



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:07 AM UTC

PDB ID : 4P42 / pdb_00004p42
Title : Extended-Synaptotagmin 2, SMP - C2A - C2B Domains
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Deposited on : 2014-03-10
Resolution : 2.44 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

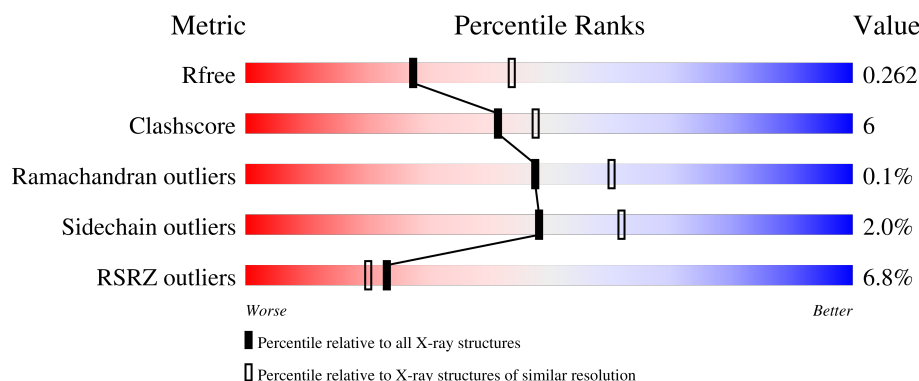
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	474	5% 81% 14% • •
1	B	474	8% 72% 19% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PEE	A	702	X	-	-	-
3	PEE	B	702	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7493 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.

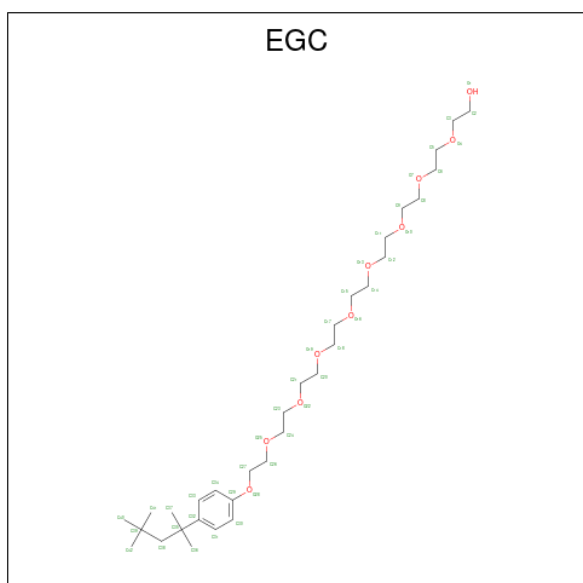
- Molecule 1 is a protein called Extended synaptotagmin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3666	2353	621	680	12			
1	B	431	Total	C	N	O	S	0	0	0
			3477	2239	591	635	12			

There are 4 discrepancies between the modelled and reference sequences:

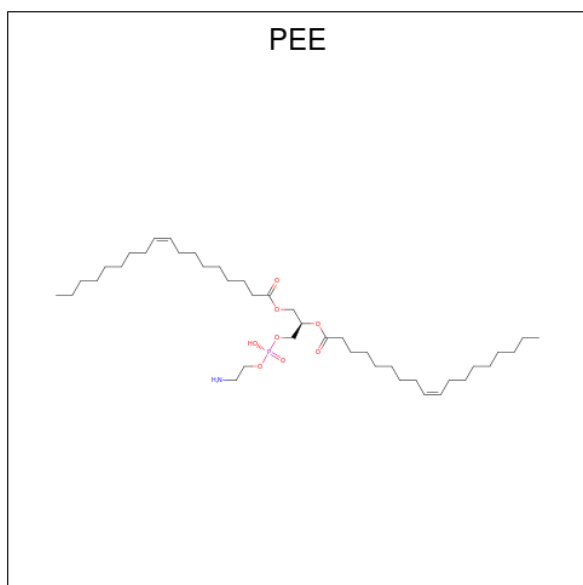
Chain	Residue	Modelled	Actual	Comment	Reference
A	161	GLY	-	expression tag	UNP A0FGR8
A	162	SER	-	expression tag	UNP A0FGR8
B	161	GLY	-	expression tag	UNP A0FGR8
B	162	SER	-	expression tag	UNP A0FGR8

- Molecule 2 is 2-(2-{2-[2-(2-{2-[2-(2-{4-(1,1,3,3-TETRAMETHYL-BUTYL)-PHEN OXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (CCD ID: EGC) (formula: C₃₂H₅₈O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			29	24	5		
2	B	1	Total	C	O	0	0
			25	21	4		

- Molecule 3 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			42	37	5		
3	B	1	Total	C	O	0	0
			42	37	5		

