



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 19, 2021 – 10:11 AM EST

PDB ID : 6W8C
Title : K2P2.1 (TREK-1):ML335 complex, 1 mM K+
Authors : Lolicato, M.; Minor, D.L.
Deposited on : 2020-03-20
Resolution : 2.60 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 : 2.16
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) : 2.16

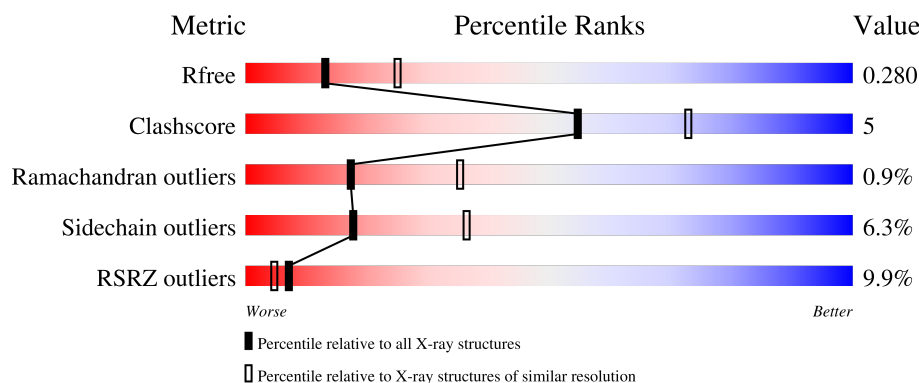
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	312	<div> <div>7%</div> <div>74%</div> <div>13%</div> <div>12%</div> </div>
1	B	312	<div> <div>11%</div> <div>76%</div> <div>13%</div> <div>10%</div> </div>

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 4741 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 Potassium channel subfamily K member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2159	1438	341	375	5			
1	B	281	Total	C	N	O	S	0	0	0
			2182	1453	345	379	5			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	expression tag	UNP P97438
A	84	ARG	LYS	engineered mutation	UNP P97438
A	85	GLU	GLN	engineered mutation	UNP P97438
A	86	LYS	THR	engineered mutation	UNP P97438
A	88	LEU	ILE	engineered mutation	UNP P97438
A	89	ARG	ALA	engineered mutation	UNP P97438
A	90	ALA	GLN	engineered mutation	UNP P97438
A	92	PRO	ALA	engineered mutation	UNP P97438
A	95	SER	ASN	engineered mutation	UNP P97438
A	96	ASP	SER	engineered mutation	UNP P97438
A	97	GLN	THR	engineered mutation	UNP P97438
A	119	ALA	ASN	engineered mutation	UNP P97438
A	300	ALA	SER	engineered mutation	UNP P97438
A	306	ALA	GLU	engineered mutation	UNP P97438
A	323	SER	-	expression tag	UNP P97438
A	324	ASN	-	expression tag	UNP P97438
A	325	SER	-	expression tag	UNP P97438
A	326	LEU	-	expression tag	UNP P97438
A	327	GLU	-	expression tag	UNP P97438
A	328	VAL	-	expression tag	UNP P97438
A	329	LEU	-	expression tag	UNP P97438
A	330	PHE	-	expression tag	UNP P97438
A	331	GLN	-	expression tag	UNP P97438
B	20	MET	-	expression tag	UNP P97438
B	84	ARG	LYS	engineered mutation	UNP P97438

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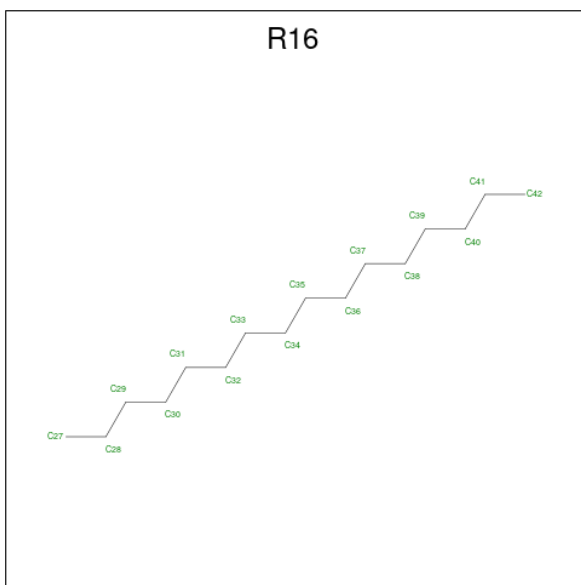
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Chain	Residue	Modelled	Actual	Comment	Reference
B	85	GLU	GLN	engineered mutation	UNP P97438
B	86	LYS	THR	engineered mutation	UNP P97438
B	88	LEU	ILE	engineered mutation	UNP P97438
B	89	ARG	ALA	engineered mutation	UNP P97438
B	90	ALA	GLN	engineered mutation	UNP P97438
B	92	PRO	ALA	engineered mutation	UNP P97438
B	95	SER	ASN	engineered mutation	UNP P97438
B	96	ASP	SER	engineered mutation	UNP P97438
B	97	GLN	THR	engineered mutation	UNP P97438
B	119	ALA	ASN	engineered mutation	UNP P97438
B	300	ALA	SER	engineered mutation	UNP P97438
B	306	ALA	GLU	engineered mutation	UNP P97438
B	323	SER	-	expression tag	UNP P97438
B	324	ASN	-	expression tag	UNP P97438
B	325	SER	-	expression tag	UNP P97438
B	326	LEU	-	expression tag	UNP P97438
B	327	GLU	-	expression tag	UNP P97438
B	328	VAL	-	expression tag	UNP P97438
B	329	LEU	-	expression tag	UNP P97438
B	330	PHE	-	expression tag	UNP P97438
B	331	GLN	-	expression tag	UNP P97438

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

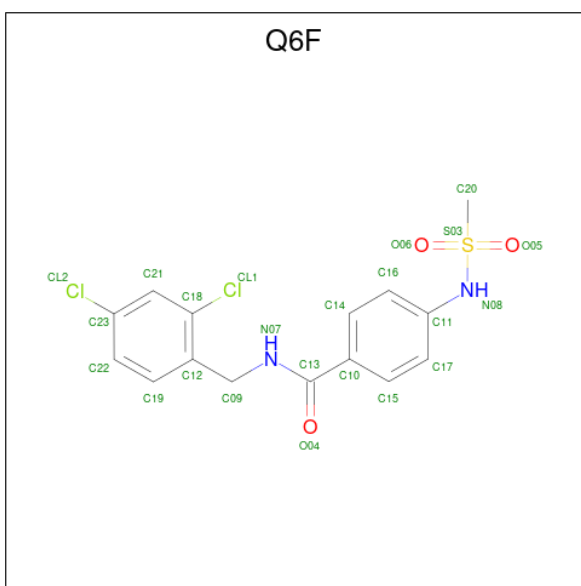
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total K 1 1	0	0
2	A	5	Total K 5 5	0	0

- Molecule 3 is HEXADECANE (three-letter code: R16) (formula: C₁₆H₃₄).



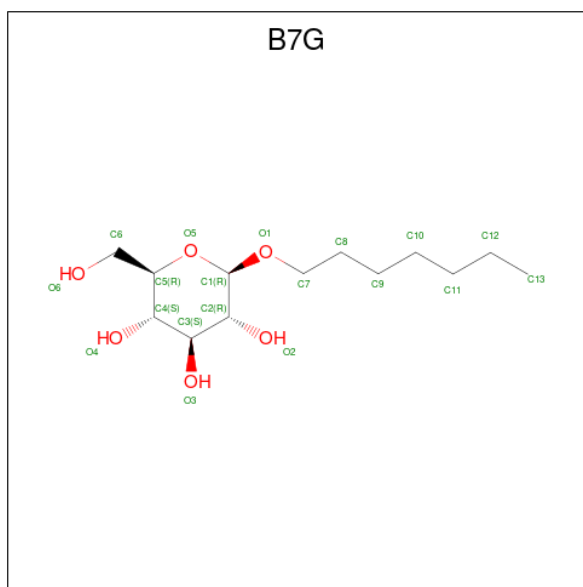
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 16 16	0	0
3	A	1	Total C 16 16	0	0
3	A	1	Total C 16 16	0	0

- Molecule 4 is N-[(2,4-dichlorophenyl)methyl]-4-[(methylsulfonyl)amino]benzamide (three-letter code: Q6F) (formula: $C_{15}H_{14}Cl_2N_2O_3S$).



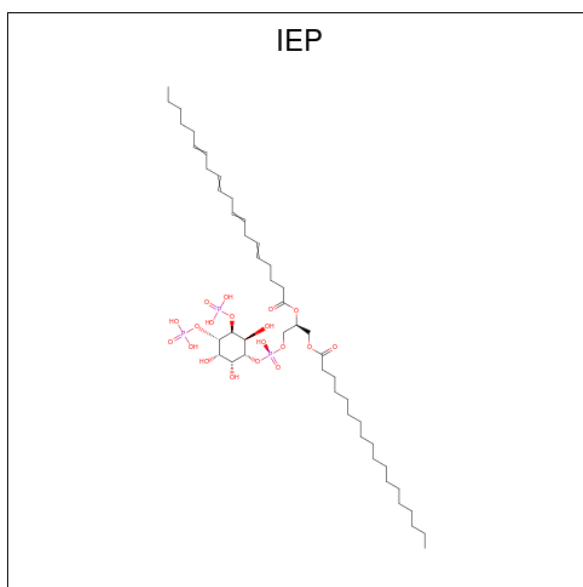
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	S	
			23	15	2	2	3	1	
4	B	1	Total	C	Cl	N	O	S	
			23	15	2	2	3	1	

- Molecule 5 is heptyl beta-D-glucopyranoside (three-letter code: B7G) (formula: C₁₃H₂₆O₆).



