



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:35 PM UTC

PDB ID : 6FOM / pdb_00006fom
Title : Copper transporter OprC
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Deposited on : 2018-02-07
Resolution : 2.90 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

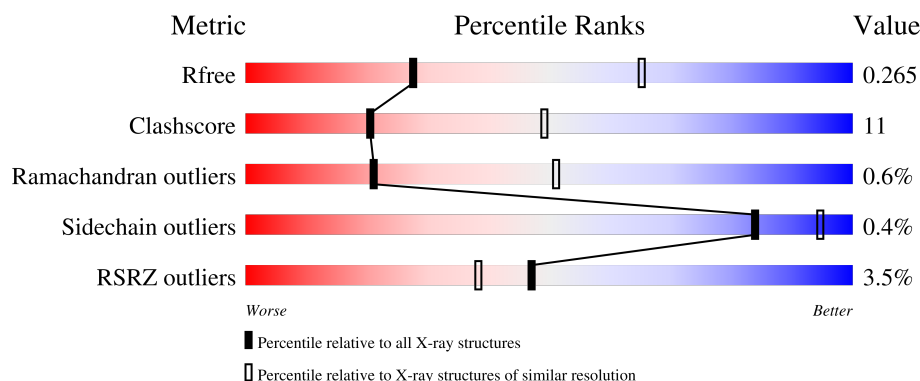
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

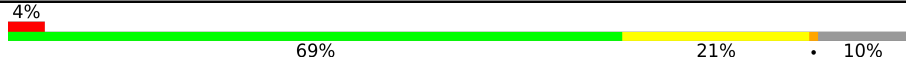
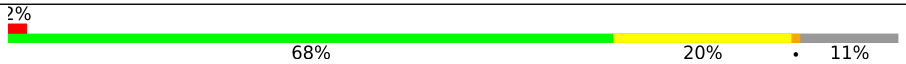
The reported resolution of this entry is 2.90 Å.

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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	723	
1	B	723	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 10133 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.

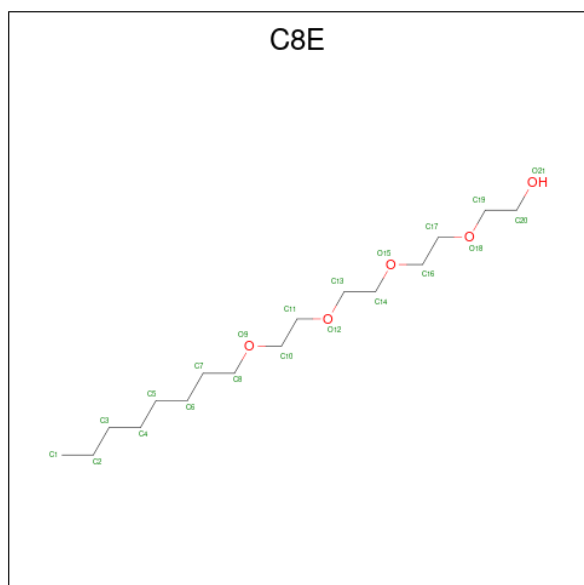
- Molecule 1 is a protein called Putative copper transport outer membrane porin OprC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	651	Total	C	N	O	S	0	1	0
			5055	3175	893	972	15			
1	B	644	Total	C	N	O	S	0	0	0
			5003	3144	884	961	14			

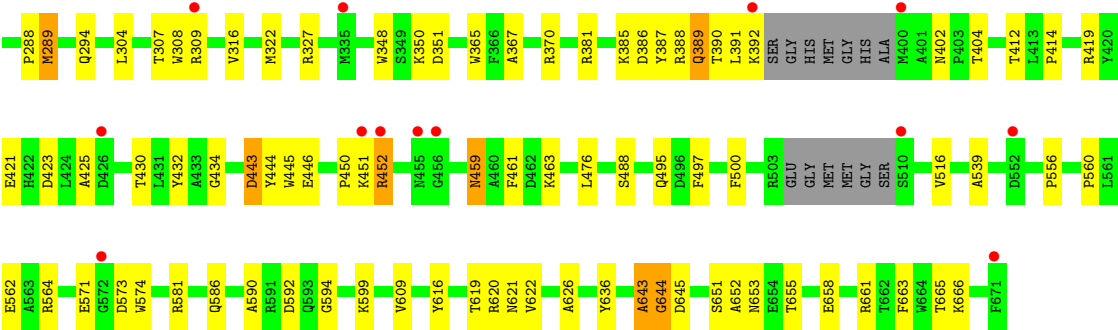
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	91	ALA	CYS	engineered mutation	UNP G3XD89
A	95	ALA	MET	engineered mutation	UNP G3XD89
B	91	ALA	CYS	engineered mutation	UNP G3XD89
B	95	ALA	MET	engineered mutation	UNP G3XD89