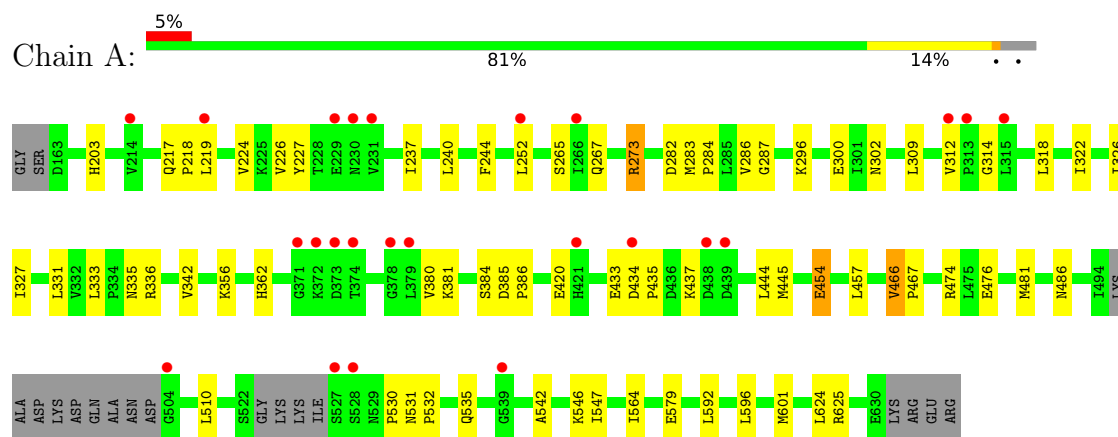
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	110	Total	O	0	0
			110	110		
4	B	102	Total	O	0	0
			102	102		

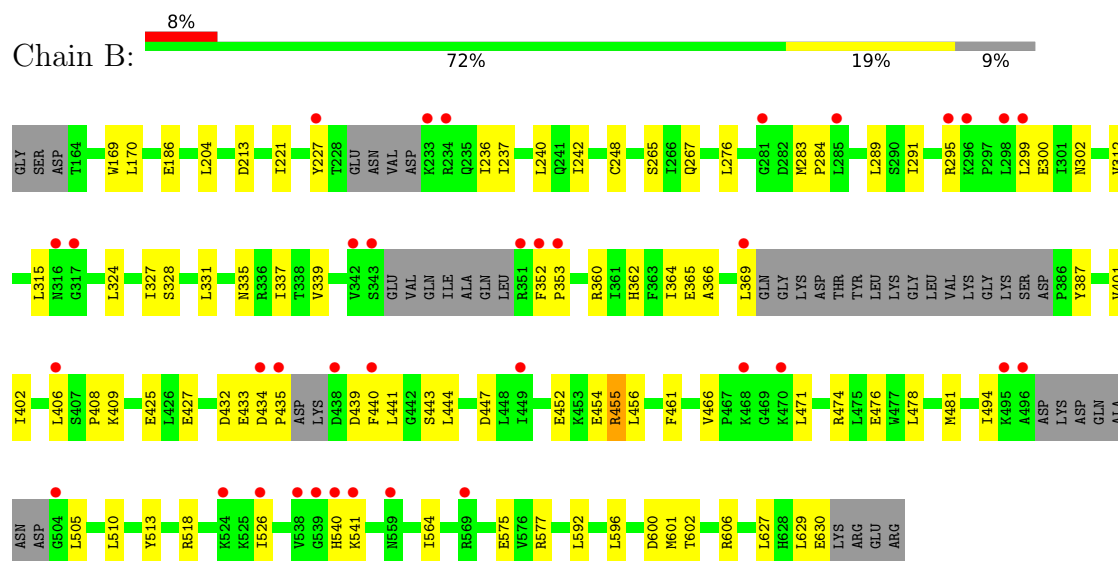
3 Residue-property plots

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

• Molecule 1: Extended synaptotagmin-2



• Molecule 1: Extended synaptotagmin-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.33Å 88.38Å 167.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.14 – 2.44 47.14 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.14-2.44) 96.1 (47.14-2.44)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1452)	Depositor
R, R_{free}	0.210 , 0.256 0.221 , 0.262	Depositor DCC
R_{free} test set	2000 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 32.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7493	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: EGC, PEE

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	0.28	0/3739	0.72	0/5068
1	B	0.28	0/3546	0.69	1/4801 (0.0%)
All	All	0.28	0/7285	0.71	1/9869 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	295	ARG	CB-CA-C	-5.83	109.84	116.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3666	0	3731	43	0
1	B	3477	0	3554	53	0
2	A	29	0	39	1	0
2	B	25	0	33	1	0
3	A	42	0	68	4	0
3	B	42	0	68	4	0
4	A	110	0	0	3	0
4	B	102	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7493	0	7493	95	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 6.

