Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2020 – 11:16 AM BST

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

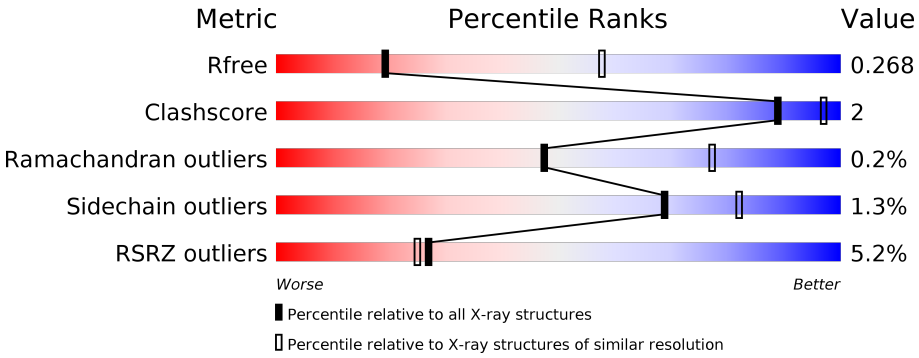
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	4% 88% 5% 6%
1	B	318	2% 88% 7%
1	C	318	3% 89% 5%
1	D	318	3% 90% 6%
1	E	318	2% 90% 5% 5%
1	F	318	3% 89% 7%

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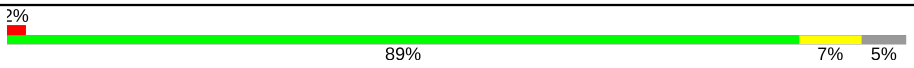
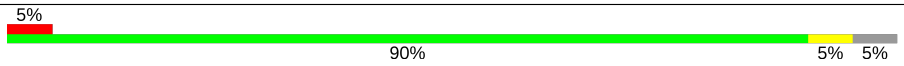
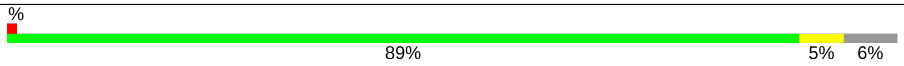
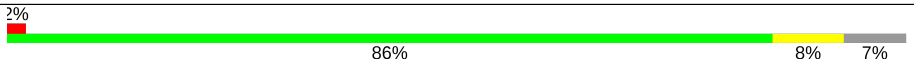
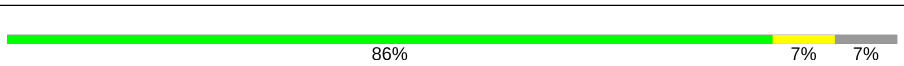
Mol	Chain	Length	Quality of chain
1	G	318	
1	H	318	
1	I	318	
1	J	318	
2	K	139	
2	L	139	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26239 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cys-loop ligand-gated ion channel.

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

There are 60 discrepancies between the modelled and reference sequences:

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

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

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

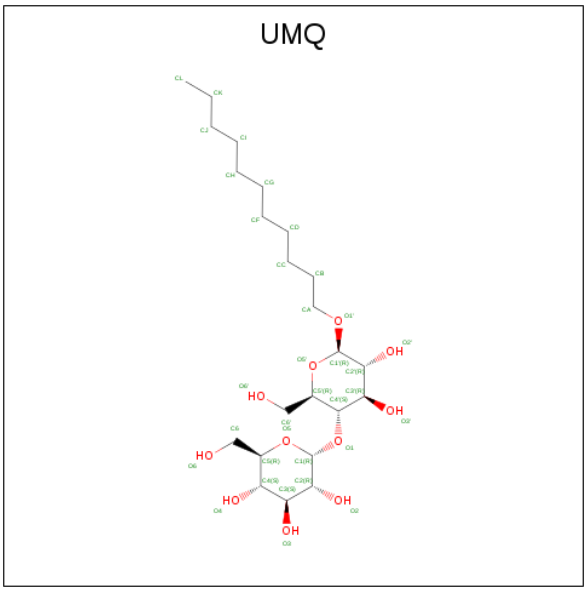
- Molecule 2 is a protein called NANOBODY 21.

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: $C_{23}H_{44}O_{11}$).



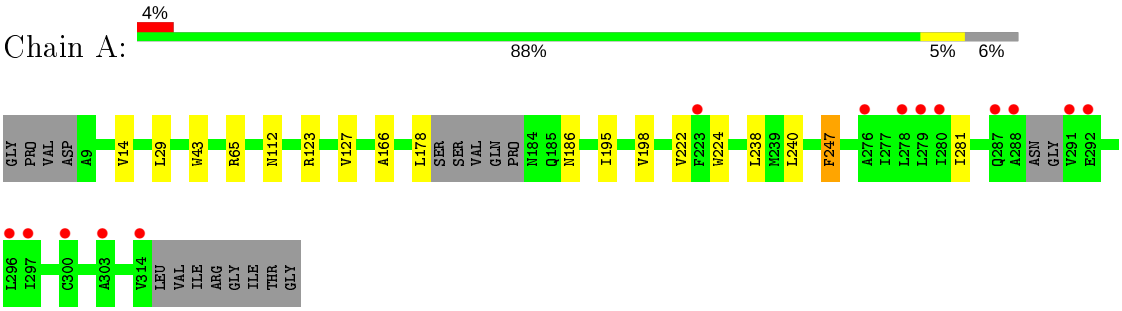
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 32 21 11	0	0
4	B	1	Total C O 32 21 11	0	0
4	B	1	Total C O 32 21 11	0	0
4	C	1	Total C O 32 21 11	0	0
4	E	1	Total C O 32 21 11	0	0
4	F	1	Total C O 32 21 11	0	0
4	G	1	Total C O 32 21 11	0	0
4	G	1	Total C O 32 21 11	0	0
4	I	1	Total C O 32 21 11	0	0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

3 Residue-property plots

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

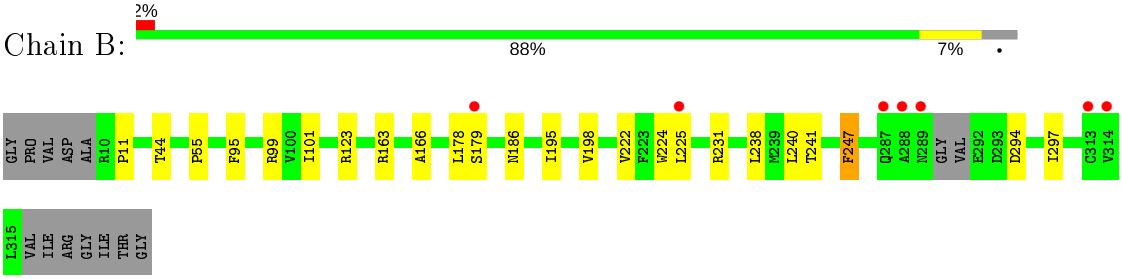
- Molecule 1: Cys-loop ligand-gated ion channel

Chain A:



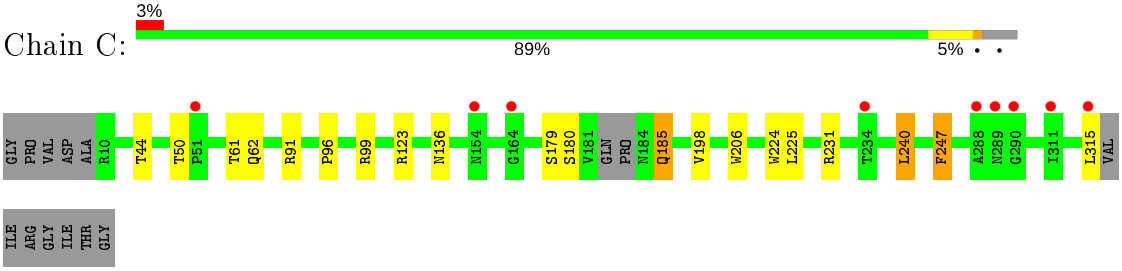
- Molecule 1: Cys-loop ligand-gated ion channel

Chain B:



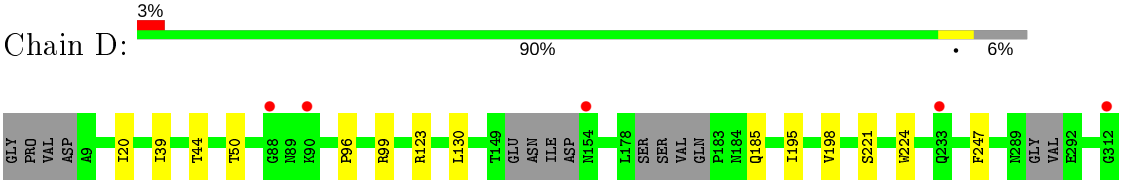
- Molecule 1: Cys-loop ligand-gated ion channel

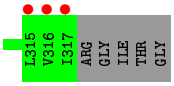
Chain C:



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

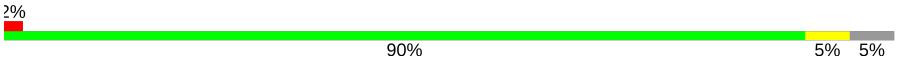
Chain D:

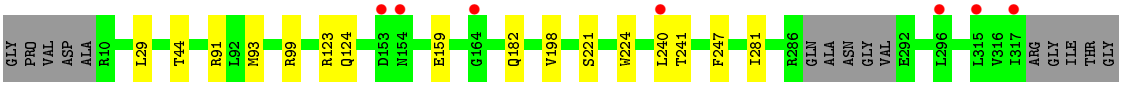




- Molecule 1: Cys-loop ligand-gated ion channel

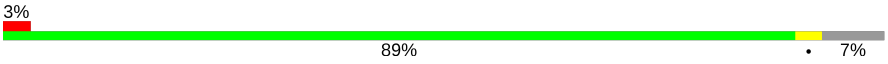
Chain E:

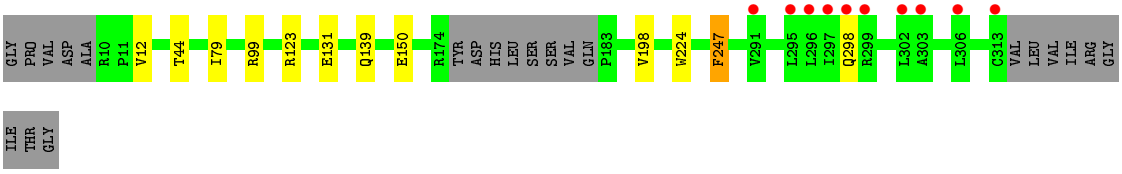




- Molecule 1: Cys-loop ligand-gated ion channel

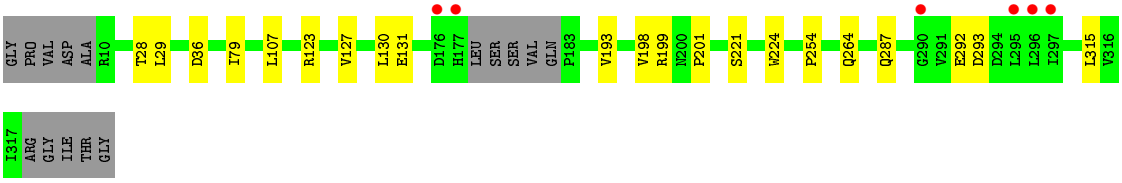
Chain F:





