



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:34 PM UTC

PDB ID : 5IVA / pdb_00005iva
Title : The LPS Transporter LptDE from Pseudomonas aeruginosa, core complex
Authors : Botos, I.; Buchanan, S.K.
Deposited on : 2016-03-20
Resolution : 2.99 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

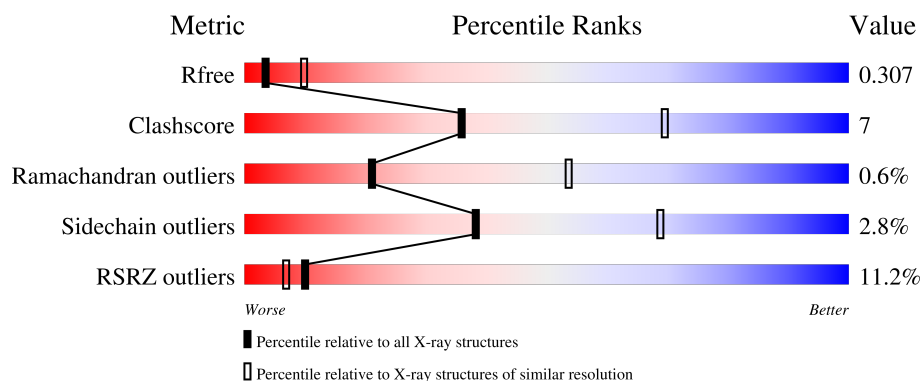
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	646	11% 70% 19% 10%
2	B	192	7% 67% 10% 21%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6104 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 LPS-assembly protein LptD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	579	4761	3013	820	918	10	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q9I5U2
A	2	SER	-	expression tag	UNP Q9I5U2
A	3	ASN	-	expression tag	UNP Q9I5U2
A	4	HIS	-	expression tag	UNP Q9I5U2
A	5	HIS	-	expression tag	UNP Q9I5U2
A	6	HIS	-	expression tag	UNP Q9I5U2
A	7	HIS	-	expression tag	UNP Q9I5U2
A	8	HIS	-	expression tag	UNP Q9I5U2
A	9	HIS	-	expression tag	UNP Q9I5U2
A	10	HIS	-	expression tag	UNP Q9I5U2
A	11	HIS	-	expression tag	UNP Q9I5U2
A	12	HIS	-	expression tag	UNP Q9I5U2
A	13	HIS	-	expression tag	UNP Q9I5U2
A	14	GLU	-	expression tag	UNP Q9I5U2
A	15	ASN	-	expression tag	UNP Q9I5U2
A	16	LEU	-	expression tag	UNP Q9I5U2
A	17	TYR	-	expression tag	UNP Q9I5U2
A	18	PHE	-	expression tag	UNP Q9I5U2
A	19	GLN	-	expression tag	UNP Q9I5U2
A	20	SER	-	expression tag	UNP Q9I5U2
A	21	MET	-	expression tag	UNP Q9I5U2

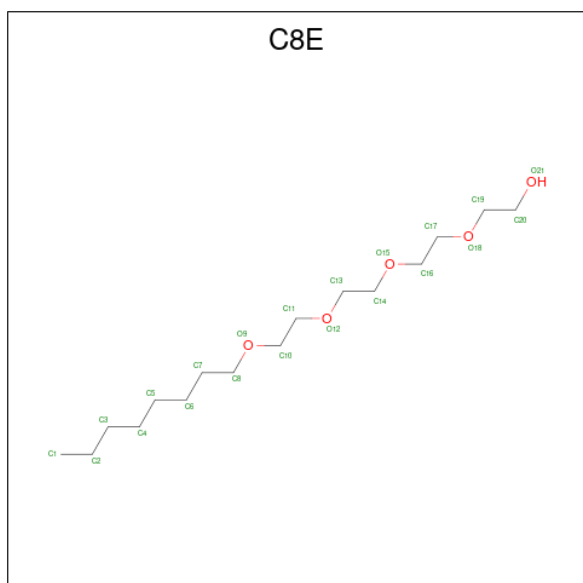
- Molecule 2 is a protein called LPS-assembly lipoprotein LptE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	152	Total	C	N	O	S	0	0	0
			1192	730	218	241	3			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	ALA	-	expression tag	UNP A0A0A8RAG8
B	2	PRO	-	expression tag	UNP A0A0A8RAG8
B	3	ASN	-	expression tag	UNP A0A0A8RAG8
B	4	THR	-	expression tag	UNP A0A0A8RAG8
B	5	SER	-	expression tag	UNP A0A0A8RAG8

- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (CCD ID: C8E) (formula: C₁₆H₃₄O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			21	16	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	16	5		