All (95) 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:510:LEU:HB2	1:A:564:ILE:HD11	1.59	0.82
1:B:510:LEU:HB2	1:B:564:ILE:HD11	1.65	0.79
1:A:335:ASN:HB3	2:A:701:EGC:H241	1.69	0.75
1:B:452:GLU:O	1:B:455:ARG:NH1	2.20	0.74
1:A:327:ILE:HG23	3:A:702:PEE:H62	1.70	0.72
1:B:366:ALA:HB3	1:B:408:PRO:HD2	1.72	0.71
1:B:455:ARG:HG3	1:B:630:GLU:HG2	1.72	0.71
1:A:336:ARG:NH1	4:A:801:HOH:O	2.24	0.71
1:A:546:LYS:NZ	1:B:186:GLU:OE2	2.24	0.70
1:B:369:LEU:HB2	1:B:406:LEU:HD22	1.73	0.70
1:B:402:ILE:HD12	1:B:408:PRO:HB2	1.74	0.69
1:B:444:LEU:HD12	1:B:471:LEU:HD23	1.79	0.65
1:B:362:HIS:HB2	1:B:474:ARG:HB3	1.79	0.63
1:B:364:ILE:HG22	1:B:365:GLU:HG3	1.82	0.62
1:A:326:ILE:HD13	3:A:702:PEE:H13	1.82	0.61
1:B:283:MET:HG3	1:B:284:PRO:HA	1.83	0.61
1:A:385:ASP:HB2	1:A:433:GLU:HB3	1.82	0.60
1:A:227:TYR:HB3	1:A:237:ILE:HB	1.86	0.57
1:A:564:ILE:HD13	1:A:592:LEU:HD13	1.85	0.57
1:A:531:ASN:HB2	1:A:579:GLU:HG3	1.86	0.57
1:B:478:LEU:HD23	1:B:627:LEU:HB3	1.85	0.57
1:A:267:GLN:HB2	1:A:300:GLU:HB2	1.87	0.57
1:A:362:HIS:HB2	1:A:474:ARG:HB3	1.87	0.57
1:B:425:GLU:HG2	1:B:447:ASP:HA	1.86	0.56
1:B:365:GLU:HG2	1:B:409:LYS:HG3	1.88	0.56
1:B:236:ILE:HB	1:B:276:LEU:HB2	1.89	0.55
1:A:283:MET:HG3	1:A:284:PRO:HA	1.89	0.55
1:A:265:SER:OG	1:A:302:ASN:ND2	2.32	0.54
1:A:433:GLU:O	1:A:435:PRO:HD3	2.08	0.54
1:B:564:ILE:HD13	1:B:592:LEU:HD13	1.91	0.53
1:B:335:ASN:HB3	2:B:701:EGC:H241	1.90	0.53
1:B:454:GLU:O	1:B:456:LEU:N	2.43	0.52
1:A:356:LYS:HD2	1:A:420:GLU:OE2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:LEU:HA	1:A:601:MET:HE3	1.92	0.52
1:A:331:LEU:HD21	3:A:702:PEE:H68	1.91	0.52
1:B:265:SER:OG	1:B:302:ASN:ND2	2.40	0.51
1:B:267:GLN:HB2	1:B:300:GLU:HB3	1.91	0.51
1:B:596:LEU:HA	1:B:601:MET:HE3	1.93	0.51
1:B:432:ASP:HB3	1:B:439:ASP:HB3	1.91	0.51
1:B:444:LEU:HD11	1:B:461:PHE:HB2	1.93	0.51
1:A:381:LYS:NZ	1:A:434:ASP:O	2.44	0.50
1:A:481:MET:SD	1:A:486:ASN:ND2	2.84	0.50
1:B:227:TYR:HB3	1:B:237:ILE:HB	1.92	0.50
1:A:625:ARG:NH1	4:A:842:HOH:O	2.33	0.50
1:B:518:ARG:NH2	4:B:802:HOH:O	2.44	0.49
1:B:352:PHE:CE1	1:B:513:TYR:HB2	2.47	0.49
1:A:287:GLY:HA2	1:A:342:VAL:HG22	1.94	0.48
1:B:204:LEU:HD21	1:B:315:LEU:HD11	1.95	0.48
1:A:474:ARG:NH1	1:A:476:GLU:OE2	2.47	0.48
1:B:312:VAL:HB	1:B:315:LEU:HD12	1.96	0.48
1:A:318:LEU:HD22	1:A:322:ILE:HG21	1.95	0.47
1:B:221:ILE:HD13	1:B:240:LEU:HD23	1.96	0.47
1:B:369:LEU:HD22	1:B:441:LEU:HB3	1.96	0.47
1:A:457:LEU:HD22	1:B:526:ILE:HD12	1.96	0.47
1:A:454:GLU:HG3	1:B:526:ILE:HD11	1.97	0.47
1:B:365:GLU:O	1:B:471:LEU:HD12	2.14	0.47
1:B:352:PHE:N	1:B:353:PRO:HD3	2.30	0.47
1:B:434:ASP:HB3	1:B:435:PRO:HD3	1.97	0.47
1:A:226:VAL:HG23	1:B:169:TRP:HB2	1.97	0.47
1:B:474:ARG:NH1	1:B:476:GLU:OE2	2.48	0.46
1:B:540:HIS:ND1	1:B:541:LYS:HG3	2.31	0.46
1:A:273:ARG:NH2	4:A:803:HOH:O	2.43	0.46
1:B:600:ASP:O	1:B:602:THR:HG23	2.15	0.46
1:A:282:ASP:OD1	1:A:283:MET:N	2.48	0.46
1:B:299:LEU:HD21	1:B:328:SER:HB2	1.96	0.45
1:B:331:LEU:HD21	3:B:702:PEE:H66	1.96	0.45
1:A:312:VAL:HG12	1:A:314:GLY:H	1.82	0.45
1:B:289:LEU:HB2	1:B:339:VAL:HB	1.98	0.45
1:B:213:ASP:O	1:B:248:CYS:HB2	2.17	0.45
1:A:217:GLN:HA	1:A:218:PRO:HD3	1.73	0.45
3:B:702:PEE:H34	3:B:702:PEE:H57	1.98	0.44
1:A:203:HIS:HB2	1:A:314:GLY:HA3	1.98	0.44
1:B:387:TYR:HB3	1:B:401:VAL:HG22	1.99	0.44
1:B:327:ILE:HG23	3:B:702:PEE:H56	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:ILE:HB	1:B:337:ILE:HB	2.00	0.44
1:B:432:ASP:HB2	1:B:441:LEU:HD11	1.99	0.44
1:A:252:LEU:HD12	1:A:309:LEU:HD11	1.99	0.43
1:B:494:ILE:HG23	1:B:505:LEU:HB2	1.99	0.43
1:B:360:ARG:HD2	1:B:476:GLU:OE1	2.19	0.43
1:A:384:SER:O	1:A:386:PRO:HD3	2.18	0.43
3:A:702:PEE:H53	3:A:702:PEE:H58	1.92	0.42
1:A:437:LYS:HD2	1:A:437:LYS:HA	1.82	0.42
1:A:535:GLN:OE1	1:A:542:ALA:HB1	2.20	0.42
1:A:219:LEU:HD12	1:A:244:PHE:CD1	2.55	0.42
1:B:170:LEU:HD23	1:B:170:LEU:HA	1.94	0.41
3:B:702:PEE:H72	3:B:702:PEE:H67	1.55	0.41
1:A:224:VAL:HG22	1:A:240:LEU:HD22	2.02	0.41
1:B:575:GLU:HG3	1:B:577:ARG:HG3	2.02	0.41
1:A:265:SER:HG	1:A:302:ASN:HD22	1.59	0.41
1:A:530:PRO:O	1:A:532:PRO:HD3	2.21	0.41
1:B:440:PHE:HZ	1:B:443:SER:HB3	1.87	0.40
1:A:284:PRO:C	1:A:286:VAL:H	2.29	0.40
1:A:466:VAL:HA	1:A:467:PRO:HD3	1.95	0.40
1:A:547:ILE:HG21	1:A:579:GLU:HG2	2.03	0.40
1:B:299:LEU:HG	1:B:324:LEU:HD22	2.04	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	449/474 (95%)	431 (96%)	18 (4%)	0	100	100
1	B	419/474 (88%)	401 (96%)	17 (4%)	1 (0%)	43	53
All	All	868/948 (92%)	832 (96%)	35 (4%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	455	ARG

