



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:26 AM UTC

PDB ID : 6BWJ / pdb_00006bwj
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

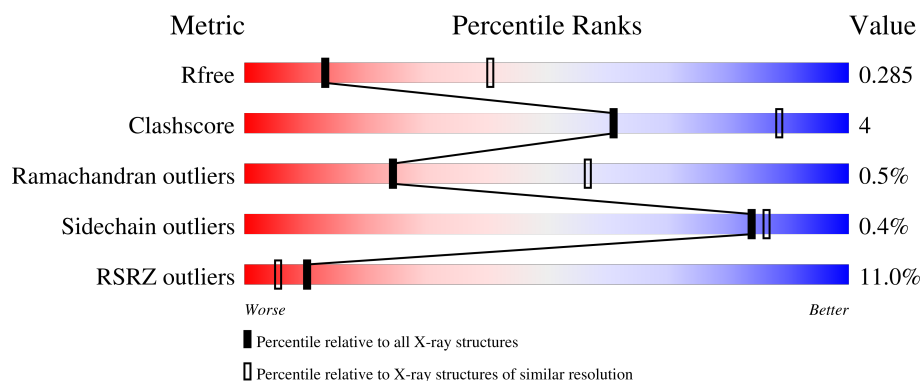
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 $\leq 5\%$. 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	776	9% 70% 8% 21%
1	B	776	9% 73% 7% 20%

2 Entry composition

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

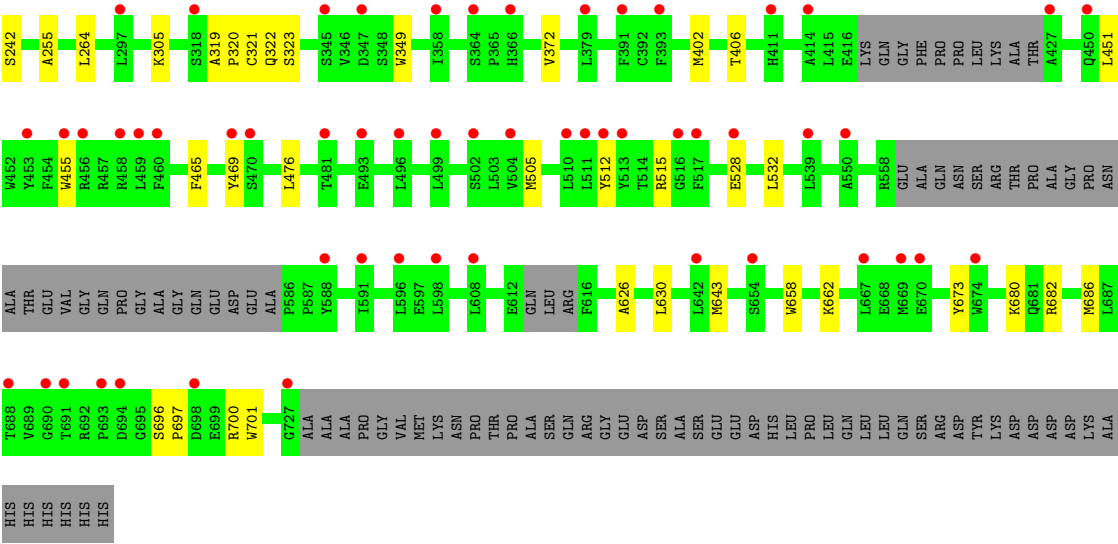
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Chain	Residue	Modelled	Actual	Comment	Reference
B	764	TYR	-	expression tag	UNP G1SNM3
B	765	LYS	-	expression tag	UNP G1SNM3
B	766	ASP	-	expression tag	UNP G1SNM3
B	767	ASP	-	expression tag	UNP G1SNM3
B	768	ASP	-	expression tag	UNP G1SNM3
B	769	ASP	-	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

- [illegible]