- Molecule 2 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (CCD ID: C8E) (formula: C₁₆H₃₄O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			15	10	5		
2	A	1	Total	C	O	0	0
			18	13	5		
2	B	1	Total	C	O	0	0
			21	16	5		
2	B	1	Total	C	O	0	0
			21	16	5		



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	62.13Å 170.56Å 197.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.26 – 2.90 49.26 – 2.90	Depositor EDS
% Data completeness (in resolution range)	88.9 (49.26-2.90) 88.9 (49.26-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.214 , 0.270 (Not available) , 0.265	Depositor DCC
R_{free} test set	2025 reflections (4.26%)	wwPDB-VP
Wilson B-factor (Å ²)	49.2	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 21.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10133	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.68 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5220e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.44	0/5182	0.70	0/7024
1	B	0.45	0/5126	0.77	6/6949 (0.1%)
All	All	0.44	0/10308	0.74	6/13973 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	452	ARG	CG-CD-NE	7.59	128.69	112.00
1	B	452	ARG	NE-CZ-NH1	-6.97	114.53	121.50
1	B	452	ARG	CD-NE-CZ	-6.89	114.75	124.40
1	B	452	ARG	CA-CB-CG	-6.56	100.99	114.10
1	B	452	ARG	NE-CZ-NH2	6.07	124.67	119.20
1	B	309	ARG	CB-CG-CD	5.24	123.36	111.30

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	5055	0	4833	116	0
1	B	5003	0	4786	112	0
2	A	33	0	43	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	42	0	66	4	0
All	All	10133	0	9728	223	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 11.

