	1/6/14/14	0/1/1/1
5	GOL	B	403	-	-	2/4/4/4	-
3	ABU	E	401	-	-	2/4/4/4	-

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

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	ABU	O-C	2.91	1.31	1.22
3	E	401	ABU	O-C	2.90	1.31	1.22
3	D	401	ABU	O-C	2.83	1.31	1.22
3	E	401	ABU	OXT-C	-2.76	1.21	1.30
3	A	401	ABU	O-C	2.64	1.30	1.22
4	E	402	MES	C8-S	-2.60	1.73	1.77
3	C	401	ABU	OXT-C	-2.58	1.22	1.30
3	D	401	ABU	OXT-C	-2.55	1.22	1.30
3	A	401	ABU	OXT-C	-2.52	1.22	1.30
4	B	402	MES	C8-S	2.47	1.81	1.77
4	C	402	MES	C8-S	2.42	1.81	1.77
4	B	402	MES	C7-N4	2.19	1.52	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	ABU	OXT-C-CG	3.42	125.01	114.03
3	A	401	ABU	O-C-CG	-3.41	112.14	123.08
3	D	401	ABU	O-C-CG	-3.07	113.20	123.08
3	D	401	ABU	OXT-C-CG	3.03	123.78	114.03
3	E	401	ABU	OXT-C-CG	2.78	122.95	114.03
3	E	401	ABU	O-C-CG	-2.77	114.19	123.08
3	C	401	ABU	OXT-C-CG	2.55	122.21	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	401	ABU	O-C-CG	-2.33	115.59	123.08
8	E	408	UMQ	C3'-C4'-C5'	2.16	115.88	110.93
8	E	408	UMQ	O5'-C5'-C4'	2.13	114.25	109.75
8	B	407	UMQ	O2'-C2'-C1'	-2.02	105.15	110.05

There are no chirality outliers.

All (74) 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	406	UMQ	O5'-C1'-O1'-CA
8	E	409	UMQ	C2'-C1'-O1'-CA
8	E	409	UMQ	O5'-C1'-O1'-CA
8	B	407	UMQ	O5-C1-O1-C4'
8	E	408	UMQ	C3'-C4'-O1-C1
7	D	404	PG4	O3-C5-C6-O4
8	E	408	UMQ	C5'-C4'-O1-C1
8	E	408	UMQ	O5'-C5'-C6'-O6'
7	C	404	PG4	O3-C5-C6-O4
7	D	404	PG4	C6-C5-O3-C4
7	B	404	PG4	O2-C3-C4-O3
8	C	406	UMQ	O5-C1-O1-C4'
7	C	404	PG4	O4-C7-C8-O5
8	B	407	UMQ	O1'-CA-CB-CC
5	E	404	GOL	O1-C1-C2-C3
5	E	404	GOL	C1-C2-C3-O3
8	E	408	UMQ	O5-C5-C6-O6
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-C1-O1-C4'
8	E	408	UMQ	CA-CB-CC-CD
7	E	405	PG4	O2-C3-C4-O3
7	D	404	PG4	O2-C3-C4-O3
7	D	404	PG4	O1-C1-C2-O2
8	E	409	UMQ	C4-C5-C6-O6
8	E	409	UMQ	O5'-C5'-C6'-O6'
8	B	406	UMQ	CF-CG-CH-CI
8	B	407	UMQ	O5'-C5'-C6'-O6'

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

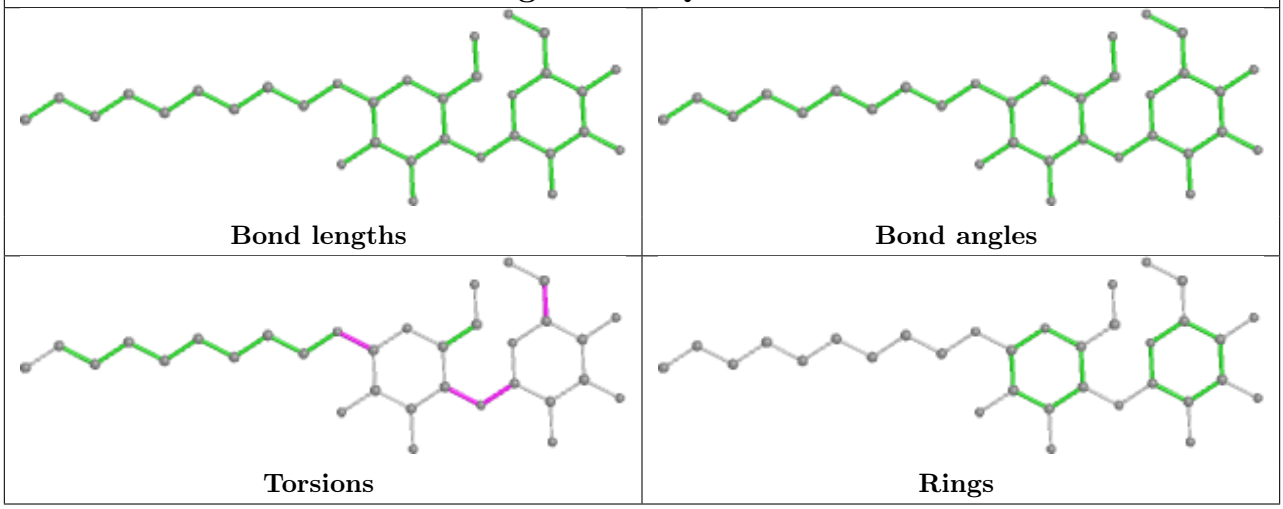
There are no ring outliers.