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	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 47.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.00-3.10) 87.1 (47.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.55 (at 3.13Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.247 , 0.272 0.249 , 0.285	Depositor DCC
R_{free} test set	2003 reflections (5.32%)	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)	0.33 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.15	0/4803	0.37	0/6542
1	B	0.16	0/4712	0.36	0/6431
All	All	0.16	0/9515	0.37	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	40	0
1	B	4608	4337	4368	37	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	76	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 (76) 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:B:476:LEU:HG	1:B:505:MET:HE1	1.92	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:643:MET:HE1	1:B:643:MET:CB	2.43	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:690:GLY:O	1:A:698:ASP:HB3	2.22	0.40
1:B:465:PHE:CD2	1:B:465:PHE:C	2.99	0.40
1:A:637:ASN:OD1	1:A:637:ASN:C	2.65	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	602/776 (78%)	580 (96%)	18 (3%)	4 (1%)	18	49
1	B	609/776 (78%)	586 (96%)	21 (3%)	2 (0%)	36	67
All	All	1211/1552 (78%)	1166 (96%)	39 (3%)	6 (0%)	24	57

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

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%)	471 (100%)	2 (0%)	84	86
1	B	449/666 (67%)	447 (100%)	2 (0%)	84	86
All	All	922/1332 (69%)	918 (100%)	4 (0%)	84	86

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	472	ILE
1	A	673	TYR
1	B	84	ARG
1	B	232	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	200	ASN
1	A	322	GLN
1	A	361	HIS
1	A	381	GLN
1	A	661	GLN
1	B	314	GLN
1	B	352	ASN
1	B	381	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	A	1001	-	45,52,52	3.91	17 (37%)	44,83,83	1.41	5 (11%)
2	6EU	B	803	-	45,52,52	3.97	16 (35%)	44,83,83	1.62	5 (11%)

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

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	803	6EU	CAS-CAX	17.15	1.60	1.33
2	A	1001	6EU	CAS-CAX	16.73	1.59	1.33
2	B	803	6EU	CAW-CBA	9.12	1.52	1.33
2	A	1001	6EU	CAW-CBA	9.01	1.51	1.33
2	B	803	6EU	CAM-CAL	8.05	1.66	1.54
2	B	803	6EU	CAK-CAS	7.90	1.68	1.50
2	A	1001	6EU	CAM-CAL	7.76	1.66	1.54
2	A	1001	6EU	CAK-CAS	7.62	1.67	1.50
2	A	1001	6EU	OAB-CAL	-7.40	1.32	1.43
2	B	803	6EU	OAB-CAL	-7.18	1.33	1.43
2	A	1001	6EU	CAJ-CAO	5.38	1.63	1.54
2	B	803	6EU	CAJ-CAO	5.33	1.63	1.54
2	B	803	6EU	CAY-CBE	4.12	1.58	1.51
2	A	1001	6EU	CAY-CBE	4.09	1.57	1.51
2	B	803	6EU	OAF-CBK	3.96	1.44	1.33
2	A	1001	6EU	OAF-CBK	3.83	1.44	1.33
2	B	803	6EU	OAB-CAQ	-3.28	1.35	1.41
2	A	1001	6EU	OAB-CAQ	-3.21	1.35	1.41
2	A	1001	6EU	OAE-CAZ	-3.07	1.17	1.22
2	B	803	6EU	OAE-CAZ	-3.05	1.17	1.22
2	A	1001	6EU	OAH-CBQ	2.85	1.41	1.37
2	A	1001	6EU	CBM-CBN	2.84	1.56	1.51
2	B	803	6EU	CBM-CBN	2.74	1.56	1.51
2	B	803	6EU	OAH-CBQ	2.69	1.41	1.37
2	B	803	6EU	CBC-CAX	2.66	1.57	1.50
2	A	1001	6EU	CBC-CAX	2.60	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	803	6EU	CAT-CAN	2.48	1.58	1.53
2	A	1001	6EU	CAT-CAN	2.32	1.58	1.53
2	A	1001	6EU	OAD-CAR	-2.30	1.38	1.43
2	B	803	6EU	OAD-CAR	-2.19	1.38	1.43
2	A	1001	6EU	OAI-CBS	2.10	1.40	1.36
2	A	1001	6EU	CBO-CBQ	2.05	1.42	1.38
2	B	803	6EU	OAI-CBS	2.02	1.40	1.36

