Full wwPDB X-ray Structure Validation Report (i)

Sep 26, 2023 – 04:54 PM EDT

PDB ID	:	6BWJ
Title	:	Crystal structure of the TRPV2 ion channel in complex with RTx
Authors	:	Zubcevic, L.; Le, S.; Yang, H.; Lee, S.Y.
Deposited on	:	2017-12-15
Resolution	:	3.10 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

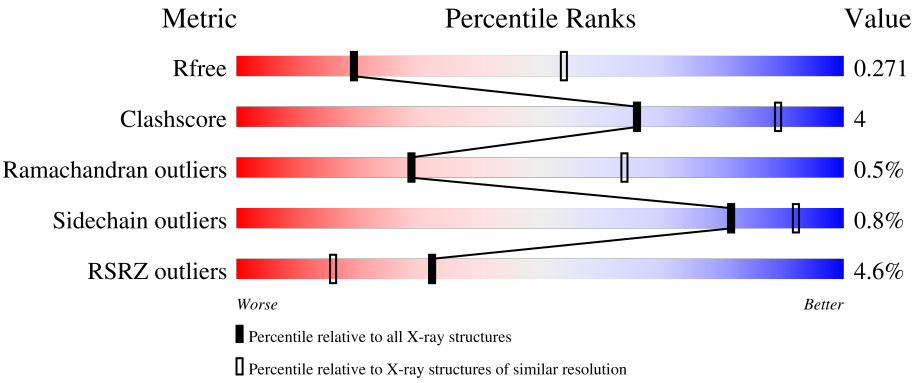
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	776	3% 70% 8% 21%
1	B	776	4% 72% 7% 20%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18348 atoms, of which 8952 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 Transient receptor potential cation channel subfamily V member 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	610	Total	C	H	N	O	S	0	0	0
			9229	3046	4535	790	830	28			
1	B	617	Total	C	H	N	O	S	0	0	0
			8945	2985	4337	776	819	28			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	470	SER	PHE	engineered mutation	UNP G1SNM3
A	505	MET	LEU	engineered mutation	UNP G1SNM3
A	508	THR	LEU	engineered mutation	UNP G1SNM3
A	528	GLU	GLN	engineered mutation	UNP G1SNM3
A	763	ASP	-	expression tag	UNP G1SNM3
A	764	TYR	-	expression tag	UNP G1SNM3
A	765	LYS	-	expression tag	UNP G1SNM3
A	766	ASP	-	expression tag	UNP G1SNM3
A	767	ASP	-	expression tag	UNP G1SNM3
A	768	ASP	-	expression tag	UNP G1SNM3
A	769	ASP	-	expression tag	UNP G1SNM3
A	770	LYS	-	expression tag	UNP G1SNM3
A	771	ALA	-	expression tag	UNP G1SNM3
A	772	HIS	-	expression tag	UNP G1SNM3
A	773	HIS	-	expression tag	UNP G1SNM3
A	774	HIS	-	expression tag	UNP G1SNM3
A	775	HIS	-	expression tag	UNP G1SNM3
A	776	HIS	-	expression tag	UNP G1SNM3
A	777	HIS	-	expression tag	UNP G1SNM3
B	470	SER	PHE	engineered mutation	UNP G1SNM3
B	505	MET	LEU	engineered mutation	UNP G1SNM3
B	508	THR	LEU	engineered mutation	UNP G1SNM3
B	528	GLU	GLN	engineered mutation	UNP G1SNM3
B	763	ASP	-	expression tag	UNP G1SNM3

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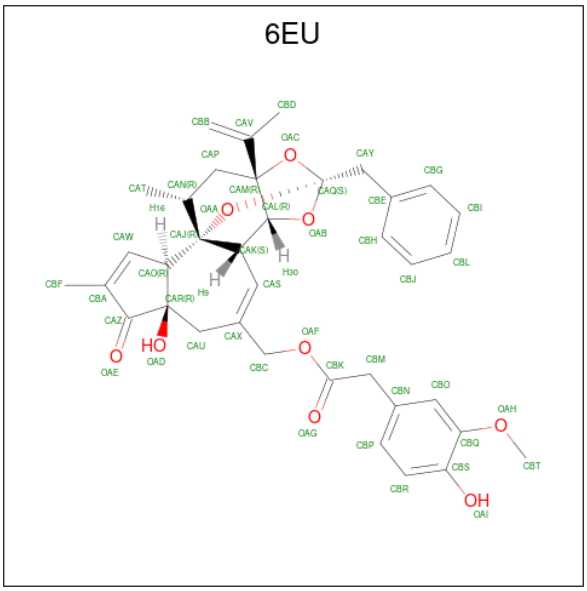
Chain	Residue	Modelled	Actual	Comment	Reference
B	764	TYR	-	expression tag	UNP G1SNM3
B	765	LYS	-	expression tag	UNP G1SNM3
B	766	ASP	-	expression tag	UNP G1SNM3
B	767	ASP	-	expression tag	UNP G1SNM3
B	768	ASP	-	expression tag	UNP G1SNM3
B	769	ASP	-	expression tag	UNP G1SNM3
B	770	LYS	-	expression tag	UNP G1SNM3
B	771	ALA	-	expression tag	UNP G1SNM3
B	772	HIS	-	expression tag	UNP G1SNM3
B	773	HIS	-	expression tag	UNP G1SNM3
B	774	HIS	-	expression tag	UNP G1SNM3
B	775	HIS	-	expression tag	UNP G1SNM3
B	776	HIS	-	expression tag	UNP G1SNM3
B	777	HIS	-	expression tag	UNP G1SNM3