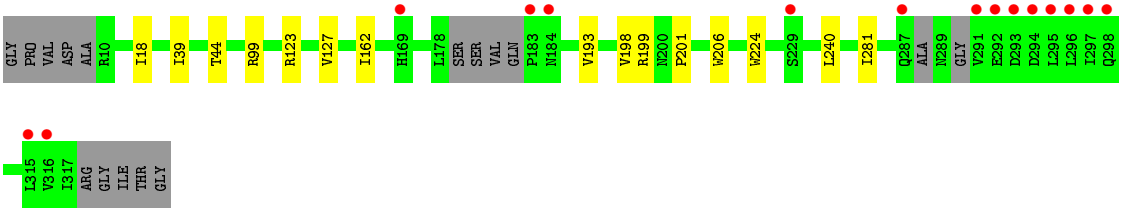
- Molecule 1: Cys-loop ligand-gated ion channel

Chain G:



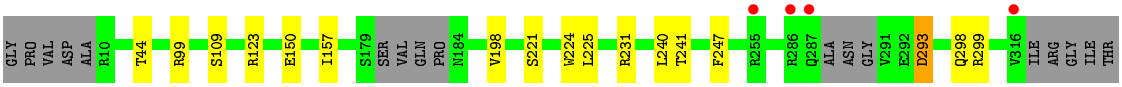
- Molecule 1: Cys-loop ligand-gated ion channel

Chain H:



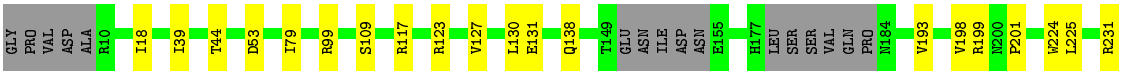
- Molecule 1: Cys-loop ligand-gated ion channel

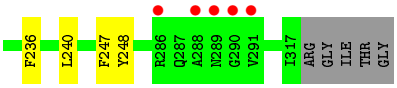
Chain I:



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

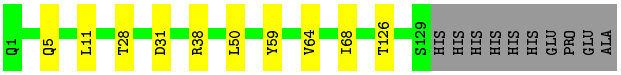
Chain J:





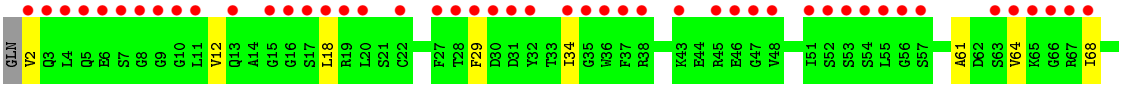
- Molecule 2: NANOBODY 21

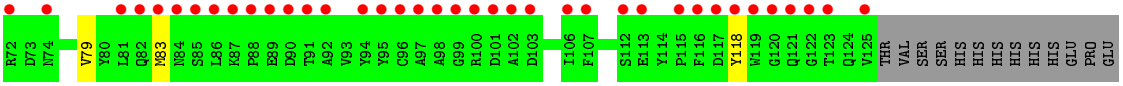
Chain K:



- Molecule 2: NANOBODY 21

Chain L:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	121.80Å 122.35Å 128.22Å 71.02° 64.19° 61.66°	Depositor
Resolution (Å)	48.32 – 3.25 48.32 – 3.25	Depositor EDS
% Data completeness (in resolution range)	89.9 (48.32-3.25) 89.9 (48.32-3.25)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.16-3549, BUSTER 2.10.3	Depositor
R, R_{free}	0.248 , 0.264 0.262 , 0.268	Depositor DCC
R_{free} test set	4097 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	97.6	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 40.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.018 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	26239	wwPDB-VP
Average B, all atoms (Å^2)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.42	0/2452	0.65	2/3348 (0.1%)
1	B	0.41	0/2492	0.65	2/3406 (0.1%)
1	C	0.38	0/2513	0.58	0/3431
1	D	0.38	0/2451	0.56	0/3347
1	E	0.40	0/2436	0.61	0/3334
1	F	0.39	0/2421	0.61	0/3306
1	G	0.39	0/2474	0.61	0/3381
1	H	0.38	0/2488	0.60	0/3397
1	I	0.40	0/2480	0.62	2/3385 (0.1%)
1	J	0.39	0/2449	0.60	0/3344
2	K	0.36	0/992	0.64	1/1346 (0.1%)
2	L	0.38	0/961	0.60	0/1303
All	All	0.39	0/26609	0.61	7/36328 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	163	ARG	NE-CZ-NH1	-10.09	115.26	120.30
1	B	163	ARG	NE-CZ-NH2	9.62	125.11	120.30
1	A	65	ARG	NE-CZ-NH1	-5.65	117.47	120.30
1	I	293	ASP	N-CA-C	-5.40	96.42	111.00
2	K	38	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	I	299	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	A	65	ARG	NE-CZ-NH2	5.08	122.84	120.30

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	2387	0	2298	13	0
1	B	2425	0	2320	15	0
1	C	2444	0	2359	14	0
1	D	2386	0	2315	9	0
1	E	2371	0	2262	11	0
1	F	2356	0	2271	6	0
1	G	2407	0	2332	10	0
1	H	2423	0	2342	7	0
1	I	2415	0	2345	7	0
1	J	2384	0	2315	13	0
2	K	972	0	917	4	0
2	L	941	0	893	7	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	F	2	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	32	0	37	0	0
4	B	64	0	74	2	0
4	C	32	0	37	1	0
4	E	32	0	37	0	0
4	F	32	0	37	0	0
4	G	64	0	74	0	0
4	I	32	0	37	1	0
4	J	32	0	37	0	0
All	All	26239	0	25339	98	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (98) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:79:ILE:HD11	1:G:131:GLU:HB2	1.66	0.76
2:L:34:ILE:HG21	2:L:79:VAL:HG21	1.69	0.74
1:A:123:ARG:HG2	1:A:198:VAL:HG12	1.74	0.69
1:I:123:ARG:HG2	1:I:198:VAL:HG22	1.75	0.68
1:B:294:ASP:HB2	1:B:297:ILE:HG22	1.77	0.67
4:B:403:UMQ:HC1	1:C:315:LEU:HD13	1.78	0.63
1:H:18:ILE:HG12	1:H:39:ILE:HD12	1.82	0.61
1:B:95:PHE:HE1	1:B:101:ILE:HD12	1.65	0.61
1:D:20:ILE:CD1	1:D:195:ILE:HD11	2.32	0.59
1:B:178:LEU:HD22	1:B:186:ASN:HA	1.87	0.56
1:B:95:PHE:CE1	1:B:101:ILE:HD12	2.41	0.55
1:G:221:SER:HB2	1:H:281:ILE:HD11	1.90	0.54
1:D:20:ILE:HD12	1:D:195:ILE:HD11	1.90	0.54
1:B:166:ALA:HB2	1:B:195:ILE:CD1	2.39	0.53
1:C:206:TRP:CZ2	4:C:402:UMQ:H5'1	2.45	0.51
2:L:61:ALA:HB3	2:L:64:VAL:HG22	1.92	0.51
2:K:64:VAL:HB	2:K:68:ILE:HD12	1.92	0.50
1:A:281:ILE:HD11	1:E:221:SER:HB2	1.94	0.50
1:C:61:THR:HG23	1:C:62:GLN:HE21	1.77	0.49
1:C:123:ARG:HG2	1:C:198:VAL:HG22	1.95	0.49
1:G:28:THR:HG21	1:G:254:PRO:HB2	1.93	0.49
1:B:101:ILE:HD13	1:C:179:SER:HB3	1.95	0.49
2:L:64:VAL:HB	2:L:68:ILE:HD12	1.95	0.49
1:A:178:LEU:HD11	1:A:186:ASN:HB3	1.94	0.49
4:B:403:UMQ:HC1	1:C:315:LEU:CD1	2.41	0.49
1:A:29:LEU:HD11	1:E:159:GLU:CD	2.33	0.48
1:F:123:ARG:HG2	1:F:198:VAL:HG22	1.96	0.48
1:B:101:ILE:HD13	1:C:179:SER:CB	2.43	0.48
1:J:123:ARG:HG2	1:J:198:VAL:HG22	1.95	0.48
1:C:136:ASN:ND2	1:C:185:GLN:HG3	2.29	0.48
1:F:79:ILE:HD11	1:F:131:GLU:HB3	1.94	0.48
1:A:166:ALA:HB2	1:A:195:ILE:HD13	1.96	0.47
1:J:79:ILE:HD11	1:J:131:GLU:HB3	1.95	0.47
1:A:240:LEU:HD21	1:E:240:LEU:HD22	1.95	0.47
1:A:166:ALA:HB2	1:A:195:ILE:CD1	2.44	0.47
1:I:157:ILE:HD11	1:J:117:ARG:NE	2.29	0.47
1:G:123:ARG:HG2	1:G:198:VAL:HG22	1.96	0.46
2:K:11:LEU:HD23	2:K:126:THR:HB	1.96	0.46
1:B:123:ARG:HG2	1:B:198:VAL:HG22	1.97	0.46
1:G:264:GLN:HB3	1:G:315:LEU:HD11	1.98	0.46
2:L:29:PHE:CE1	2:L:34:ILE:HD11	2.50	0.46
1:D:44:THR:HA	1:D:99:ARG:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:PHE:HE2	1:E:247:PHE:CG	2.35	0.45
1:B:247:PHE:CD2	1:C:247:PHE:HE2	2.34	0.45
1:D:39:ILE:HD11	1:D:130:LEU:HD11	1.98	0.45
1:E:123:ARG:HG2	1:E:198:VAL:HG22	1.98	0.45
1:J:18:ILE:HG12	1:J:39:ILE:HD12	1.98	0.45
1:F:44:THR:HA	1:F:99:ARG:HA	1.99	0.45
1:G:287:GLN:OE1	1:G:292:GLU:CB	2.65	0.45
1:B:241:THR:OG1	1:C:240:LEU:HD12	2.17	0.44
1:D:50:THR:HG22	1:D:96:PRO:HB3	1.99	0.44
1:G:36:ASP:HB2	1:G:107:LEU:HD13	1.99	0.44
1:H:206:TRP:CZ2	4:I:401:UMQ:H5'1	2.51	0.44
2:K:50:LEU:HD12	2:K:59:TYR:HD1	1.83	0.44
1:C:50:THR:OG1	1:C:96:PRO:HG3	2.17	0.44
1:J:79:ILE:CD1	1:J:131:GLU:HB3	2.48	0.44
2:L:2:VAL:HG21	2:L:118:TYR:CZ	2.53	0.43
1:J:44:THR:HA	1:J:99:ARG:HA	2.00	0.43
1:G:199:ARG:O	1:G:201:PRO:HD3	2.19	0.43
1:J:199:ARG:O	1:J:201:PRO:HD3	2.18	0.43
1:D:20:ILE:CD1	1:D:195:ILE:CD1	2.97	0.43
1:A:240:LEU:HD13	1:E:241:THR:HA	2.01	0.43
1:H:123:ARG:HG2	1:H:198:VAL:HG22	2.00	0.43
1:E:44:THR:HA	1:E:99:ARG:HA	2.00	0.42
1:B:294:ASP:HB2	1:B:297:ILE:CG2	2.46	0.42
1:B:222:VAL:HG13	1:B:238:LEU:HD21	2.00	0.42
1:C:247:PHE:CD2	1:D:247:PHE:HE2	2.37	0.42
1:E:91:ARG:NH1	1:E:93:MET:HB2	2.35	0.42
1:H:199:ARG:O	1:H:201:PRO:HD3	2.20	0.42
1:A:247:PHE:HE2	1:E:247:PHE:CD2	2.37	0.42
1:A:14:VAL:HG22	1:A:43:TRP:HB3	2.02	0.42
1:B:222:VAL:HG13	1:B:238:LEU:CD2	2.50	0.42
1:B:44:THR:HA	1:B:99:ARG:HA	2.02	0.42
1:D:123:ARG:HG2	1:D:198:VAL:HG22	2.01	0.42
1:H:44:THR:HA	1:H:99:ARG:HA	2.01	0.42
2:L:2:VAL:HG11	2:L:118:TYR:CG	2.54	0.42
1:J:127:VAL:HA	1:J:193:VAL:O	2.20	0.41
1:D:221:SER:HB2	1:E:281:ILE:HD11	2.02	0.41
1:E:29:LEU:HA	1:E:29:LEU:HD12	1.94	0.41
1:G:29:LEU:HD12	1:G:29:LEU:HA	1.92	0.41
1:F:247:PHE:HA	1:J:248:TYR:HD1	1.85	0.41
1:F:247:PHE:HE2	1:J:247:PHE:CD2	2.38	0.41
1:C:44:THR:HA	1:C:99:ARG:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:LEU:HB2	1:C:231:ARG:HG3	2.03	0.41
1:J:225:LEU:HB2	1:J:231:ARG:HG3	2.03	0.41
1:I:221:SER:OG	1:J:236:PHE:HZ	2.04	0.41
1:I:225:LEU:HB2	1:I:231:ARG:HG3	2.03	0.41
1:I:44:THR:HA	1:I:99:ARG:HA	2.02	0.41
2:K:28:THR:HB	2:K:31:ASP:OD1	2.20	0.41
1:I:241:THR:OG1	1:J:240:LEU:HD12	2.21	0.41
1:B:225:LEU:HB2	1:B:231:ARG:HG3	2.02	0.40
2:L:12:VAL:HG21	2:L:18:LEU:HG	2.03	0.40
1:A:112:ASN:HB2	1:A:127:VAL:HG22	2.02	0.40
1:G:127:VAL:HA	1:G:193:VAL:O	2.21	0.40
1:A:222:VAL:HG13	1:A:238:LEU:HD21	2.03	0.40
1:F:12:VAL:HG12	1:F:139:GLN:O	2.22	0.40
1:H:127:VAL:HA	1:H:193:VAL:O	2.21	0.40
1:I:293:ASP:O	1:I:298:GLN:NE2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	293/318 (92%)	287 (98%)	6 (2%)	0	100	100
1	B	300/318 (94%)	291 (97%)	8 (3%)	1 (0%)	41	72
1	C	301/318 (95%)	289 (96%)	10 (3%)	2 (1%)	22	56
1	D	291/318 (92%)	284 (98%)	7 (2%)	0	100	100
1	E	299/318 (94%)	288 (96%)	10 (3%)	1 (0%)	41	72
1	F	292/318 (92%)	279 (96%)	13 (4%)	0	100	100
1	G	299/318 (94%)	284 (95%)	14 (5%)	1 (0%)	41	72
1	H	295/318 (93%)	288 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	294/318 (92%)	282 (96%)	12 (4%)	0	100	100
1	J	291/318 (92%)	285 (98%)	6 (2%)	0	100	100
2	K	127/139 (91%)	119 (94%)	8 (6%)	0	100	100
2	L	122/139 (88%)	115 (94%)	7 (6%)	0	100	100
All	All	3204/3458 (93%)	3091 (96%)	108 (3%)	5 (0%)	47	77