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	803	6EU	OAF-CBK-CBM	5.94	120.48	111.21
2	A	1001	6EU	OAF-CBK-CBM	5.16	119.28	111.21
2	B	803	6EU	OAC-CAM-CAP	-4.25	105.73	109.40
2	A	1001	6EU	OAH-CBQ-CBS	3.70	120.10	114.55
2	B	803	6EU	OAH-CBQ-CBS	3.36	119.59	114.55
2	B	803	6EU	CAQ-CAY-CBE	-3.23	109.81	113.60
2	A	1001	6EU	OAC-CAM-CAP	-3.15	106.68	109.40
2	A	1001	6EU	OAA-CAJ-CAN	2.68	109.82	106.34
2	B	803	6EU	OAA-CAJ-CAN	2.56	109.66	106.34
2	A	1001	6EU	OAH-CBQ-CBO	-2.10	120.46	124.08

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	B	803	6EU	CBM-CBK-OAF-CBC
2	A	1001	6EU	OAG-CBK-OAF-CBC
2	B	803	6EU	OAG-CBK-OAF-CBC
2	B	803	6EU	OAA-CAQ-CAY-CBE
2	B	803	6EU	OAB-CAQ-CAY-CBE
2	A	1001	6EU	CAP-CAM-CAV-CBB

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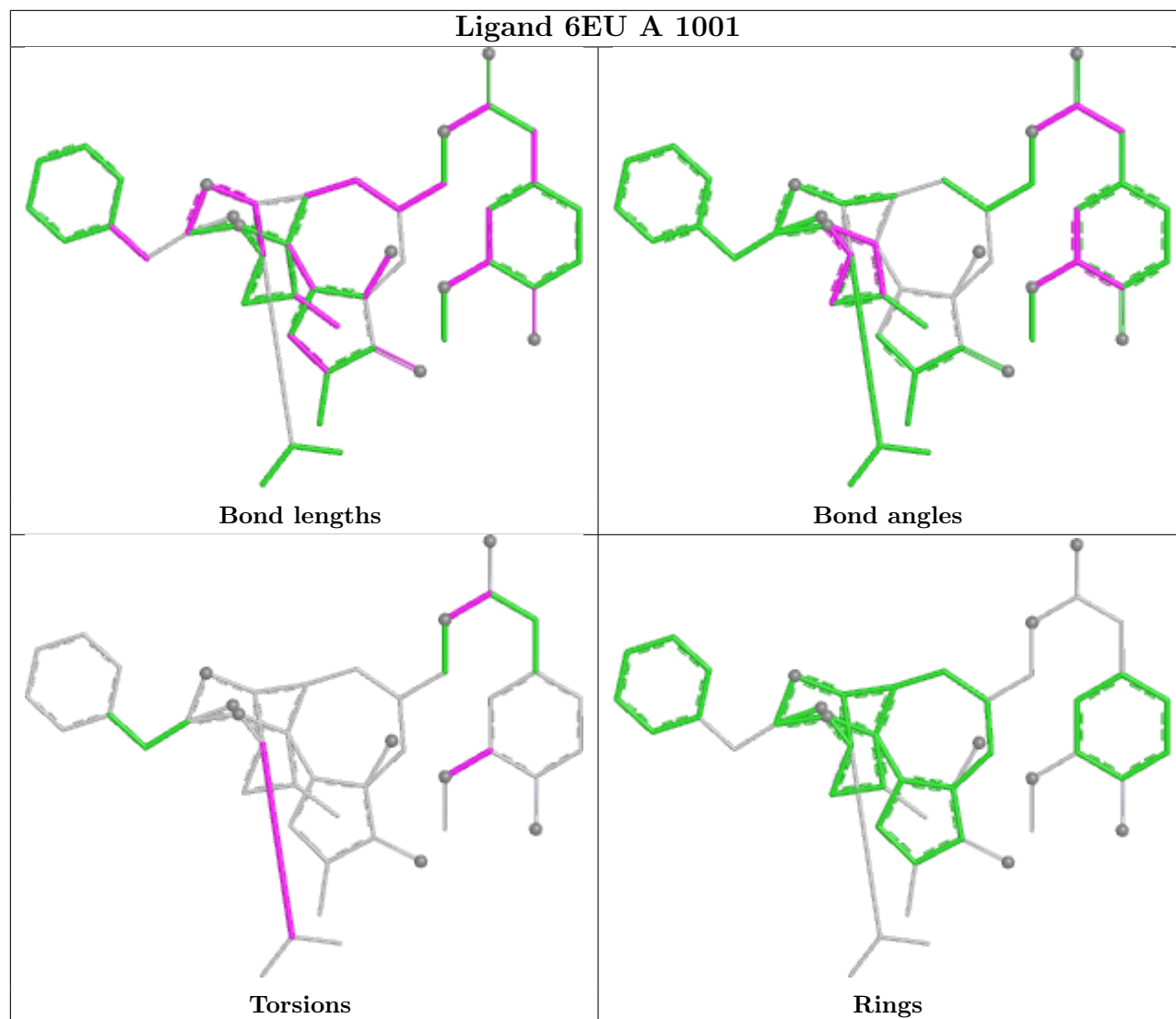
Mol	Chain	Res	Type	Atoms
2	B	803	6EU	CAP-CAM-CAV-CBB
2	B	803	6EU	OAF-CBK-CBM-CBN
2	A	1001	6EU	CAP-CAM-CAV-CBD
2	B	803	6EU	CAP-CAM-CAV-CBD
2	B	803	6EU	OAG-CBK-CBM-CBN