- Molecule 2 is resiniferatoxin (three-letter code: 6EU) (formula: $C_{37}H_{40}O_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			86	37	40	9		
2	B	1	Total	C	H	O	0	0
			86	37	40	9		

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

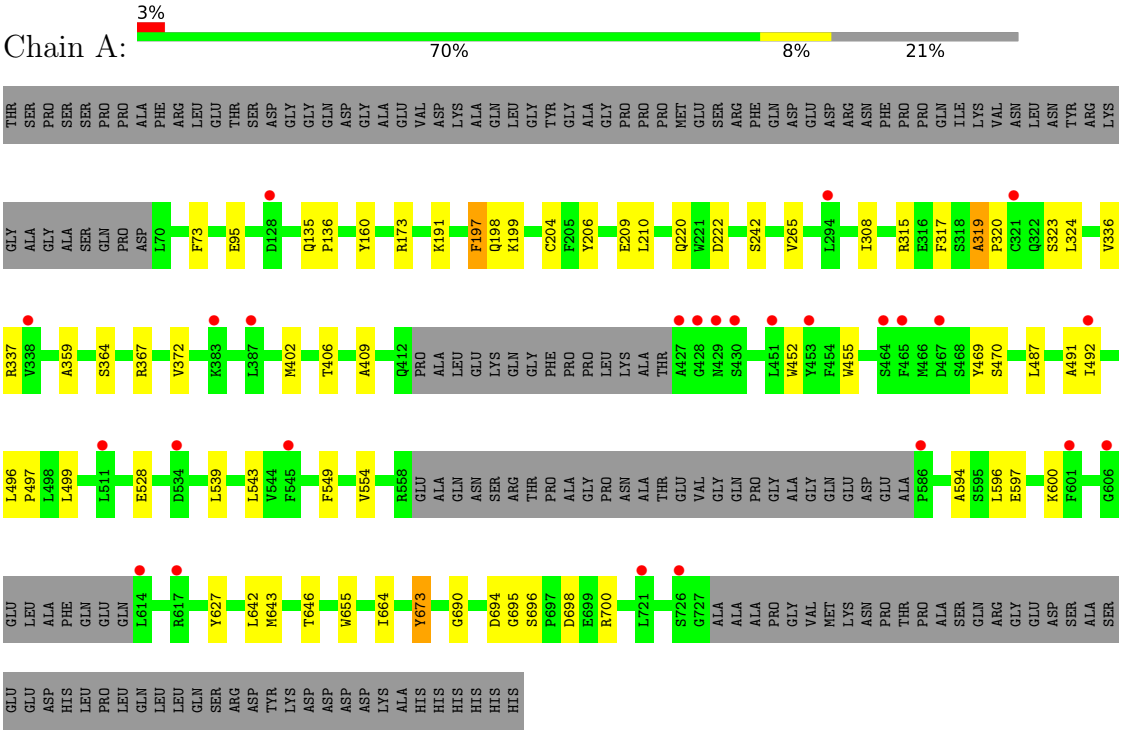
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Ca 2 2	0	0

3 Residue-property plots (i)

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

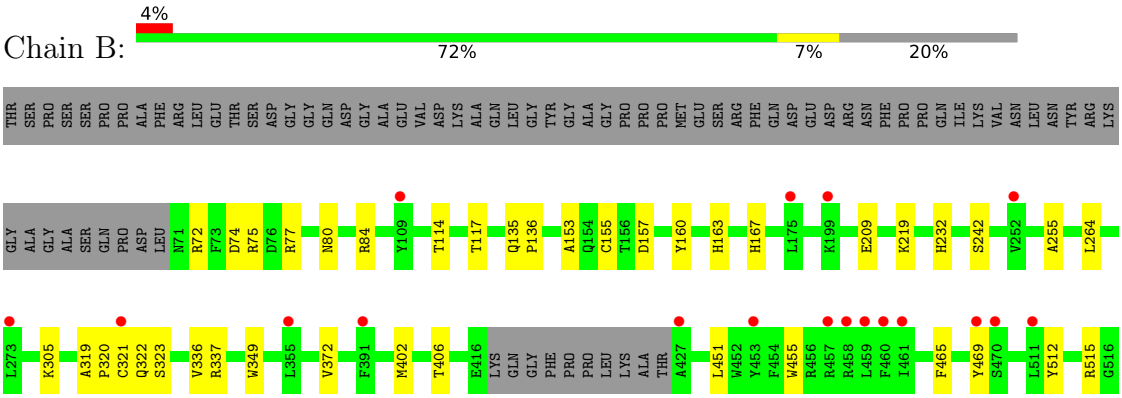
• Molecule 1: Transient receptor potential cation channel subfamily V member 2

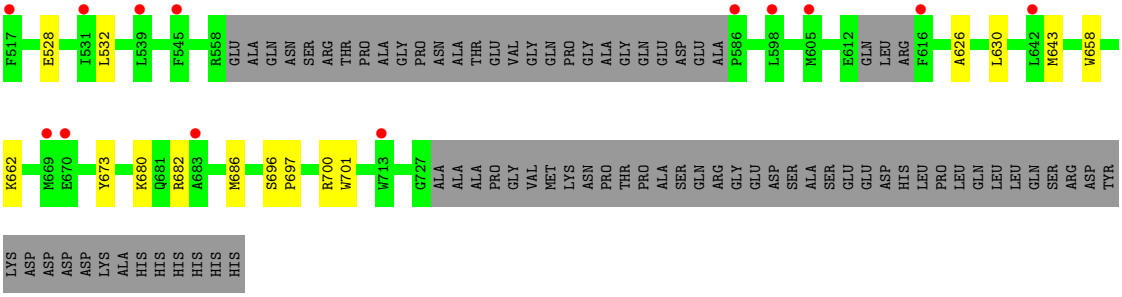
Chain A:



• Molecule 1: Transient receptor potential cation channel subfamily V member 2

Chain B:




F517 E528 I531 L532 L539 F545 R558 GLU ALA GLN ASN SER ARG THR PRO ALA GLY PRO ASN ALA THR GLU VAL GLY GLN PRO GLY ALA GLY GLN GLU ASP GLU ALA P586 L598 M605 E612 GLN LEU ARG F616 A626 L630 L642 M643 W658
K662 M669 E670 Y673 K680 Q681 R682 A683 M686 S696 P697 R700 W701 W713 G727 ALA ALA ALA PRO GLY VAL MET LYS ASN PRO THR PRO ALA SER GLN ARG GLY GLU ASP SER ALA SER GLU GLU ASP HIS LEU PRO LEU GLN LEU LEU GLN SER ARG ASP TYR
LYS ASP ASP ASP ASP LYS ALA HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	90.05Å 121.23Å 185.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.00 – 3.10 101.49 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.00-3.10) 87.1 (101.49-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.55 (at 3.13Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.247 , 0.272 0.248 , 0.271	Depositor DCC
R_{free} test set	2003 reflections (5.33%)	wwPDB-VP
Wilson B-factor (Å^2)	72.7	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 41.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	18348	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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, 6EU

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	0.26	0/4803	0.46	0/6542
1	B	0.26	0/4712	0.45	0/6431
All	All	0.26	0/9515	0.45	0/12973

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4694	4535	4542	39	0
1	B	4608	4337	4368	36	0
2	A	46	40	0	1	0
2	B	46	40	0	0	0
3	B	2	0	0	0	0
All	All	9396	8952	8910	74	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 4.