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	418/433 (96%)	409 (98%)	9 (2%)	45	59
1	B	396/433 (92%)	389 (98%)	7 (2%)	51	64
All	All	814/866 (94%)	798 (98%)	16 (2%)	48	62

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	273	ARG
1	A	296	LYS
1	A	333	LEU
1	A	380	VAL
1	A	444	LEU
1	A	445	MET
1	A	454	GLU
1	A	466	VAL
1	A	624	LEU
1	B	242	ILE
1	B	427	GLU
1	B	433	GLU
1	B	466	VAL
1	B	481	MET
1	B	606	ARG
1	B	629	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	316	ASN
1	A	540	HIS
1	A	587	ASN
1	A	611	ASN
1	B	235	GLN
1	B	241	GLN
1	B	267	GLN
1	B	587	ASN
1	B	611	ASN

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](#)

4 ligands are modelled in this entry.

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	EGC	A	701	-	29,29,42	0.98	1 (3%)	37,37,50	0.62	0
3	PEE	A	702	-	41,41,50	1.17	4 (9%)	43,43,55	1.07	3 (6%)
3	PEE	B	702	-	41,41,50	1.16	4 (9%)	43,43,55	1.09	2 (4%)
2	EGC	B	701	-	25,25,42	1.05	1 (4%)	33,33,50	0.61	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEE	B	702	-	1/1/3/8	23/43/43/54	-
2	EGC	A	701	-	-	5/27/27/40	0/1/1/1
3	PEE	A	702	-	1/1/3/8	24/43/43/54	-
2	EGC	B	701	-	-	3/23/23/40	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	PEE	C18-C19	3.94	1.54	1.31
3	B	702	PEE	C18-C19	3.93	1.54	1.31
3	A	702	PEE	C39-C38	3.64	1.52	1.31
3	B	702	PEE	C39-C38	3.61	1.52	1.31
3	A	702	PEE	O2-C10	3.24	1.43	1.34
2	B	701	EGC	O28-C29	3.24	1.45	1.37
2	A	701	EGC	O28-C29	3.20	1.44	1.37
3	B	702	PEE	O2-C10	3.19	1.43	1.34
3	A	702	PEE	O3-C30	2.98	1.42	1.33
3	B	702	PEE	O3-C30	2.85	1.41	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	PEE	O2-C10-C11	4.10	120.36	111.48
3	A	702	PEE	O2-C10-C11	3.83	119.76	111.48
3	B	702	PEE	O3-C30-C31	2.56	119.63	111.83
3	A	702	PEE	O3-C30-C31	2.46	119.34	111.83
3	A	702	PEE	O2-C10-O4	-2.05	118.90	123.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	702	PEE	C2
3	B	702	PEE	C2