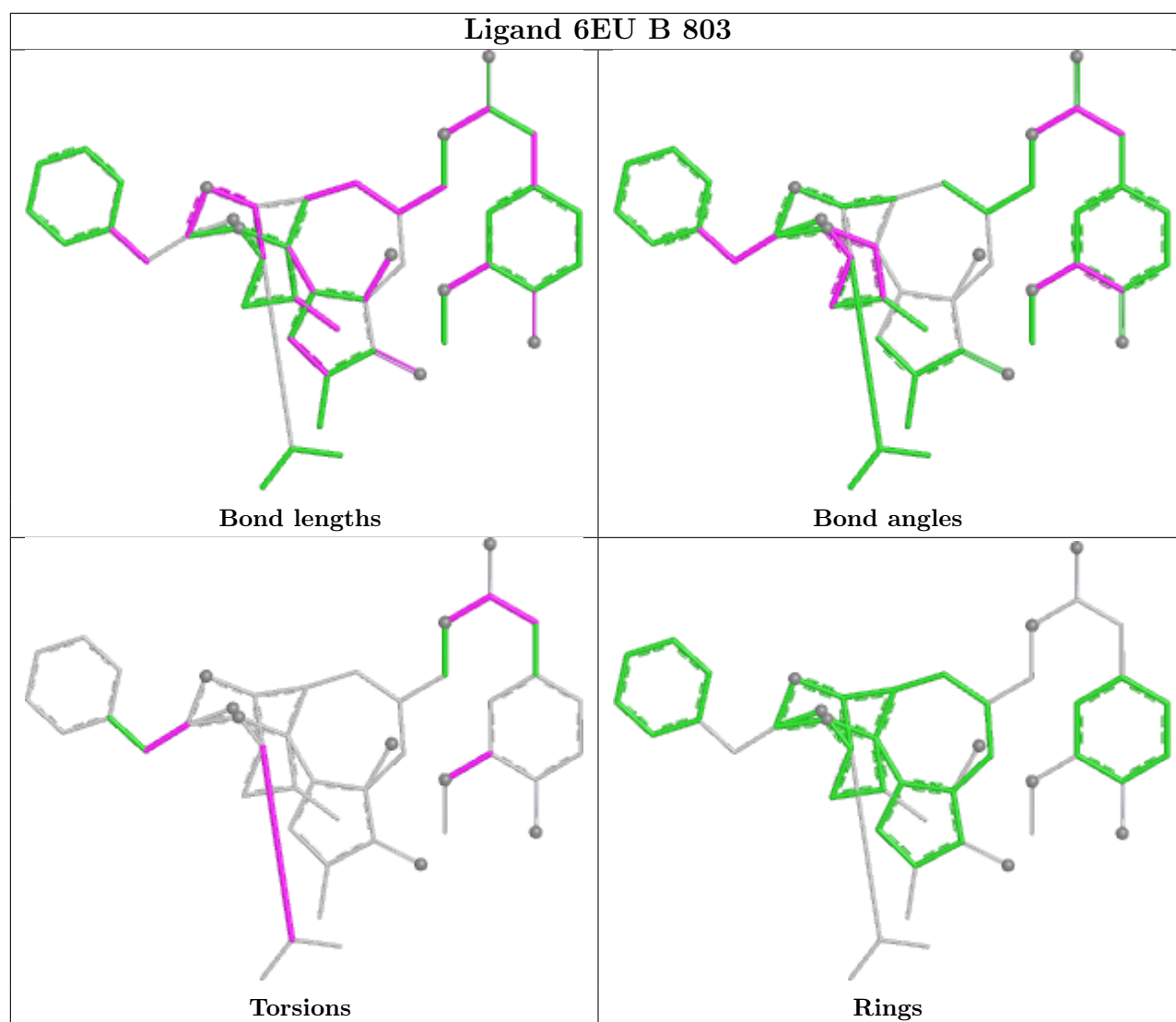
There are no ring outliers.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	610/776 (78%)	0.67	69 (11%)	10 5	47, 88, 158, 192	0
1	B	617/776 (79%)	0.67	66 (10%)	11 6	45, 93, 161, 202	0
All	All	1227/1552 (79%)	0.67	135 (11%)	10 5	45, 90, 160, 202	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	427	ALA	8.6
1	A	465	PHE	6.0
1	B	654	SER	5.5
1	A	453	TYR	5.5
1	A	471	GLU	5.0
1	B	366	HIS	4.9
1	A	451	LEU	4.8
1	B	694	ASP	4.7
1	A	450	GLN	4.6
1	B	469	TYR	4.3
1	B	470	SER	4.3
1	A	664	ILE	4.2
1	A	467	ASP	4.1
1	A	499	LEU	4.1
1	B	179	LYS	4.0
1	A	448	LEU	4.0
1	B	175	LEU	3.9
1	A	321	CYS	3.9
1	A	466	MET	3.9
1	A	444	VAL	3.8
1	A	721	LEU	3.8
1	A	512	TYR	3.8
1	B	364	SER	3.8
1	A	374	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	453	TYR	3.8
1	B	208	GLY	3.7
1	B	517	PHE	3.7
1	A	428	GLY	3.6
1	A	429	ASN	3.6
1	B	459	LEU	3.6
1	B	670	GLU	3.6
1	B	513	TYR	3.4
1	B	318	SER	3.3
1	A	464	SER	3.3
1	A	472	ILE	3.2
1	A	589	ARG	3.2
1	A	668	GLU	3.2
1	B	669	MET	3.1
1	A	238	GLN	3.0
1	A	486	VAL	3.0
1	A	586	PRO	3.0
1	B	502	SER	3.0
1	B	698	ASP	3.0
1	B	690	GLY	3.0
1	A	666	VAL	3.0
1	B	588	TYR	3.0
1	B	183	GLU	3.0
1	A	387	LEU	2.9
1	B	345	SER	2.9
1	B	460	PHE	2.9
1	B	393	PHE	2.8
1	A	412	GLN	2.8
1	A	447	LEU	2.8
1	B	591	ILE	2.8
1	A	319	ALA	2.7
1	B	427	ALA	2.7
1	B	177	CYS	2.7
1	A	727	GLY	2.7
1	B	414	ALA	2.7
1	A	318	SER	2.7