All (5) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (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	250/282 (89%)	248 (99%)	2 (1%)	81	89
1	B	257/282 (91%)	252 (98%)	5 (2%)	57	76
1	C	261/282 (93%)	257 (98%)	4 (2%)	65	80
1	D	252/282 (89%)	250 (99%)	2 (1%)	81	89
1	E	246/282 (87%)	244 (99%)	2 (1%)	81	89
1	F	247/282 (88%)	243 (98%)	4 (2%)	62	79
1	G	253/282 (90%)	251 (99%)	2 (1%)	81	89
1	H	259/282 (92%)	256 (99%)	3 (1%)	71	83
1	I	259/282 (92%)	254 (98%)	5 (2%)	57	76
1	J	254/282 (90%)	249 (98%)	5 (2%)	55	76
2	K	101/113 (89%)	100 (99%)	1 (1%)	76	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	L	97/113 (86%)	96 (99%)	1 (1%)	76 85
All	All	2736/3046 (90%)	2700 (99%)	36 (1%)	69 82

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	224	TRP
1	A	247	PHE
1	B	11	PRO
1	B	55	PRO
1	B	224	TRP
1	B	240	LEU
1	B	247	PHE
1	C	91	ARG
1	C	224	TRP
1	C	240	LEU
1	C	247	PHE
1	D	185	GLN
1	D	224	TRP
1	E	124	GLN
1	E	224	TRP
1	F	150	GLU
1	F	224	TRP
1	F	247	PHE
1	F	298	GLN
1	G	130	LEU
1	G	224	TRP
1	H	162	ILE
1	H	224	TRP
1	H	240	LEU
1	I	109	SER
1	I	150	GLU
1	I	224	TRP
1	I	240	LEU
1	I	247	PHE
1	J	53	ASP
1	J	109	SER
1	J	130	LEU
1	J	138	GLN
1	J	224	TRP
2	K	5	GLN
2	L	83	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	C	103	ASN
1	D	138	GLN
1	E	124	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	UMQ	E	401	-	33,33,35	0.24	0	44,44,46	0.54	0
4	UMQ	J	401	-	33,33,35	0.23	0	44,44,46	0.49	0
4	UMQ	B	402	-	33,33,35	0.25	0	44,44,46	0.77	1 (2%)
4	UMQ	G	402	-	33,33,35	0.23	0	44,44,46	0.69	0
4	UMQ	G	403	-	33,33,35	0.21	0	44,44,46	0.47	0
4	UMQ	A	402	-	33,33,35	0.21	0	44,44,46	0.51	0
4	UMQ	I	401	-	33,33,35	0.25	0	44,44,46	0.47	0
4	UMQ	F	403	-	33,33,35	0.21	0	44,44,46	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	UMQ	B	403	-	33,33,35	0.22	0	44,44,46	0.53	0
4	UMQ	C	402	-	33,33,35	0.25	0	44,44,46	0.46	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
4	UMQ	E	401	-	-	7/18/58/60	0/2/2/2
4	UMQ	J	401	-	-	7/18/58/60	0/2/2/2
4	UMQ	B	402	-	-	9/18/58/60	0/2/2/2
4	UMQ	G	402	-	-	9/18/58/60	0/2/2/2
4	UMQ	G	403	-	-	5/18/58/60	0/2/2/2
4	UMQ	A	402	-	-	6/18/58/60	0/2/2/2
4	UMQ	I	401	-	-	6/18/58/60	0/2/2/2
4	UMQ	F	403	-	-	5/18/58/60	0/2/2/2
4	UMQ	B	403	-	-	6/18/58/60	0/2/2/2
4	UMQ	C	402	-	-	8/18/58/60	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	402	UMQ	C3'-C4'-C5'	2.13	115.80	110.93

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	403	UMQ	C2'-C1'-O1'-CA
4	G	403	UMQ	O5'-C1'-O1'-CA
4	A	402	UMQ	C2'-C1'-O1'-CA
4	A	402	UMQ	O5'-C1'-O1'-CA
4	F	403	UMQ	C2'-C1'-O1'-CA
4	F	403	UMQ	O5'-C1'-O1'-CA
4	B	403	UMQ	C2'-C1'-O1'-CA
4	B	403	UMQ	O5'-C1'-O1'-CA
4	E	401	UMQ	O5-C1-O1-C4'

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

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

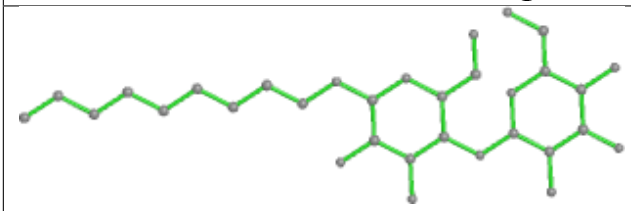
There are no ring outliers.

3 monomers are involved in 4 short contacts:

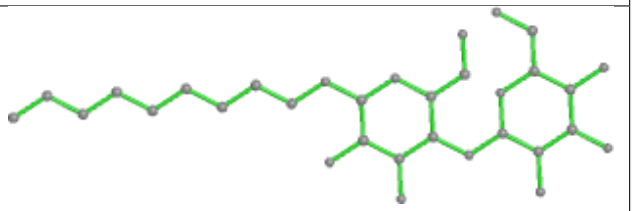
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	401	UMQ	1	0
4	B	403	UMQ	2	0
4	C	402	UMQ	1	0