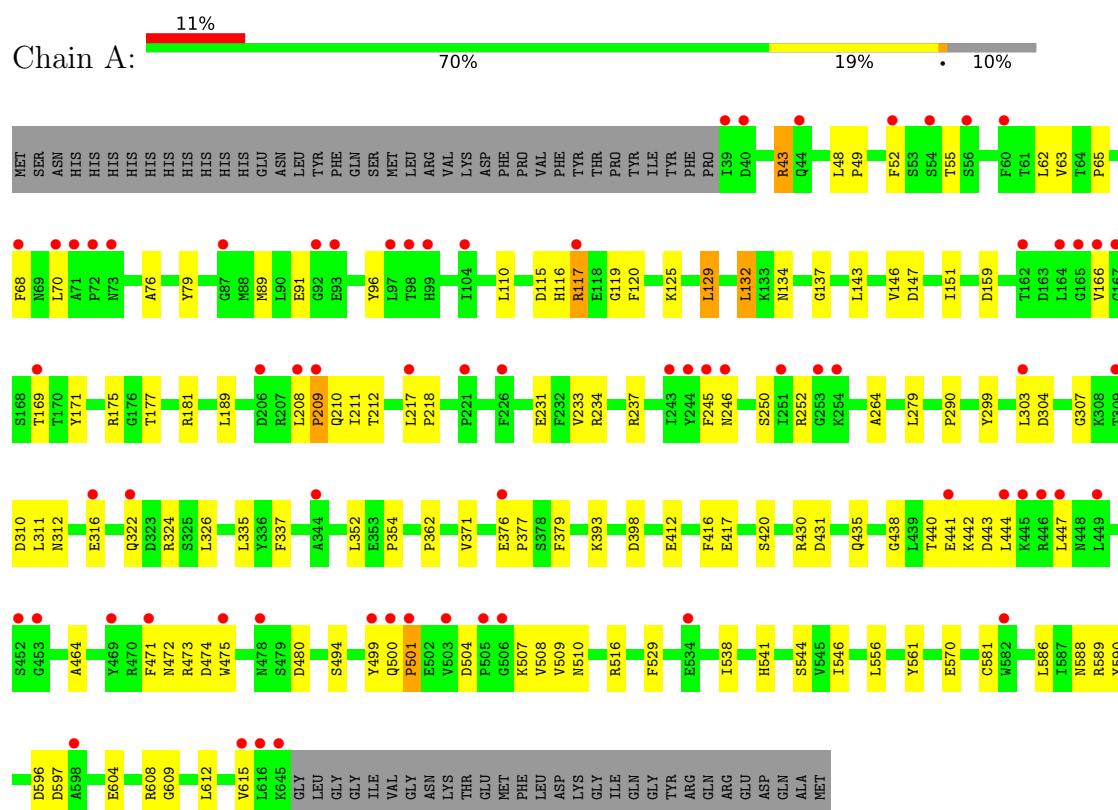
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	B	1	Total	O	0	0
			1	1		

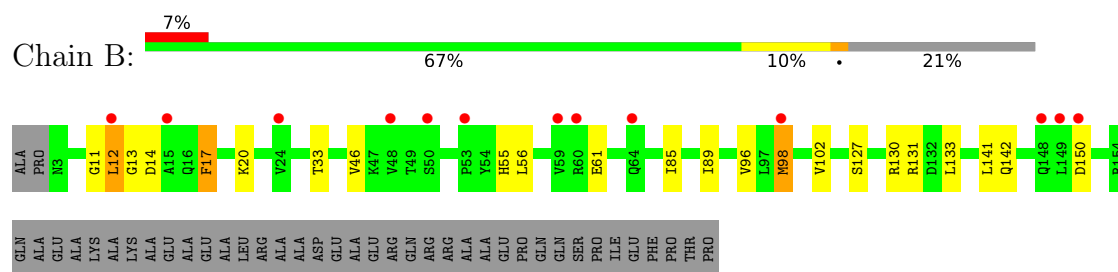
3 Residue-property plots [i](#)

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: LPS-assembly protein LptD



• Molecule 2: LPS-assembly lipoprotein LptE



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	148.92Å 155.99Å 115.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.09 – 2.99 49.09 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.09-2.99) 91.9 (49.09-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.248 , 0.295 0.259 , 0.307	Depositor DCC
R_{free} test set	1385 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	67.1	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6104	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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: C8E

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	0/4893	0.71	3/6643 (0.0%)
2	B	0.26	0/1204	0.67	0/1628
All	All	0.27	0/6097	0.71	3/8271 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	ARG	N-CA-C	-6.05	105.21	112.59
1	A	49	PRO	CA-C-N	5.07	126.17	119.84
1	A	49	PRO	C-N-CA	5.07	126.17	119.84

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	4761	0	4472	76	0
2	B	1192	0	1174	9	0
3	A	147	0	238	7	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
All	All	6104	0	5884	88	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 7.