3 monomers are involved in 3 short contacts:

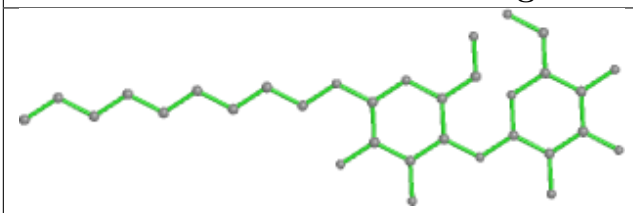
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	404	PG4	2	0
3	E	401	ABU	1	0
5	E	404	GOL	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

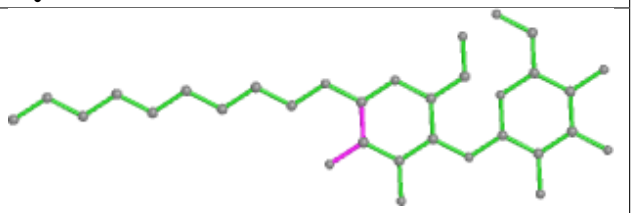
Ligand UMQ C 406



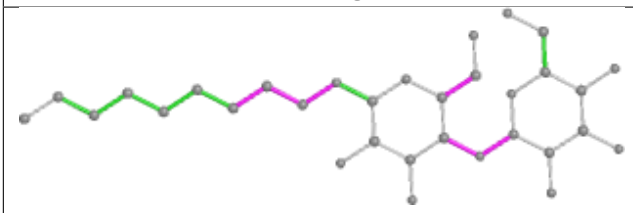
Ligand UMQ B 407



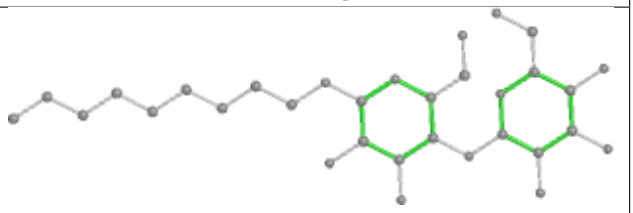
Bond lengths



Bond angles

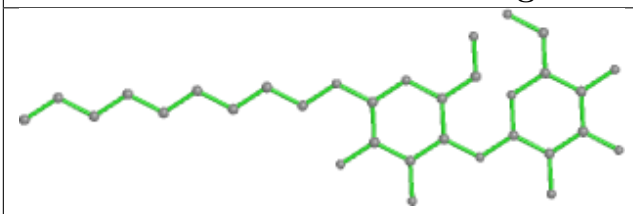


Torsions

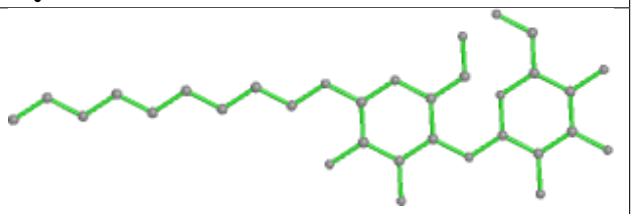


Rings

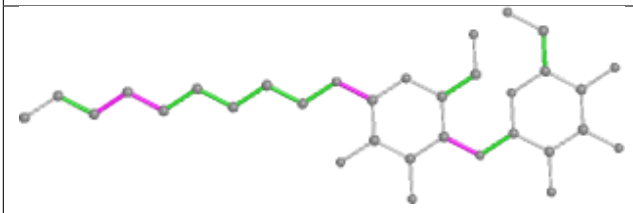
Ligand UMQ B 406



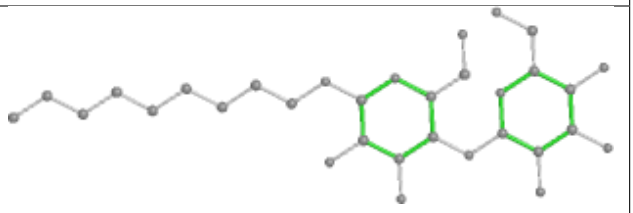
Bond lengths



Bond angles

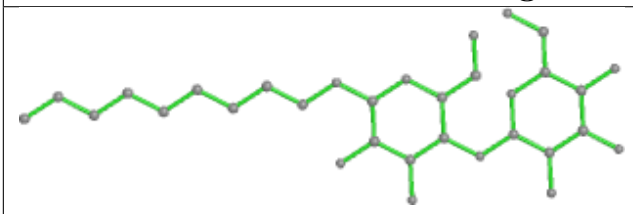


Torsions

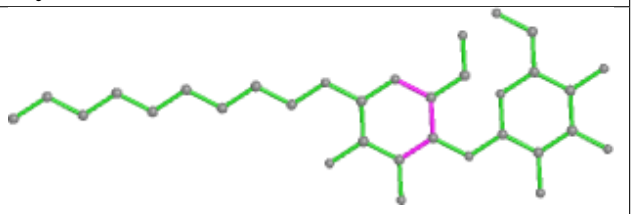


Rings

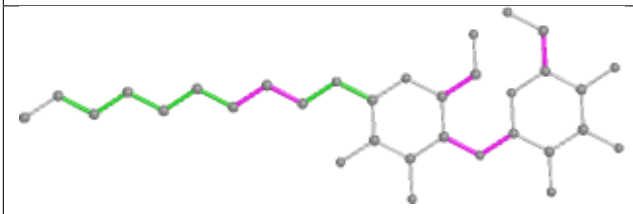
Ligand UMQ E 408



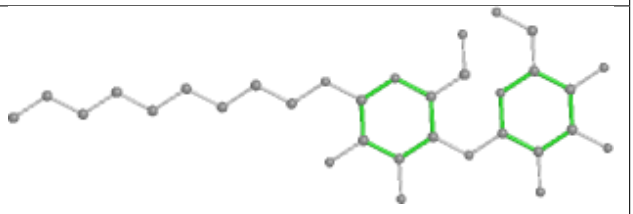
Bond lengths



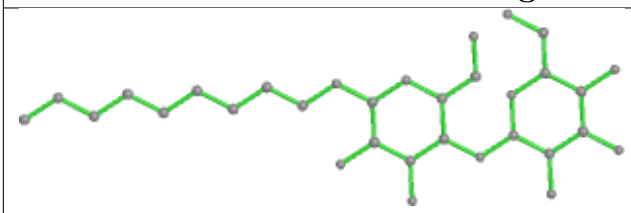
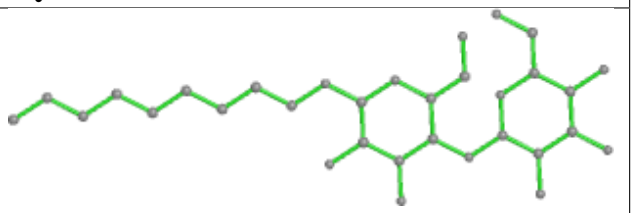
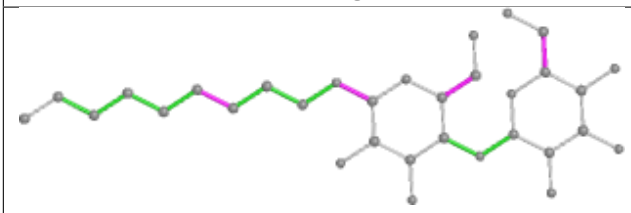
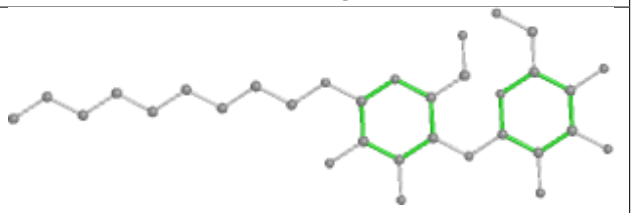