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

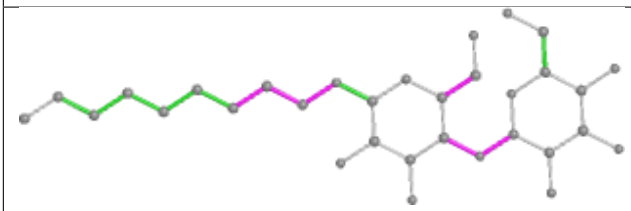
Ligand UMQ E 401



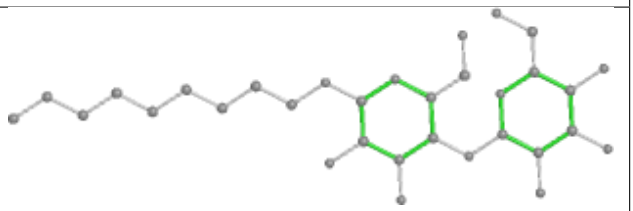
Bond lengths



Bond angles

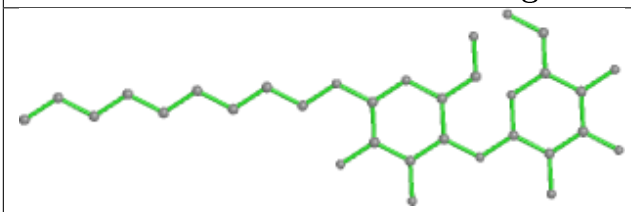


Torsions

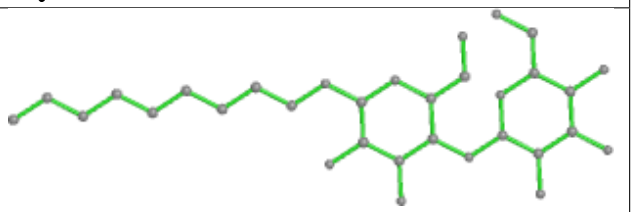


Rings

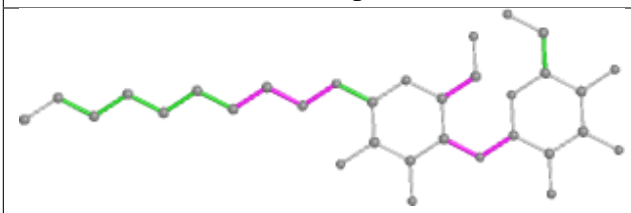
Ligand UMQ J 401



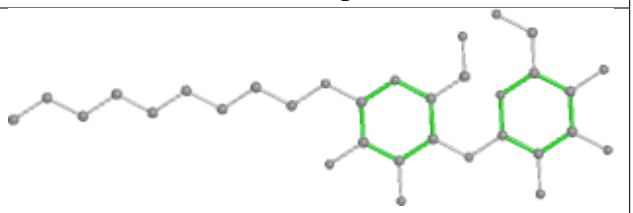
Bond lengths



Bond angles

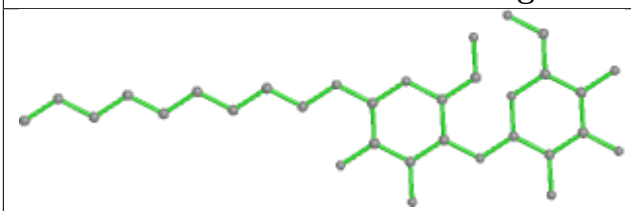


Torsions

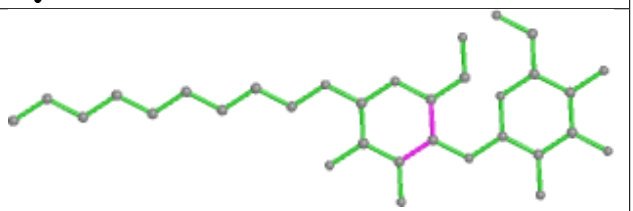


Rings

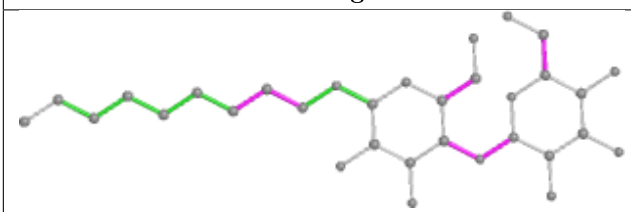
Ligand UMQ B 402



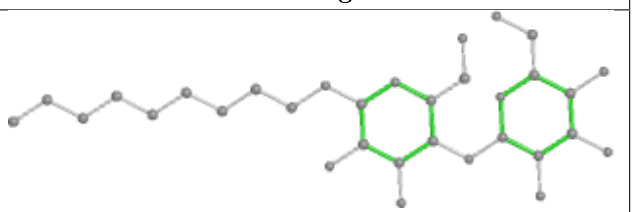
Bond lengths



Bond angles

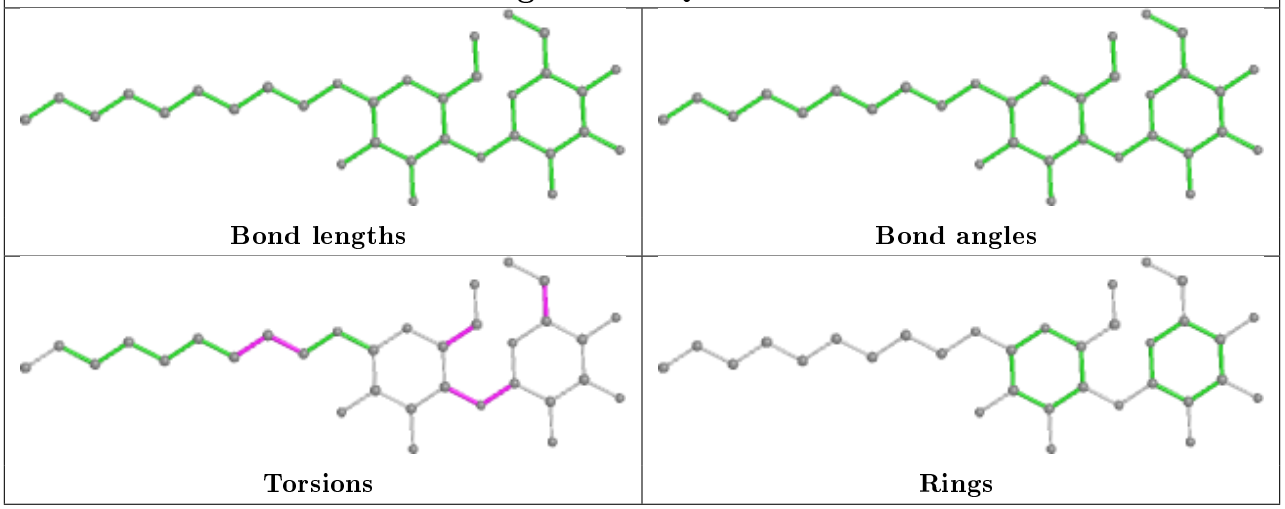


Torsions

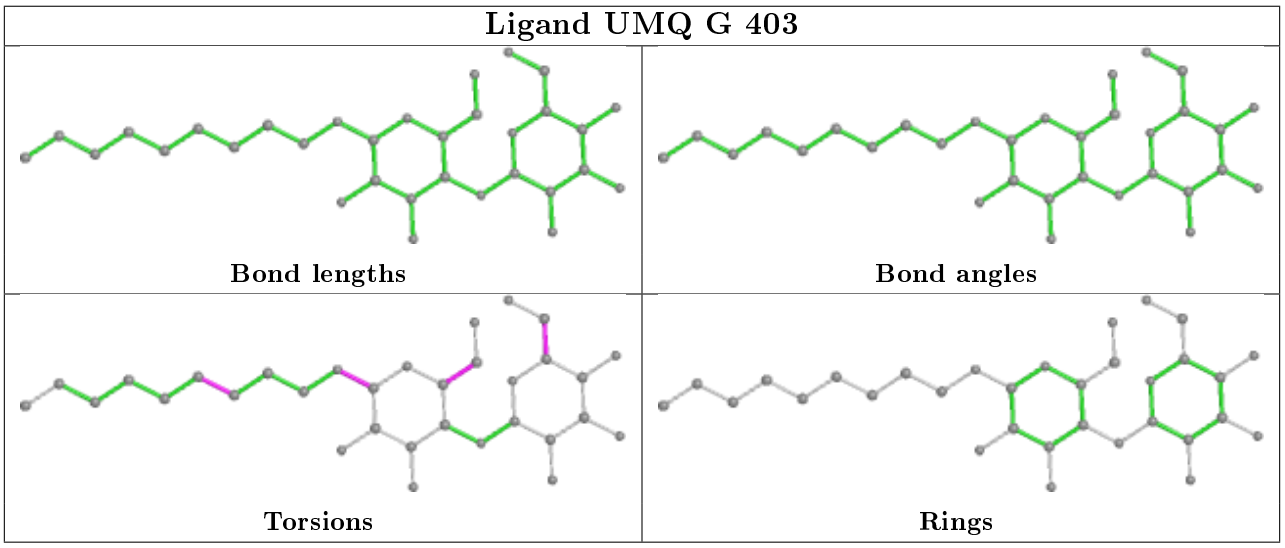


Rings

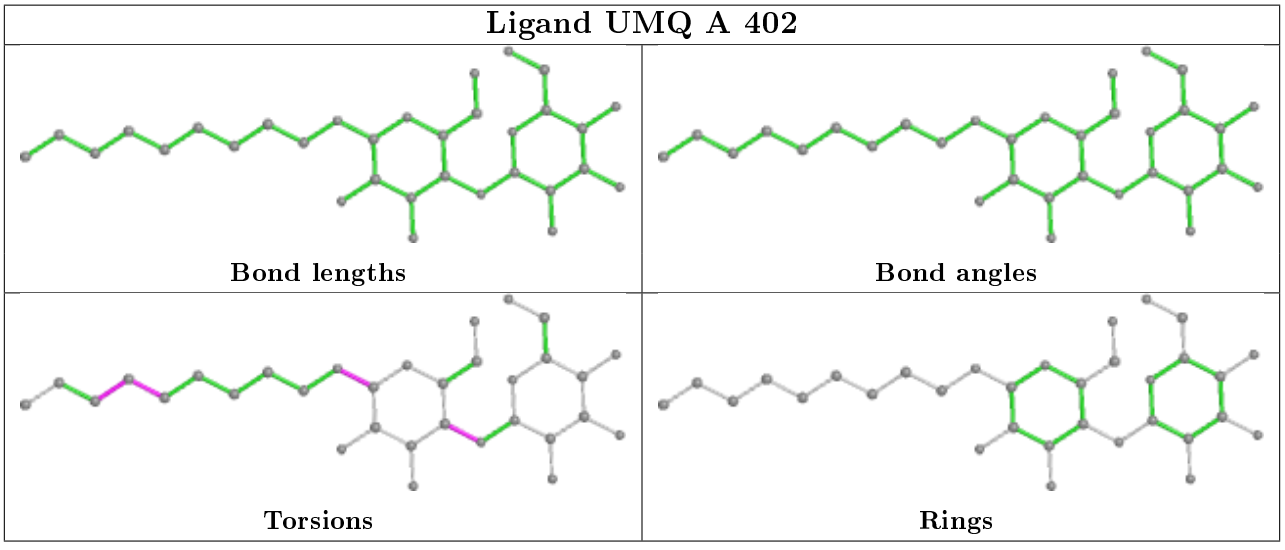
Ligand UMQ G 402



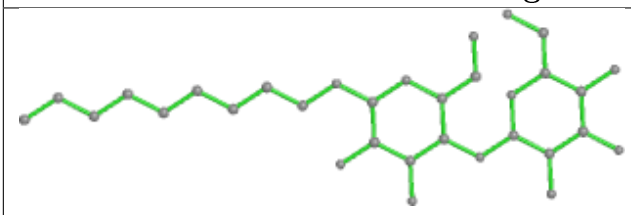
Ligand UMQ G 403



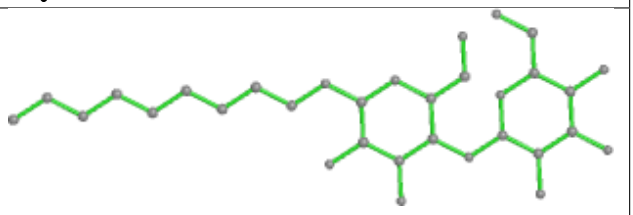
Ligand UMQ A 402



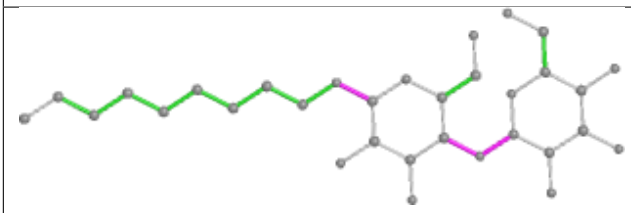
Ligand UMQ I 401



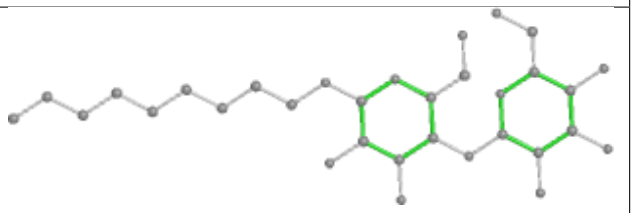
Bond lengths



Bond angles

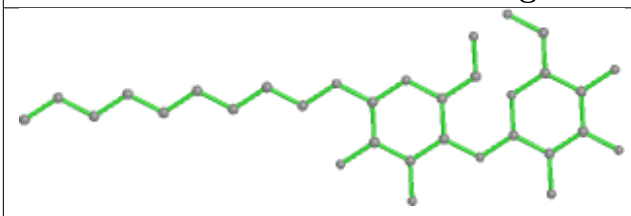


Torsions

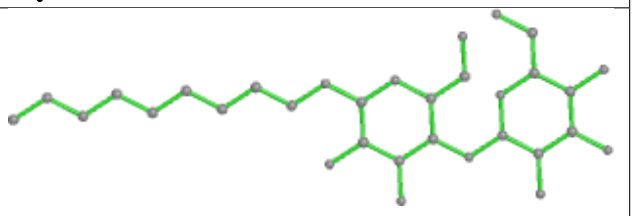


Rings

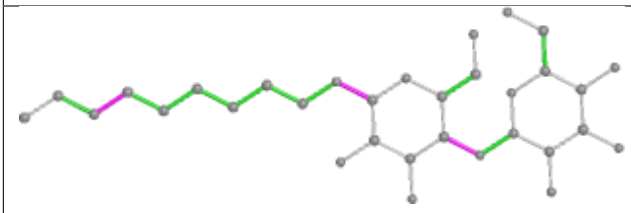
Ligand UMQ F 403



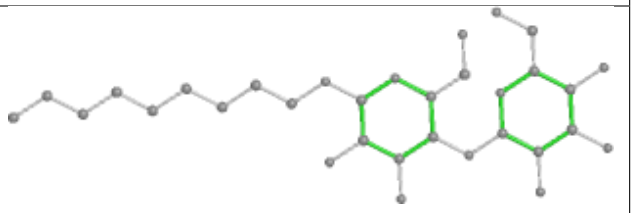
Bond lengths



Bond angles

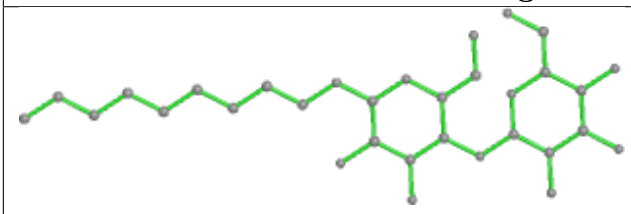


Torsions

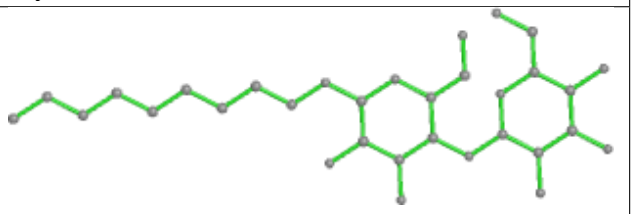


Rings

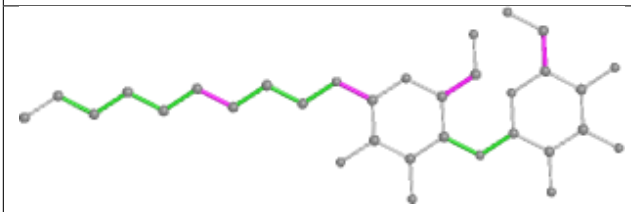
Ligand UMQ B 403



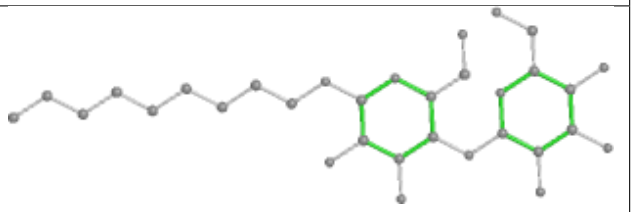
Bond lengths



Bond angles

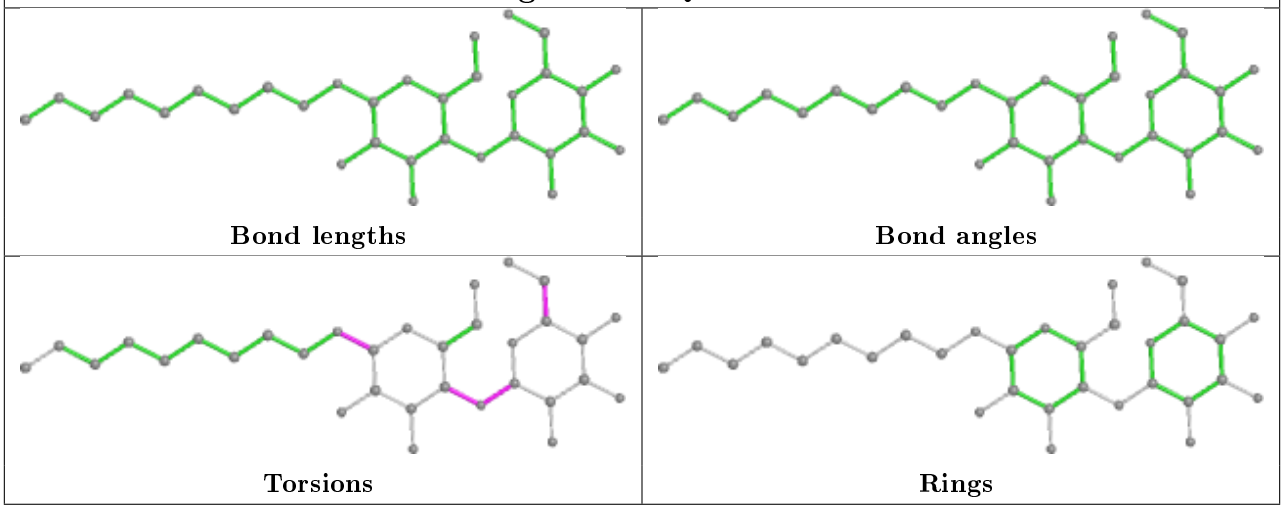


Torsions



Rings

Ligand UMQ C 402



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	299/318 (94%)	-0.13	14 (4%) 31 28	56, 96, 170, 196	0
1	B	304/318 (95%)	-0.31	7 (2%) 60 58	53, 91, 164, 188	0
1	C	304/318 (95%)	-0.37	9 (2%) 50 48	73, 106, 160, 183	0
1	D	299/318 (94%)	-0.26	8 (2%) 54 51	77, 112, 168, 185	0
1	E	303/318 (95%)	-0.44	7 (2%) 60 58	63, 103, 155, 184	0
1	F	296/318 (93%)	-0.17	10 (3%) 45 42	75, 109, 169, 184	0
1	G	303/318 (95%)	-0.27	6 (1%) 65 63	74, 108, 173, 201	0
1	H	302/318 (94%)	-0.22	15 (4%) 28 26	65, 100, 178, 208	0
1	I	300/318 (94%)	-0.36	4 (1%) 77 75	55, 90, 168, 190	0
1	J	297/318 (93%)	-0.36	5 (1%) 70 67	63, 95, 155, 188	0
2	K	129/139 (92%)	-0.58	0 100 100	63, 81, 110, 113	0
2	L	124/139 (89%)	3.61	85 (68%) 0 0	53, 72, 83, 84	124 (100%)
All	All	3260/3458 (94%)	-0.15	170 (5%) 27 25	53, 100, 166, 208	124 (3%)

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	291	VAL	15.3
2	L	3	GLN	10.5
2	L	2	VAL	10.3
2	L	120	GLY	10.0
2	L	121	GLN	9.9
2	L	4	LEU	9.0
1	A	288	ALA	8.6
2	L	117	ASP	8.6
2	L	55	LEU	8.4
2	L	118	TYR	8.2
2	L	54	SER	7.8

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Mol	Chain	Res	Type	RSRZ