All (88) 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:299:TYR:HB2	1:A:322:GLN:HB2	1.59	0.84
1:A:89:MET:HB3	1:A:110:LEU:HD12	1.69	0.75
1:A:208:LEU:HB3	1:A:209:PRO:HD3	1.70	0.73
1:A:443:ASP:HA	1:A:447:LEU:HB2	1.75	0.68
1:A:570:GLU:OE1	1:A:589:ARG:NH1	2.29	0.65
1:A:501:PRO:HG2	1:A:504:ASP:HB3	1.79	0.65
1:A:147:ASP:HB3	1:A:175:ARG:HG2	1.80	0.63
1:A:471:PHE:HB3	1:A:475:TRP:HB3	1.82	0.62
1:A:175:ARG:NH1	1:A:177:THR:OG1	2.33	0.61
1:A:335:LEU:HB2	1:A:354:PRO:HG2	1.82	0.61
1:A:129:LEU:HD23	1:A:151:ILE:HG22	1.82	0.60
1:A:516:ARG:HB3	1:A:538:ILE:HB	1.83	0.60
1:A:209:PRO:HD2	1:A:234:ARG:HB3	1.83	0.60
2:B:33:THR:HG22	2:B:130:ARG:HG3	1.84	0.59
1:A:326:LEU:HD12	1:A:362:PRO:HG2	1.83	0.59
2:B:61:GLU:HG3	2:B:85:ILE:HG12	1.85	0.58
1:A:480:ASP:HB3	1:A:494:SER:HB3	1.84	0.57
1:A:417:GLU:OE1	1:A:420:SER:OG	2.20	0.57
1:A:473:ARG:HH22	1:A:475:TRP:HE3	1.51	0.56
1:A:246:ASN:N	1:A:250:SER:O	2.36	0.56
1:A:210:GLN:HG3	1:A:233:VAL:HG22	1.87	0.55
1:A:508:VAL:HG22	1:A:546:ILE:HB	1.89	0.55
1:A:337:PHE:HB2	1:A:352:LEU:HB3	1.87	0.55
1:A:117:ARG:NH2	1:A:159:ASP:OD1	2.40	0.55
1:A:312:ASN:O	1:A:316:GLU:N	2.40	0.55
1:A:398:ASP:OD2	1:A:430:ARG:NH1	2.39	0.54
1:A:132:LEU:HD22	1:A:134:ASN:HB2	1.88	0.54
1:A:169:THR:OG1	1:A:171:TYR:O	2.24	0.54
1:A:212:THR:HG22	1:A:231:GLU:HG3	1.89	0.54
1:A:499:TYR:HB3	1:A:509:VAL:HB	1.90	0.54
1:A:588:ASN:HD21	3:A:702:C8E:H41	1.73	0.54
1:A:608:ARG:HD3	3:A:702:C8E:H52	1.91	0.53
1:A:48:LEU:HB3	1:A:65:PRO:HB2	1.89	0.53
1:A:510:ASN:HB2	1:A:544:SER:HB2	1.91	0.53
1:A:590:TYR:HD1	1:A:608:ARG:HG2	1.73	0.52
2:B:89:ILE:HB	2:B:98:MET:HG2	1.90	0.52
1:A:79:TYR:HB2	1:A:91:GLU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:HIS:CD2	1:A:561:TYR:HB3	2.46	0.51
1:A:440:THR:OG1	1:A:441:GLU:N	2.44	0.50
1:A:119:GLY:O	1:A:252:ARG:NH1	2.45	0.50
1:A:474:ASP:HB2	1:A:500:GLN:HB2	1.94	0.49
1:A:324:ARG:NH2	1:A:393:LYS:O	2.37	0.49
1:A:120:PHE:HE2	1:A:597:ASP:HA	1.77	0.48
3:A:707:C8E:H52	3:A:707:C8E:H21	1.45	0.48
1:A:438:GLY:H	1:A:442:LYS:HD2	1.78	0.48
2:B:14:ASP:O	2:B:142:GLN:NE2	2.47	0.48
1:A:472:ASN:C	1:A:474:ASP:H	2.22	0.47
1:A:68:PHE:HB2	1:A:76:ALA:HB3	1.96	0.47
1:A:473:ARG:NH1	1:A:500:GLN:O	2.48	0.47
1:A:55:THR:HA	1:A:609:GLY:HA3	1.96	0.46
1:A:310:ASP:N	1:A:310:ASP:OD1	2.49	0.46
1:A:237:ARG:NH2	1:A:264:ALA:O	2.48	0.45
1:A:398:ASP:N	1:A:398:ASP:OD1	2.48	0.45
1:A:245:PHE:O	1:A:252:ARG:NH2	2.48	0.45
1:A:189:LEU:HD23	1:A:211:ILE:HG13	1.99	0.45
1:A:307:GLY:O	1:A:312:ASN:ND2	2.41	0.44
1:A:52:PHE:CE2	1:A:62:LEU:HD13	2.53	0.44
1:A:501:PRO:HG3	1:A:507:LYS:HD2	1.99	0.44
1:A:43:ARG:H	1:A:43:ARG:HG3	1.49	0.44
1:A:430:ARG:NH1	1:A:431:ASP:O	2.51	0.44
1:A:561:TYR:CZ	3:A:701:C8E:H62	2.52	0.44
1:A:412:GLU:HG3	1:A:416:PHE:HB2	2.00	0.43
2:B:127:SER:HB3	2:B:131:ARG:HH12	1.83	0.43
1:A:96:TYR:OH	1:A:134:ASN:OD1	2.29	0.43
3:A:703:C8E:H171	3:A:703:C8E:H141	1.78	0.43
1:A:311:LEU:H	1:A:311:LEU:HG	1.55	0.43
1:A:125:LYS:HE2	1:A:125:LYS:HB3	1.90	0.43
1:A:143:LEU:HB2	1:A:181:ARG:CZ	2.48	0.43
1:A:443:ASP:OD1	1:A:444:LEU:N	2.52	0.43
1:A:546:ILE:HG12	1:A:556:LEU:HG	2.01	0.42
2:B:20:LYS:HA	2:B:46:VAL:HG22	2.00	0.42
1:A:137:GLY:O	1:A:181:ARG:NH2	2.52	0.42
1:A:379:PHE:CE2	1:A:464:ALA:HB2	2.55	0.42
1:A:115:ASP:CG	1:A:116:HIS:H	2.28	0.42
1:A:209:PRO:CD	1:A:234:ARG:HB3	2.47	0.41
2:B:56:LEU:HD22	2:B:141:LEU:HD21	2.01	0.41
1:A:279:LEU:O	1:A:290:PRO:HD2	2.20	0.41
1:A:586:LEU:HD12	1:A:612:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:PRO:HD3	1:A:507:LYS:O	2.20	0.41
3:A:706:C8E:H41	3:A:706:C8E:H13	1.79	0.41
1:A:217:LEU:HA	1:A:218:PRO:HD3	1.95	0.41
1:A:608:ARG:HB3	3:A:702:C8E:H61	2.02	0.41
2:B:11:GLY:O	2:B:13:GLY:N	2.54	0.41
1:A:371:VAL:HG21	1:A:529:PHE:HE2	1.85	0.41
1:A:134:ASN:HB3	1:A:146:VAL:HB	2.03	0.40
1:A:376:GLU:HA	1:A:377:PRO:HD2	1.94	0.40
1:A:435:GLN:HB2	1:A:440:THR:HB	2.03	0.40
2:B:102:VAL:HG22	2:B:133: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	577/646 (89%)	531 (92%)	44 (8%)	2 (0%)	36	67
2	B	150/192 (78%)	142 (95%)	6 (4%)	2 (1%)	9	36
All	All	727/838 (87%)	673 (93%)	50 (7%)	4 (1%)	21	53