All (74) 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:B:469:TYR:HB3	1:B:528:GLU:OE2	1.52	1.09
1:A:469:TYR:HB3	1:A:528:GLU:OE2	1.59	1.02
1:B:512:TYR:O	1:B:515:ARG:NH1	2.14	0.80
1:B:323:SER:O	1:B:700:ARG:NH2	2.20	0.73
1:B:114:THR:HG23	1:B:155:CYS:HB3	1.76	0.68
1:B:74:ASP:OD1	1:B:75:ARG:N	2.28	0.66
1:B:469:TYR:CB	1:B:528:GLU:OE2	2.39	0.66
1:A:323:SER:O	1:A:700:ARG:NH2	2.31	0.64
1:B:349:TRP:CZ3	1:B:680:LYS:O	2.51	0.64
1:A:469:TYR:CB	1:A:528:GLU:OE2	2.44	0.61
1:B:451:LEU:O	1:B:455:TRP:N	2.33	0.58
1:B:72:ARG:O	1:B:77:ARG:NH1	2.36	0.57
1:A:198:GLN:HA	1:A:206:TYR:CD1	2.39	0.56
1:A:197:PHE:O	1:A:199:LYS:HG2	2.07	0.54
1:A:319:ALA:CB	1:A:320:PRO:CD	2.85	0.54
1:B:319:ALA:HB1	1:B:320:PRO:CD	2.37	0.54
1:A:470:SER:HB3	2:A:1001:6EU:OAI	2.07	0.53
1:A:690:GLY:O	1:A:698:ASP:N	2.32	0.53
1:A:324:LEU:HD12	1:A:324:LEU:O	2.09	0.53
1:B:209:GLU:OE2	1:B:242:SER:OG	2.26	0.52
1:A:315:ARG:HD2	1:A:317:PHE:HE2	1.74	0.51
1:A:209:GLU:OE2	1:A:242:SER:OG	2.26	0.51
1:A:317:PHE:CD2	1:A:324:LEU:HD12	2.46	0.50
1:B:349:TRP:CE3	1:B:682:ARG:HG3	2.47	0.49
1:A:135:GLN:HB3	1:A:136:PRO:HD3	1.96	0.48
1:B:135:GLN:HB3	1:B:136:PRO:HD3	1.95	0.48
1:A:191:LYS:HG2	1:A:210:LEU:CD2	2.44	0.48
1:B:320:PRO:O	1:B:322:GLN:N	2.39	0.47
1:A:173:ARG:HA	1:A:220:GLN:OE1	2.15	0.46
1:B:255:ALA:O	1:B:305:LYS:CE	2.63	0.46
1:A:452:TRP:CD1	1:A:455:TRP:HE3	2.34	0.46
1:B:80:ASN:O	1:B:84:ARG:HG2	2.16	0.46
1:A:549:PHE:CD1	1:A:627:TYR:HB2	2.51	0.46
1:A:315:ARG:NH1	1:A:324:LEU:O	2.49	0.46
1:B:372:VAL:O	1:B:372:VAL:HG12	2.16	0.45
1:B:465:PHE:HE2	1:B:532:LEU:HD13	1.81	0.45
1:B:163:HIS:CE1	1:B:167:HIS:HB3	2.51	0.45
1:B:114:THR:HG22	1:B:114:THR:O	2.17	0.44
1:B:349:TRP:CZ3	1:B:682:ARG:HG3	2.52	0.44
1:A:95:GLU:OE1	1:A:95:GLU:N	2.48	0.44
1:B:402:MET:O	1:B:406:THR:N	2.44	0.44
1:A:487:LEU:O	1:A:491:ALA:O	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:THR:OG1	1:B:157:ASP:HB3	2.18	0.43
1:A:317:PHE:CE2	1:A:324:LEU:HD12	2.54	0.43
1:B:696:SER:OG	1:B:697:PRO:HD2	2.19	0.43
1:B:686:MET:HB3	1:B:701:TRP:CE2	2.53	0.43
1:B:219:LYS:HB3	1:B:264:LEU:HD11	2.00	0.43
1:A:359:ALA:HB1	1:A:664:ILE:HD13	2.01	0.42
1:A:402:MET:O	1:A:406:THR:N	2.44	0.42
1:A:265:VAL:HG12	1:A:308:ILE:HD12	2.00	0.42
1:B:658:TRP:CZ2	1:B:662:LYS:HD2	2.54	0.42
1:A:596:LEU:O	1:A:600:LYS:HG2	2.20	0.42
1:A:539:LEU:O	1:A:543:LEU:HG	2.20	0.42
1:B:349:TRP:CH2	1:B:680:LYS:O	2.73	0.42
1:A:319:ALA:HB3	1:A:320:PRO:CD	2.50	0.41
1:A:642:LEU:O	1:A:646:THR:HG23	2.20	0.41
1:B:349:TRP:CE3	1:B:682:ARG:CG	3.03	0.41
1:B:117:THR:HG21	1:B:153:ALA:CB	2.51	0.41
1:B:686:MET:HA	1:B:700:ARG:O	2.21	0.41
1:A:372:VAL:HG11	1:A:655:TRP:CZ3	2.55	0.41
1:A:222:ASP:OD1	1:A:222:ASP:N	2.54	0.41
1:A:554:VAL:CG2	1:A:594:ALA:CB	2.98	0.41
1:A:336:VAL:HG12	1:A:337:ARG:N	2.35	0.41
1:A:409:ALA:HA	1:A:499:LEU:HD21	2.02	0.41
1:B:255:ALA:O	1:B:305:LYS:HE3	2.21	0.41
1:A:364:SER:O	1:A:367:ARG:HG3	2.21	0.41
1:B:626:ALA:O	1:B:630:LEU:HG	2.21	0.41
1:B:336:VAL:HG12	1:B:337:ARG:N	2.37	0.40
1:A:694:ASP:O	1:A:696:SER:N	2.55	0.40
1:A:496:LEU:HB3	1:A:497:PRO:HD3	2.02	0.40
1:A:594:ALA:O	1:A:597:GLU:N	2.54	0.40
1:A:643:MET:HE1	1:B:643:MET:CB	2.51	0.40
1:A:690:GLY:O	1:A:698:ASP:HB3	2.22	0.40
1:B:219:LYS:HG3	1:B:219:LYS:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	602/776 (78%)	580 (96%)	18 (3%)	4 (1%)	22 57
1	B	609/776 (78%)	586 (96%)	21 (3%)	2 (0%)	41 73
All	All	1211/1552 (78%)	1166 (96%)	39 (3%)	6 (0%)	29 64

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	ALA
1	A	492	ILE
1	A	695	GLY
1	B	321	CYS
1	B	673	TYR
1	A	673	TYR

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	473/666 (71%)	468 (99%)	5 (1%)	73 89
1	B	449/666 (67%)	447 (100%)	2 (0%)	91 96
All	All	922/1332 (69%)	915 (99%)	7 (1%)	81 92

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	PHE
1	A	160	TYR
1	A	197	PHE
1	A	204	CYS
1	A	673	TYR
1	B	160	TYR

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Mol	Chain	Res	Type
1	B	232	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	HIS
1	A	200	ASN
1	A	322	GLN
1	A	361	HIS
1	A	450	GLN
1	B	314	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
2	6EU	B	803	-	43,52,52	3.90	14 (32%)	42,83,83	1.74	5 (11%)
2	6EU	A	1001	-	43,52,52	3.83	16 (37%)	42,83,83	1.55	6 (14%)

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
2	6EU	B	803	-	-	15/20/101/101	0/8/7/7
2	6EU	A	1001	-	-	6/20/101/101	0/8/7/7