2	L	63	SER	7.6
2	L	90	ASP	7.5
2	L	85	SER	7.4
2	L	92	ALA	7.3
2	L	5	GLN	7.2
2	L	38	ARG	7.0
2	L	31	ASP	6.9
1	D	315	LEU	6.9
2	L	9	GLY	6.9
2	L	83	MET	6.8
2	L	18	LEU	6.7
2	L	30	ASP	6.3
2	L	37	PHE	6.2
2	L	67	ARG	5.9
2	L	8	GLY	5.9
2	L	100	ARG	5.9
2	L	119	TRP	5.8
2	L	6	GLU	5.7
2	L	99	GLY	5.7
2	L	56	GLY	5.6
1	A	296	LEU	5.4
1	B	179	SER	5.4
1	F	297	ILE	5.4
2	L	45	ARG	5.3
2	L	34	ILE	5.1
2	L	94	TYR	5.1
1	G	296	LEU	5.0
2	L	53	SER	5.0
1	H	295	LEU	4.9
1	G	297	ILE	4.9
2	L	15	GLY	4.8
1	A	287	GLN	4.7
2	L	84	ASN	4.6
2	L	19	ARG	4.6
2	L	91	THR	4.6
2	L	98	ALA	4.5
2	L	113	GLU	4.5
2	L	82	GLN	4.5
1	F	296	LEU	4.5
2	L	35	GLY	4.4
1	H	183	PRO	4.4
1	G	295	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	H	315	LEU	4.2
2	L	7	SER	4.2
2	L	95	TYR	4.2
1	J	288	ALA	4.1
2	L	115	PRO	4.1
1	J	289	ASN	4.1
2	L	125	VAL	4.1
1	G	290	GLY	4.0
2	L	123	THR	4.0
1	H	292	GLU	4.0
1	B	288	ALA	4.0
2	L	29	PHE	4.0
1	E	315	LEU	4.0
1	D	154	ASN	3.9
2	L	122	GLY	3.9
2	L	68	ILE	3.9
1	G	177	HIS	3.9
1	A	314	VAL	3.9
2	L	16	GLY	3.9
1	C	288	ALA	3.6
1	F	299	ARG	3.6
1	D	88	GLY	3.6
2	L	32	TYR	3.6
1	C	234	THR	3.6
1	B	289	ASN	3.6
1	H	294	ASP	3.6
1	H	296	LEU	3.5
2	L	86	LEU	3.5
2	L	72	ARG	3.5
2	L	46	GLU	3.5
2	L	10	GLY	3.5
1	F	303	ALA	3.5
2	L	13	GLN	3.4
1	F	302	LEU	3.4
1	I	287	GLN	3.4
1	F	295	LEU	3.4
1	H	316	VAL	3.4
2	L	88	PRO	3.3
2	L	48	VAL	3.3
2	L	116	PHE	3.2
2	L	17	SER	3.2
1	B	314	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	154	ASN	3.1
1	J	290	GLY	3.1
1	H	291	VAL	3.1
1	E	164	GLY	3.1
2	L	57	SER	3.1
2	L	97	ALA	3.0
2	L	66	GLY	3.0
2	L	52	SER	2.9
2	L	89	GLU	2.9
1	B	287	GLN	2.9
1	B	313	CYS	2.9
2	L	81	LEU	2.9
1	E	154	ASN	2.9
1	G	176	ASP	2.9
1	I	286	ARG	2.8
2	L	64	VAL	2.8
1	A	297	ILE	2.8
2	L	74	ASN	2.8
1	H	297	ILE	2.8
2	L	43	LYS	2.8
1	A	292	GLU	2.7
2	L	20	LEU	2.7
1	D	233	GLN	2.7
1	E	153	ASP	2.6
1	C	289	ASN	2.6
1	B	225	LEU	2.6
1	D	316	VAL	2.6
2	L	65	LYS	2.6
2	L	22	CYS	2.6
1	E	296	LEU	2.5
1	A	303	ALA	2.5
2	L	96	CYS	2.5
2	L	47	GLY	2.5
2	L	36	TRP	2.5
2	L	87	LYS	2.5
2	L	28	THR	2.5
2	L	103	ASP	2.4
2	L	27	PHE	2.4
1	A	278	LEU	2.4
1	J	291	VAL	2.4
1	H	169	HIS	2.4
1	F	291	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	317	ILE	2.3
1	H	184	ASN	2.3
1	D	312	GLY	2.3
2	L	51	ILE	2.3
1	A	280	ILE	2.3
2	L	112	SER	2.3
1	A	300	CYS	2.3
2	L	11	LEU	2.3
1	C	290	GLY	2.3
1	C	51	PRO	2.2
1	H	229	SER	2.2
1	H	287	GLN	2.2
2	L	106	ILE	2.2
2	L	102	ALA	2.2
1	D	90	LYS	2.2
2	L	101	ASP	2.2
1	J	286	ARG	2.2
1	F	306	LEU	2.2
1	C	311	ILE	2.2
1	A	276	ALA	2.2
1	C	315	LEU	2.2
1	I	316	VAL	2.2
1	H	293	ASP	2.1
1	A	279	LEU	2.1
1	I	255	ARG	2.1
1	C	164	GLY	2.1
1	F	313	CYS	2.1
1	D	317	ILE	2.1
1	H	298	GLN	2.1
1	A	223	PHE	2.0
1	F	298	GLN	2.0
2	L	107	PHE	2.0
1	E	240	LEU	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