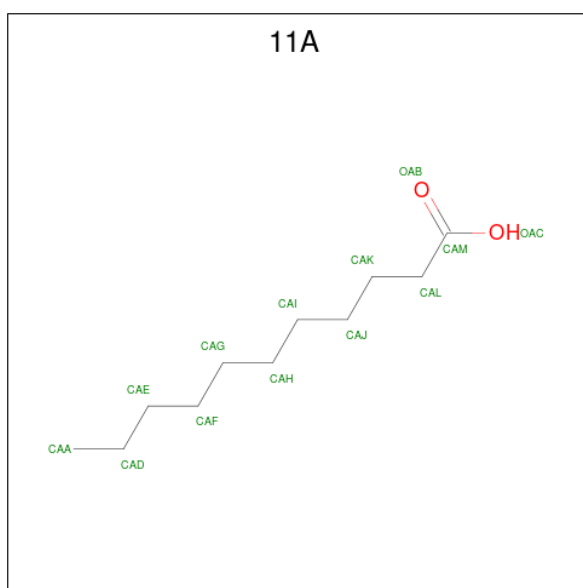
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O		
			19	13	6	0	0
5	B	1	Total	C	O		
			19	13	6	0	0
5	B	1	Total	C	O		
			19	13	6	0	0
5	B	1	Total	C	O		
			19	13	6	0	0

- Molecule 6 is [(2 {S})-1-octadecanoyloxy-3-[oxidanyl-[(1 {R},2 {R},3 {S},4 {S},5 {S},6 {S})-2,3,6-tris(oxidanyl)-4,5-diphosphonoxy-cyclohexyl]oxy-phosphoryl]oxy-propan-2-yl] icos-5,8,11,14-tetraenoate (three-letter code: IEP) (formula: C₄₇H₈₅O₁₉P₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	P	0	0
			69	47	19	3		
6	B	1	Total	C	O	P	0	0
			69	47	19	3		

- Molecule 7 is UNDECANOIC ACID (three-letter code: 11A) (formula: $C_{11}H_{22}O_2$).

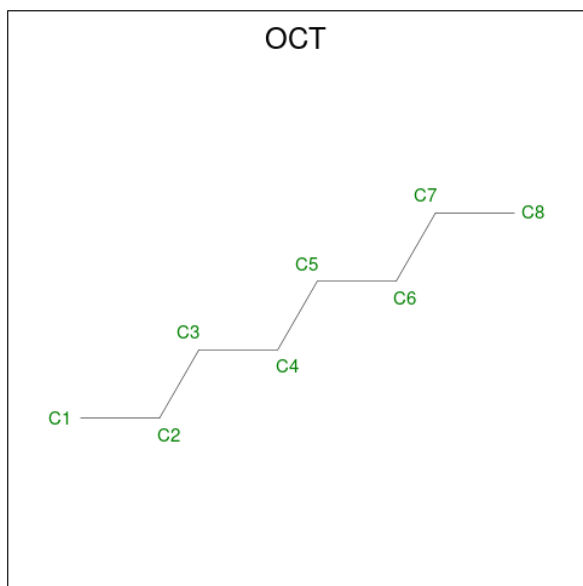


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O		0	0
			13	11	2			
7	B	1	Total	C	O		0	0
			13	11	2			

- Molecule 8 is CADMIUM ION (three-letter code: CD) (formula: Cd).

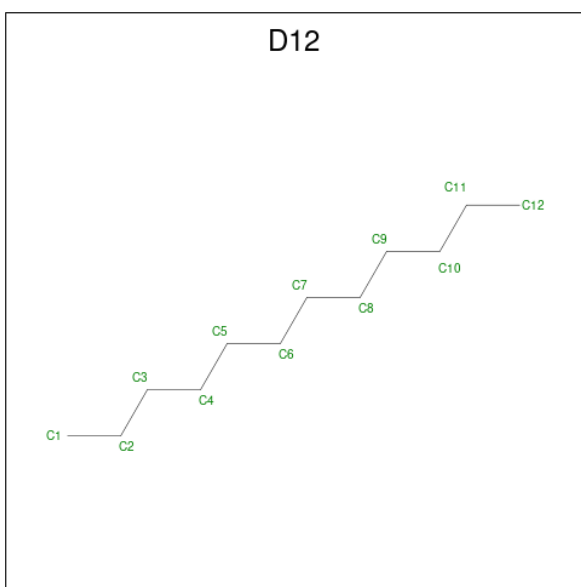
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	3	Total	Cd	0	0
			3	3		

- Molecule 9 is N-OCTANE (three-letter code: OCT) (formula: C₈H₁₈).



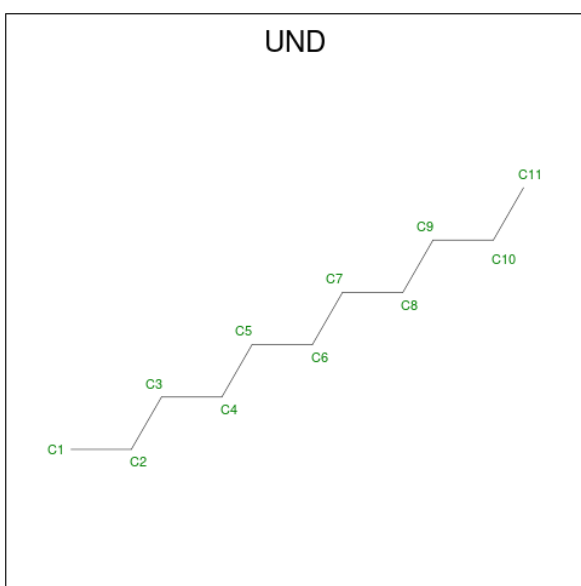
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	C	0	0
			8	8		
9	B	1	Total	C	0	0
			8	8		

- Molecule 10 is DODECANE (three-letter code: D12) (formula: C₁₂H₂₆).



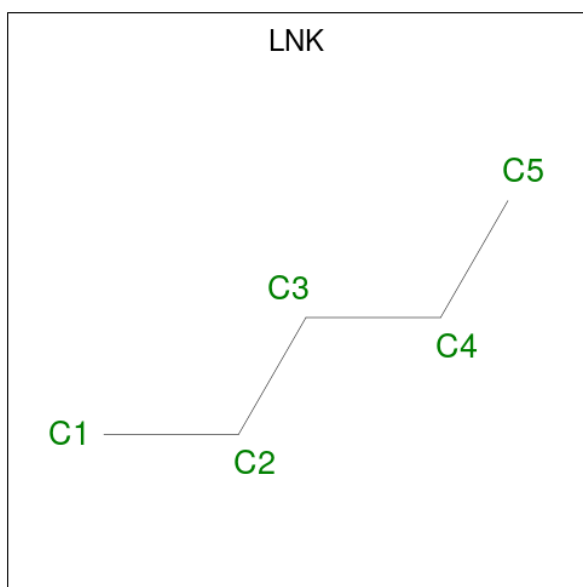
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	C	0	0
			12	12		
10	B	1	Total	C	0	0
			12	12		

- Molecule 11 is UNDECANE (three-letter code: UND) (formula: $C_{11}H_{24}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	1	Total	C	0	0
			11	11		

- Molecule 12 is PENTANE (three-letter code: LNK) (formula: C_5H_{12}).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total C 5 5	0	0

- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total O 1 1	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.13Å 119.78Å 128.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.97 – 2.60 14.97 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (14.97-2.60) 100.0 (14.97-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.10.3 (6-FEB-2020)	Depositor
R, R_{free}	0.251 , 0.263 0.261 , 0.280	Depositor DCC
R_{free} test set	1581 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	81.9	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 107.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4741	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: R16, 11A, D12, IEP, Q6F, CD, UND, LNK, B7G, OCT, K

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	0.62	0/2212	0.75	0/3008
1	B	0.59	0/2234	0.76	0/3037
All	All	0.61	0/4446	0.75	0/6045

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	268	ASP	Peptide
1	B	268	ASP	Peptide

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	2159	0	2207	26	0
1	B	2182	0	2242	27	0
2	A	5	0	0	0	0
2	B	1	0	0	0	0
3	A	48	0	102	0	0
4	A	23	0	0	1	0
4	B	23	0	0	1	0
5	A	19	0	26	0	0
5	B	57	0	78	1	0
6	A	69	0	0	1	0
6	B	69	0	0	3	0
7	A	13	0	21	0	0
7	B	13	0	21	1	0
8	B	3	0	0	0	0
9	B	16	0	36	0	0
10	B	24	0	52	2	0
11	B	11	0	24	0	0
12	B	5	0	12	0	0
13	A	1	0	0	1	0
All	All	4741	0	4821	50	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 5.

All (50) 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:317:TRP:NE1	13:A:501:HOH:O	1.96	0.77
6:B:413:IEP:O43	6:B:413:IEP:O46	2.09	0.70
1:A:107:VAL:HG22	1:B:110:ILE:HD11	1.77	0.65
1:B:273:VAL:HG12	10:B:408:D12:H22	1.79	0.65
1:A:197:ILE:HD11	1:A:206:ILE:HD13	1.82	0.61
1:A:197:ILE:HD11	1:A:206:ILE:HG21	1.85	0.58
1:B:37:SER:O	1:B:41:VAL:HG23	2.04	0.57
1:B:303:THR:HG22	5:B:411:B7G:H92	1.87	0.56
1:B:261:GLY:HA2	4:B:415:Q6F:C20	2.35	0.56
1:A:37:SER:O	1:A:41:VAL:HG23	2.07	0.55
1:B:201:VAL:HB	1:B:206:ILE:HD11	1.89	0.55
1:A:45:LYS:O	1:A:49:THR:HG22	2.07	0.55
1:A:80:ILE:HG12	1:B:114:ILE:HD13	1.88	0.54
1:B:85:GLU:HA	1:B:88:LEU:HD12	1.89	0.53
1:B:46:THR:HG23	6:B:413:IEP:O28	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:LEU:HD21	1:B:280:VAL:HG13	1.91	0.52
1:B:49:THR:O	1:B:53:VAL:HG23	2.10	0.52
1:A:181:LEU:HD21	1:A:280:VAL:HG13	1.92	0.52
1:A:197:ILE:O	1:A:197:ILE:HG22	2.09	0.51
1:A:278:ILE:CD1	4:A:408:Q6F:C21	2.88	0.51
1:A:57:TYR:CE2	1:B:162:TYR:CE1	2.99	0.51
1:A:110:ILE:HD11	1:B:107:VAL:HG22	1.92	0.51
1:B:197:ILE:HG22	1:B:197:ILE:O	2.11	0.50
1:A:49:THR:O	1:A:53:VAL:HG23	2.12	0.50
1:A:197:ILE:N	1:A:197:ILE:HD12	2.27	0.49
1:A:267:LEU:HD12	1:A:269:PHE:HE2	1.76	0.49
1:B:135:PHE:CZ	1:B:150:PRO:HD3	2.48	0.49
6:B:413:IEP:O46	6:B:413:IEP:P42	2.70	0.49
1:A:193:GLU:HA	1:A:197:ILE:HD13	1.95	0.48
1:A:197:ILE:CD1	1:A:206:ILE:HD13	2.43	0.48
1:B:273:VAL:HG12	10:B:408:D12:C2	2.42	0.48
1:B:114:ILE:HD12	1:B:116:PRO:CG	2.45	0.46
1:B:222:PHE:CE1	1:B:280:VAL:HG12	2.51	0.46
1:A:135:PHE:CZ	1:A:150:PRO:HD3	2.51	0.46
1:A:196:PHE:C	1:A:197:ILE:HD12	2.36	0.46
1:B:84:ARG:HG3	1:B:88:LEU:HG	1.99	0.45
1:B:210:SER:O	1:B:213:ILE:HG22	2.17	0.45
1:B:268:ASP:OD1	7:B:414:11A:OAB	2.35	0.45
1:A:267:LEU:HD12	1:A:269:PHE:CE2	2.51	0.44
1:A:222:PHE:CE1	1:A:280:VAL:HG12	2.53	0.43
1:B:114:ILE:HD12	1:B:116:PRO:HG3	2.01	0.43
1:A:87:PHE:CZ	1:B:102:LEU:HD22	2.53	0.42
1:B:123:GLN:N	1:B:123:GLN:HE21	2.18	0.42
6:A:410:IEP:P25	6:A:410:IEP:O47	2.78	0.42
1:A:152:THR:HG22	1:A:154:GLY:H	1.84	0.41
1:A:206:ILE:HA	1:A:209:ILE:HD12	2.02	0.41
1:B:59:ILE:O	1:B:63:THR:HG23	2.20	0.41
1:B:152:THR:HG22	1:B:154:GLY:H	1.85	0.41
1:A:126:HIS:O	1:A:131:SER:HB3	2.22	0.40
1:A:243:TYR:HA	1:B:160:ILE:HD11	2.03	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	272/312 (87%)	254 (93%)	15 (6%)	3 (1%)	14	30
1	B	277/312 (89%)	255 (92%)	20 (7%)	2 (1%)	22	43
All	All	549/624 (88%)	509 (93%)	35 (6%)	5 (1%)	17	35