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	PEE	C11-C10-O2-C2
3	A	702	PEE	C1-C2-O2-C10
3	A	702	PEE	O2-C2-C3-O3
3	B	702	PEE	C11-C10-O2-C2
3	B	702	PEE	O4-C10-O2-C2
3	A	702	PEE	O4-C10-O2-C2
3	A	702	PEE	C31-C30-O3-C3
3	B	702	PEE	C12-C13-C14-C15
2	A	701	EGC	O19-C20-C21-O22
3	A	702	PEE	O5-C30-O3-C3
3	B	702	PEE	C40-C41-C42-C43
3	B	702	PEE	C10-C11-C12-C13
3	B	702	PEE	C17-C18-C19-C20
3	B	702	PEE	O5-C30-O3-C3
3	B	702	PEE	C32-C33-C34-C35
3	B	702	PEE	C42-C43-C44-C45
3	B	702	PEE	C33-C34-C35-C36
3	B	702	PEE	C41-C42-C43-C44
3	A	702	PEE	C35-C36-C37-C38
3	B	702	PEE	C15-C16-C17-C18
3	A	702	PEE	C34-C35-C36-C37
3	B	702	PEE	C31-C30-O3-C3
3	B	702	PEE	C36-C37-C38-C39
3	B	702	PEE	C19-C20-C21-C22
3	A	702	PEE	C41-C42-C43-C44
3	A	702	PEE	C10-C11-C12-C13
3	B	702	PEE	C1-C2-C3-O3
3	A	702	PEE	C43-C44-C45-C46
3	A	702	PEE	C12-C13-C14-C15
3	A	702	PEE	C21-C22-C23-C24
3	A	702	PEE	C31-C32-C33-C34
3	B	702	PEE	C11-C12-C13-C14
3	A	702	PEE	C14-C15-C16-C17
3	A	702	PEE	C42-C43-C44-C45
2	B	701	EGC	O19-C20-C21-O22
3	A	702	PEE	C44-C45-C46-C47
3	A	702	PEE	C1-C2-C3-O3
3	A	702	PEE	C17-C18-C19-C20
3	B	702	PEE	O2-C2-C3-O3
2	B	701	EGC	C27-C26-O25-C24
2	A	701	EGC	C34-C29-O28-C27
2	A	701	EGC	C30-C29-O28-C27
3	A	702	PEE	C20-C21-C22-C23