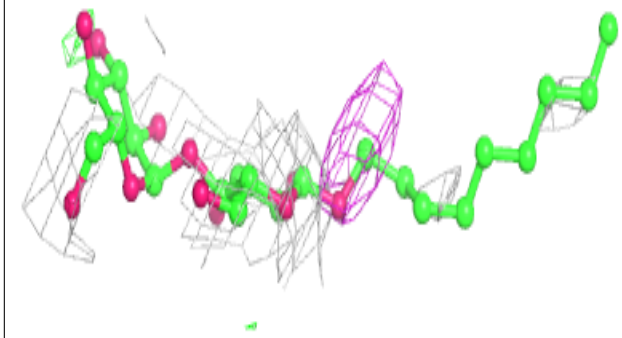
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

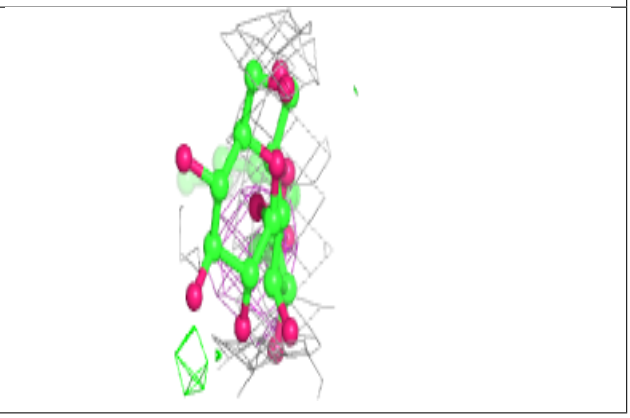
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CA	F	402	1/1	0.23	0.24	148,148,148,148	0
4	UMQ	B	403	32/34	0.68	0.33	119,143,145,147	0
3	CA	F	401	1/1	0.70	0.17	112,112,112,112	0
4	UMQ	A	402	32/34	0.75	0.25	117,139,146,147	0
3	CA	G	401	1/1	0.76	0.14	117,117,117,117	0
3	CA	B	401	1/1	0.79	0.11	115,115,115,115	0
4	UMQ	E	401	32/34	0.79	0.23	120,147,150,150	0
3	CA	D	401	1/1	0.80	0.12	124,124,124,124	0
4	UMQ	B	402	32/34	0.80	0.27	119,137,153,155	0
4	UMQ	C	402	32/34	0.81	0.24	122,135,147,149	0
4	UMQ	F	403	32/34	0.81	0.23	122,142,149,150	0
4	UMQ	J	401	32/34	0.81	0.36	121,142,145,147	0
4	UMQ	I	401	32/34	0.81	0.21	121,135,145,146	0
4	UMQ	G	403	32/34	0.83	0.20	121,143,151,153	0
3	CA	A	401	1/1	0.83	0.09	111,111,111,111	0
4	UMQ	G	402	32/34	0.84	0.27	130,148,156,157	0
3	CA	H	401	1/1	0.87	0.12	102,102,102,102	0
3	CA	C	401	1/1	0.98	0.16	95,95,95,95	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 403:

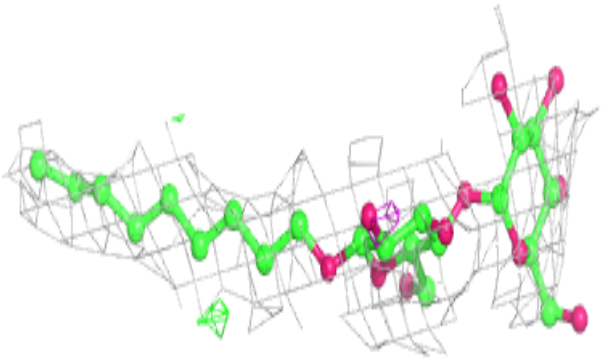
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

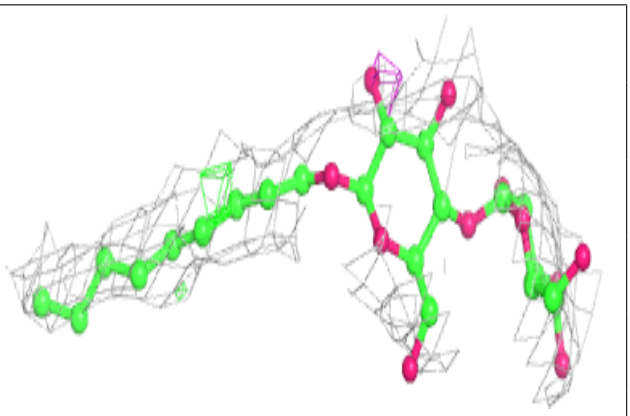




Electron density around UMQ A 402:

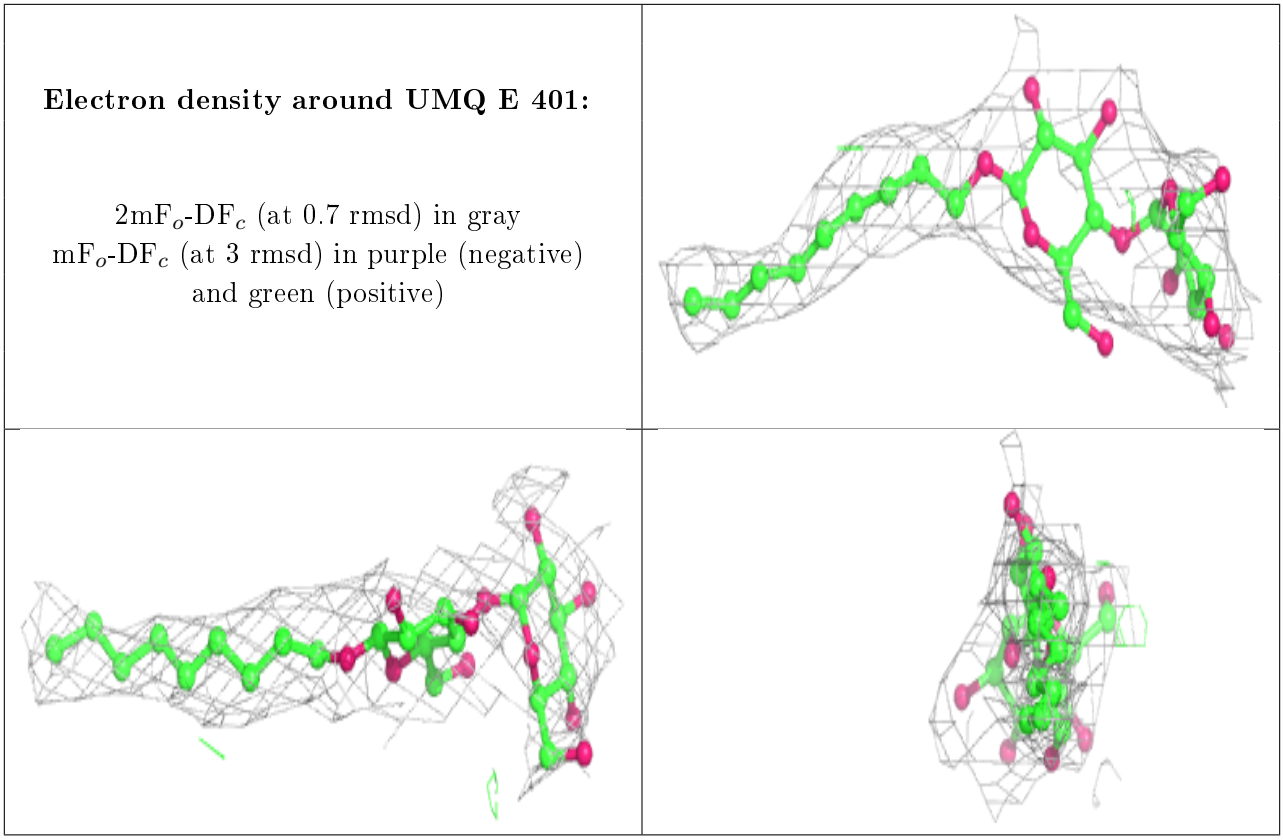
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