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	ALA
1	B	266	TYR
1	A	204	THR
1	B	264	ILE
1	A	199	TRP

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	227/260 (87%)	209 (92%)	18 (8%)	12	24
1	B	230/260 (88%)	219 (95%)	11 (5%)	25	49
All	All	457/520 (88%)	428 (94%)	29 (6%)	18	36

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	SER

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Mol	Chain	Res	Type
1	A	37	SER
1	A	49	THR
1	A	56	LEU
1	A	70	GLN
1	A	86	LYS
1	A	88	LEU
1	A	100	ASP
1	A	110	ILE
1	A	210	SER
1	A	216	LEU
1	A	225	LEU
1	A	265	GLU
1	A	267	LEU
1	A	269	PHE
1	A	304	LYS
1	A	316	GLU
1	A	321	VAL
1	B	42	MET
1	B	56	LEU
1	B	70	GLN
1	B	93	CYS
1	B	100	ASP
1	B	110	ILE
1	B	123	GLN
1	B	216	LEU
1	B	268	ASP
1	B	278	ILE
1	B	301	LYS

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

Mol	Chain	Res	Type
1	B	40	ASN
1	B	123	GLN

5.3.3 RNA ⓘ

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 28 ligands modelled in this entry, 9 are monoatomic - leaving 19 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	$\# Z > 2$
3	R16	A	407	-	15,15,15	0.37	0	14,14,14	0.58	0
12	LNK	B	416	-	4,4,4	0.44	0	3,3,3	0.33	0
9	OCT	B	405	-	7,7,7	0.42	0	6,6,6	0.38	0
10	D12	B	407	-	11,11,11	0.40	0	10,10,10	0.55	0
6	IEP	A	410	-	69,69,69	0.99	3 (4%)	83,87,87	1.21	6 (7%)
5	B7G	B	410	-	19,19,19	1.35	3 (15%)	24,24,24	2.42	8 (33%)
3	R16	A	406	-	15,15,15	0.35	0	14,14,14	0.70	0
10	D12	B	408	-	11,11,11	0.39	0	10,10,10	0.51	0
4	Q6F	A	408	-	24,24,24	1.67	5 (20%)	34,34,34	2.90	9 (26%)
4	Q6F	B	415	-	24,24,24	1.69	5 (20%)	34,34,34	2.56	6 (17%)
6	IEP	B	413	-	69,69,69	1.10	5 (7%)	83,87,87	1.32	12 (14%)
3	R16	A	405	-	15,15,15	0.37	0	14,14,14	0.72	0
11	UND	B	412	-	10,10,10	0.40	0	9,9,9	0.56	0
7	11A	B	414	-	9,12,12	0.47	0	8,12,12	0.48	0
5	B7G	B	409	-	19,19,19	1.23	2 (10%)	24,24,24	1.21	1 (4%)
7	11A	A	411	-	9,12,12	0.39	0	8,12,12	0.59	0
5	B7G	B	411	-	19,19,19	1.28	3 (15%)	24,24,24	1.57	2 (8%)
9	OCT	B	406	-	7,7,7	0.39	0	6,6,6	0.57	0
5	B7G	A	409	-	19,19,19	1.23	2 (10%)	24,24,24	0.94	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	R16	A	407	-	-	7/13/13/13	-
12	LNK	B	416	-	-	2/2/2/2	-
9	OCT	B	405	-	-	3/5/5/5	-
10	D12	B	407	-	-	4/9/9/9	-
6	IEP	A	410	-	-	19/66/90/90	0/1/1/1
5	B7G	B	410	-	-	6/10/30/30	0/1/1/1
3	R16	A	406	-	-	6/13/13/13	-
10	D12	B	408	-	-	6/9/9/9	-
4	Q6F	A	408	-	-	1/14/14/14	0/2/2/2
4	Q6F	B	415	-	-	3/14/14/14	0/2/2/2
6	IEP	B	413	-	-	36/58/90/90	-
3	R16	A	405	-	-	6/13/13/13	-
11	UND	B	412	-	-	2/8/8/8	-
7	11A	B	414	-	-	4/8/10/10	-
5	B7G	B	409	-	-	3/10/30/30	0/1/1/1
7	11A	A	411	-	-	2/8/10/10	-
5	B7G	B	411	-	-	5/10/30/30	0/1/1/1
9	OCT	B	406	-	-	1/5/5/5	-
5	B7G	A	409	-	-	6/10/30/30	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	415	Q6F	C13-N07	4.92	1.44	1.33
4	A	408	Q6F	C13-N07	4.84	1.44	1.33
6	B	413	IEP	P42-O41	4.41	1.67	1.59
6	B	413	IEP	O20-C18	4.40	1.46	1.33
6	A	410	IEP	O20-C18	4.18	1.45	1.33
6	A	410	IEP	O48-C49	4.03	1.45	1.34
6	B	413	IEP	O48-C49	3.97	1.45	1.34
5	B	410	B7G	O5-C1	3.71	1.51	1.41
5	B	411	B7G	O5-C1	3.36	1.50	1.41
5	A	409	B7G	O5-C1	3.32	1.50	1.41
4	A	408	Q6F	S03-N08	3.23	1.67	1.63
5	B	409	B7G	O5-C1	3.11	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	415	Q6F	C10-C13	2.96	1.56	1.50
4	B	415	Q6F	C11-N08	2.86	1.47	1.43
6	A	410	IEP	P42-O41	2.79	1.64	1.59
5	B	410	B7G	O3-C3	2.69	1.49	1.43
4	B	415	Q6F	S03-N08	2.68	1.66	1.63
5	B	411	B7G	O5-C5	2.57	1.50	1.44
4	A	408	Q6F	C10-C13	2.53	1.55	1.50
4	A	408	Q6F	C20-S03	2.45	1.81	1.75
5	B	410	B7G	C1-C2	2.40	1.59	1.52
5	B	409	B7G	O3-C3	2.34	1.48	1.43
4	A	408	Q6F	C11-N08	2.31	1.46	1.43
6	B	413	IEP	P37-O36	2.29	1.63	1.59
5	B	411	B7G	O3-C3	2.26	1.48	1.43
6	B	413	IEP	C33-C32	2.12	1.56	1.52
5	A	409	B7G	O5-C5	2.11	1.49	1.44
4	B	415	Q6F	C18-CL1	2.07	1.78	1.73

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	408	Q6F	C20-S03-N08	10.71	118.84	106.63
4	B	415	Q6F	O06-S03-O05	-9.71	104.88	118.85
4	B	415	Q6F	C20-S03-N08	7.58	115.28	106.63
4	A	408	Q6F	O06-S03-O05	-6.73	109.17	118.85
4	A	408	Q6F	C17-C11-N08	-5.87	107.41	120.09
5	B	410	B7G	C3-C4-C5	-5.27	100.83	110.24
5	B	410	B7G	O1-C1-C2	5.17	116.37	108.30
5	B	411	B7G	O1-C1-C2	5.15	116.34	108.30
4	A	408	Q6F	C16-C11-N08	5.01	130.94	120.09
5	B	410	B7G	O4-C4-C3	4.66	121.13	110.35
6	A	410	IEP	O48-C49-C51	4.46	121.12	111.50
5	B	410	B7G	O5-C5-C4	-4.43	101.65	109.69
4	B	415	Q6F	C12-C09-N07	-4.42	103.70	113.03
6	B	413	IEP	O41-C32-C33	4.29	118.80	108.69
6	A	410	IEP	O28-C29-C30	4.15	118.31	108.66
5	B	411	B7G	C7-O1-C1	4.15	120.72	113.84
6	B	413	IEP	C33-C34-C29	3.75	116.74	108.96
6	A	410	IEP	O41-C32-C31	3.62	117.09	108.66
4	A	408	Q6F	C12-C09-N07	-3.55	105.53	113.03
6	B	413	IEP	O48-C49-C51	3.48	118.99	111.50
5	B	410	B7G	C6-C5-C4	2.99	120.02	113.00
5	B	409	B7G	C7-O1-C1	2.95	118.74	113.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	410	B7G	C7-O1-C1	2.85	118.57	113.84
5	A	409	B7G	O1-C1-C2	2.75	112.60	108.30
5	B	410	B7G	O4-C4-C5	2.73	116.07	109.30
6	B	413	IEP	O46-C31-C30	2.68	116.53	110.35
4	B	415	Q6F	C10-C13-N07	2.67	122.82	117.09
4	A	408	Q6F	C21-C18-C12	-2.66	120.06	122.42
6	B	413	IEP	O43-P42-O41	2.55	117.42	105.99
6	B	413	IEP	O48-C49-O50	-2.53	117.60	123.70
6	A	410	IEP	C52-C51-C49	-2.52	104.44	113.62
6	B	413	IEP	C22-O48-C49	-2.52	111.60	117.79
6	A	410	IEP	P25-O28-C29	2.51	128.53	119.41
4	B	415	Q6F	O04-C13-C10	-2.50	116.47	120.94
6	B	413	IEP	O20-C21-C22	2.44	115.54	108.43
4	A	408	Q6F	C18-C21-C23	2.33	121.32	118.71
6	B	413	IEP	C31-C32-C33	-2.32	106.37	111.66
4	A	408	Q6F	C14-C10-C15	2.32	121.89	118.59
6	B	413	IEP	O47-C30-C31	2.31	115.68	110.35
4	A	408	Q6F	C12-C18-CL1	2.29	123.44	119.73
6	B	413	IEP	C34-C33-C32	2.27	116.84	111.66
5	B	410	B7G	C1-C2-C3	2.20	114.57	110.00
6	B	413	IEP	O20-C18-C17	2.12	118.56	111.91
6	A	410	IEP	C31-C30-C29	2.06	114.39	109.68
4	B	415	Q6F	C19-C22-C23	2.01	121.37	119.24

There are no chirality outliers.