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	803	6EU	CAS-CAX	16.63	1.60	1.33
2	A	1001	6EU	CAS-CAX	16.22	1.59	1.33
2	B	803	6EU	CAM-CAL	9.40	1.66	1.54
2	A	1001	6EU	CAM-CAL	9.07	1.66	1.54
2	B	803	6EU	CAW-CBA	8.27	1.52	1.33
2	A	1001	6EU	CAW-CBA	8.17	1.51	1.33
2	A	1001	6EU	OAB-CAL	-7.33	1.32	1.43
2	B	803	6EU	CAK-CAS	7.12	1.68	1.50
2	B	803	6EU	OAB-CAL	-7.11	1.33	1.43
2	A	1001	6EU	CAK-CAS	6.87	1.67	1.50
2	B	803	6EU	OAF-CBK	3.95	1.44	1.33
2	B	803	6EU	CAY-CBE	3.88	1.58	1.51
2	A	1001	6EU	CAY-CBE	3.85	1.57	1.51
2	A	1001	6EU	OAF-CBK	3.83	1.44	1.33
2	B	803	6EU	OAB-CAQ	-3.15	1.35	1.41
2	A	1001	6EU	OAB-CAQ	-3.09	1.35	1.41
2	A	1001	6EU	OAE-CAZ	-3.00	1.17	1.22
2	B	803	6EU	OAE-CAZ	-2.97	1.17	1.22
2	B	803	6EU	CBC-CAX	2.94	1.57	1.50
2	A	1001	6EU	OAH-CBQ	2.91	1.41	1.37
2	A	1001	6EU	CBC-CAX	2.88	1.57	1.50
2	A	1001	6EU	CBM-CBN	2.81	1.56	1.51
2	B	803	6EU	OAH-CBQ	2.75	1.41	1.37
2	B	803	6EU	CBM-CBN	2.72	1.56	1.51
2	B	803	6EU	CAT-CAN	2.47	1.58	1.53
2	A	1001	6EU	CAT-CAN	2.32	1.58	1.53
2	A	1001	6EU	OAD-CAR	-2.18	1.38	1.42
2	B	803	6EU	OAD-CAR	-2.07	1.38	1.42
2	A	1001	6EU	OAI-CBS	2.05	1.40	1.36
2	A	1001	6EU	CAR-CAO	-2.04	1.50	1.55

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	803	6EU	OAC-CAM-CAP	-6.06	105.73	109.59
2	B	803	6EU	OAF-CBK-CBM	5.55	120.48	111.07
2	A	1001	6EU	OAF-CBK-CBM	4.84	119.28	111.07
2	A	1001	6EU	OAC-CAM-CAP	-4.57	106.68	109.59
2	A	1001	6EU	OAH-CBQ-CBS	3.82	120.10	114.57
2	B	803	6EU	OAH-CBQ-CBS	3.47	119.59	114.57
2	A	1001	6EU	OAA-CAJ-CAN	3.22	109.82	106.13
2	B	803	6EU	OAA-CAJ-CAN	3.09	109.66	106.13
2	B	803	6EU	CAW-CBA-CAZ	-2.78	106.54	108.66
2	A	1001	6EU	CAW-CBA-CAZ	-2.15	107.02	108.66
2	A	1001	6EU	OAH-CBQ-CBO	-2.13	120.46	124.12

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	6EU	CAP-CAM-CAV-CBB
2	B	803	6EU	CAP-CAM-CAV-CBB
2	B	803	6EU	OAC-CAM-CAV-CBB
2	B	803	6EU	OAC-CAM-CAV-CBD
2	B	803	6EU	CAL-CAM-CAV-CBB
2	B	803	6EU	CAL-CAM-CAV-CBD
2	B	803	6EU	OAC-CAQ-CAY-CBE
2	A	1001	6EU	CBO-CBQ-OAH-CBT
2	B	803	6EU	CBS-CBQ-OAH-CBT
2	A	1001	6EU	CBS-CBQ-OAH-CBT
2	A	1001	6EU	CBM-CBK-OAF-CBC
2	B	803	6EU	CBO-CBQ-OAH-CBT
2	A	1001	6EU	OAG-CBK-OAF-CBC
2	B	803	6EU	CBM-CBK-OAF-CBC
2	B	803	6EU	OAG-CBK-OAF-CBC
2	B	803	6EU	OAF-CBK-CBM-CBN
2	B	803	6EU	OAA-CAQ-CAY-CBE
2	B	803	6EU	OAB-CAQ-CAY-CBE
2	B	803	6EU	CAP-CAM-CAV-CBD
2	A	1001	6EU	CAP-CAM-CAV-CBD
2	B	803	6EU	OAG-CBK-CBM-CBN

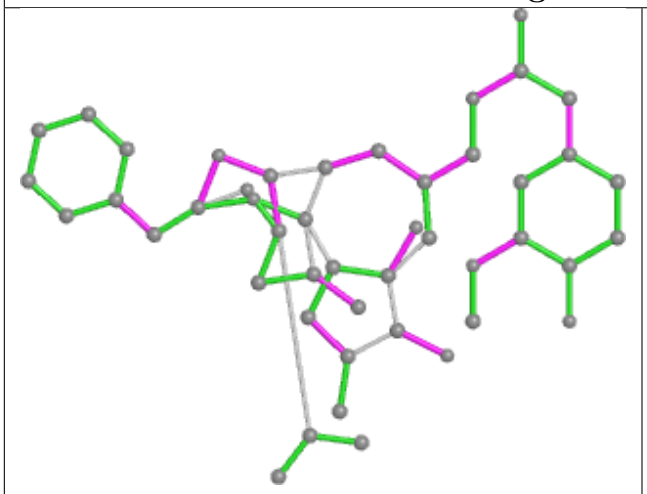
There are no ring outliers.

1 monomer is involved in 1 short contact:

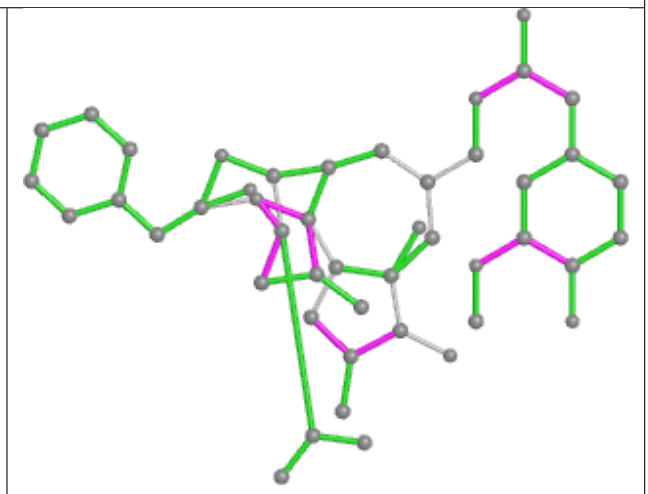
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	6EU	1	0

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.