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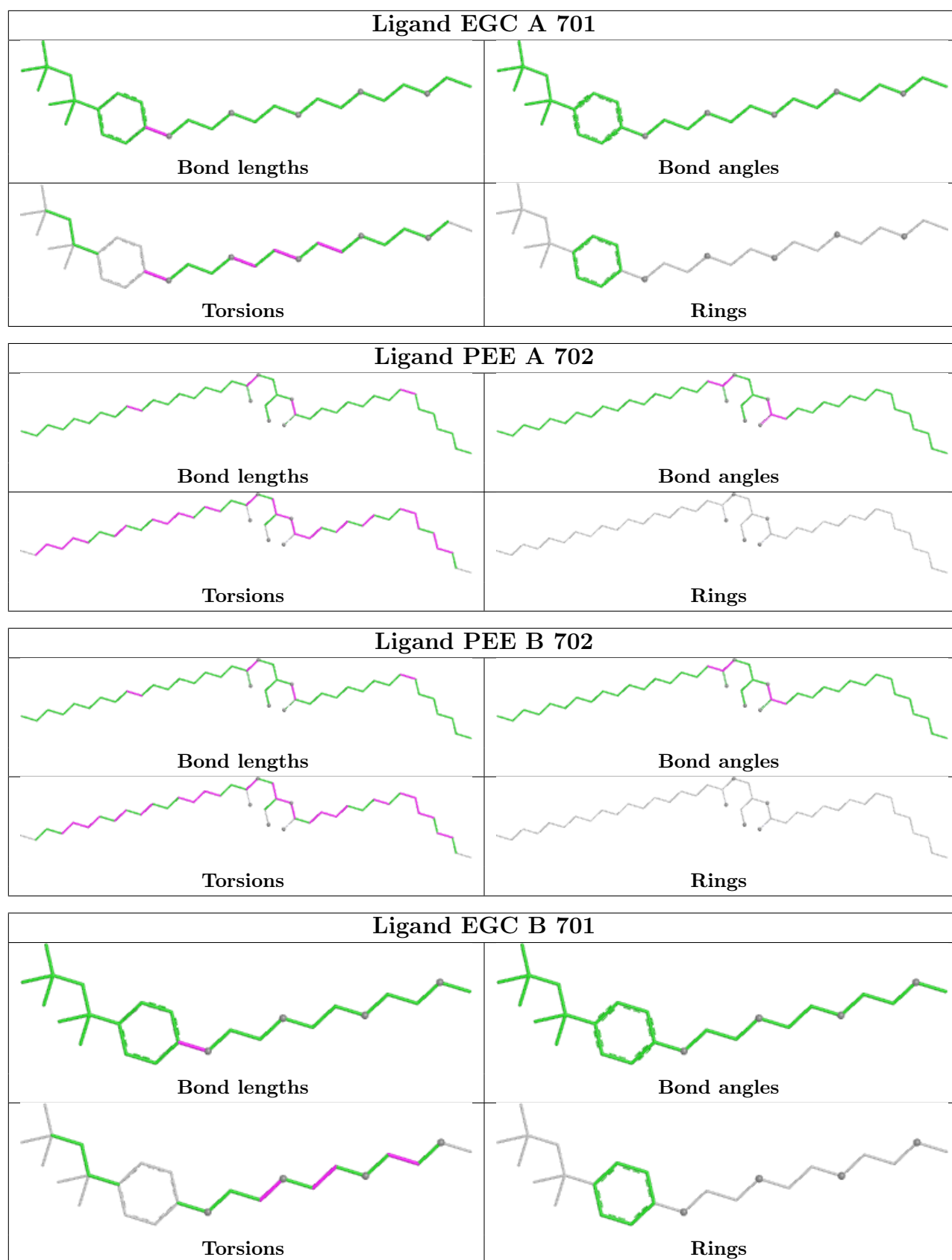
Mol	Chain	Res	Type	Atoms
3	B	702	PEE	C3-C2-O2-C10
2	A	701	EGC	C23-C24-O25-C26
3	B	702	PEE	C18-C19-C20-C21
3	B	702	PEE	C31-C32-C33-C34
3	B	702	PEE	C38-C39-C40-C41
3	A	702	PEE	C18-C19-C20-C21
3	B	702	PEE	C21-C22-C23-C24
2	B	701	EGC	O22-C23-C24-O25
3	A	702	PEE	C38-C39-C40-C41
3	A	702	PEE	O2-C10-C11-C12
2	A	701	EGC	C24-C23-O22-C21
3	A	702	PEE	C33-C34-C35-C36

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	EGC	1	0
3	A	702	PEE	4	0
3	B	702	PEE	4	0
2	B	701	EGC	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	455/474 (95%)	0.35	24 (5%) 32 29	30, 46, 72, 115	0
1	B	431/474 (90%)	0.48	36 (8%) 17 14	29, 46, 95, 139	0
All	All	886/948 (93%)	0.41	60 (6%) 23 20	29, 46, 86, 139	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	352	PHE	8.3
1	B	496	ALA	5.4
1	A	504	GLY	4.9
1	B	540	HIS	4.9
1	B	369	LEU	4.6
1	B	504	GLY	4.6
1	B	435	PRO	4.1
1	A	219	LEU	4.1
1	B	343	SER	4.1
1	B	406	LEU	4.0
1	B	541	LYS	3.9
1	B	295	ARG	3.7
1	B	316	ASN	3.7
1	A	231	VAL	3.6
1	B	351	ARG	3.6
1	B	233	LYS	3.5
1	A	379	LEU	3.4
1	B	298	LEU	3.4
1	A	439	ASP	3.3
1	A	374	THR	3.3
1	B	538	VAL	3.3
1	A	371	GLY	3.1
1	B	296	LYS	3.1
1	A	527	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	526	ILE	3.1
1	A	252	LEU	3.0
1	B	524	LYS	3.0
1	A	230	ASN	3.0
1	B	438	ASP	3.0
1	B	353	PRO	2.8
1	A	372	LYS	2.8
1	B	468	LYS	2.8
1	A	421	HIS	2.7
1	B	227	TYR	2.7
1	A	229	GLU	2.7
1	B	495	LYS	2.6
1	A	214	VAL	2.5
1	A	315	LEU	2.5
1	B	342	VAL	2.5
1	B	470	LYS	2.4
1	B	440	PHE	2.4
1	A	266	ILE	2.3
1	B	234	ARG	2.3
1	B	281	GLY	2.3
1	A	378	GLY	2.3
1	B	569	ARG	2.3
1	B	317	GLY	2.3
1	A	528	SER	2.2
1	B	285	LEU	2.2
1	B	449	ILE	2.2
1	A	434	ASP	2.2
1	A	539	GLY	2.1
1	B	539	GLY	2.1
1	A	373	ASP	2.1
1	A	438	ASP	2.1
1	B	559	ASN	2.1
1	B	299	LEU	2.1
1	B	434	ASP	2.1
1	A	313	PRO	2.0
1	A	312	VAL	2.0