All (122) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	413	IEP	C30-C29-O28-P25
6	B	413	IEP	C34-C29-O28-P25
6	B	413	IEP	C31-C32-O41-P42
6	B	413	IEP	C32-C33-O36-P37
6	B	413	IEP	C34-C33-O36-P37
6	B	413	IEP	O50-C49-O48-C22
6	B	413	IEP	C57-C58-C59-C60
6	B	413	IEP	C58-C59-C60-C61
6	B	413	IEP	C23-O24-P25-O28
6	B	413	IEP	C29-O28-P25-O24
6	A	410	IEP	C30-C29-O28-P25
6	A	410	IEP	C31-C32-O41-P42
6	A	410	IEP	C34-C33-O36-P37
6	A	410	IEP	C51-C49-O48-C22

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Mol	Chain	Res	Type	Atoms
6	A	410	IEP	O50-C49-O48-C22
4	B	415	Q6F	C11-N08-S03-O06
5	B	411	B7G	C8-C7-O1-C1
5	B	409	B7G	C8-C7-O1-C1
5	A	409	B7G	O5-C1-O1-C7
5	A	409	B7G	C2-C1-O1-C7
6	B	413	IEP	C51-C49-O48-C22
5	B	411	B7G	O5-C5-C6-O6
5	B	411	B7G	C4-C5-C6-O6
5	A	409	B7G	C4-C5-C6-O6
5	B	410	B7G	C4-C5-C6-O6
6	B	413	IEP	O20-C21-C22-O48
5	B	410	B7G	O5-C5-C6-O6
5	A	409	B7G	O5-C5-C6-O6
6	B	413	IEP	C15-C16-C17-C18
6	A	410	IEP	C07-C08-C09-C10
5	B	409	B7G	C4-C5-C6-O6
6	A	410	IEP	C15-C16-C17-C18
7	B	414	11A	CAF-CAG-CAH-CAI
6	A	410	IEP	C10-C11-C12-C13
7	A	411	11A	CAG-CAH-CAI-CAJ
3	A	405	R16	C28-C29-C30-C31
9	B	405	OCT	C4-C5-C6-C7
6	B	413	IEP	C10-C11-C12-C13
3	A	407	R16	C33-C34-C35-C36
6	A	410	IEP	C05-C06-C07-C08
3	A	405	R16	C35-C36-C37-C38
5	B	410	B7G	C7-C8-C9-C10
6	B	413	IEP	C02-C03-C04-C05
5	B	411	B7G	C11-C10-C9-C8
10	B	408	D12	C4-C5-C6-C7
10	B	408	D12	C5-C6-C7-C8
3	A	405	R16	C37-C38-C39-C40
6	B	413	IEP	C51-C52-C53-C54
3	A	406	R16	C38-C39-C40-C41
10	B	407	D12	C2-C3-C4-C5
10	B	408	D12	C3-C4-C5-C6
5	A	409	B7G	C9-C10-C11-C12
6	B	413	IEP	C49-C51-C52-C53
5	B	411	B7G	C2-C1-O1-C7
6	A	410	IEP	C22-C23-O24-P25
6	B	413	IEP	C06-C07-C08-C09

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Mol	Chain	Res	Type	Atoms
6	A	410	IEP	C1-C2-C3-C4
3	A	407	R16	C32-C33-C34-C35
7	B	414	11A	CAG-CAH-CAI-CAJ
6	A	410	IEP	C2-C3-C4-C5
3	A	407	R16	C37-C38-C39-C40
7	B	414	11A	CAI-CAJ-CAK-CAL
6	A	410	IEP	C13-C14-C15-C16
9	B	406	OCT	C2-C3-C4-C5
6	B	413	IEP	C08-C09-C10-C11
10	B	408	D12	C7-C8-C9-C10
3	A	406	R16	C30-C31-C32-C33
5	B	410	B7G	C8-C7-O1-C1
3	A	407	R16	C36-C37-C38-C39
3	A	406	R16	C32-C33-C34-C35
6	B	413	IEP	O20-C21-C22-C23
6	B	413	IEP	C12-C13-C14-C15
6	B	413	IEP	C29-O28-P25-O26
6	B	413	IEP	C29-O28-P25-O27
3	A	405	R16	C30-C31-C32-C33
10	B	408	D12	C9-C10-C11-C12
6	A	410	IEP	C11-C12-C13-C14
5	B	409	B7G	O5-C5-C6-O6
10	B	407	D12	C11-C10-C9-C8
6	A	410	IEP	C03-C04-C05-C06
11	B	412	UND	C7-C8-C9-C10
6	B	413	IEP	C17-C18-O20-C21
11	B	412	UND	C1-C2-C3-C4
6	B	413	IEP	C33-O36-P37-O38
7	B	414	11A	CAD-CAE-CAF-CAG
6	B	413	IEP	C23-O24-P25-O27
10	B	408	D12	C11-C10-C9-C8
3	A	406	R16	C37-C38-C39-C40
6	B	413	IEP	O19-C18-O20-C21
9	B	405	OCT	C1-C2-C3-C4
3	A	407	R16	C28-C29-C30-C31
4	A	408	Q6F	C11-N08-S03-O05
3	A	405	R16	C31-C32-C33-C34
6	B	413	IEP	C05-C06-C07-C08
7	A	411	11A	CAI-CAJ-CAK-CAL
10	B	407	D12	C7-C8-C9-C10
12	B	416	LNK	C1-C2-C3-C4
6	A	410	IEP	C02-C03-C04-C05

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Mol	Chain	Res	Type	Atoms
5	B	410	B7G	C11-C10-C9-C8
6	A	410	IEP	C09-C10-C11-C12
6	B	413	IEP	C60-C61-C62-C63
6	B	413	IEP	C61-C62-C63-C64
5	A	409	B7G	O1-C7-C8-C9
12	B	416	LNK	C2-C3-C4-C5
6	B	413	IEP	C11-C12-C13-C14
6	A	410	IEP	C12-C13-C14-C15
9	B	405	OCT	C2-C3-C4-C5
3	A	407	R16	C29-C30-C31-C32
3	A	406	R16	C36-C37-C38-C39
6	A	410	IEP	C2-C1-C64-C63
3	A	405	R16	C27-C28-C29-C30
4	B	415	Q6F	C17-C11-N08-S03
4	B	415	Q6F	C16-C11-N08-S03
6	B	413	IEP	C22-C23-O24-P25
5	B	410	B7G	C10-C11-C12-C13
6	B	413	IEP	C09-C10-C11-C12
3	A	406	R16	C28-C29-C30-C31
10	B	407	D12	C4-C5-C6-C7
3	A	407	R16	C38-C39-C40-C41
6	B	413	IEP	C14-C15-C16-C17
6	B	413	IEP	O48-C49-C51-C52
6	B	413	IEP	O50-C49-C51-C52

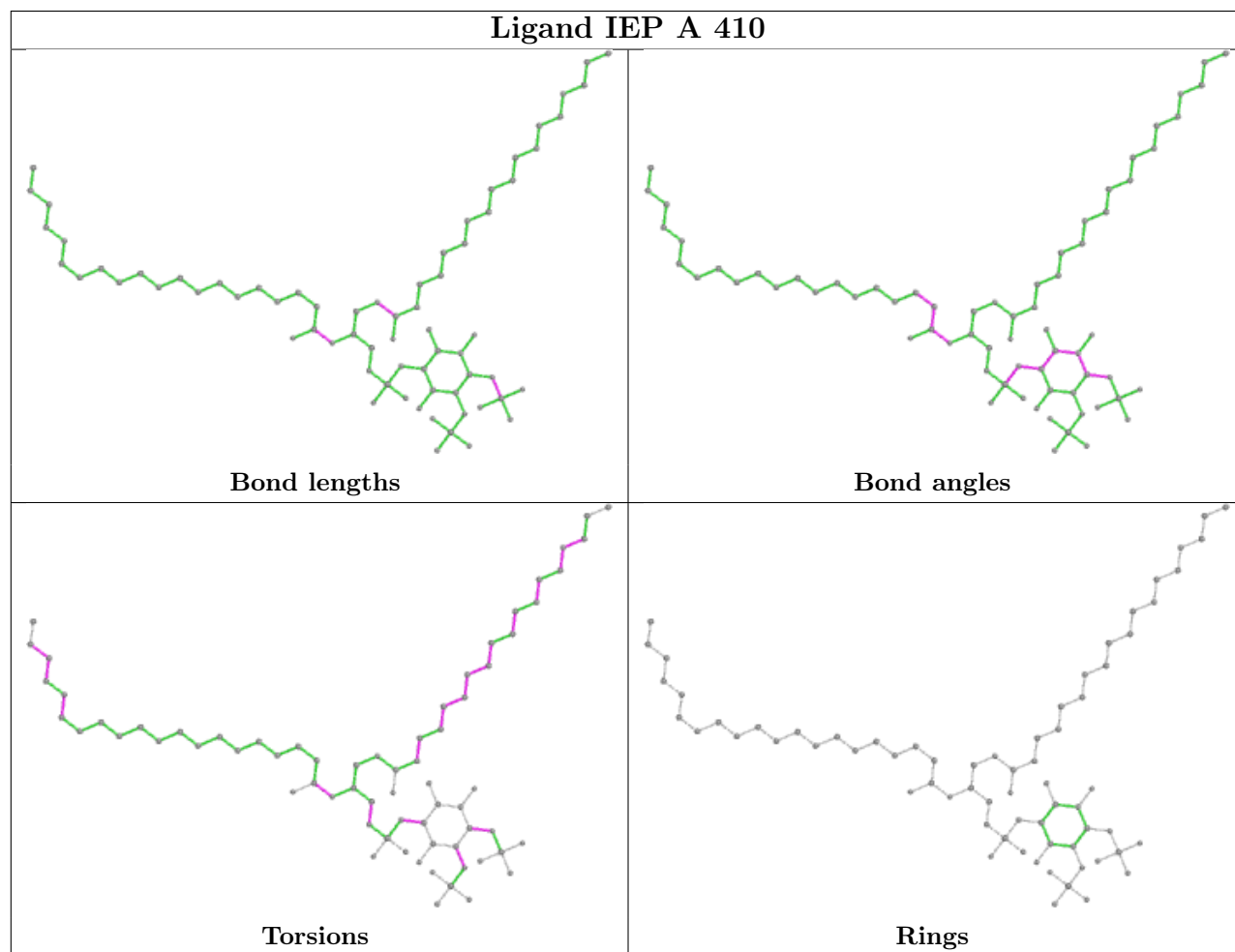
There are no ring outliers.