1	B	297	LEU	2.7
1	B	693	PRO	2.6
1	B	391	PHE	2.6
1	B	691	THR	2.6
1	B	496	LEU	2.6
1	A	430	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	510	LEU	2.6
1	A	601	PHE	2.6
1	A	70	LEU	2.6
1	A	481	THR	2.6
1	A	445	TYR	2.6
1	A	709	ASN	2.6
1	B	511	LEU	2.6
1	B	481	THR	2.6
1	B	727	GLY	2.5
1	B	499	LEU	2.5
1	A	513	TYR	2.5
1	A	485	GLN	2.5
1	A	203	THR	2.5
1	B	458	ARG	2.5
1	B	101	SER	2.5
1	B	539	LEU	2.5
1	A	695	GLY	2.5
1	A	605	MET	2.4
1	B	642	LEU	2.4
1	A	455	TRP	2.4
1	B	199	LYS	2.4
1	B	667	LEU	2.4
1	B	504	VAL	2.4
1	A	463	ILE	2.4
1	A	294	LEU	2.4
1	A	452	TRP	2.4
1	A	643	MET	2.4
1	B	596	LEU	2.4
1	B	528	GLU	2.4
1	B	164	SER	2.4
1	A	621	LEU	2.3
1	B	379	LEU	2.3
1	B	450	GLN	2.3
1	A	528	GLU	2.3
1	A	435	GLY	2.3
1	B	550	ALA	2.3
1	A	536	LEU	2.3
1	B	516	GLY	2.2
1	A	511	LEU	2.2
1	A	665	SER	2.2
1	A	210	LEU	2.2
1	A	494	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	674	TRP	2.2
1	B	688	THR	2.2
1	A	283	VAL	2.2
1	B	184	ASN	2.2
1	A	687	LEU	2.1
1	B	608	LEU	2.1
1	A	675	TRP	2.1
1	B	358	ILE	2.1
1	B	347	ASP	2.1
1	B	598	LEU	2.1
1	A	515	ARG	2.1
1	A	484	SER	2.1
1	A	557	SER	2.1
1	B	411	HIS	2.1
1	B	455	TRP	2.1
1	A	461	ILE	2.1
1	B	232	HIS	2.1
1	A	114	THR	2.1
1	B	512	TYR	2.1
1	A	606	GLY	2.1
1	A	726	SER	2.0
1	A	706	GLY	2.0
1	B	493	GLU	2.0
1	A	440	LEU	2.0
1	A	678	ARG	2.0
1	B	180	LEU	2.0
1	B	456	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