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	PRO
2	B	12	LEU
1	A	501	PRO
2	B	17	PHE

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	510/571 (89%)	498 (98%)	12 (2%)	43	72
2	B	130/158 (82%)	124 (95%)	6 (5%)	24	57
All	All	640/729 (88%)	622 (97%)	18 (3%)	38	69

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	63	VAL
1	A	70	LEU
1	A	129	LEU
1	A	132	LEU
1	A	166	VAL
1	A	303	LEU
1	A	304	ASP
1	A	581	CYS
1	A	596	ASP
1	A	604	GLU
1	A	615	VAL
2	B	12	LEU
2	B	17	PHE
2	B	55	HIS
2	B	96	VAL
2	B	98	MET
2	B	150	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	482	ASN
1	A	566	ASN
2	B	63	ASN

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Mol	Chain	Res	Type
2	B	110	HIS

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](#)

7 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	$\# Z > 2$
3	C8E	A	701	-	20,20,20	0.38	0	19,19,19	0.41	0
3	C8E	A	706	-	20,20,20	0.38	0	19,19,19	0.34	0
3	C8E	A	704	-	20,20,20	0.38	0	19,19,19	0.34	0
3	C8E	A	703	-	20,20,20	0.38	0	19,19,19	0.37	0
3	C8E	A	705	-	20,20,20	0.38	0	19,19,19	0.39	0
3	C8E	A	707	-	20,20,20	0.38	0	19,19,19	0.40	0
3	C8E	A	702	-	20,20,20	0.38	0	19,19,19	0.58	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	C8E	A	701	-	-	13/18/18/18	-
3	C8E	A	706	-	-	10/18/18/18	-
3	C8E	A	704	-	-	11/18/18/18	-
3	C8E	A	703	-	-	13/18/18/18	-
3	C8E	A	705	-	-	14/18/18/18	-
3	C8E	A	707	-	-	12/18/18/18	-
3	C8E	A	702	-	-	10/18/18/18	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	C8E	O12-C13-C14-O15
3	A	707	C8E	O15-C16-C17-O18
3	A	707	C8E	C2-C3-C4-C5
3	A	704	C8E	O12-C13-C14-O15
3	A	704	C8E	O15-C16-C17-O18
3	A	701	C8E	O12-C13-C14-O15
3	A	703	C8E	O12-C13-C14-O15
3	A	705	C8E	O12-C13-C14-O15
3	A	706	C8E	O18-C19-C20-O21
3	A	703	C8E	C17-C16-O15-C14
3	A	702	C8E	C6-C7-C8-O9
3	A	704	C8E	C6-C7-C8-O9
3	A	702	C8E	O18-C19-C20-O21
3	A	704	C8E	O18-C19-C20-O21
3	A	705	C8E	O18-C19-C20-O21
3	A	701	C8E	O18-C19-C20-O21
3	A	703	C8E	O18-C19-C20-O21
3	A	707	C8E	O18-C19-C20-O21
3	A	701	C8E	O9-C10-C11-O12
3	A	701	C8E	C2-C3-C4-C5
3	A	702	C8E	C3-C4-C5-C6
3	A	705	C8E	C2-C3-C4-C5
3	A	705	C8E	C3-C4-C5-C6
3	A	705	C8E	C6-C7-C8-O9
3	A	702	C8E	C2-C3-C4-C5
3	A	707	C8E	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
3	A	706	C8E	C4-C5-C6-C7
3	A	703	C8E	C6-C7-C8-O9
3	A	703	C8E	C2-C3-C4-C5
3	A	704	C8E	C2-C3-C4-C5
3	A	706	C8E	C2-C3-C4-C5
3	A	706	C8E	O12-C13-C14-O15
3	A	702	C8E	C4-C5-C6-C7
3	A	704	C8E	C1-C2-C3-C4
3	A	707	C8E	O12-C13-C14-O15
3	A	706	C8E	C1-C2-C3-C4
3	A	705	C8E	C4-C5-C6-C7
3	A	707	C8E	C1-C2-C3-C4
3	A	704	C8E	C17-C16-O15-C14
3	A	701	C8E	C6-C7-C8-O9
3	A	701	C8E	C1-C2-C3-C4
3	A	702	C8E	O9-C10-C11-O12
3	A	703	C8E	C4-C5-C6-C7
3	A	705	C8E	C1-C2-C3-C4
3	A	704	C8E	C16-C17-O18-C19
3	A	707	C8E	O9-C10-C11-O12
3	A	703	C8E	C3-C4-C5-C6
3	A	707	C8E	C20-C19-O18-C17
3	A	701	C8E	C10-C11-O12-C13
3	A	705	C8E	C20-C19-O18-C17
3	A	703	C8E	C13-C14-O15-C16
3	A	701	C8E	C16-C17-O18-C19
3	A	701	C8E	C20-C19-O18-C17
3	A	702	C8E	C17-C16-O15-C14
3	A	705	C8E	C14-C13-O12-C11
3	A	705	C8E	C10-C11-O12-C13
3	A	703	C8E	C10-C11-O12-C13
3	A	701	C8E	C13-C14-O15-C16
3	A	704	C8E	C20-C19-O18-C17
3	A	707	C8E	C5-C6-C7-C8
3	A	703	C8E	C20-C19-O18-C17
3	A	706	C8E	C14-C13-O12-C11
3	A	707	C8E	C17-C16-O15-C14
3	A	701	C8E	C4-C5-C6-C7
3	A	702	C8E	C10-C11-O12-C13
3	A	706	C8E	C10-C11-O12-C13
3	A	704	C8E	C10-C11-O12-C13
3	A	707	C8E	C14-C13-O12-C11