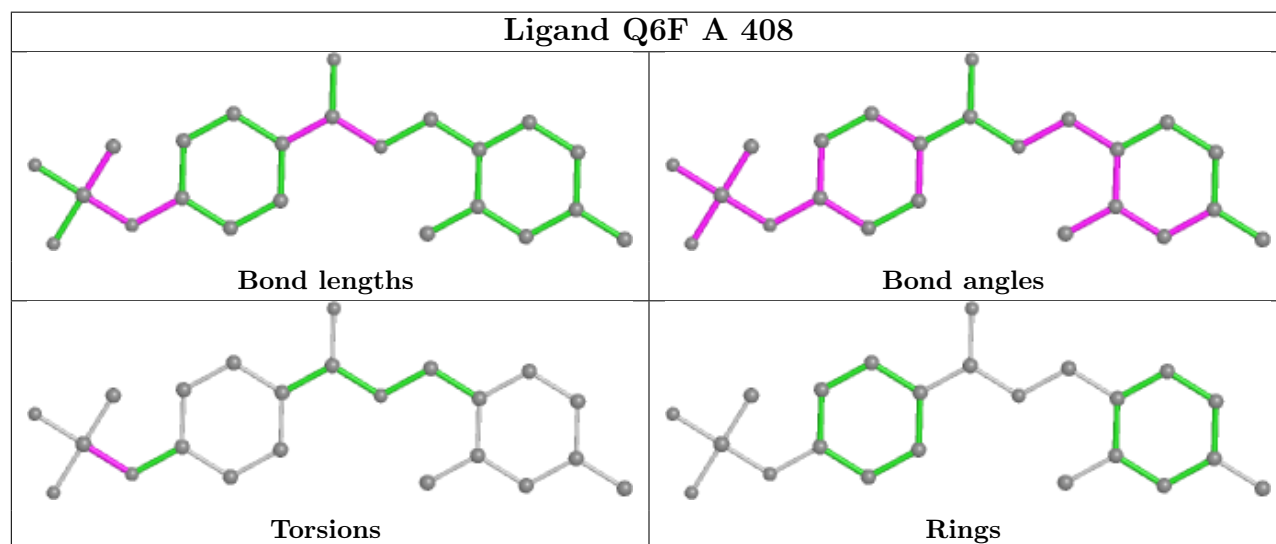
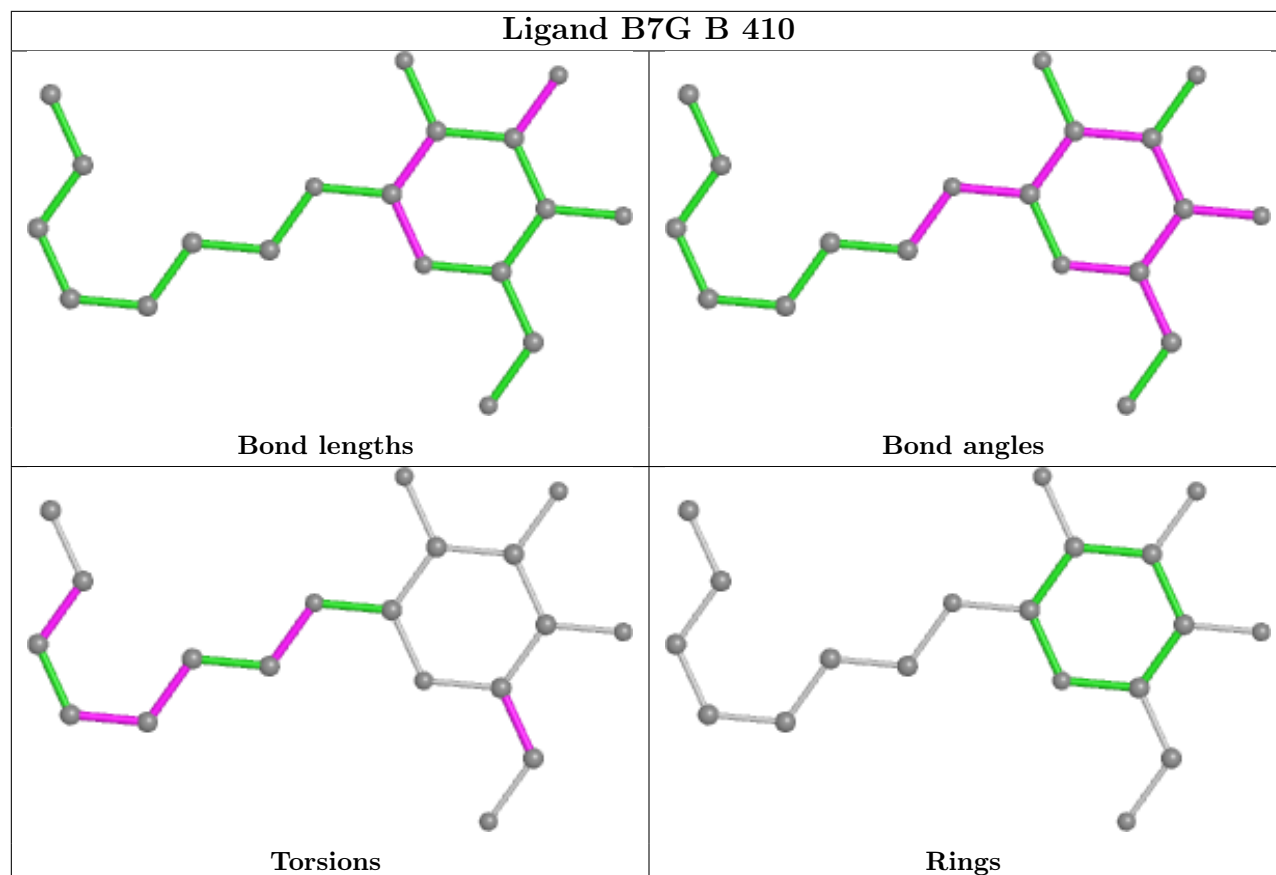
7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	410	IEP	1	0
10	B	408	D12	2	0
4	A	408	Q6F	1	0
4	B	415	Q6F	1	0
6	B	413	IEP	3	0
7	B	414	11A	1	0
5	B	411	B7G	1	0

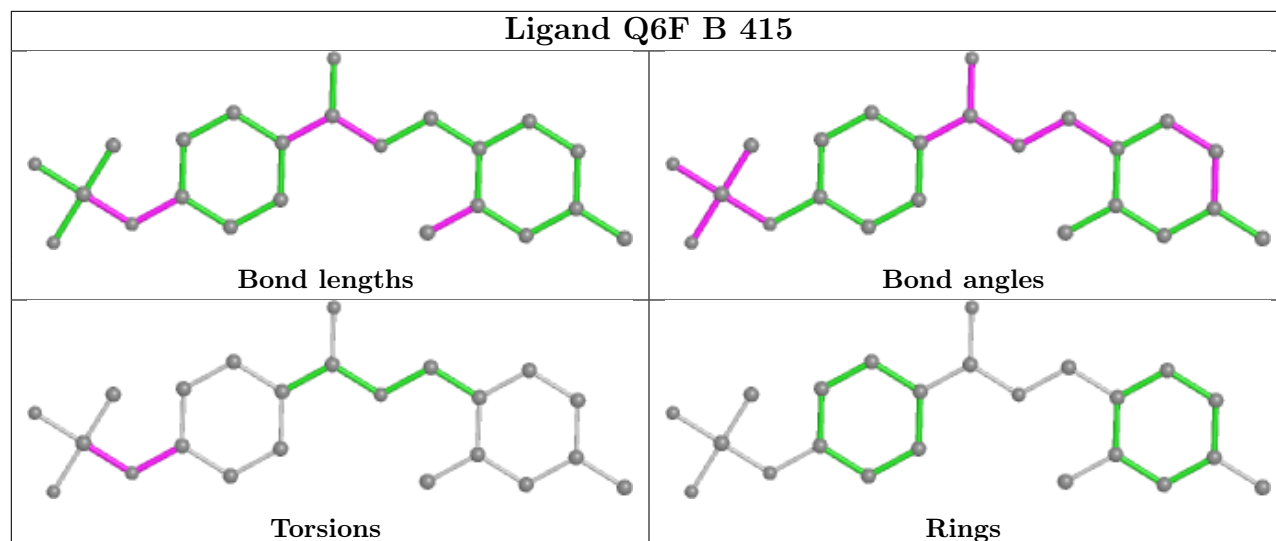
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