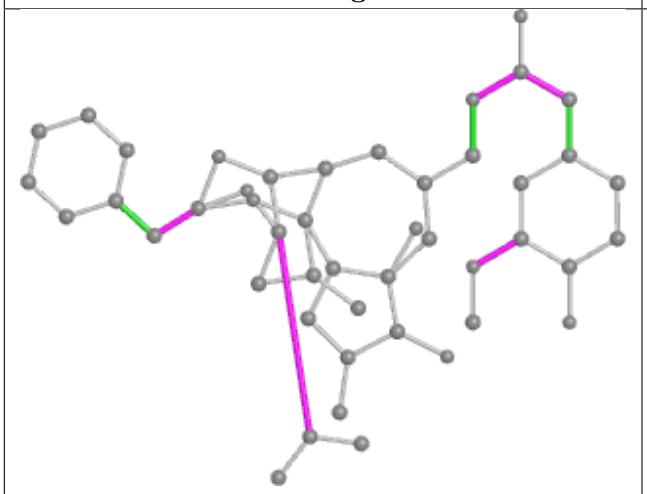
Ligand 6EU B 803



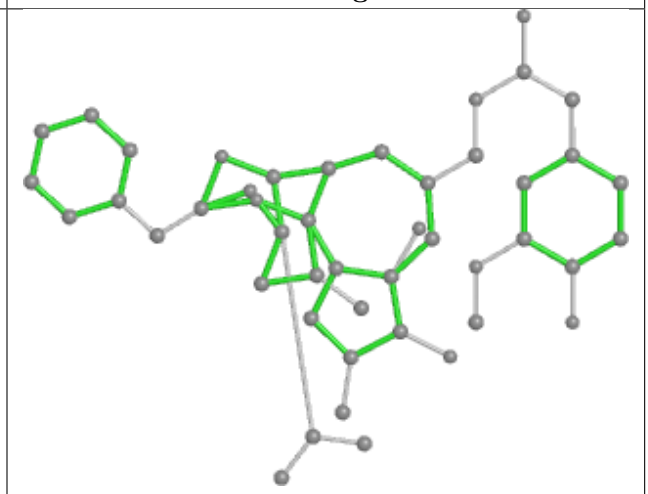
Bond lengths



Bond angles

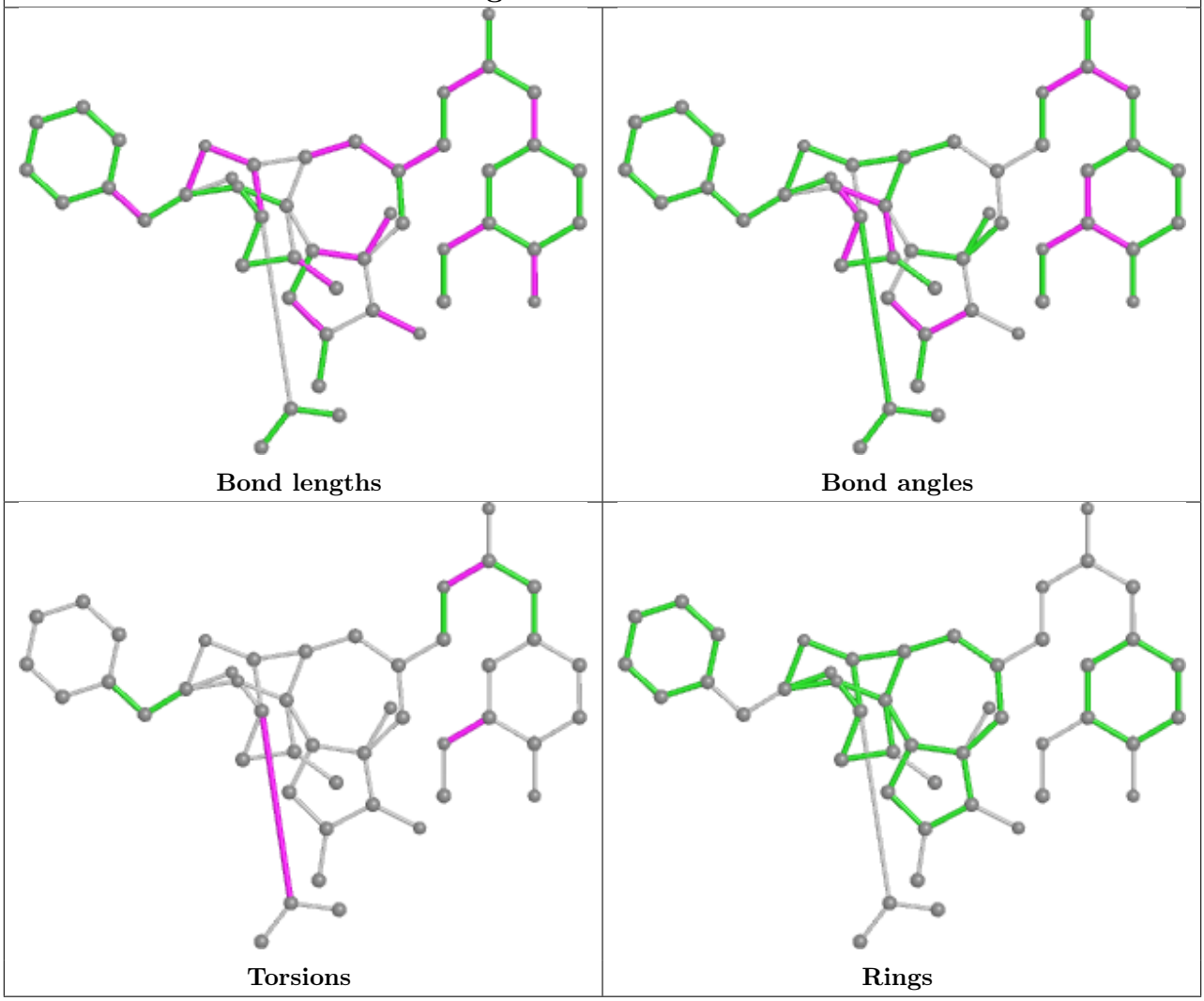


Torsions



Rings

Ligand 6EU A 1001



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, 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	610/776 (78%)	0.38	26 (4%)	35	17	41, 81, 146, 177	0
1	B	617/776 (79%)	0.44	31 (5%)	28	13	43, 85, 152, 190	0
All	All	1227/1552 (79%)	0.41	57 (4%)	32	16	41, 83, 149, 190	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	427	ALA	13.1
1	B	460	PHE	11.4
1	A	429	ASN	6.1
1	A	428	GLY	6.0
1	B	459	LEU	5.8
1	A	586	PRO	5.6
1	A	606	GLY	4.5
1	B	427	ALA	4.3
1	B	469	TYR	4.0
1	A	721	LEU	3.9
1	B	586	PRO	3.7
1	A	614	LEU	3.5
1	A	465	PHE	3.2
1	A	430	SER	3.2
1	B	616	PHE	3.2
1	B	461	ILE	3.2
1	B	458	ARG	3.1
1	A	726	SER	3.1
1	B	598	LEU	2.9
1	B	531	ILE	2.8
1	B	273	LEU	2.8
1	B	517	PHE	2.7
1	B	683	ALA	2.7