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 [i](#)

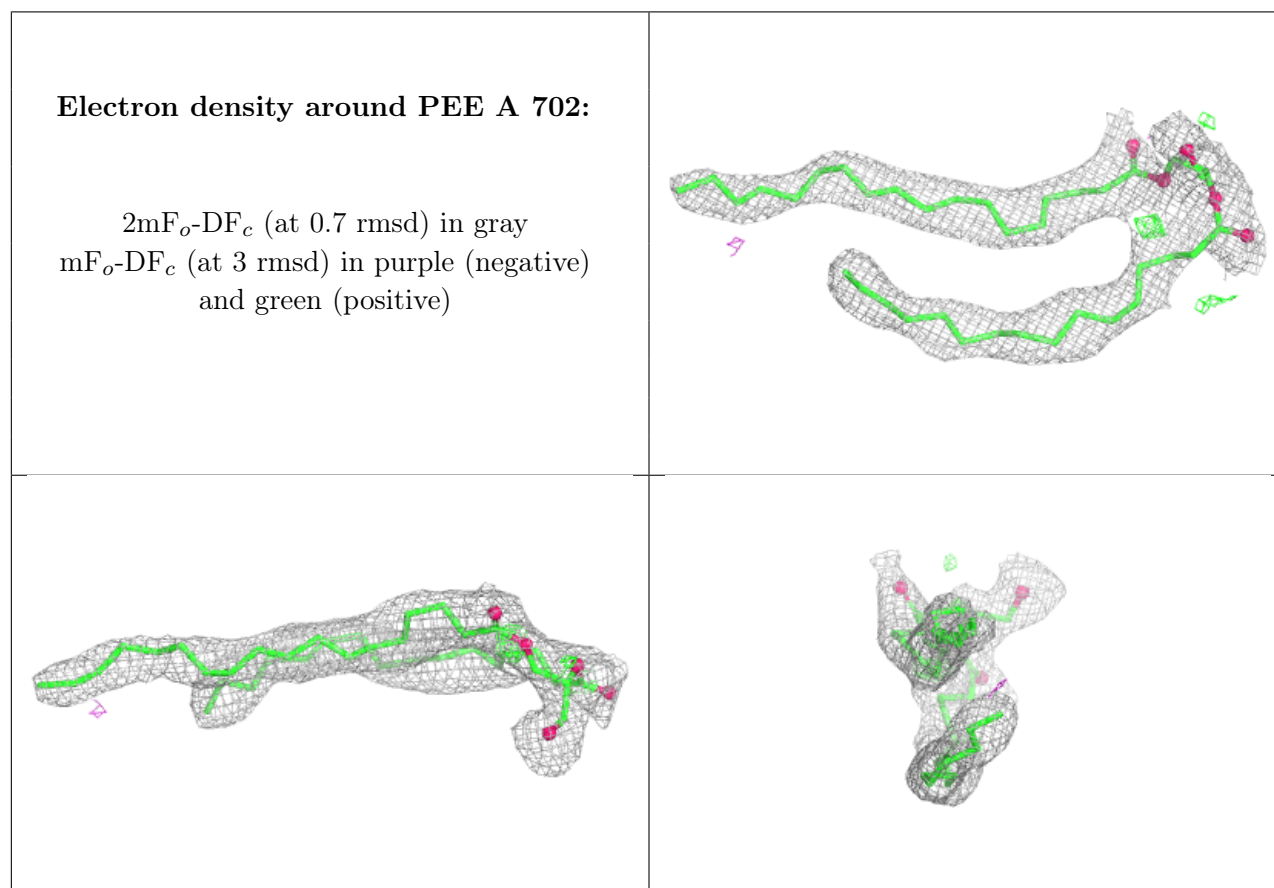
There are no oligosaccharides in this entry.

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.

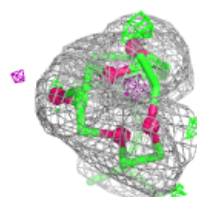
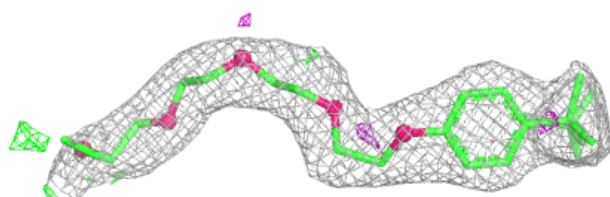
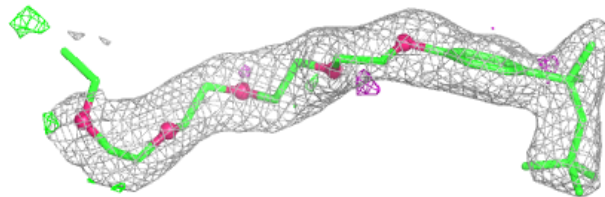
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PEE	A	702	42/51	0.85	0.17	37,57,80,81	0
2	EGC	A	701	29/42	0.87	0.15	26,43,68,73	0
3	PEE	B	702	42/51	0.87	0.18	41,55,78,81	0
2	EGC	B	701	25/42	0.88	0.11	28,39,48,50	0

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.