All (223) 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:495:GLN:OE1	1:B:381:ARG:NH1	1.82	1.12
1:A:201:ASN:HD22	1:A:241:ARG:HH21	1.14	0.90
1:A:151:LEU:HB2	1:A:666:LYS:HE3	1.53	0.89
1:A:126:SER:HB2	1:A:469:THR:HG21	1.56	0.87
1:A:412:THR:HG23	1:B:495:GLN:HE21	1.40	0.85
1:A:150:LEU:HD23	2:A:702:C8E:H132	1.62	0.81
1:B:619:THR:HG23	1:B:621:ASN:H	1.43	0.81
1:A:160:LYS:HD3	2:A:702:C8E:H141	1.61	0.81
1:B:663:PHE:HB3	2:B:702:C8E:H112	1.63	0.79
1:B:106:THR:HG22	1:B:134:ARG:HH12	1.46	0.79
1:B:40:PRO:HG2	1:B:42:PRO:N	1.98	0.78
1:B:619:THR:HG22	1:B:622:VAL:HG12	1.65	0.77
1:A:495:GLN:NE2	1:B:412:THR:OG1	2.18	0.77
1:A:619:THR:HG23	1:A:621:ASN:H	1.47	0.77
1:B:432:TYR:OH	1:B:488:SER:OG	2.02	0.77
1:A:20:THR:HG22	1:A:39:GLN:HB2	1.67	0.76
1:A:414:PRO:HG2	1:B:414:PRO:HG2	1.68	0.76
1:A:99:THR:HA	1:A:102:ILE:HD12	1.66	0.76
1:A:412:THR:HG23	1:B:495:GLN:NE2	2.00	0.75
1:A:30:ILE:HD11	1:A:114:LYS:HE2	1.69	0.75
1:A:619:THR:HG22	1:A:622:VAL:HG12	1.70	0.74
1:B:30:ILE:HD11	1:B:114:LYS:HE2	1.73	0.69
1:B:592:ASP:HA	1:B:599:LYS:HD2	1.73	0.69
1:B:43:ALA:H	1:B:157:ARG:HH12	1.38	0.69
1:B:151:LEU:HD12	1:B:666:LYS:HB2	1.75	0.69
1:A:479:ASN:HB2	1:A:484:GLN:NE2	2.09	0.67
1:B:19:VAL:HG22	1:B:38:ARG:HG2	1.73	0.67
1:A:39:GLN:HB3	1:A:40:PRO:HD3	1.77	0.66
1:B:240:LYS:HB3	1:B:270:ASP:HB3	1.78	0.66
1:A:140:GLY:O	1:A:169:ARG:NH1	2.29	0.65
1:B:111:THR:HG23	1:B:131:LEU:HB2	1.77	0.65
1:A:459:ASN:ND2	1:A:461:PHE:HB3	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:LYS:O	1:B:452:ARG:HG3	1.95	0.65
1:A:532:THR:OG1	1:A:535:TRP:N	2.26	0.64
1:A:14:LEU:O	1:A:617:ARG:NH2	2.31	0.64
1:A:196:ARG:HD3	1:A:228:ARG:NH2	2.13	0.64
1:B:20:THR:HG22	1:B:39:GLN:HB3	1.79	0.63
1:A:404:THR:HG21	1:A:459:ASN:ND2	2.13	0.63
1:B:140:GLY:O	1:B:169:ARG:NH1	2.32	0.63
1:B:620:ARG:HG2	1:B:620:ARG:HH11	1.64	0.63
1:A:282:ASP:HB2	1:A:283:PRO:HD3	1.81	0.63
1:B:386:ASP:OD1	1:B:388:ARG:HG3	1.99	0.63
1:B:144:SER:C	1:B:145:ARG:HD3	2.24	0.62
1:B:560:PRO:HB3	1:B:586:GLN:HB2	1.81	0.62
1:A:20:THR:HG22	1:A:39:GLN:CB	2.29	0.62
1:B:307:THR:HG23	1:B:316:VAL:HG22	1.82	0.61
1:A:560:PRO:HB3	1:A:586:GLN:HB2	1.81	0.61
1:B:288:PRO:HD2	1:B:289:MET:HE2	1.83	0.61
1:A:208:TRP:CE2	1:A:210:PRO:HG3	2.36	0.61
1:A:645:ASP:O	1:A:647:GLY:N	2.31	0.61
1:A:31:VAL:HG22	1:A:111:THR:HG23	1.82	0.60
1:A:469:THR:HB	1:A:494:VAL:HG22	1.84	0.60
1:A:651:SER:OG	1:A:652:ALA:N	2.35	0.59
1:B:385:LYS:HD3	1:B:387:TYR:CZ	2.38	0.59
1:B:651:SER:O	1:B:653:ASN:N	2.35	0.59