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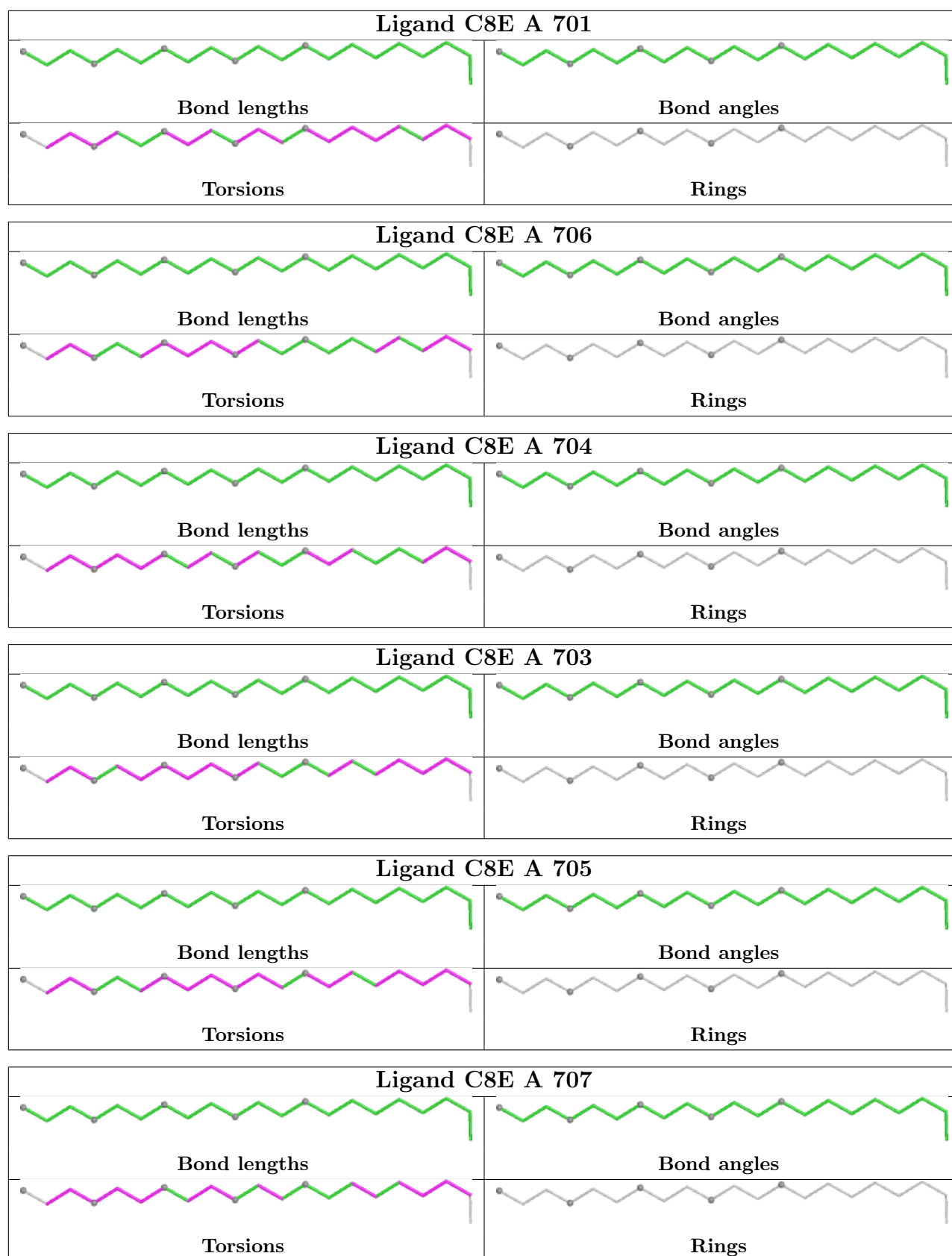
Mol	Chain	Res	Type	Atoms
3	A	705	C8E	C13-C14-O15-C16
3	A	705	C8E	C17-C16-O15-C14
3	A	703	C8E	O15-C16-C17-O18
3	A	703	C8E	C14-C13-O12-C11
3	A	705	C8E	O9-C10-C11-O12
3	A	701	C8E	C5-C6-C7-C8
3	A	702	C8E	C7-C8-O9-C10
3	A	706	C8E	C17-C16-O15-C14
3	A	703	C8E	C1-C2-C3-C4
3	A	704	C8E	C7-C8-O9-C10
3	A	705	C8E	C7-C8-O9-C10
3	A	707	C8E	C16-C17-O18-C19
3	A	706	C8E	C13-C14-O15-C16
3	A	701	C8E	C7-C8-O9-C10
3	A	706	C8E	C20-C19-O18-C17