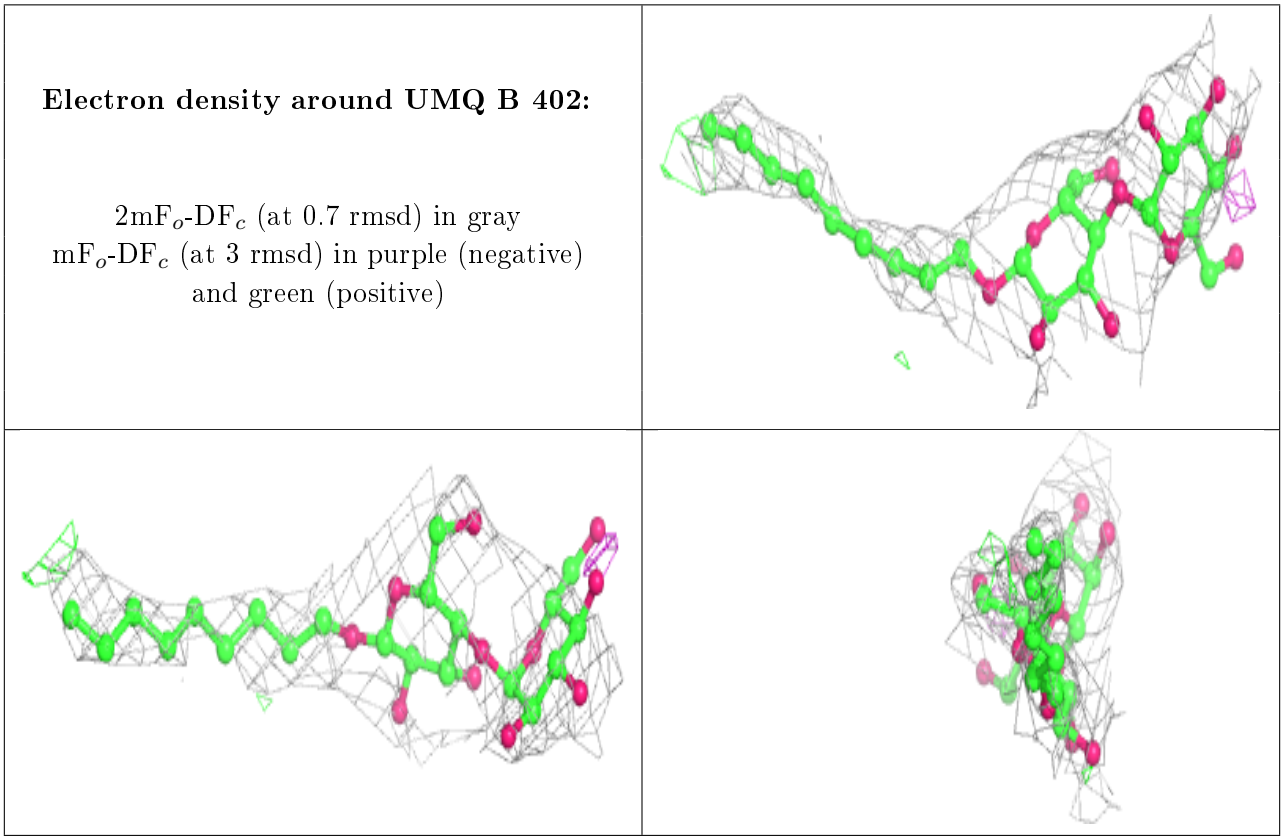
Electron density around UMQ E 401:

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



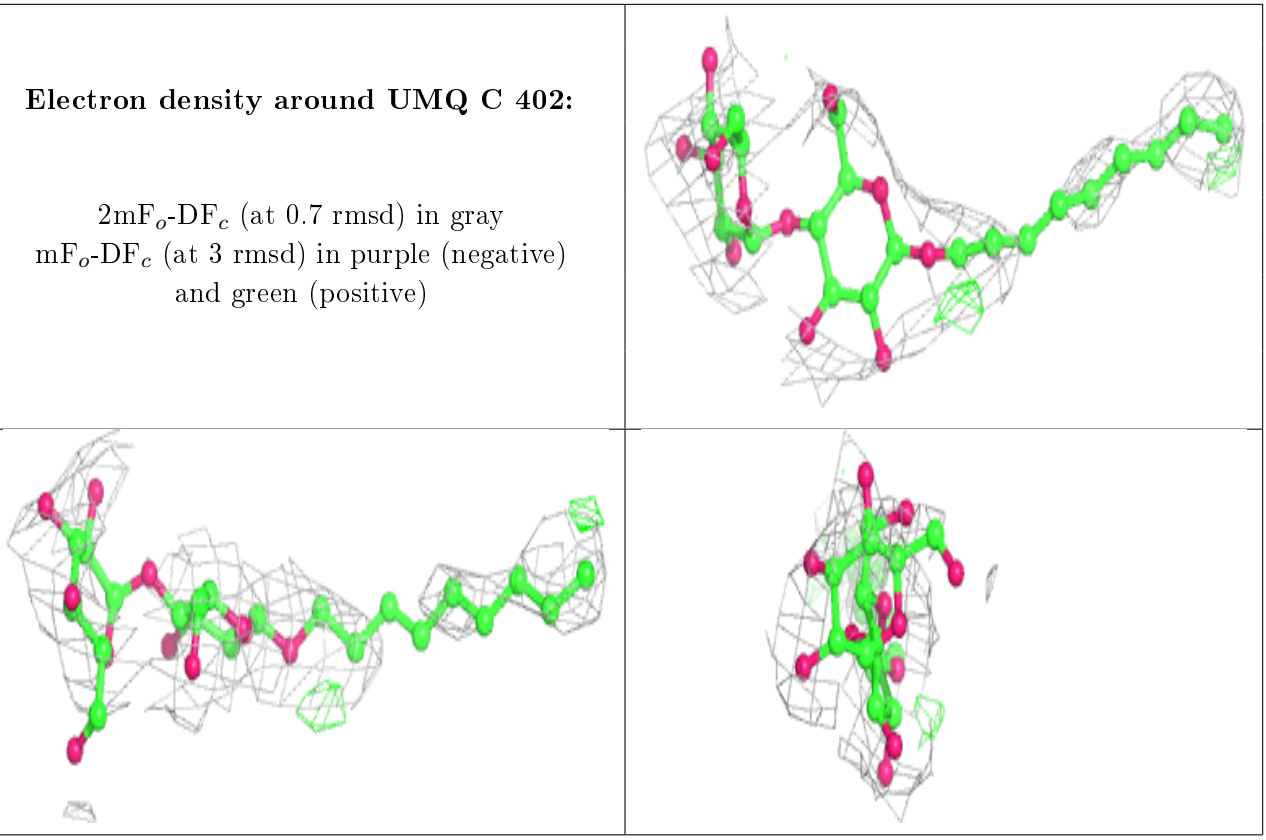
Electron density around UMQ B 402:

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



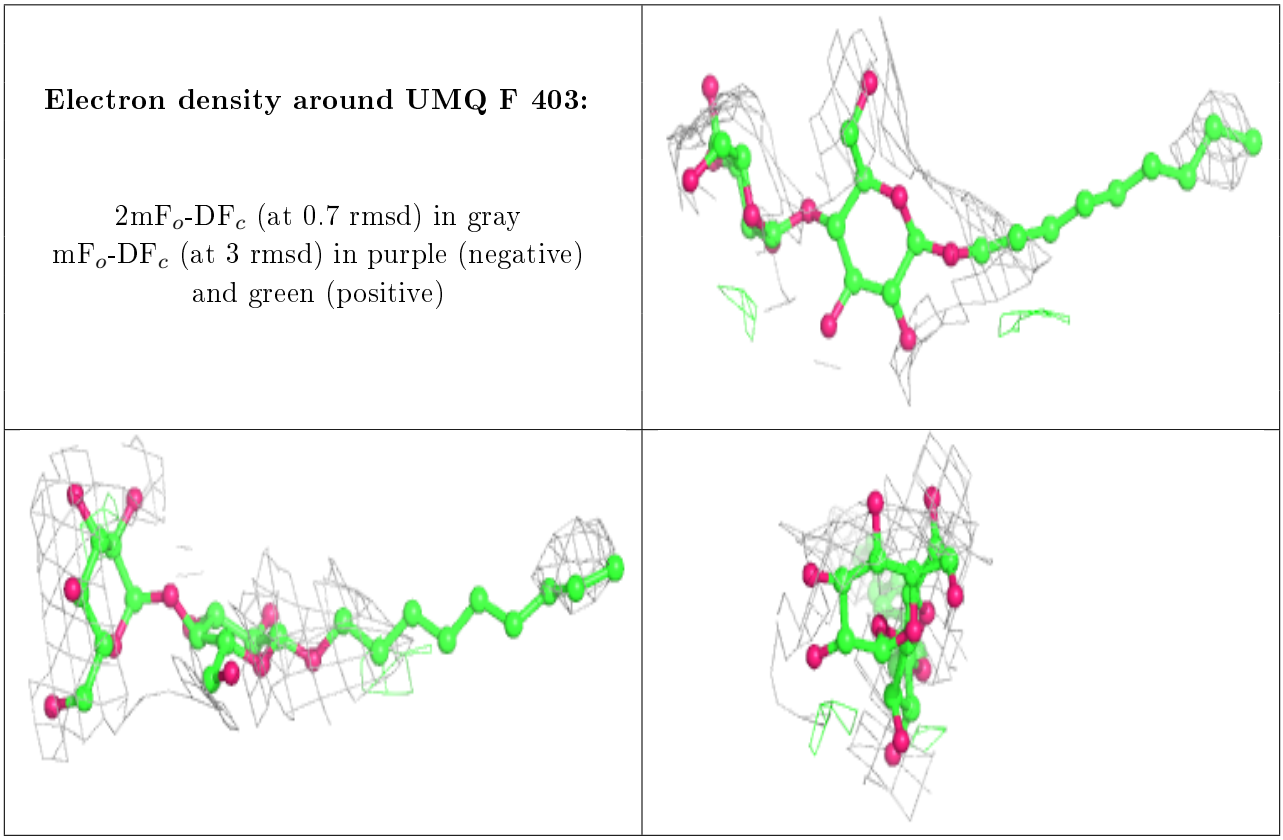
Electron density around UMQ C 402:

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



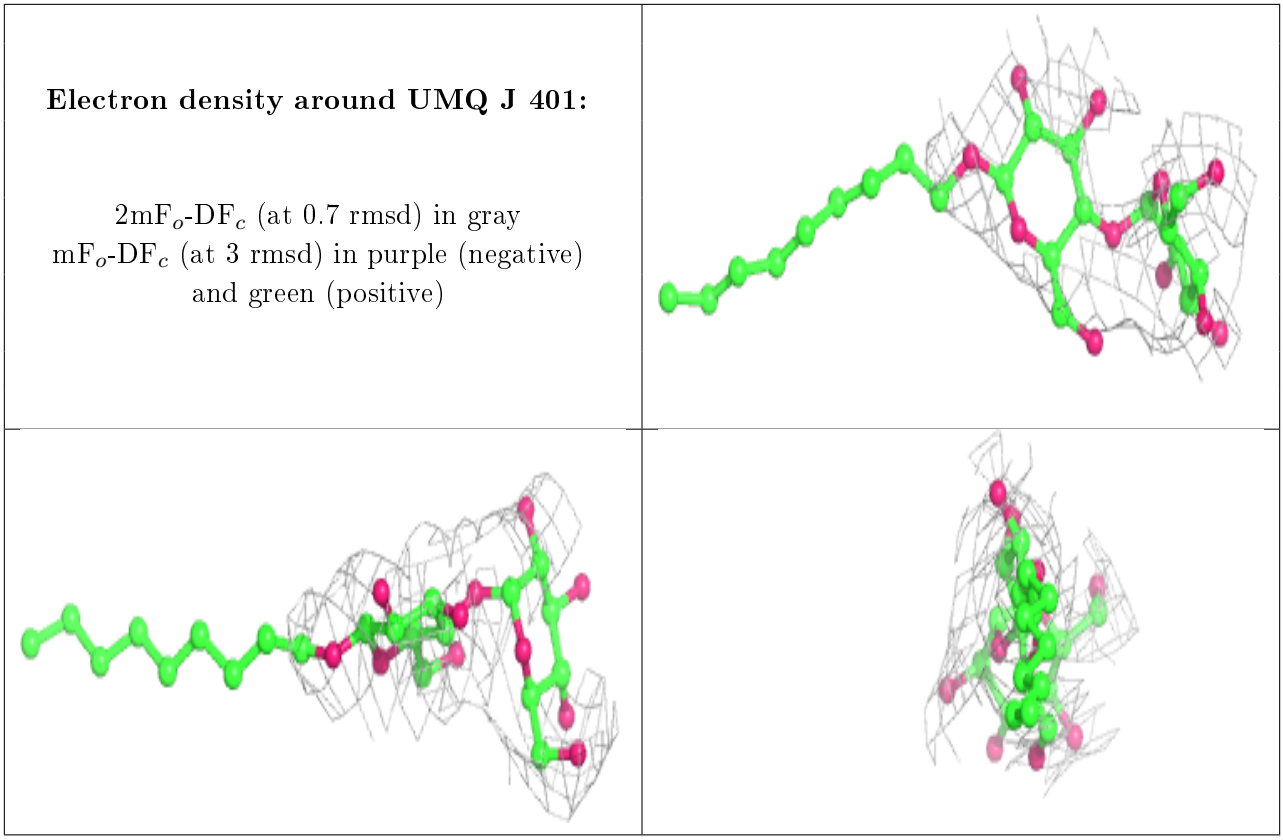
Electron density around UMQ F 403:

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



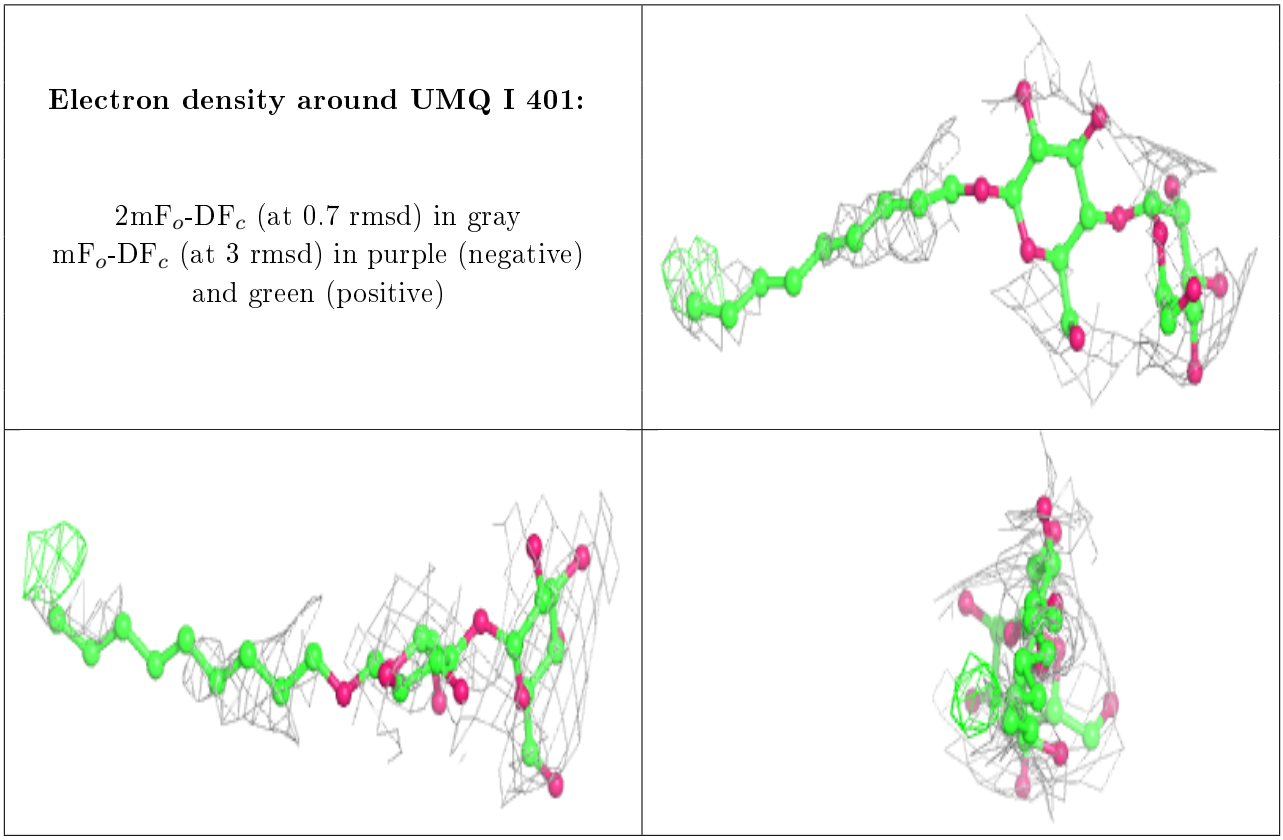
Electron density around UMQ J 401:

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



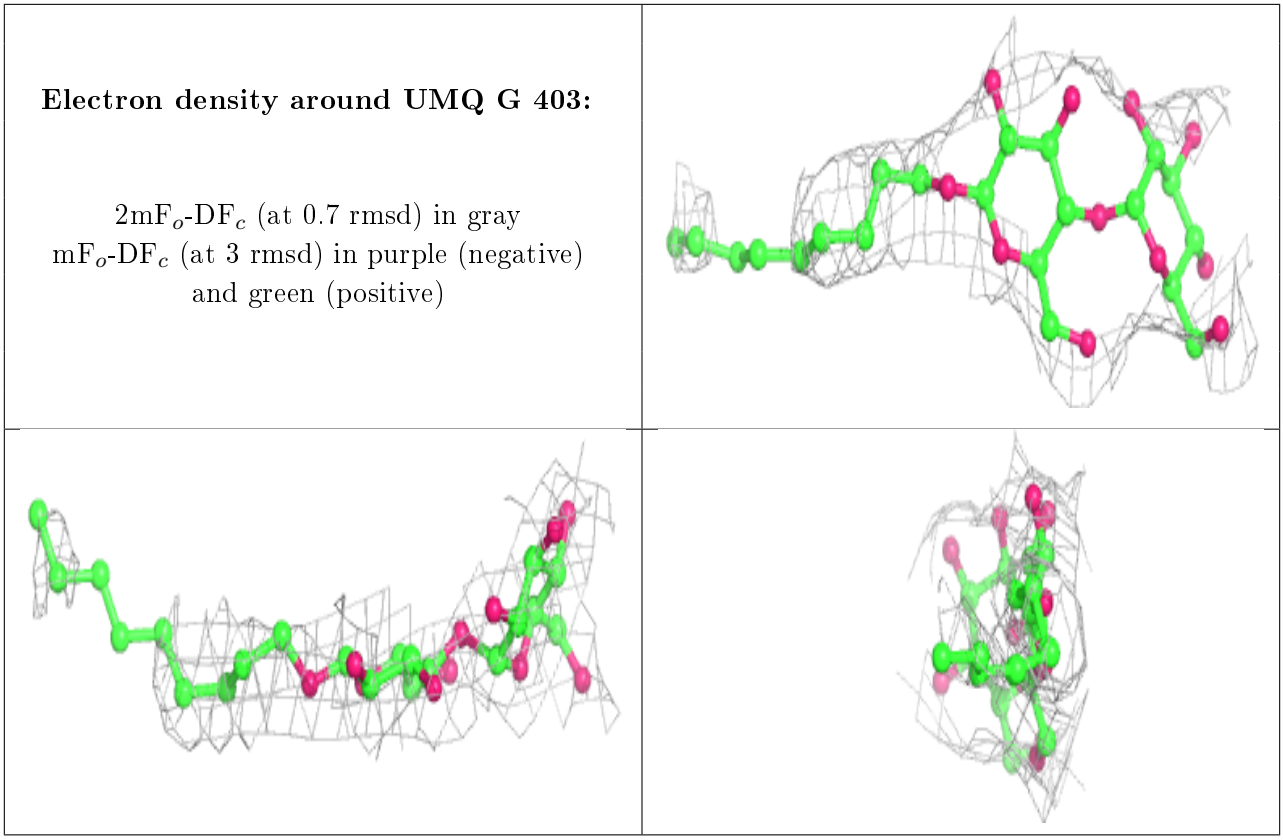
Electron density around UMQ I 401:

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



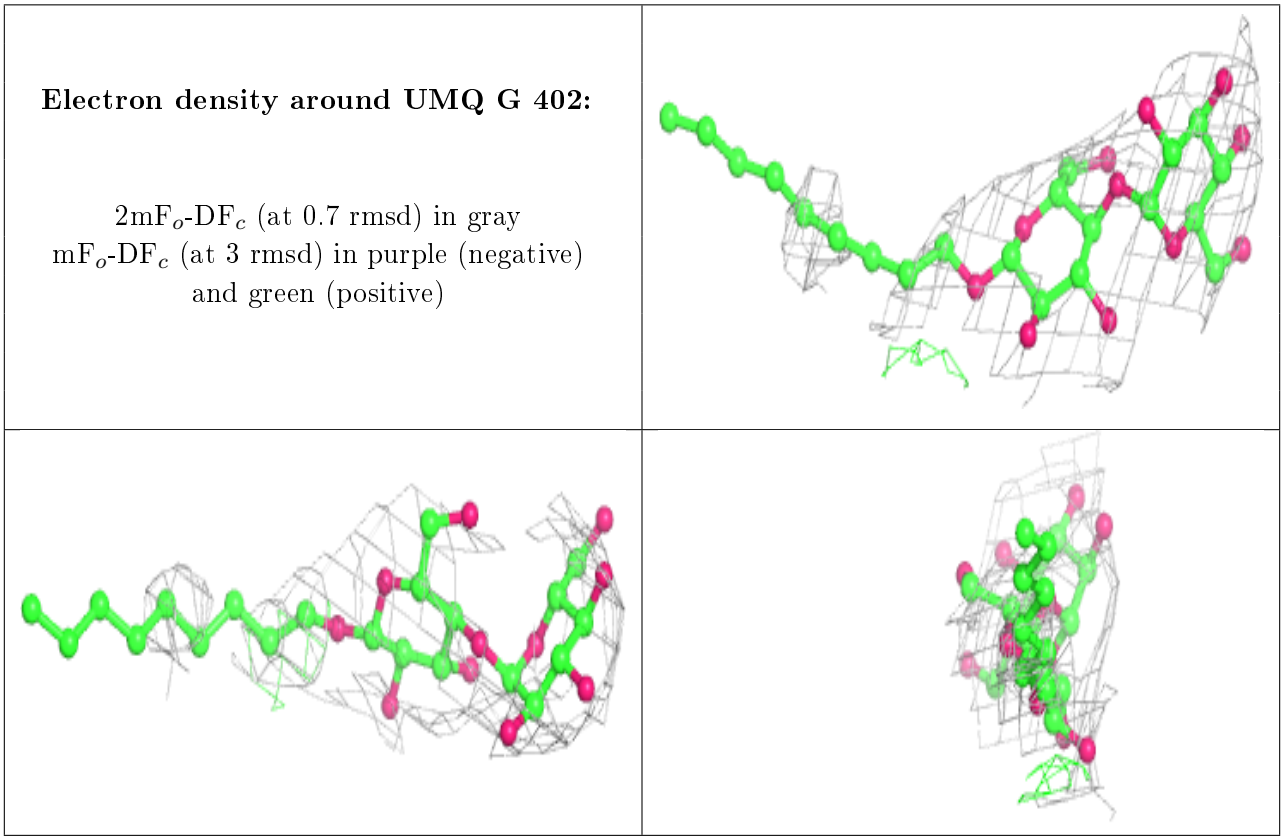
Electron density around UMQ G 403:

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



Electron density around UMQ G 402:

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



6.5 Other polymers (i)

There are no such residues in this entry.