Bond angles



Torsions



Rings

Ligand UMQ E 409	
 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 (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%)	0.61	30 (9%)	7	5	48, 74, 113, 155	0
1	B	308/318 (96%)	0.85	49 (15%)	1	1	46, 71, 127, 158	0
1	C	307/318 (96%)	0.81	45 (14%)	2	1	46, 71, 119, 143	0
1	D	305/318 (95%)	0.82	40 (13%)	3	2	43, 74, 124, 149	0
1	E	304/318 (95%)	0.73	38 (12%)	3	2	48, 74, 112, 155	0
2	F	110/121 (90%)	1.79	42 (38%)	0	0	64, 97, 130, 138	0
2	G	111/121 (91%)	0.30	5 (4%)	33	26	50, 64, 87, 117	0
2	H	112/121 (92%)	0.27	0	100	100	47, 62, 91, 105	0
2	I	111/121 (91%)	0.93	23 (20%)	1	0	54, 75, 116, 134	0
2	J	110/121 (90%)	1.32	28 (25%)	0	0	61, 99, 129, 138	0
All	All	2081/2195 (94%)	0.81	300 (14%)	2	1	43, 74, 123, 158	0

All (300) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	VAL	10.1
1	C	314	VAL	9.6
1	D	7	VAL	8.5
2	J	107	VAL	8.5
1	A	314	VAL	7.9
2	F	12	ALA	7.6
1	E	313	CYS	7.5
2	F	109	VAL	7.5
1	B	297	ILE	7.3
1	A	317	ILE	7.2
1	A	288	ALA	7.1
1	C	7	VAL	6.6
2	F	90	THR	6.6