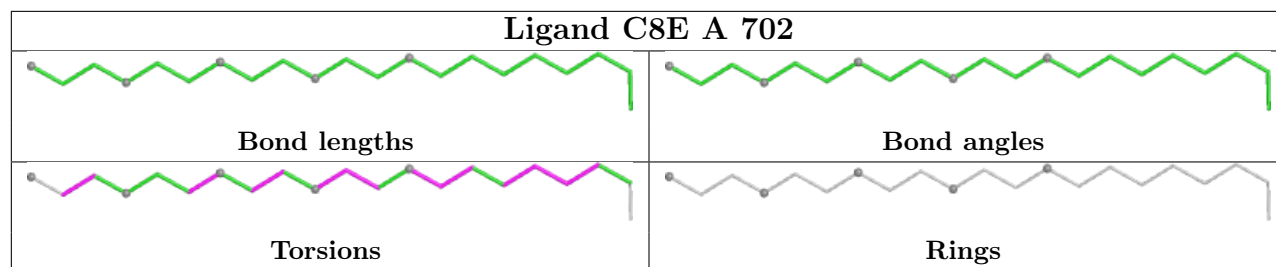
There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	C8E	1	0
3	A	706	C8E	1	0
3	A	703	C8E	1	0
3	A	707	C8E	1	0
3	A	702	C8E	3	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	579/646 (89%)	0.74	69 (11%) 9 6	39, 74, 135, 224	0
2	B	152/192 (79%)	0.67	13 (8%) 16 10	41, 75, 115, 144	0
All	All	731/838 (87%)	0.73	82 (11%) 10 7	39, 75, 131, 224	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	208	LEU	6.6
1	A	164	LEU	6.3
1	A	616	LEU	5.3
1	A	72	PRO	5.2
1	A	444	LEU	4.8
1	A	453	GLY	4.7
2	B	149	LEU	4.5
1	A	245	PHE	3.6
1	A	309	THR	3.5
1	A	254	LYS	3.5
1	A	471	PHE	3.5
1	A	253	GLY	3.4
1	A	452	SER	3.4
1	A	376	GLU	3.4
1	A	445	LYS	3.4
1	A	73	ASN	3.3
1	A	475	TRP	3.3
1	A	447	LEU	3.1
1	A	503	VAL	3.1
1	A	243	ILE	3.1
1	A	582	TRP	3.1
1	A	60	PHE	3.0
1	A	165	GLY	3.0
2	B	24	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	244	TYR	2.9
1	A	598	ALA	2.9
1	A	221	PRO	2.9
1	A	441	GLU	2.9
1	A	645	LYS	2.9
1	A	206	ASP	2.9
2	B	148	GLN	2.8
1	A	246	ASN	2.8
1	A	166	VAL	2.7
1	A	499	TYR	2.7
2	B	98	MET	2.7
1	A	478	ASN	2.7
2	B	15	ALA	2.7
2	B	150	ASP	2.7
1	A	217	LEU	2.7
2	B	59	VAL	2.6
1	A	39	ILE	2.6
1	A	162	THR	2.6
1	A	316	GLU	2.5
1	A	68	PHE	2.5
1	A	54	SER	2.5
1	A	501	PRO	2.5
1	A	92	GLY	2.5
1	A	97	LEU	2.5
1	A	505	PRO	2.4
1	A	169	THR	2.4
1	A	251	ILE	2.4
2	B	60	ARG	2.3
1	A	500	GLN	2.3
1	A	469	TYR	2.3
1	A	226	PHE	2.3
2	B	53	PRO	2.2
1	A	534	GLU	2.2
1	A	446	ARG	2.2
1	A	70	LEU	2.2
2	B	64	GLN	2.2
1	A	98	THR	2.2
1	A	56	SER	2.2
1	A	104	ILE	2.1
1	A	44	GLN	2.1
1	A	209	PRO	2.1
1	A	40	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	167	GLY	2.1
1	A	117	ARG	2.1
1	A	344	ALA	2.1
1	A	93	GLU	2.1
1	A	449	LEU	2.1
2	B	12	LEU	2.1
1	A	52	PHE	2.1
1	A	303	LEU	2.1
1	A	87	GLY	2.1
1	A	99	HIS	2.0
1	A	322	GLN	2.0
1	A	506	GLY	2.0
2	B	48	VAL	2.0
2	B	50	SER	2.0
1	A	71	ALA	2.0
1	A	615	VAL	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](#)