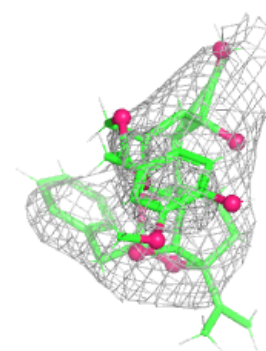
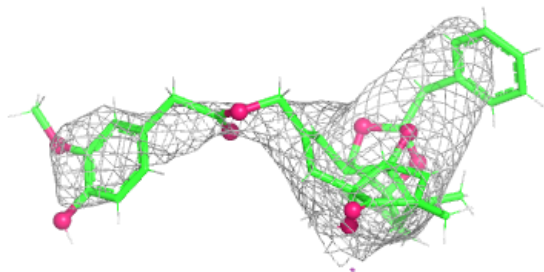
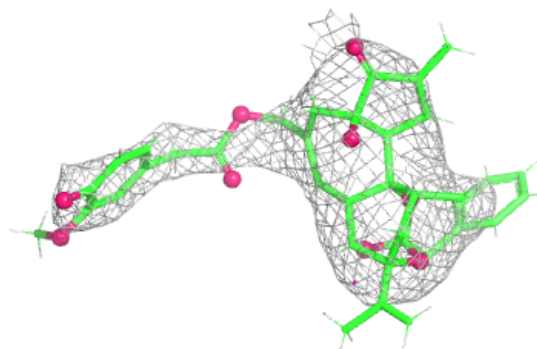
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