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Mol	Chain	Res	Type	RSRZ
2	F	13	GLN	6.5
2	F	110	SER	6.2
1	A	313	CYS	6.1
2	G	111	SER	6.1
1	E	312	GLY	6.1
1	B	306	LEU	6.1
1	C	316	VAL	6.0
1	D	163	ARG	6.0
1	B	8	ASP	6.0
2	F	18	MET	5.9
2	F	17	SER	5.8
2	F	40	ALA	5.6
2	F	14	ALA	5.5
2	F	15	GLY	5.4
2	F	108	THR	5.4
1	D	8	ASP	5.4
2	F	93	TYR	5.4
2	J	40	ALA	5.4
1	E	314	VAL	5.3
1	E	316	VAL	5.3
1	C	315	LEU	5.3
1	D	157	ILE	5.3
1	E	317	ILE	5.3
1	C	308	PHE	5.2
1	B	310	ALA	5.2
1	C	154	ASN	5.2
1	B	317	ILE	5.1
2	F	85	LEU	5.1
1	E	311	ILE	5.1
1	B	183	PRO	5.0
1	C	287	GLN	5.0
2	F	87	SER	5.0
1	C	288	ALA	5.0
1	B	314	VAL	5.0
1	E	290	GLY	4.9
1	D	286	ARG	4.9
1	A	247	PHE	4.9
1	D	315	LEU	4.8
1	D	198	VAL	4.8
1	B	282	PHE	4.8
2	I	42	GLY	4.7
1	D	282	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	315	LEU	4.6
2	F	16	GLY	4.6
1	B	308	PHE	4.6
1	E	179	SER	4.5
1	E	302	LEU	4.5
2	F	82	MET	4.5
1	D	313	CYS	4.4
1	A	310	ALA	4.4
2	F	83	SER	4.4
2	F	64	LYS	4.4
1	D	285	HIS	4.3
1	C	317	ILE	4.3
1	D	247	PHE	4.3
2	J	13	GLN	4.2
2	J	41	PRO	4.2
1	B	316	VAL	4.2
1	B	247	PHE	4.2
1	B	244	ALA	4.2
1	A	316	VAL	4.2
1	D	314	VAL	4.1
1	C	8	ASP	4.1
2	I	41	PRO	4.1
1	D	289	ASN	4.1
1	B	302	LEU	4.0
2	J	10	GLY	4.0
1	A	287	GLN	4.0
2	I	14	ALA	4.0
1	B	287	GLN	4.0
2	F	41	PRO	4.0
1	C	289	ASN	4.0
2	F	84	THR	4.0
1	A	244	ALA	3.9
1	D	9	ALA	3.9
1	C	313	CYS	3.9
2	J	93	TYR	3.9
1	D	183	PRO	3.9
2	F	11	LEU	3.9
1	E	183	PRO	3.9
1	B	286	ARG	3.8
1	C	247	PHE	3.8
1	D	306	LEU	3.8
2	I	13	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
2	I	110	SER	3.8
1	C	306	LEU	3.7
1	B	154	ASN	3.7
1	C	293	ASP	3.7
1	B	248	TYR	3.7
2	I	109	VAL	3.6
2	J	44	GLN	3.6
1	B	307	GLY	3.6
2	J	109	VAL	3.6
1	A	315	LEU	3.6
1	C	302	LEU	3.5
2	J	108	THR	3.5
1	B	153	ASP	3.5
1	A	183	PRO	3.5
2	F	67	PHE	3.5
1	A	311	ILE	3.4
1	C	243	VAL	3.4
2	G	13	GLN	3.4
1	D	288	ALA	3.4
1	A	240	LEU	3.4
1	A	164	GLY	3.4
1	B	288	ALA	3.4
1	E	288	ALA	3.4
2	J	27	ARG	3.4
1	B	296	LEU	3.4
2	I	85	LEU	3.4
1	D	49	LYS	3.4
1	B	311	ILE	3.4
1	E	296	LEU	3.3
1	E	304	PHE	3.3
1	A	163	ARG	3.3
1	B	312	GLY	3.3
1	D	308	PHE	3.3
2	F	88	GLU	3.3
2	J	90	THR	3.3
2	F	86	GLN	3.3
1	D	162	ILE	3.3
1	E	308	PHE	3.3
1	B	164	GLY	3.3
1	B	289	ASN	3.3
1	B	163	ARG	3.3
2	I	18	MET	3.3