1:A:83:ASN:O	1:A:263:GLN:NE2	2.34	0.58
1:A:310:TRP:HD1	1:A:311:ASP:OD1	1.86	0.58
1:B:327:ARG:HG2	1:B:350:LYS:HA	1.84	0.58
1:A:77:ARG:NH1	1:A:467:GLU:OE1	2.36	0.58
1:A:149:SER:OG	1:A:668:ASP:OD2	2.22	0.58
1:B:38:ARG:O	1:B:40:PRO:HD3	2.03	0.58
1:A:181:GLN:OE1	1:A:198:LYS:NZ	2.37	0.57
1:B:106:THR:HG22	1:B:134:ARG:NH1	2.18	0.57
1:B:392:LYS:HB2	1:B:451:LYS:HZ2	1.69	0.57
1:A:365:TRP:CE2	1:A:367:ALA:HB2	2.40	0.57
1:B:262:ALA:HB2	1:B:304:LEU:HD12	1.87	0.56
1:B:49:TYR:OH	1:B:105:GLU:HG2	2.06	0.56
1:B:571:GLU:O	1:B:573:ASP:N	2.39	0.56
1:A:525:LEU:HD21	1:A:541:LEU:HD23	1.88	0.56
1:A:445:TRP:O	1:A:450:PRO:HD3	2.05	0.55
1:B:661:ARG:HD2	2:B:701:C8E:H162	1.89	0.55
1:B:42:PRO:HB2	1:B:157:ARG:HH12	1.72	0.55
1:A:438:ALA:HB3	1:A:469:THR:HG23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ASP:OD1	1:B:176:THR:HG22	2.08	0.54
1:B:144:SER:O	1:B:145:ARG:HD3	2.07	0.54
1:B:365:TRP:CE2	1:B:367:ALA:HB2	2.43	0.54
1:B:19:VAL:CG2	1:B:38:ARG:HG2	2.37	0.54
1:B:87:MET:HE3	1:B:269:ALA:HB2	1.89	0.54
1:B:254:SER:OG	1:B:255:ASP:N	2.40	0.54
1:B:106:THR:O	1:B:134:ARG:NH1	2.42	0.53
1:A:621:ASN:HB3	1:A:671:PHE:CE1	2.44	0.53
1:B:93:ASN:HB2	1:B:232:ARG:NH1	2.24	0.53
1:A:144:SER:C	1:A:145:ARG:HD3	2.34	0.53
1:B:463:LYS:HG3	1:B:463:LYS:O	2.08	0.52
1:A:154:SER:O	1:A:157:ARG:HG3	2.09	0.52
1:B:390:THR:O	1:B:391:LEU:HB2	2.09	0.52
1:A:287:MET:HE3	1:A:291:MET:SD	2.50	0.52
1:B:445:TRP:O	1:B:450:PRO:HD3	2.10	0.51
1:A:447:LEU:HD22	1:A:461:PHE:HA	1.92	0.51
1:A:641:ASN:ND2	1:A:658:GLU:OE1	2.42	0.51
1:B:500:PHE:HB2	1:B:594:GLY:O	2.11	0.50
1:A:160:LYS:HD2	2:A:702:C8E:H192	1.93	0.50
1:B:365:TRP:CZ2	1:B:367:ALA:HB2	2.47	0.50
1:A:126:SER:HB2	1:A:469:THR:CG2	2.33	0.50
1:A:32:THR:OG1	1:A:38:ARG:NH1	2.45	0.49
1:A:27:PRO:O	1:A:29:THR:HG23	2.12	0.49
1:A:442:PRO:HB2	1:A:447:LEU:HG	1.95	0.49
1:B:181:GLN:HB3	1:B:198:LYS:HG3	1.94	0.49
1:B:643:ALA:HA	1:B:655:THR:HA	1.94	0.49
1:B:93:ASN:HB2	1:B:232:ARG:HH12	1.77	0.49
1:A:138:ARG:HH22	1:A:212:GLU:HA	1.78	0.49
1:B:111:THR:CG2	1:B:131:LEU:HB2	2.42	0.49
1:B:103:SER:O	1:B:106:THR:HB	2.13	0.49
1:A:459:ASN:OD1	1:A:462:ASP:N	2.32	0.49
1:A:41:VAL:HG12	1:A:629:ASP:OD2	2.13	0.48
1:B:564:ARG:HE	1:B:581:ARG:HD2	1.77	0.48
1:A:571:GLU:O	1:A:573:ASP:N	2.40	0.48
1:B:279:ARG:HG2	1:B:280:THR:N	2.27	0.48
1:B:388:ARG:O	1:B:389:GLN:HB2	2.13	0.48
1:B:86:MET:HG2	1:B:88:LEU:HD11	1.96	0.48
1:B:644:GLY:O	1:B:645:ASP:HB3	2.13	0.48
1:A:157:ARG:NH2	1:A:662:THR:HG21	2.29	0.48
1:A:201:ASN:ND2	1:A:241:ARG:HH21	1.96	0.48