1	B	605	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	511	LEU	2.6
1	A	294	LEU	2.5
1	A	383	LYS	2.4
1	A	492	ILE	2.4
1	B	470	SER	2.4
1	A	338	VAL	2.4
1	A	387	LEU	2.4
1	B	457	ARG	2.4
1	B	199	LYS	2.4
1	A	453	TYR	2.4
1	A	617	ARG	2.3
1	A	451	LEU	2.3
1	B	109	TYR	2.3
1	A	128	ASP	2.3
1	B	252	VAL	2.3
1	B	670	GLU	2.3
1	B	669	MET	2.3
1	B	453	TYR	2.3
1	A	464	SER	2.2
1	B	713	TRP	2.2
1	B	391	PHE	2.1
1	B	539	LEU	2.1
1	B	545	PHE	2.1
1	A	545	PHE	2.1
1	B	511	LEU	2.1
1	A	534	ASP	2.1
1	B	355	LEU	2.1
1	A	321	CYS	2.0
1	B	175	LEU	2.0
1	B	642	LEU	2.0
1	A	601	PHE	2.0
1	A	467	ASP	2.0
1	B	321	CYS	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

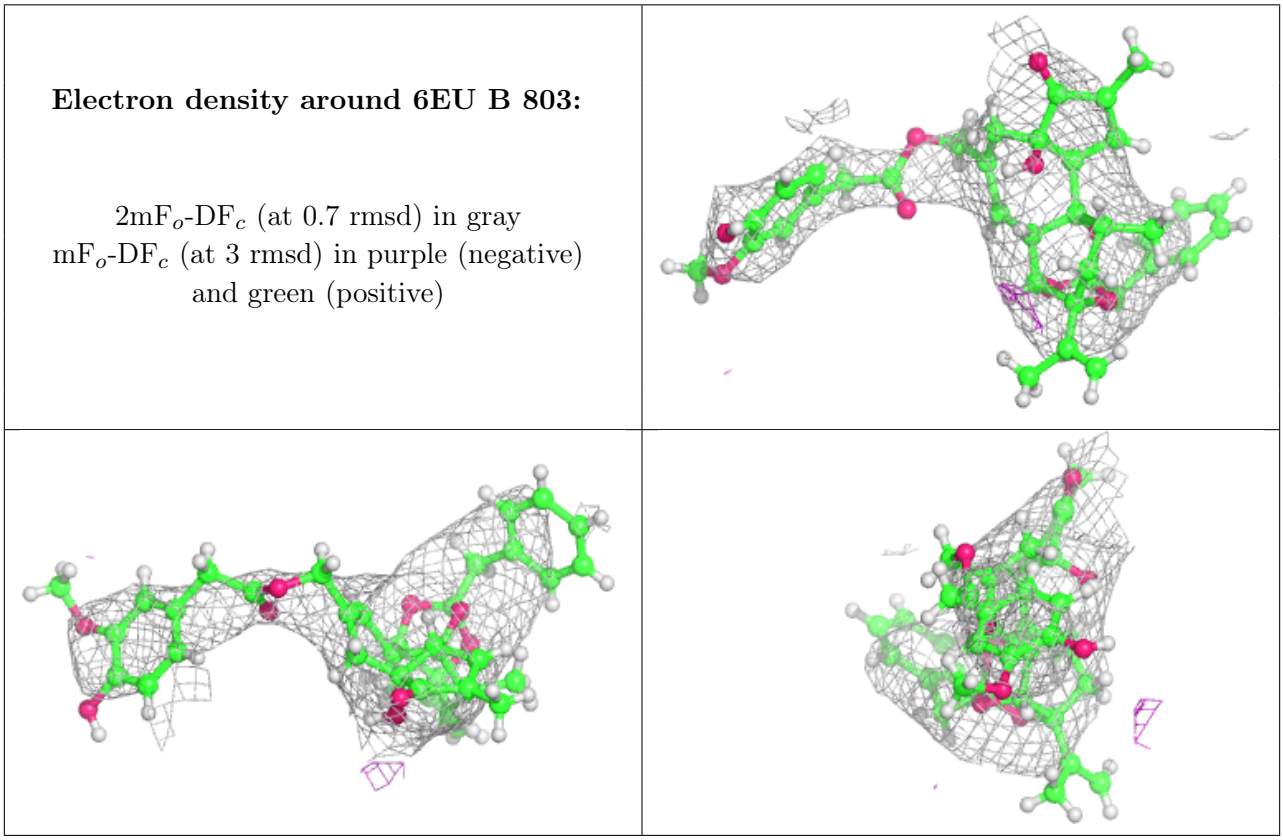
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	B	802	1/1	0.65	0.37	101,101,101,101	1
3	CA	B	801	1/1	0.81	0.41	97,97,97,97	1
2	6EU	B	803	46/46	0.89	0.47	95,124,150,160	0
2	6EU	A	1001	46/46	0.90	0.34	86,108,131,141	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.