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Mol	Chain	Res	Type	RSRZ
2	J	89	ASP	3.3
1	B	313	CYS	3.2
1	E	287	GLN	3.2
1	C	240	LEU	3.2
2	F	91	ALA	3.2
2	I	91	ALA	3.2
1	C	251	ASN	3.2
2	F	107	VAL	3.2
2	I	43	LYS	3.2
1	D	123	ARG	3.2
1	B	303	ALA	3.1
1	E	165	LYS	3.1
1	E	154	ASN	3.1
1	D	240	LEU	3.1
1	C	248	TYR	3.1
2	I	16	GLY	3.1
1	C	250	SER	3.1
2	F	89	ASP	3.1
1	B	240	LEU	3.1
2	J	105	THR	3.1
1	A	243	VAL	3.1
1	D	312	GLY	3.0
2	I	107	VAL	3.0
1	E	206	TRP	3.0
2	F	10	GLY	3.0
1	E	161	TRP	3.0
1	D	303	ALA	3.0
2	J	94	TYR	2.9
2	G	109	VAL	2.9
1	C	9	ALA	2.9
1	C	156	GLU	2.9
1	D	283	ALA	2.9
2	J	62	SER	2.9
2	F	65	GLY	2.9
2	I	10	GLY	2.9
2	F	7	SER	2.9
1	C	244	ALA	2.9
1	D	244	ALA	2.9
1	B	243	VAL	2.8
1	E	289	ASN	2.8
1	B	315	LEU	2.8
1	C	307	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	154	ASN	2.8
1	D	181	VAL	2.8
2	I	40	ALA	2.8
1	C	183	PRO	2.8
1	C	311	ILE	2.8
2	F	66	ARG	2.8
2	I	106	GLN	2.8
1	C	310	ALA	2.8
1	B	223	PHE	2.7
1	B	241	THR	2.7
1	A	251	ASN	2.7
2	J	14	ALA	2.7
1	A	248	TYR	2.7
1	E	163	ARG	2.7
1	B	294	ASP	2.7
2	F	63	VAL	2.7
1	B	161	TRP	2.7
2	F	20	LEU	2.6
2	F	38	ARG	2.6
1	A	242	VAL	2.6
2	J	87	SER	2.6
2	J	110	SER	2.6
2	J	92	VAL	2.6
1	E	240	LEU	2.6
2	F	21	SER	2.6
2	F	39	GLN	2.6
1	A	307	GLY	2.5
1	E	303	ALA	2.5
2	J	43	LYS	2.5
2	I	108	THR	2.5
2	J	65	GLY	2.5
1	A	161	TRP	2.5
1	E	164	GLY	2.5
1	B	304	PHE	2.5
1	C	161	TRP	2.5
1	D	161	TRP	2.5
1	C	163	ARG	2.5
1	B	184	ASN	2.4
2	J	39	GLN	2.4
2	G	108	THR	2.4
1	D	294	ASP	2.4
1	A	48	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	J	67	PHE	2.4
1	C	312	GLY	2.4
1	D	246	ALA	2.4
1	C	151	ASN	2.4
1	D	248	TYR	2.4
2	I	9	GLY	2.4
1	E	152	ILE	2.4
1	B	250	SER	2.4
1	B	162	ILE	2.4
2	J	1	GLN	2.4
1	C	282	PHE	2.3
1	D	160	TRP	2.3
1	C	152	ILE	2.3
1	E	185	GLN	2.3
2	F	94	TYR	2.3
2	G	110	SER	2.3
1	C	252	ILE	2.3
1	C	303	ALA	2.3
2	J	46	GLU	2.3
1	A	289	ASN	2.3
1	B	251	ASN	2.3
1	C	253	LEU	2.3
1	A	241	THR	2.3
1	A	245	TYR	2.3
1	B	123	ARG	2.2
1	B	157	ILE	2.2
1	B	236	PHE	2.2
1	D	184	ASN	2.2
1	E	198	VAL	2.2
1	E	247	PHE	2.2
1	B	156	GLU	2.2
1	C	224	TRP	2.2
1	B	246	ALA	2.2
2	I	90	THR	2.2
2	J	85	LEU	2.2
2	F	44	GLN	2.2
1	E	53	ASP	2.2
1	C	261	VAL	2.2
1	E	300	CYS	2.2
1	D	309	LEU	2.1
1	B	239	MET	2.1
1	C	283	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	246	ALA	2.1
2	F	42	GLY	2.1
2	F	61	ASP	2.1
1	A	52	GLY	2.1
1	D	182	GLN	2.1
1	C	318	ARG	2.1
1	D	251	ASN	2.1
1	A	312	GLY	2.1
1	D	243	VAL	2.1
1	E	248	TYR	2.1
2	F	60	ALA	2.1
1	A	237	THR	2.1
1	C	249	THR	2.1
1	A	250	SER	2.1
1	C	245	TYR	2.1
1	D	241	THR	2.1
2	I	93	TYR	2.1
1	E	157	ILE	2.1
1	C	164	GLY	2.1
1	E	156	GLU	2.1
1	E	305	PRO	2.1
1	E	297	ILE	2.1
1	B	245	TYR	2.0
2	I	88	GLU	2.0
1	D	316	VAL	2.0
2	F	48	VAL	2.0
2	I	92	VAL	2.0
1	C	179	SER	2.0
1	E	162	ILE	2.0
1	A	308	PHE	2.0
1	B	249	THR	2.0
2	I	17	SER	2.0
2	I	87	SER	2.0
2	J	38	ARG	2.0
2	J	106	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