1:B:423:ASP:HA	1:B:430:THR:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ARG:NH1	1:B:658:GLU:OE2	2.47	0.48
1:B:196:ARG:HD3	1:B:228:ARG:NH1	2.29	0.48
1:A:15:ALA:HB3	1:A:570:GLU:OE1	2.13	0.47
1:A:367:ALA:O	1:A:371:ASP:HB2	2.14	0.47
1:B:27:PRO:O	1:B:29:THR:HG23	2.14	0.47
1:B:40:PRO:HD2	1:B:42:PRO:HD3	1.95	0.47
1:A:22:VAL:HG11	1:A:32:THR:HB	1.96	0.47
1:A:392:LYS:HZ1	1:A:399:ALA:HB2	1.80	0.47
1:A:651:SER:HB3	1:A:654:GLU:OE1	2.14	0.47
1:A:586:GLN:HG2	1:A:639:HIS:CD2	2.50	0.47
1:A:87:MET:HE3	1:A:269:ALA:HB2	1.97	0.46
1:B:240:LYS:CB	1:B:270:ASP:HB3	2.44	0.46
1:A:282:ASP:HB2	1:A:283:PRO:CD	2.44	0.46
1:B:87:MET:CE	1:B:269:ALA:HB2	2.46	0.46
1:A:124:GLY:O	1:A:126:SER:N	2.48	0.46
1:B:73:MET:HB3	1:B:77:ARG:HD2	1.96	0.46
1:B:497:PHE:N	1:B:516:VAL:O	2.49	0.46
1:A:39:GLN:O	1:A:39:GLN:NE2	2.46	0.46
1:B:174:ARG:HE	1:B:176:THR:CG2	2.29	0.46
1:B:81:LEU:HD11	1:B:121:TRP:HB3	1.97	0.46
1:A:644:GLY:HA3	1:A:650:PHE:HB3	1.98	0.46
1:A:78:LEU:HD22	1:A:130:ILE:HD11	1.97	0.45
1:A:283:PRO:C	1:A:288:PRO:HB3	2.41	0.45
1:A:414:PRO:CG	1:B:414:PRO:HG2	2.43	0.45
1:A:564:ARG:HE	1:A:581:ARG:HD2	1.81	0.45
1:B:170:LEU:HA	1:B:209:THR:O	2.17	0.45
1:B:322:MET:HE3	1:B:322:MET:HB3	1.68	0.45
1:A:172:TYR:CE1	1:A:207:GLY:HA3	2.51	0.45
1:A:412:THR:H	1:B:495:GLN:HE22	1.63	0.45
1:A:497:PHE:N	1:A:516:VAL:O	2.50	0.45
1:A:81:LEU:HD11	1:A:121:TRP:HB3	1.99	0.45
1:B:419:ARG:HA	1:B:434:GLY:HA2	1.99	0.45
1:B:351:ASP:HB2	1:B:388:ARG:HG2	1.98	0.45
1:A:532:THR:HG1	1:A:535:TRP:H	1.62	0.45
1:A:503:ARG:HH22	1:A:512:GLN:CD	2.24	0.45
1:B:99:THR:HA	1:B:102:ILE:HD12	1.98	0.45
1:B:452:ARG:HH11	1:B:452:ARG:HD3	1.36	0.45
1:A:392:LYS:NZ	1:A:399:ALA:HB2	2.32	0.45
1:B:61:ASN:HB3	1:B:229:TYR:CD1	2.52	0.45
1:B:294:GLN:HG2	1:B:348:TRP:CH2	2.52	0.45
1:A:163:ASP:OD1	1:A:176:THR:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:MET:HB2	1:A:335:MET:HE3	1.74	0.44
1:A:144:SER:H	1:A:145:ARG:NH1	2.16	0.44
1:B:562:GLU:OE1	1:B:581:ARG:NE	2.44	0.44
1:A:151:LEU:O	1:A:158:PHE:HA	2.16	0.44
1:A:282:ASP:OD1	1:A:282:ASP:N	2.39	0.44
1:B:257:LEU:HD13	1:B:308:TRP:CZ3	2.52	0.44
1:A:350:LYS:HE3	1:A:387:TYR:CD1	2.53	0.44
2:B:701:C8E:H102	2:B:701:C8E:H71	1.58	0.44
1:A:119:VAL:HB	1:A:378:ARG:HD2	1.99	0.44
1:B:48:ASP:CG	1:B:51:LYS:HE3	2.43	0.44
1:A:386:ASP:OD2	1:A:388:ARG:HG3	2.17	0.44
1:B:289:MET:HE2	1:B:289:MET:H	1.83	0.44
1:A:149:SER:HB3	1:A:666:LYS:HE2	2.00	0.43
1:B:279:ARG:HG2	1:B:280:THR:H	1.82	0.43
1:B:574:TRP:HB3	1:B:616:TYR:HD1	1.83	0.43