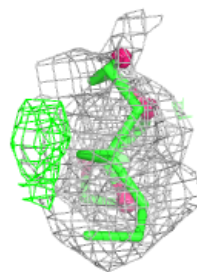
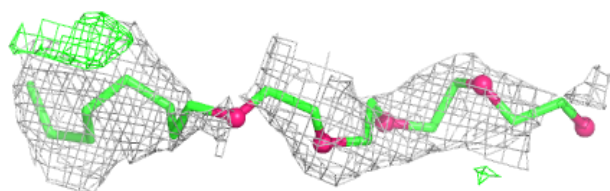
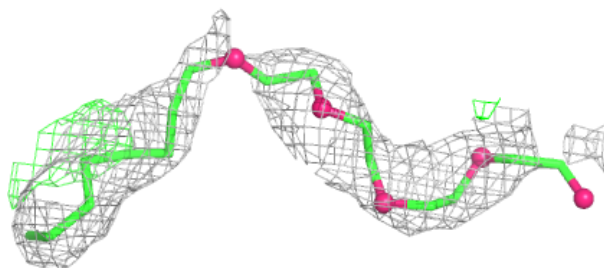
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	C8E	A	704	21/21	0.35	0.25	103,121,128,136	0
3	C8E	A	707	21/21	0.63	0.35	80,95,120,134	0
3	C8E	A	701	21/21	0.77	0.23	57,78,86,92	0
3	C8E	A	703	21/21	0.79	0.22	50,91,117,132	0
3	C8E	A	702	21/21	0.80	0.23	69,89,97,106	0
3	C8E	A	706	21/21	0.82	0.24	55,78,120,128	0
3	C8E	A	705	21/21	0.82	0.22	56,77,99,120	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.

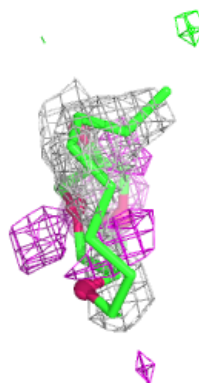
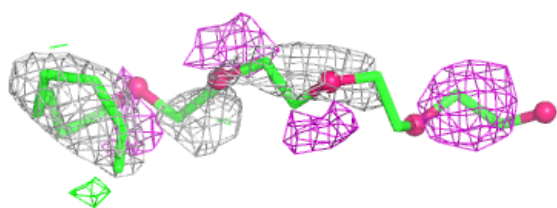
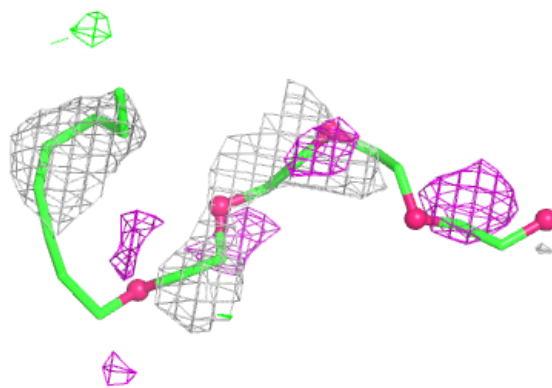
Electron density around C8E A 704:

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

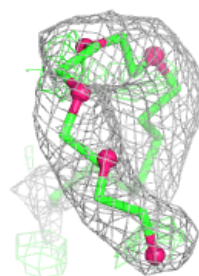
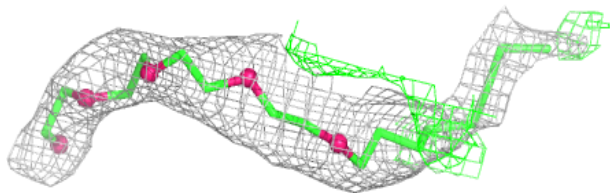


Electron density around C8E A 707:

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

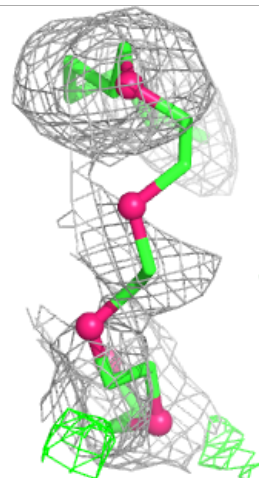
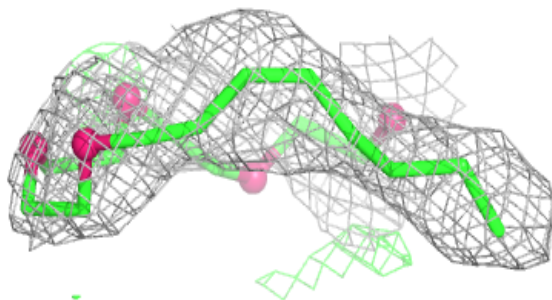
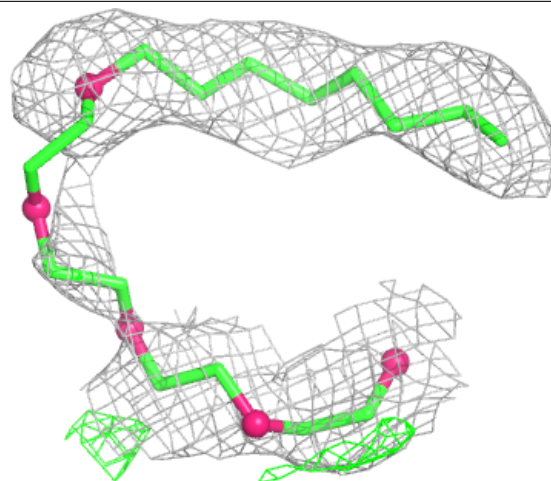
**Electron density around C8E A 701:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