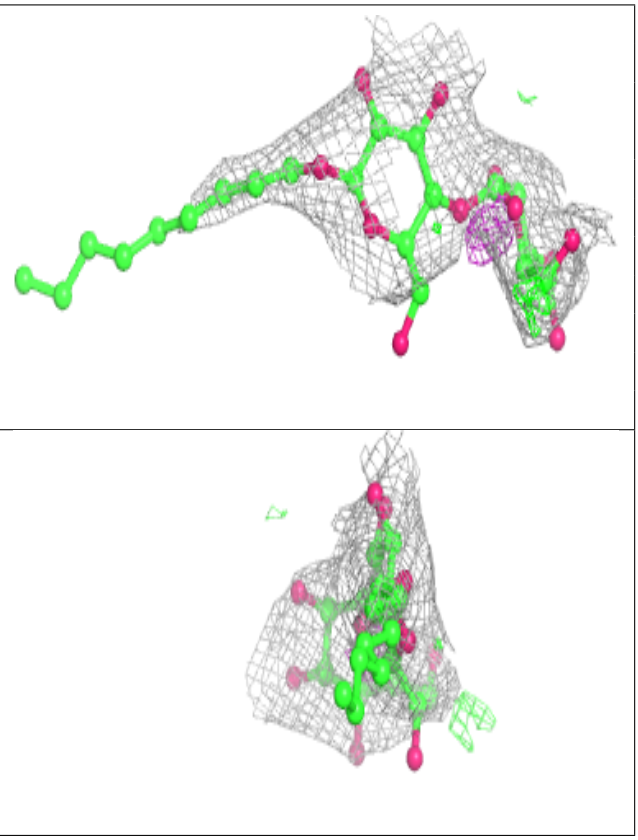
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CA	E	406	1/1	0.54	0.12	126,126,126,126	0
6	CA	C	405	1/1	0.56	0.10	110,110,110,110	0
6	CA	A	404	1/1	0.65	0.06	107,107,107,107	0
6	CA	B	405	1/1	0.69	0.12	118,118,118,118	0
5	GOL	E	404	6/6	0.70	0.28	89,91,91,92	0
4	MES	C	402	12/12	0.71	0.31	88,92,111,112	0
7	PG4	D	404	13/13	0.76	0.29	81,83,86,86	0
9	ACT	E	407	4/4	0.78	0.29	81,81,81,81	0
4	MES	A	402	12/12	0.79	0.24	87,92,116,116	0
7	PG4	C	404	13/13	0.79	0.34	97,101,103,103	0
7	PG4	E	405	13/13	0.80	0.28	82,83,86,86	0
8	UMQ	B	406	32/34	0.80	0.31	98,121,137,140	0
5	GOL	C	403	6/6	0.80	0.29	68,69,71,71	0
8	UMQ	B	407	32/34	0.81	0.31	100,114,130,135	0
5	GOL	B	403	6/6	0.82	0.23	73,77,78,78	0
8	UMQ	E	409	32/34	0.83	0.46	99,131,137,138	0
9	ACT	D	406	4/4	0.83	0.43	75,76,76,77	0
8	UMQ	E	408	32/34	0.83	0.25	95,120,134,135	0
3	ABU	A	401	7/7	0.84	0.19	68,74,83,84	0
3	ABU	E	401	7/7	0.84	0.29	63,68,76,78	0
7	PG4	B	404	13/13	0.85	0.22	82,84,86,87	0
4	MES	E	402	12/12	0.85	0.25	79,83,104,104	0
4	MES	B	402	12/12	0.87	0.27	89,92,105,106	0
5	GOL	A	403	6/6	0.87	0.31	72,73,75,75	0
4	MES	D	402	12/12	0.87	0.26	82,86,106,107	0
8	UMQ	C	406	32/34	0.87	0.27	106,122,131,134	0
3	ABU	D	401	7/7	0.88	0.20	68,70,77,77	0
5	GOL	D	403	6/6	0.89	0.31	74,76,79,81	0
3	ABU	B	401	7/7	0.90	0.16	64,69,77,77	0
5	GOL	E	403	6/6	0.91	0.22	73,74,74,75	0
3	ABU	C	401	7/7	0.92	0.24	58,62,71,72	0
6	CA	D	405	1/1	0.94	0.05	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.

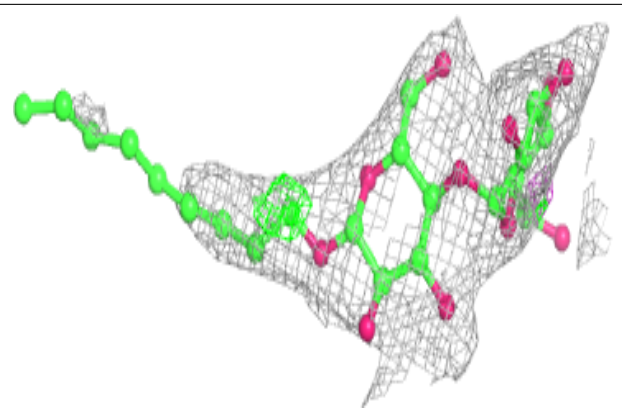
Electron density around UMQ B 406:

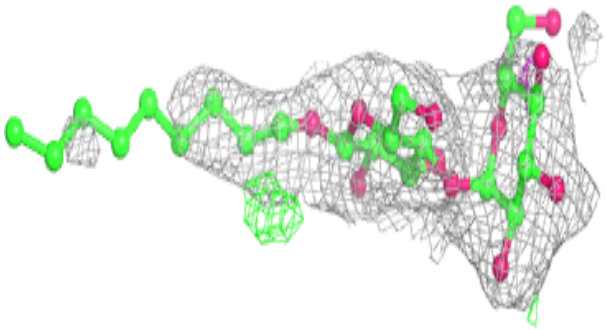
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

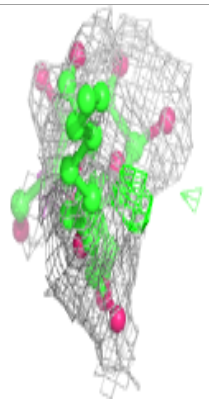


Electron density around UMQ B 407:

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

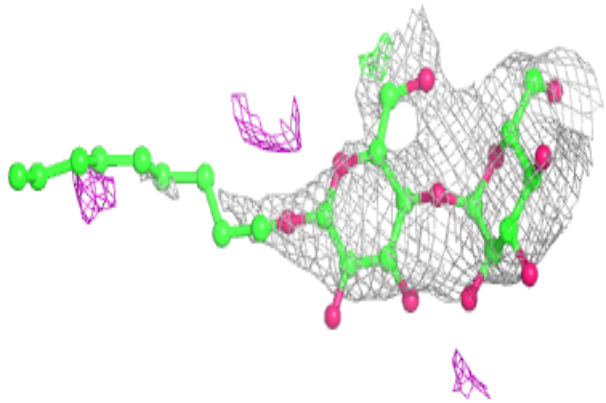


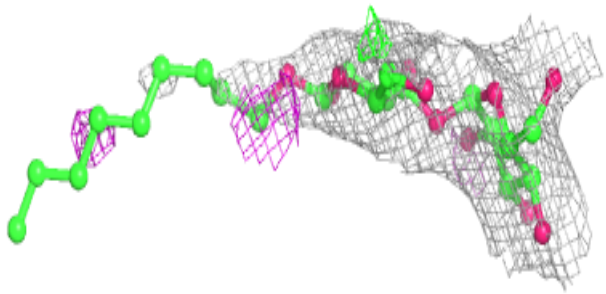


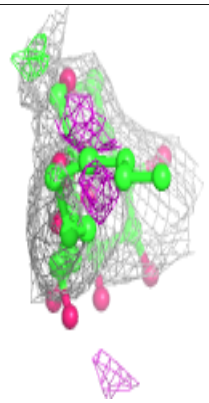


Electron density around UMQ E 409:

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

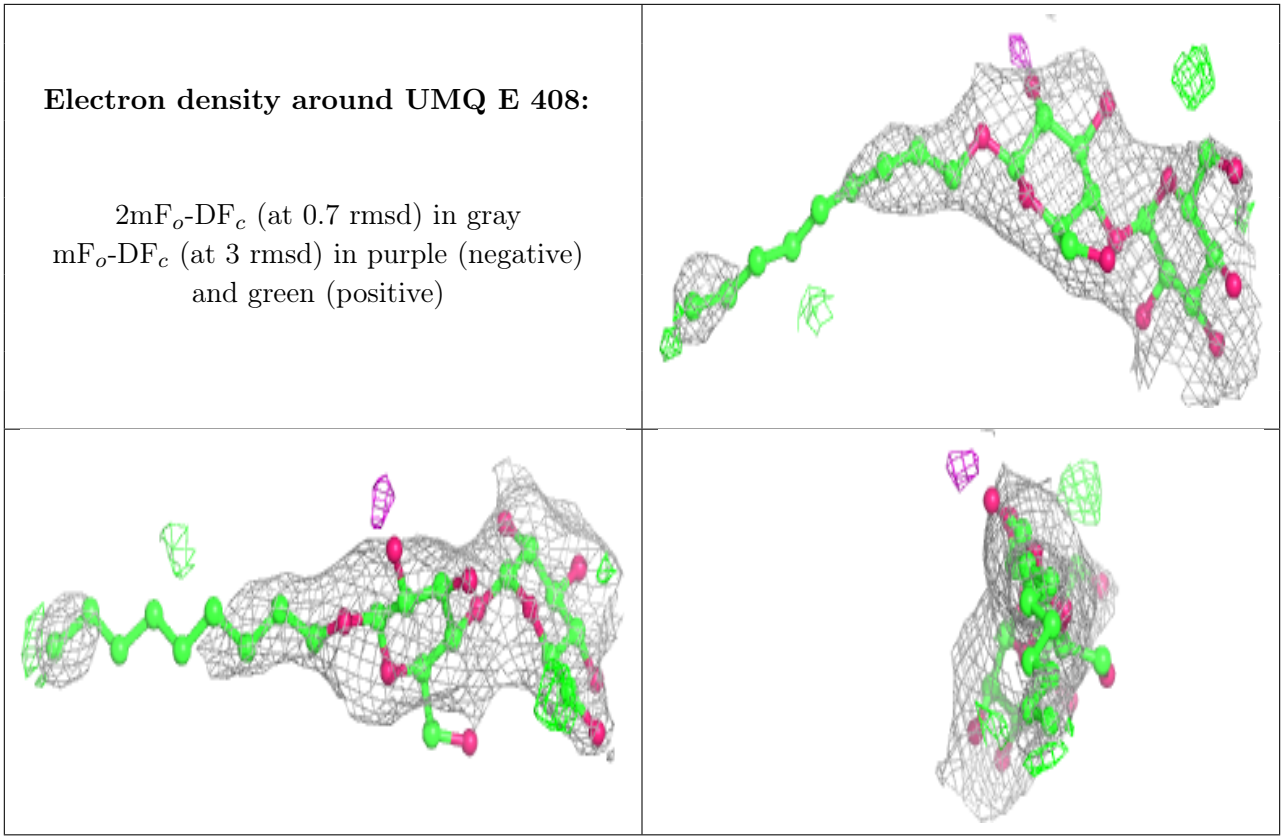






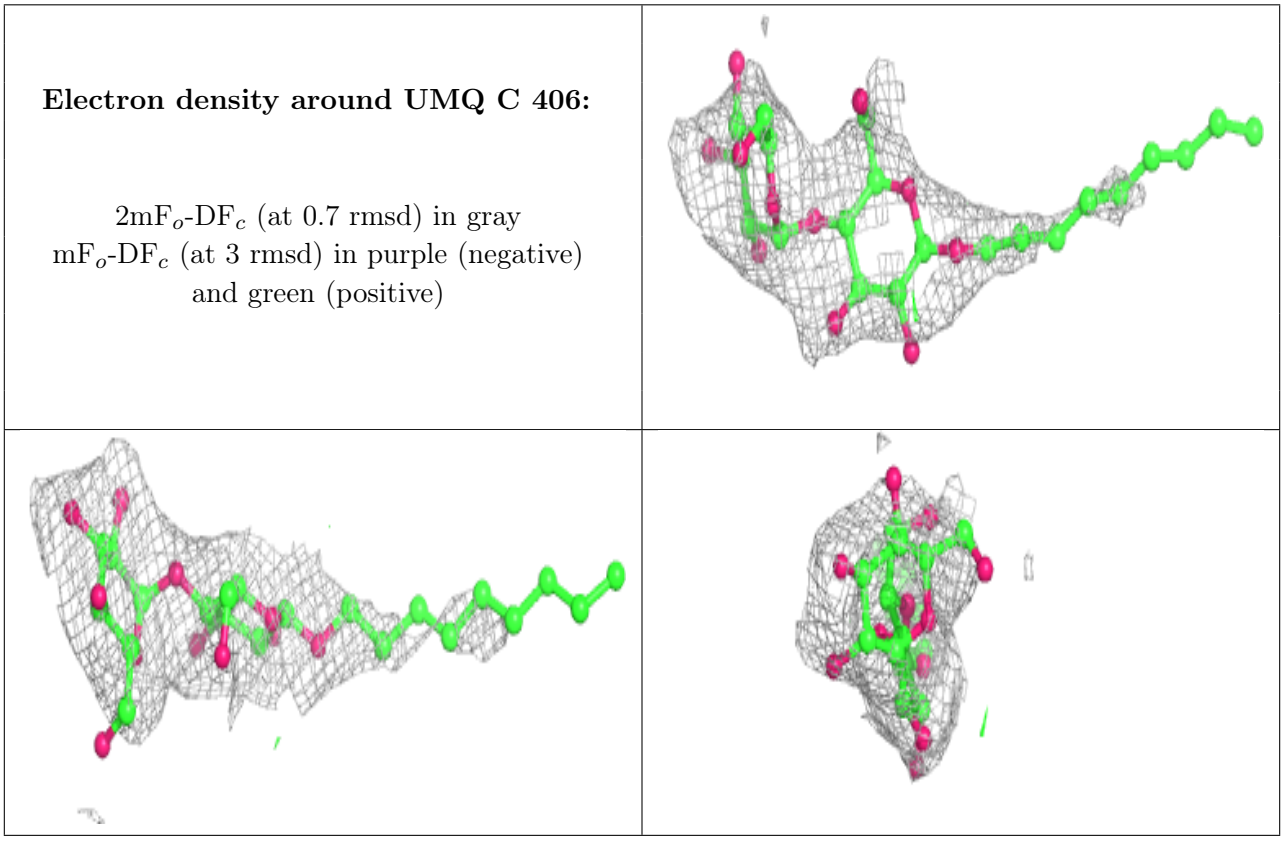
Electron density around UMQ E 408:

$2mF_o$-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)



6.5 Other polymers (i)

There are no such residues in this entry.