1:A:171:GLY:HA2	1:A:207:GLY:O	2.18	0.43
1:A:86:MET:O	1:A:267:ASN:ND2	2.39	0.43
1:B:27:PRO:HG2	1:B:421:GLU:CD	2.43	0.43
1:A:562:GLU:HG3	1:A:583:VAL:HG12	2.01	0.43
1:B:386:ASP:HB2	1:B:461:PHE:CE1	2.53	0.43
1:B:238:GLN:HB3	1:B:272:ILE:HG13	2.00	0.43
1:B:60:ARG:HH12	1:B:658:GLU:CD	2.27	0.43
1:A:42:PRO:HG2	1:A:49:TYR:CE1	2.54	0.43
1:A:149:SER:C	1:A:150:LEU:HD12	2.44	0.43
1:B:626:ALA:HB2	1:B:665:THR:HG23	2.01	0.43
1:B:112:VAL:HG22	1:B:130:ILE:HG12	2.01	0.42
1:B:157:ARG:HD2	1:B:182:SER:HB2	2.01	0.42
1:A:400:MET:HE3	1:A:400:MET:HB2	1.92	0.42
1:A:532:THR:HG1	1:A:535:TRP:N	2.16	0.42
1:B:402:ASN:OD1	1:B:404:THR:HG22	2.19	0.42
1:B:102:ILE:O	1:B:104:PRO:HD3	2.19	0.42
2:A:701:C8E:H191	2:A:701:C8E:H161	1.62	0.42
1:B:609:VAL:HG11	1:B:636:TYR:CZ	2.55	0.42
1:A:644:GLY:O	1:A:645:ASP:HB2	2.20	0.42
1:B:370:ARG:CZ	1:B:425:ALA:HB2	2.49	0.42
1:B:443:ASP:HB2	1:B:446:GLU:CG	2.50	0.42
1:A:591:ARG:NH2	1:A:601:PHE:O	2.53	0.42
1:B:539:ALA:HA	1:B:564:ARG:O	2.20	0.42
1:A:210:PRO:HD2	1:A:214:THR:HB	2.01	0.42
1:A:350:LYS:HE3	1:A:387:TYR:CE1	2.55	0.42
1:A:78:LEU:HD22	1:A:130:ILE:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:GLY:O	1:A:472:LEU:HD12	2.20	0.41
1:A:41:VAL:O	1:A:41:VAL:HG13	2.19	0.41
1:B:459:ASN:C	1:B:459:ASN:HD22	2.26	0.41
1:B:556:PRO:HB3	1:B:590:ALA:HB3	2.02	0.41
1:A:28:LEU:HG	1:A:114:LYS:O	2.20	0.41
1:A:628:VAL:HG22	1:A:663:PHE:CE2	2.55	0.41
1:A:437:HIS:ND1	1:A:470:THR:OG1	2.52	0.41
1:A:621:ASN:HB3	1:A:671:PHE:CD1	2.55	0.41
1:A:645:ASP:C	1:A:647:GLY:N	2.79	0.41
1:B:32:THR:OG1	1:B:38:ARG:NH1	2.52	0.41
1:A:638:GLU:HB2	1:A:641:ASN:OD1	2.20	0.41
1:B:388:ARG:O	1:B:389:GLN:CB	2.68	0.41
1:A:507:MET:HB3	1:A:508:GLY:H	1.59	0.41
1:B:289:MET:H	1:B:289:MET:CE	2.34	0.41
1:A:65:ASN:CG	1:A:100:SER:HB2	2.46	0.41
1:B:196:ARG:HD3	1:B:228:ARG:CZ	2.50	0.41
1:A:499:LEU:HD11	1:A:593:GLN:HB3	2.02	0.41
1:A:583:VAL:HG21	1:A:607:PHE:CZ	2.55	0.41
1:A:661:ARG:HD2	2:A:701:C8E:H172	2.03	0.41
1:B:60:ARG:NH1	1:B:658:GLU:CD	2.79	0.41
1:B:273:MET:HB2	1:B:273:MET:HE2	1.85	0.41
1:B:444:TYR:CD2	1:B:444:TYR:C	2.99	0.41
1:B:661:ARG:NH1	2:B:701:C8E:H162	2.36	0.41
1:B:476:LEU:HD12	1:B:476:LEU:C	2.45	0.41
1:A:82:THR:CG2	1:A:102:ILE:HG12	2.51	0.40
1:A:61:ASN:HB3	1:A:229:TYR:CD2	2.56	0.40
1:A:581:ARG:NH1	1:A:638:GLU:OE1	2.51	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	644/723 (89%)	605 (94%)	36 (6%)	3 (0%)	24	54
1	B	636/723 (88%)	592 (93%)	39 (6%)	5 (1%)	16	44
All	All	1280/1446 (88%)	1197 (94%)	75 (6%)	8 (1%)	21	51