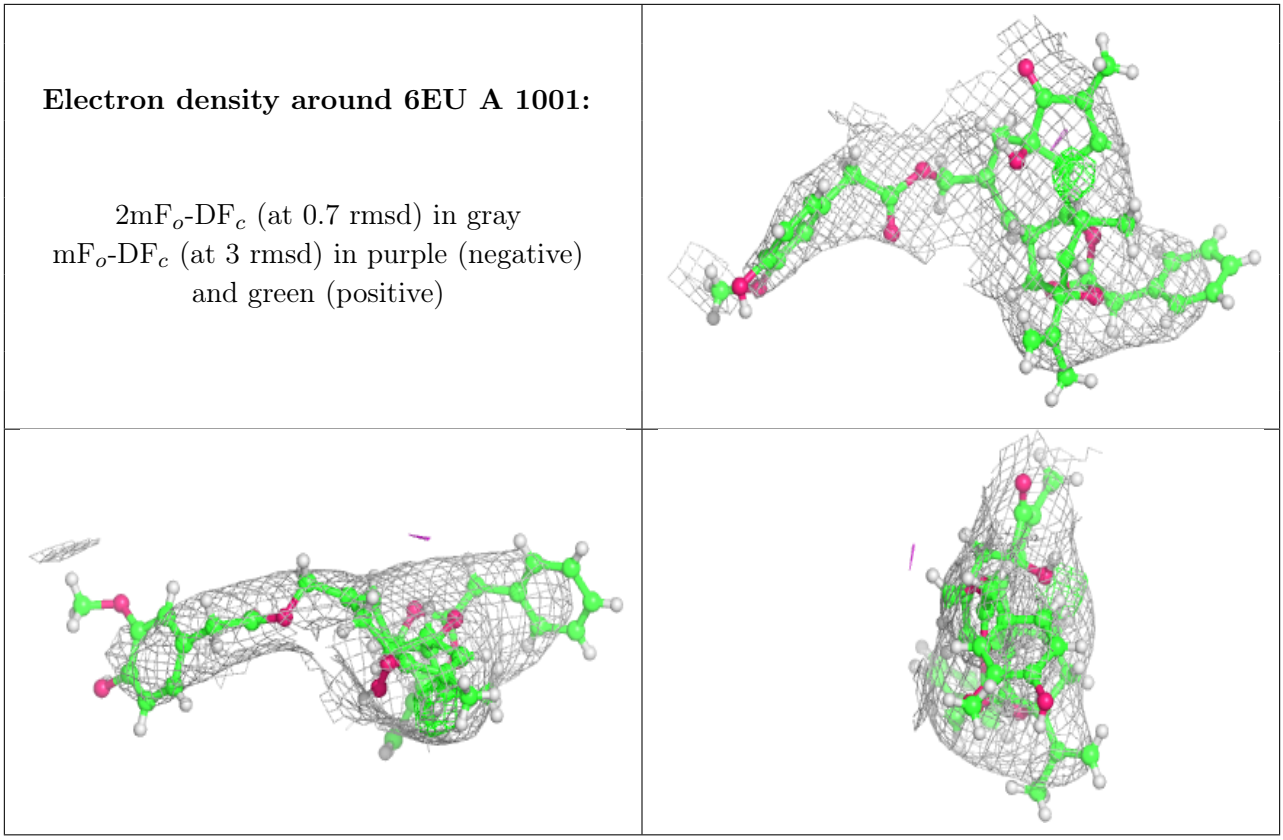
Electron density around 6EU B 803:

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



Electron density around 6EU A 1001:

$2mF_o$-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.