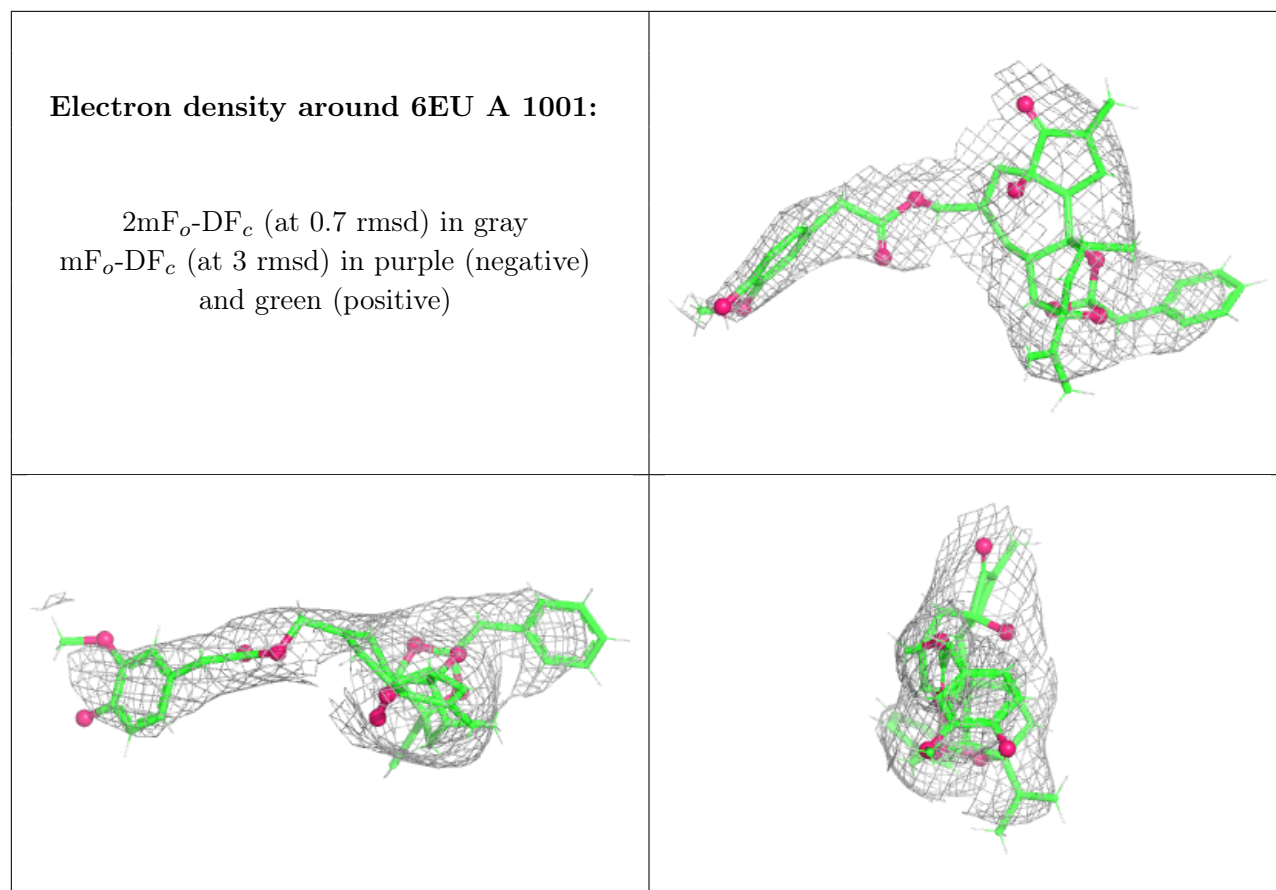
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CA	B	802	1/1	0.82	0.21	101,101,101,101	1
2	6EU	B	803	46/46	0.84	0.18	95,124,150,160	0
3	CA	B	801	1/1	0.92	0.22	97,97,97,97	1
2	6EU	A	1001	46/46	0.93	0.15	86,108,131,141	0

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)





6.5 Other polymers [i](#)

There are no such residues in this entry.