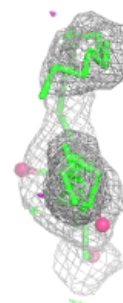
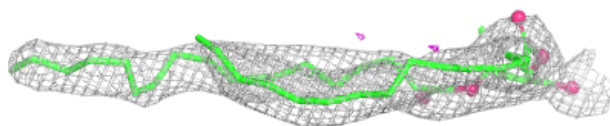
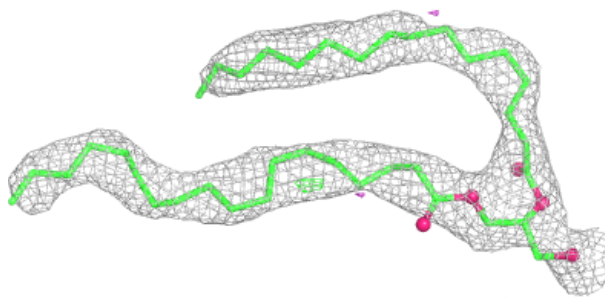


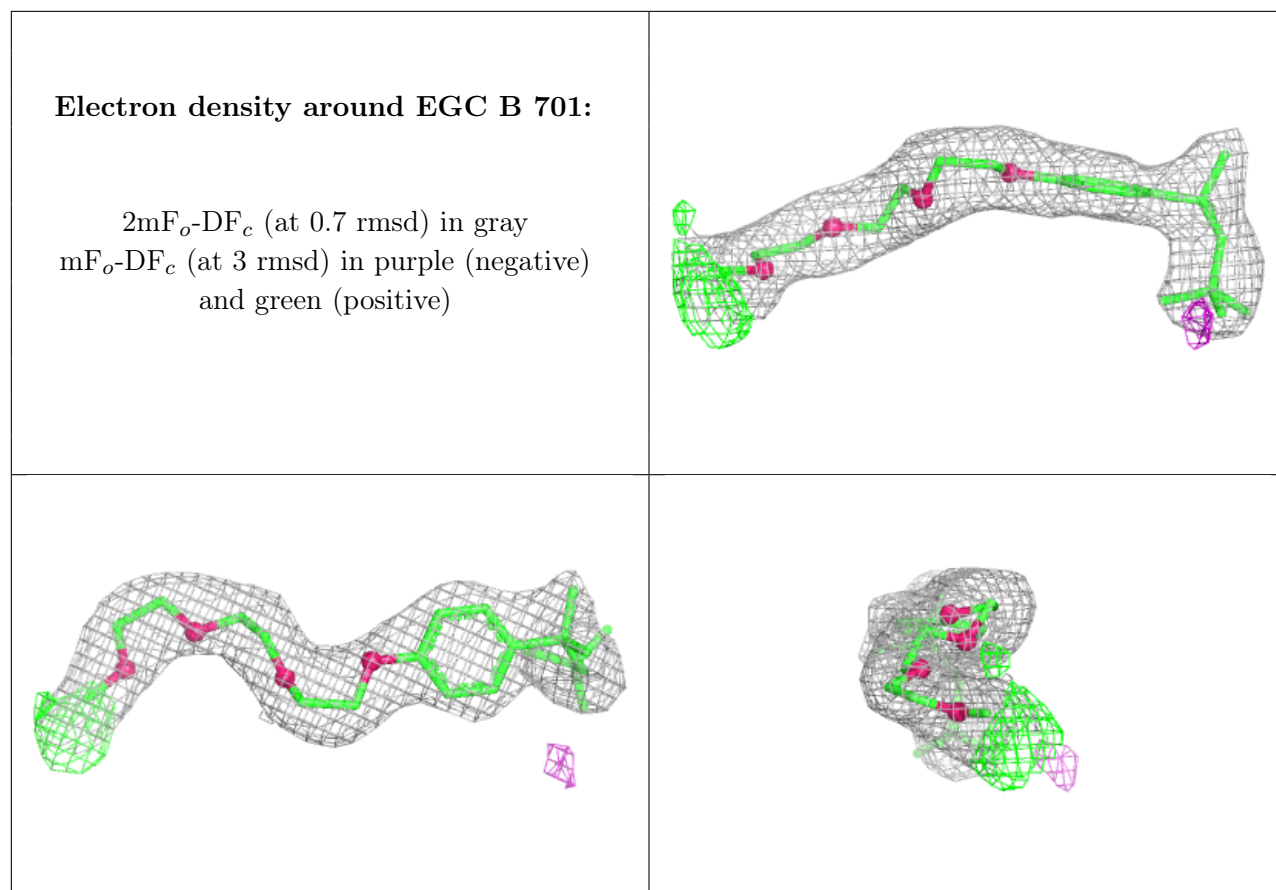
Electron density around EGC A 701:

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

**Electron density around PEE B 702:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.