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	VAL
1	A	282	ASP
1	A	645	ASP
1	B	652	ALA
1	B	389	GLN
1	B	443	ASP
1	B	643	ALA
1	B	644	GLY

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	520/571 (91%)	519 (100%)	1 (0%)	87	96
1	B	515/571 (90%)	512 (99%)	3 (1%)	78	93
All	All	1035/1142 (91%)	1031 (100%)	4 (0%)	84	94

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

Mol	Chain	Res	Type
1	A	28	LEU
1	B	284	SER
1	B	289	MET
1	B	459	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	ASN
1	A	252	ASN
1	A	406	ASN
1	A	495	GLN
1	A	512	GLN
1	A	557	GLN
1	B	389	GLN
1	B	406	ASN
1	B	422	HIS
1	B	495	GLN
1	B	653	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	C8E	B	701	-	20,20,20	0.40	0	19,19,19	0.56	0
2	C8E	B	702	-	20,20,20	0.46	0	19,19,19	0.55	0
2	C8E	A	701	-	14,14,20	0.58	0	13,13,19	0.80	0
2	C8E	A	702	-	17,17,20	0.47	0	16,16,19	0.40	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
2	C8E	B	701	-	-	10/18/18/18	-
2	C8E	B	702	-	-	15/18/18/18	-
2	C8E	A	701	-	-	8/12/12/18	-
2	C8E	A	702	-	-	5/15/15/18	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	C8E	C16-C17-O18-C19
2	B	702	C8E	O12-C13-C14-O15
2	B	702	C8E	O9-C10-C11-O12
2	A	701	C8E	O12-C13-C14-O15
2	A	702	C8E	O18-C19-C20-O21
2	B	702	C8E	O18-C19-C20-O21
2	A	701	C8E	O15-C16-C17-O18
2	B	702	C8E	C6-C7-C8-O9
2	B	702	C8E	C3-C4-C5-C6
2	B	701	C8E	C3-C4-C5-C6
2	A	701	C8E	O18-C19-C20-O21
2	B	701	C8E	O18-C19-C20-O21
2	A	701	C8E	C7-C8-O9-C10
2	B	701	C8E	C1-C2-C3-C4
2	B	701	C8E	C7-C8-O9-C10
2	B	702	C8E	C14-C13-O12-C11
2	A	701	C8E	C13-C14-O15-C16
2	B	702	C8E	C11-C10-O9-C8
2	B	701	C8E	C14-C13-O12-C11
2	B	702	C8E	C2-C3-C4-C5
2	B	702	C8E	C16-C17-O18-C19
2	B	702	C8E	C7-C8-O9-C10
2	A	701	C8E	C20-C19-O18-C17
2	B	701	C8E	C2-C3-C4-C5
2	B	702	C8E	C20-C19-O18-C17

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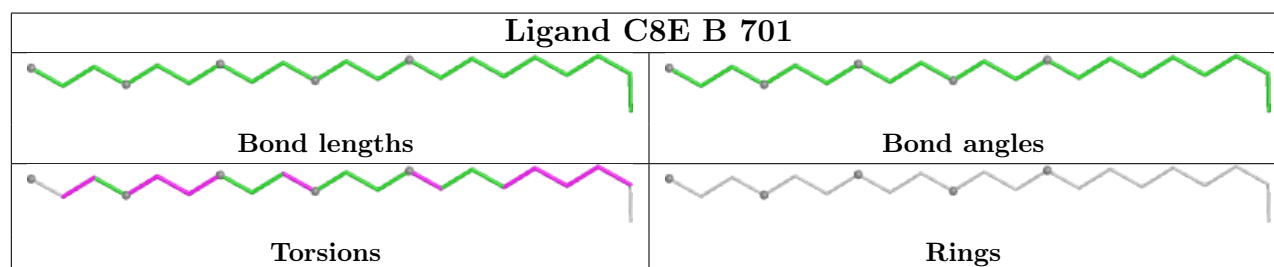
Mol	Chain	Res	Type	Atoms
2	B	702	C8E	C13-C14-O15-C16
2	A	701	C8E	C10-C11-O12-C13
2	B	701	C8E	O15-C16-C17-O18
2	A	702	C8E	C11-C10-O9-C8
2	B	701	C8E	C17-C16-O15-C14
2	A	702	C8E	C4-C5-C6-C7
2	B	701	C8E	C4-C5-C6-C7
2	B	702	C8E	C5-C6-C7-C8
2	A	702	C8E	O15-C16-C17-O18
2	B	702	C8E	C10-C11-O12-C13
2	B	701	C8E	C16-C17-O18-C19
2	A	702	C8E	O12-C13-C14-O15
2	B	702	C8E	C1-C2-C3-C4