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

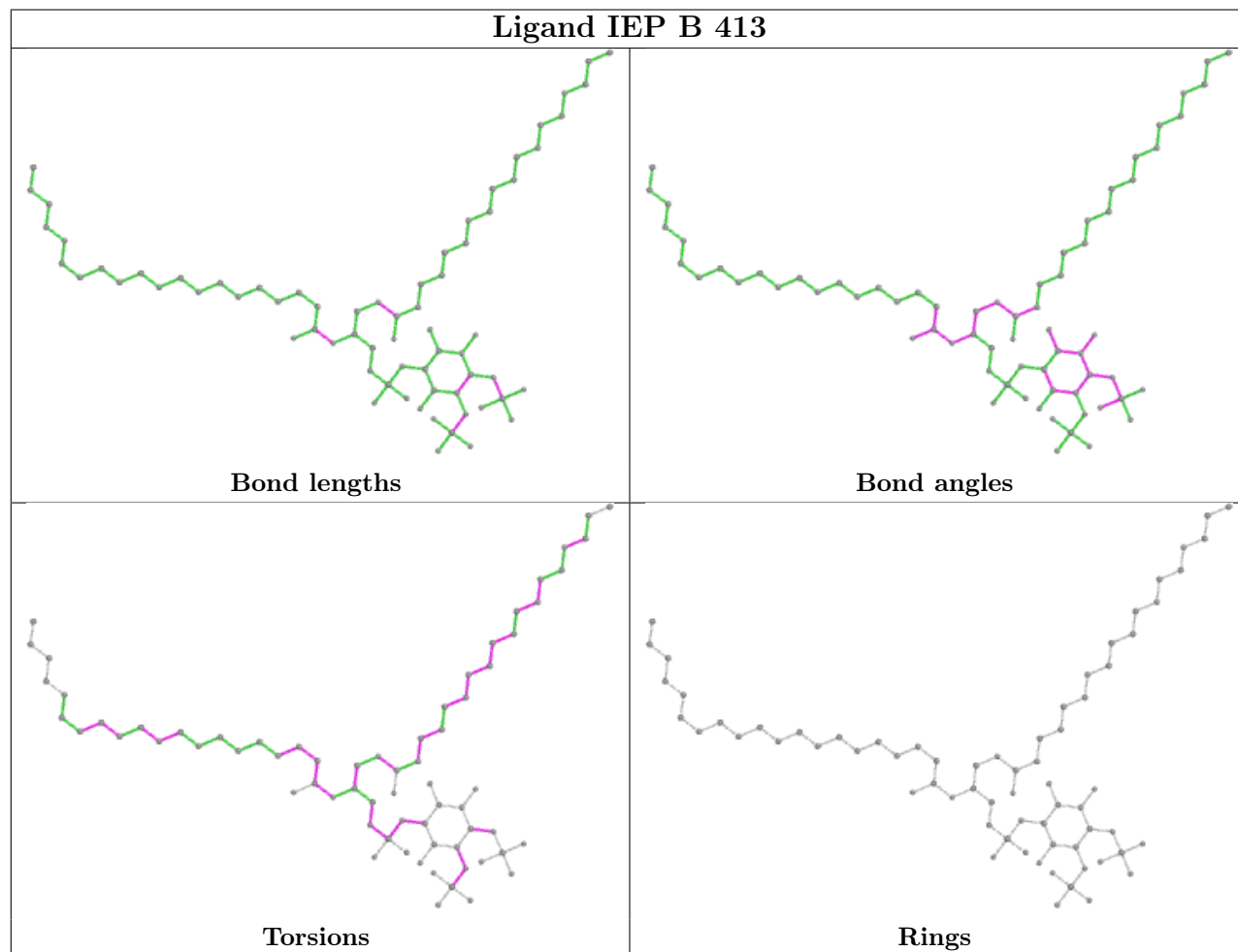




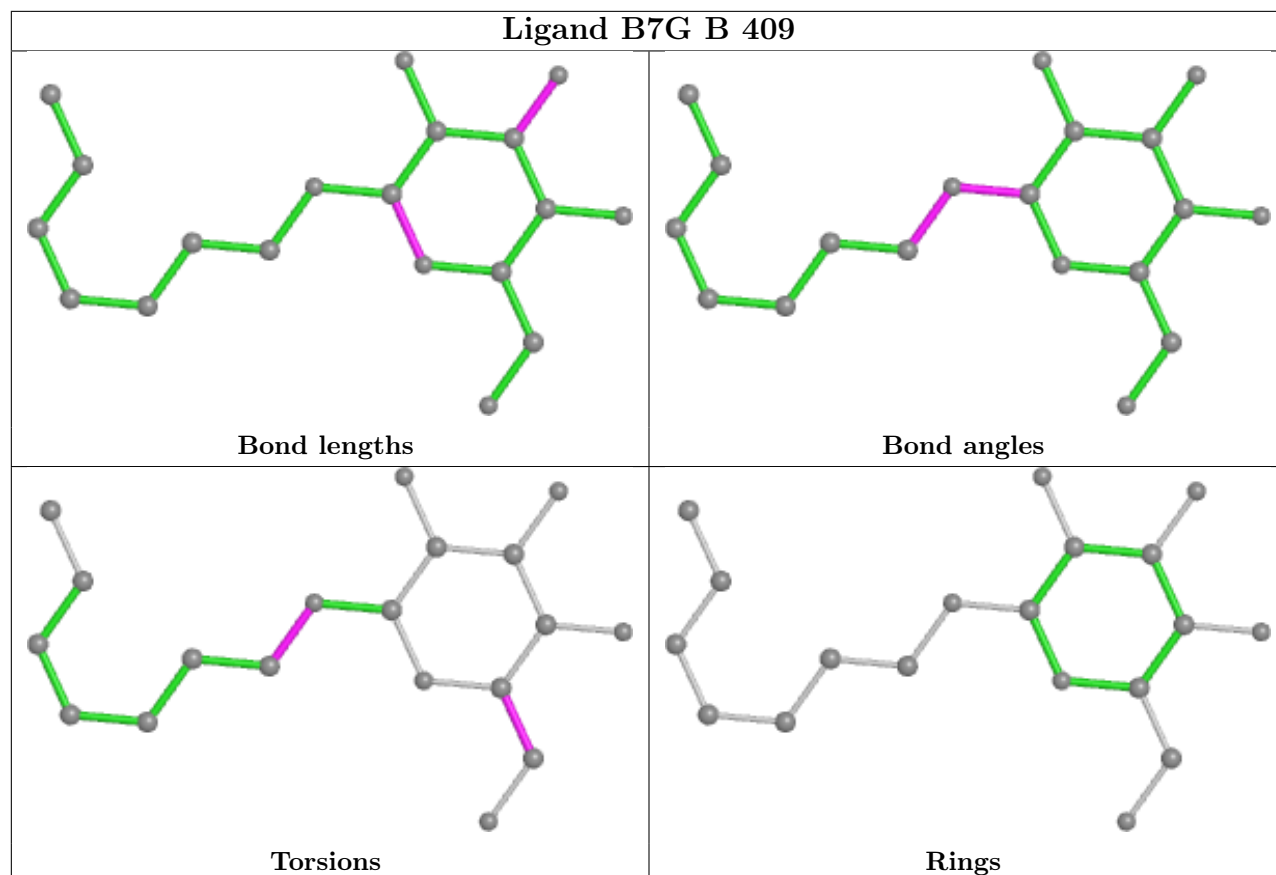
Ligand Q6F B 415



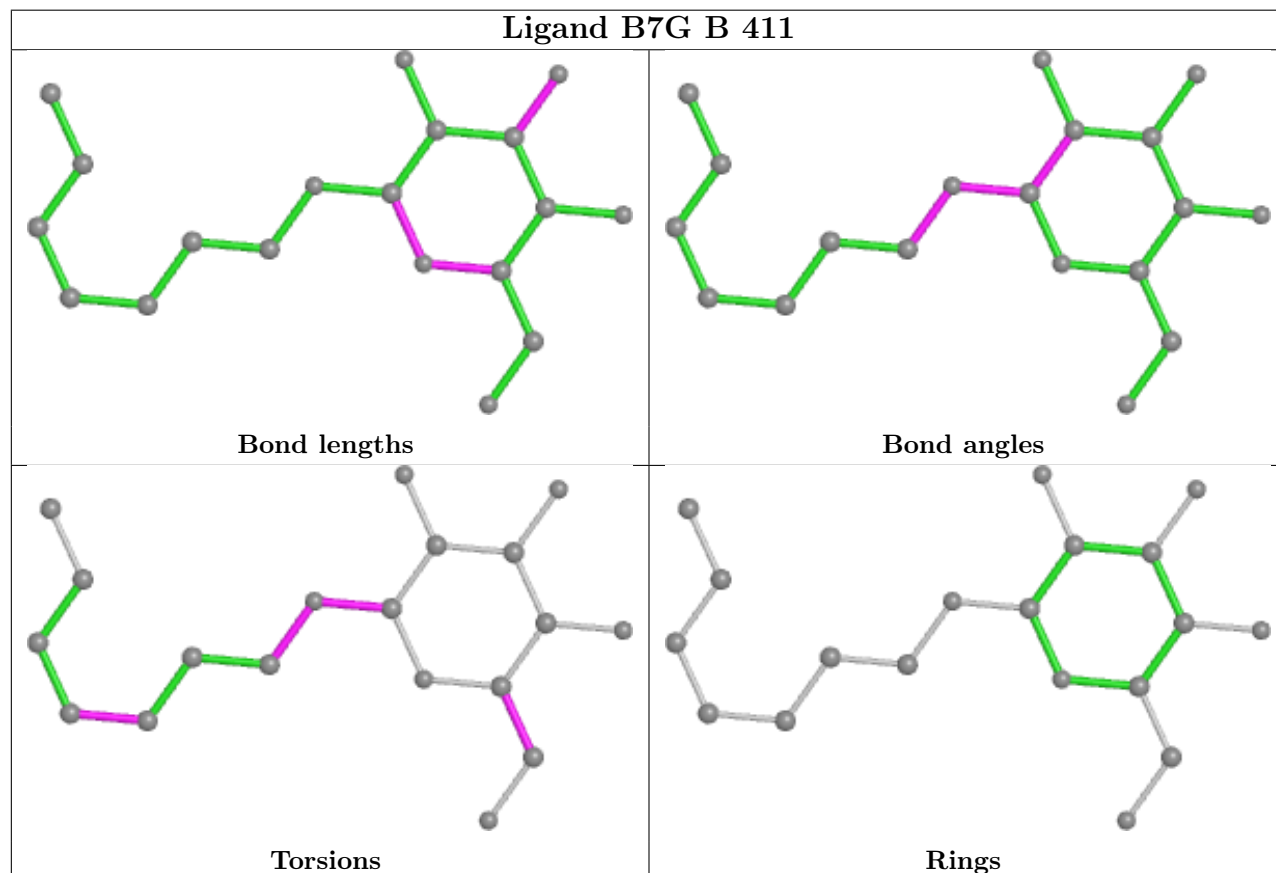
Ligand IEP B 413

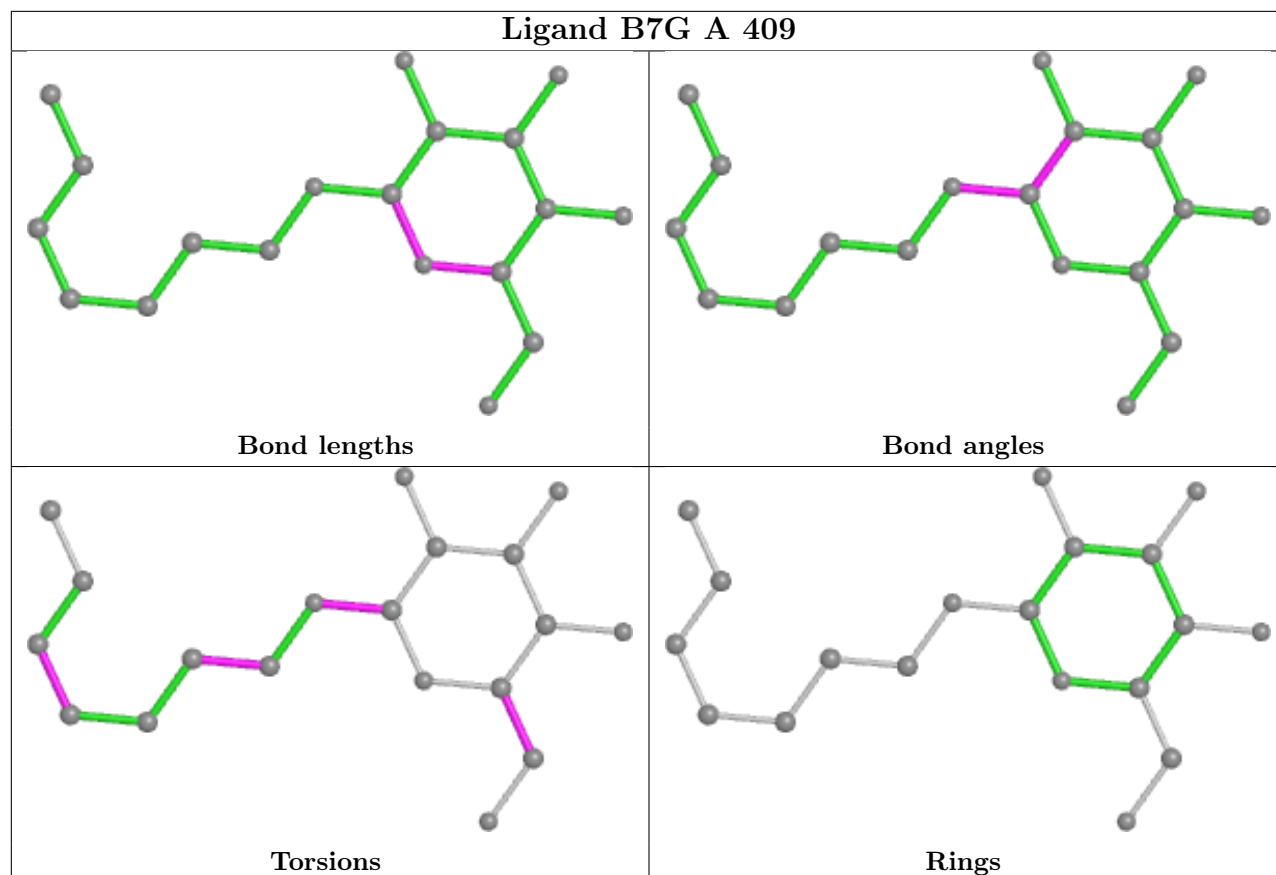


Ligand B7G B 409



Ligand B7G B 411





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	276/312 (88%)	0.25	22 (7%) 12 9	69, 104, 197, 255	0
1	B	281/312 (90%)	0.46	33 (11%) 4 3	69, 107, 212, 262	0
All	All	557/624 (89%)	0.35	55 (9%) 7 5	69, 106, 206, 262	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	199	TRP	10.5
1	A	36	ASP	10.0
1	A	198	LYS	9.9
1	B	93	CYS	8.9
1	B	35	SER	7.5
1	B	89	ARG	7.0
1	A	199	TRP	6.9
1	B	204	THR	5.5
1	B	201	VAL	5.3
1	A	196	PHE	5.2
1	B	95	SER	5.2
1	A	200	ASN	5.1
1	A	197	ILE	4.7
1	B	92	PRO	4.7
1	A	201	VAL	4.7
1	B	203	GLN	4.4
1	A	92	PRO	4.1
1	B	191	LYS	4.0
1	B	44	TRP	4.0
1	A	263	ASP	4.0
1	B	196	PHE	3.8
1	B	129	LEU	3.6
1	B	122	ASN	3.6
1	A	268	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	193	GLU	3.4
1	B	194	ASP	3.2
1	B	121	SER	3.2
1	B	36	ASP	3.2
1	B	265	GLU	3.1
1	B	113	GLY	3.1
1	A	203	GLN	3.1
1	B	86	LYS	3.0
1	A	202	SER	3.0
1	A	90	ALA	3.0
1	A	191	LYS	3.0
1	B	195	THR	2.9
1	B	268	ASP	2.8
1	A	207	ARG	2.8
1	A	190	ALA	2.7
1	B	90	ALA	2.5
1	B	205	LYS	2.5
1	A	44	TRP	2.5
1	A	320	ASN	2.3
1	A	187	LYS	2.3
1	B	97	GLN	2.3
1	A	89	ARG	2.2
1	B	190	ALA	2.2
1	A	195	THR	2.2
1	B	104	GLN	2.2
1	A	94	VAL	2.2
1	B	202	SER	2.2
1	B	120	SER	2.1
1	B	112	ALA	2.1
1	B	316	GLU	2.1
1	B	126	HIS	2.1

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