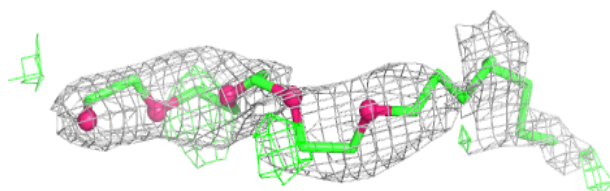
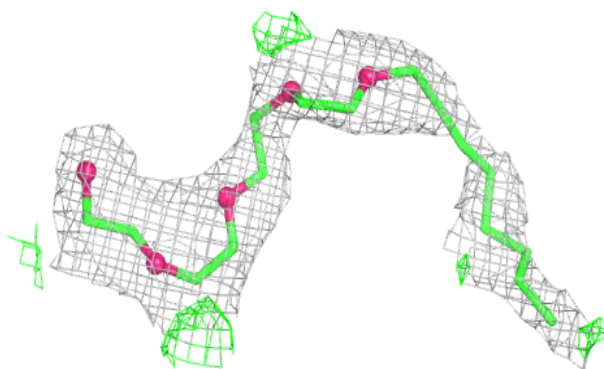
Electron density around C8E A 703:

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

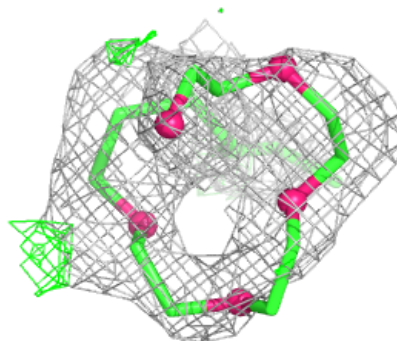
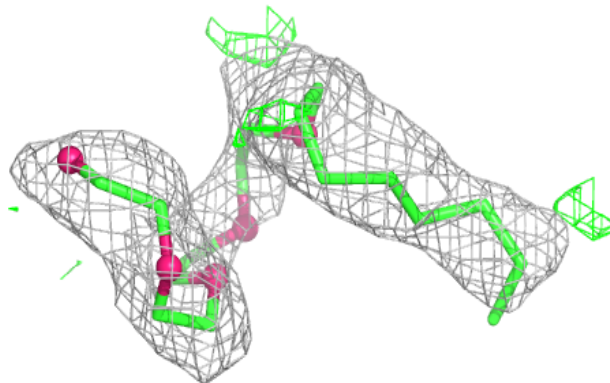
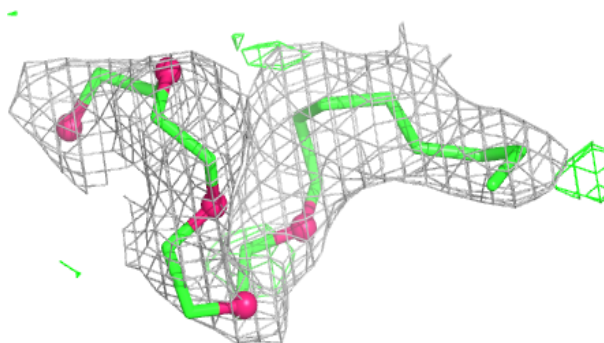


Electron density around C8E A 702:

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and green (positive)

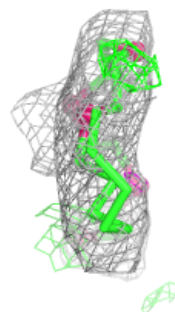
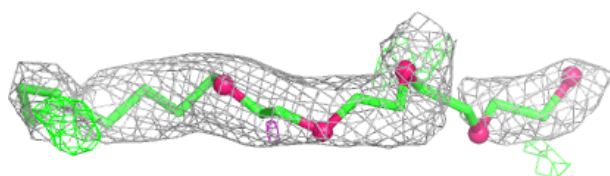
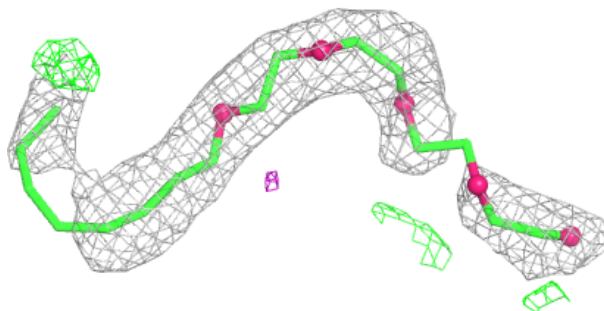
**Electron density around C8E A 706:**

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



Electron density around C8E A 705:

$2mF_o-DF_c$ (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.