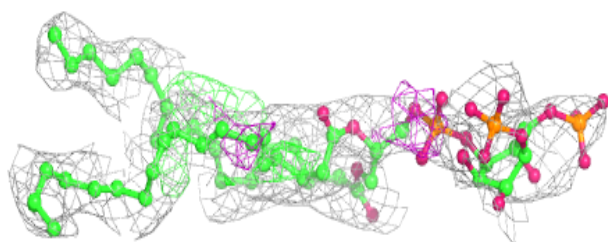
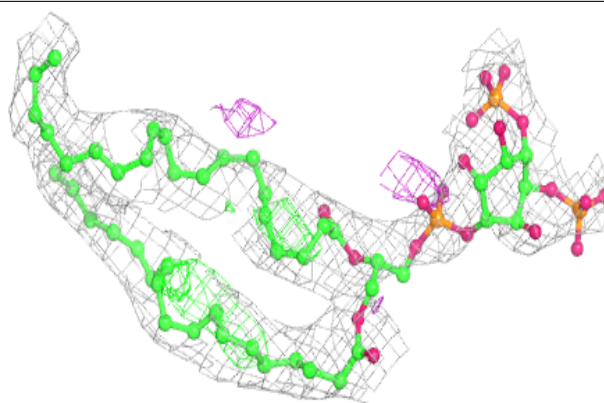
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	K	B	401	1/1	0.41	0.39	157,157,157,157	0
6	IEP	A	410	69/69	0.58	0.29	109,143,228,235	0
3	R16	A	407	16/16	0.66	0.30	122,142,155,156	0
6	IEP	B	413	69/69	0.66	0.37	99,141,205,211	0
7	11A	B	414	13/13	0.66	0.25	114,116,120,120	0
10	D12	B	408	12/12	0.70	0.29	115,132,155,158	0
11	UND	B	412	11/11	0.71	0.16	127,129,132,132	0
5	B7G	B	409	19/19	0.71	0.23	136,141,160,160	0
9	OCT	B	406	8/8	0.75	0.19	117,119,122,122	0
5	B7G	B	410	19/19	0.77	0.29	133,135,140,142	0
10	D12	B	407	12/12	0.78	0.12	130,131,132,132	0
5	B7G	B	411	19/19	0.78	0.25	134,146,148,148	0
12	LNK	B	416	5/5	0.79	0.21	96,96,96,96	0
5	B7G	A	409	19/19	0.80	0.21	146,151,156,157	0
3	R16	A	406	16/16	0.83	0.15	111,120,133,133	0
3	R16	A	405	16/16	0.83	0.14	116,124,129,129	0
9	OCT	B	405	8/8	0.85	0.12	121,121,122,123	0
7	11A	A	411	13/13	0.87	0.17	121,125,129,130	0
2	K	A	401	1/1	0.89	0.12	127,127,127,127	0
2	K	A	412	1/1	0.89	0.10	91,91,91,91	0
8	CD	B	402	1/1	0.93	0.03	203,203,203,203	0
4	Q6F	B	415	23/23	0.94	0.12	78,88,104,108	0
2	K	A	402	1/1	0.94	0.19	96,96,96,96	0
2	K	A	403	1/1	0.95	0.58	119,119,119,119	0
2	K	A	404	1/1	0.95	0.19	87,87,87,87	0
8	CD	B	404	1/1	0.95	0.06	176,176,176,176	0
4	Q6F	A	408	23/23	0.96	0.11	80,89,96,97	0
8	CD	B	403	1/1	0.97	0.02	124,124,124,124	0

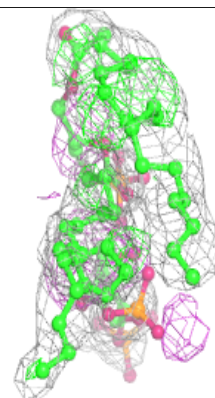
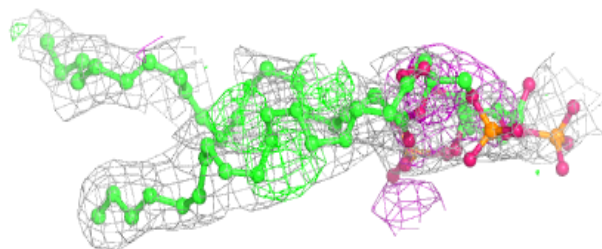
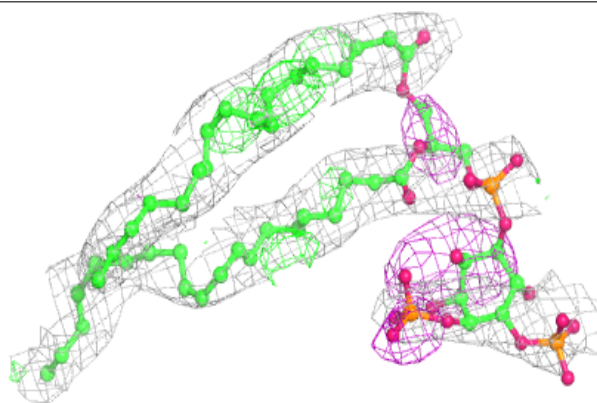
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around IEP A 410:

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

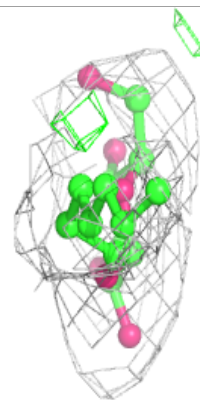
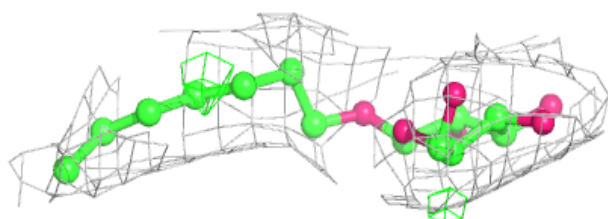
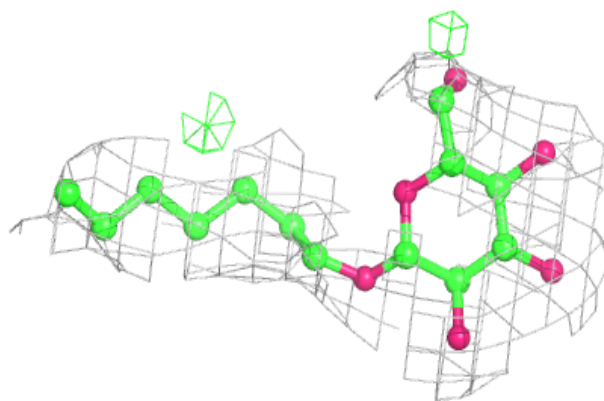
**Electron density around IEP B 413:**

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

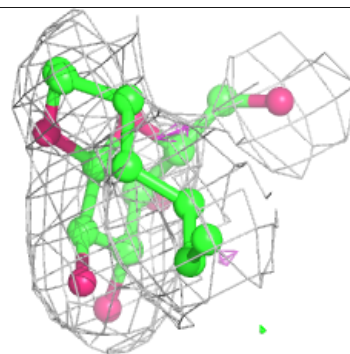
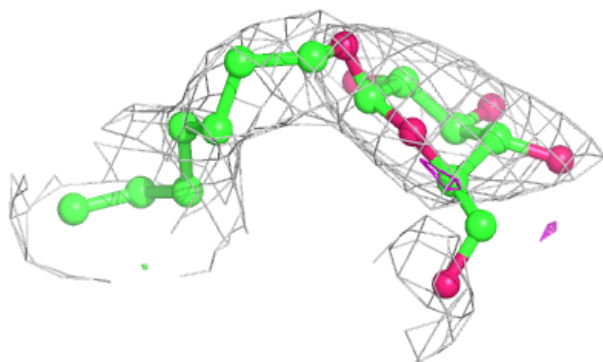
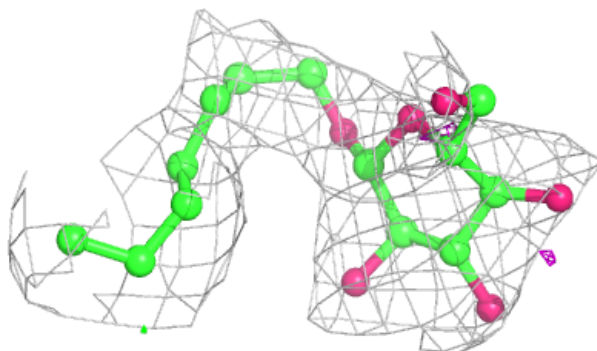


Electron density around B7G B 409:

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

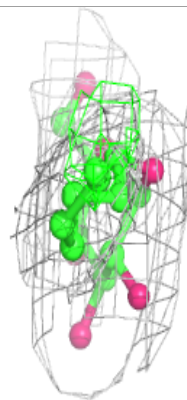
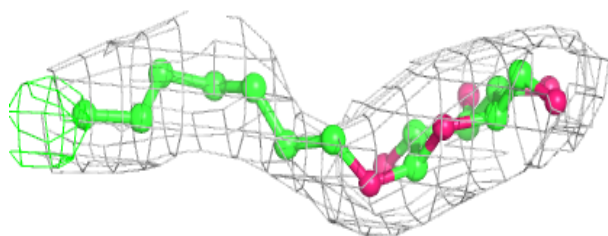
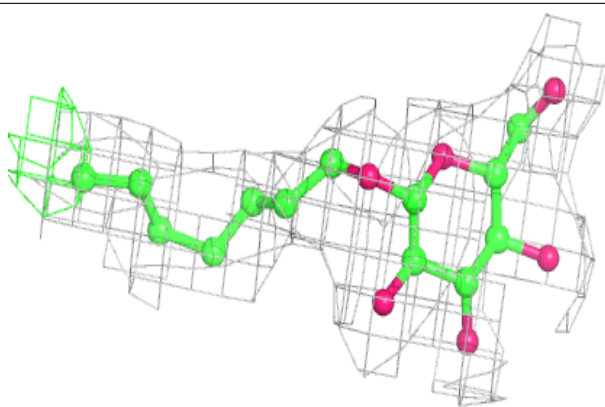
**Electron density around B7G B 410:**

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

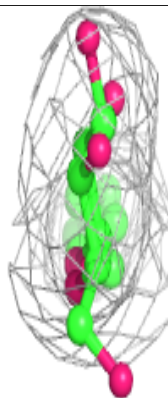
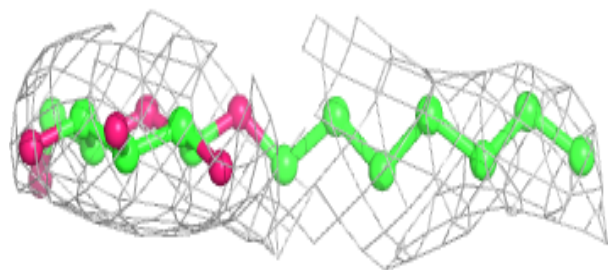
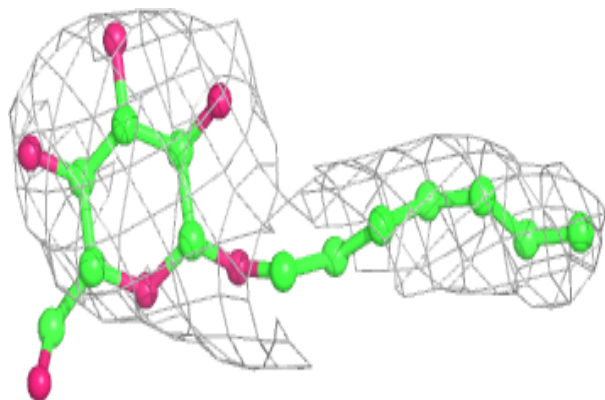


Electron density around B7G B 411:

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

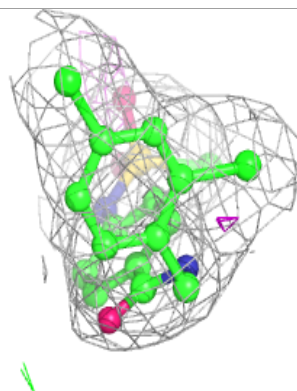
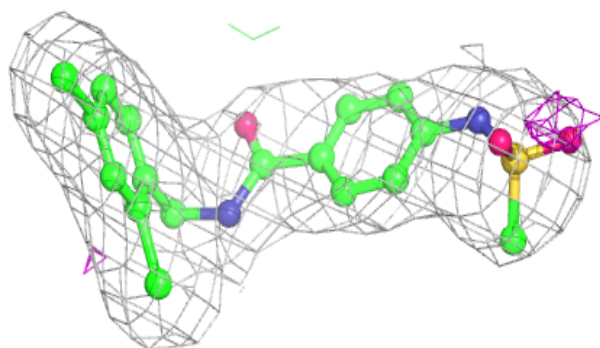
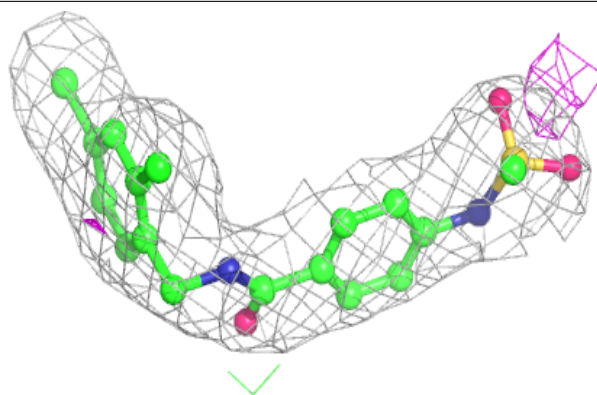
**Electron density around B7G A 409:**

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

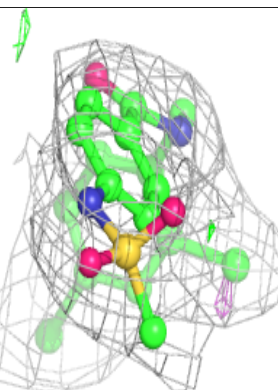
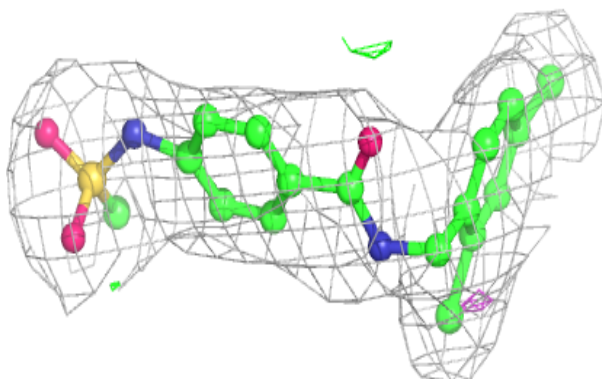
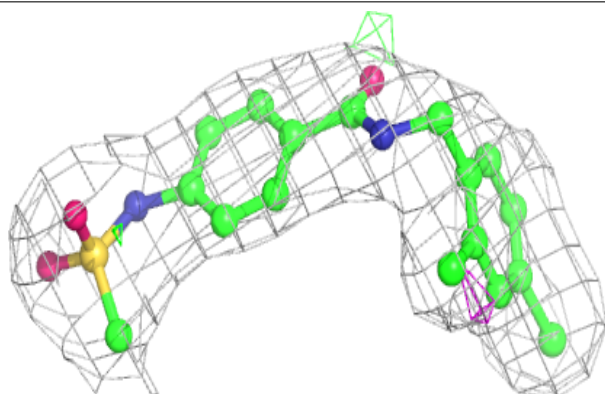


Electron density around Q6F B 415:

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

**Electron density around Q6F A 408:**

$2mF_o - DF_c$ (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.