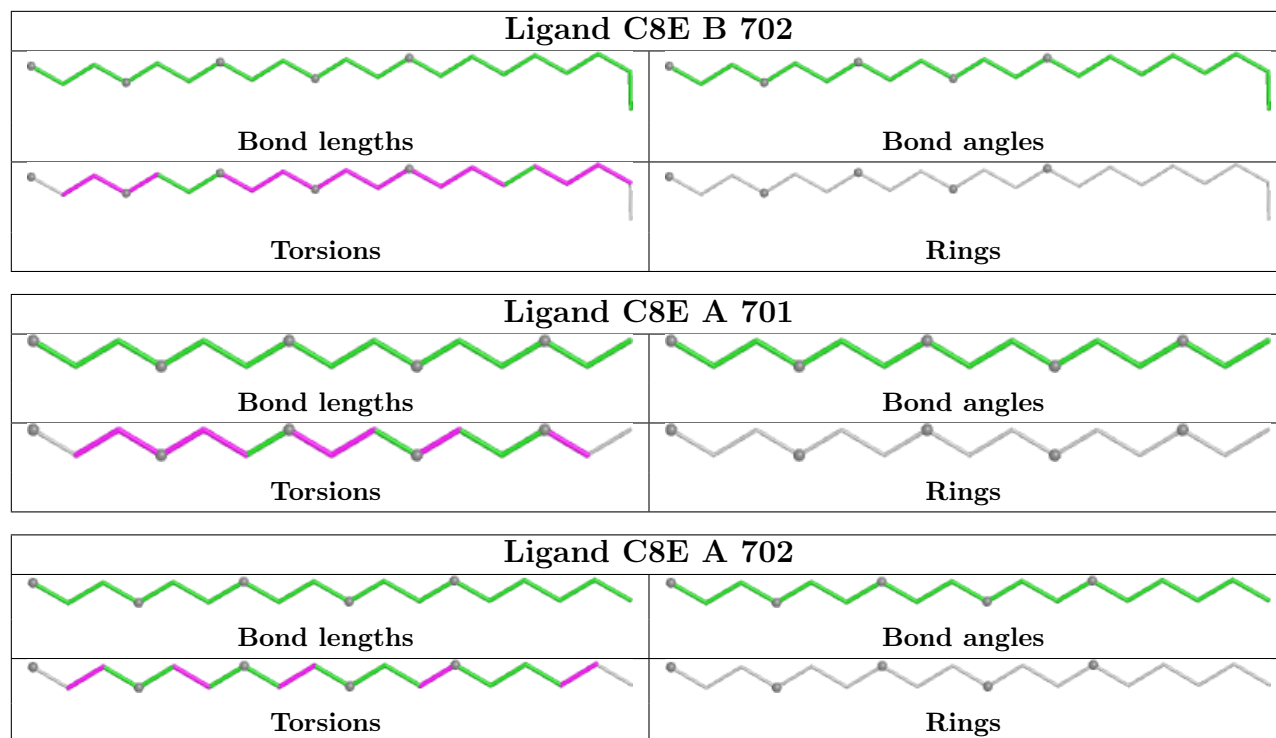
There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	C8E	3	0
2	B	702	C8E	1	0
2	A	701	C8E	2	0
2	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	651/723 (90%)	0.29	28 (4%)	40 31	26, 48, 70, 100	1 (0%)
1	B	644/723 (89%)	0.22	17 (2%)	57 48	34, 47, 68, 89	0
All	All	1295/1446 (89%)	0.25	45 (3%)	47 38	26, 47, 70, 100	1 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	507	MET	5.2
1	B	42	PRO	4.9
1	A	505	GLY	3.9
1	A	587	ASN	3.9
1	A	286	MET	3.8
1	A	586	GLN	3.8
1	A	459	ASN	3.7
1	A	601	PHE	3.7
1	B	40	PRO	3.2
1	A	589	ILE	3.1
1	A	602	ASP	3.1
1	B	335	MET	3.0
1	A	501	SER	3.0
1	A	39	GLN	2.8
1	B	456	GLY	2.8
1	B	309	ARG	2.8
1	A	14	LEU	2.8
1	A	335	MET	2.7
1	A	508	GLY	2.7
1	A	457	SER	2.6
1	A	584	ALA	2.6
1	B	455	ASN	2.6
1	B	671	PHE	2.5
1	B	552	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	603	LYS	2.4
1	B	451	LYS	2.4
1	A	333	TYR	2.4
1	A	283	PRO	2.4
1	A	342	ASP	2.3
1	B	392	LYS	2.3
1	B	452	ARG	2.3
1	B	108	ASP	2.3
1	A	338	ASP	2.2
1	A	551	ASP	2.2
1	B	510	SER	2.2
1	A	190	GLY	2.2
1	B	400	MET	2.2
1	B	572	GLY	2.2
1	B	426	ASP	2.2
1	A	159	ASP	2.1
1	A	311	ASP	2.1
1	B	33	ASN	2.1
1	A	588	ARG	2.1
1	A	646	ALA	2.1
1	A	40	PRO	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($\text{\AA}^2$)	Q<0.9
2	C8E	B	702	21/21	0.81	0.20	46,55,62,67	0
2	C8E	A	701	15/21	0.91	0.12	37,46,49,57	0

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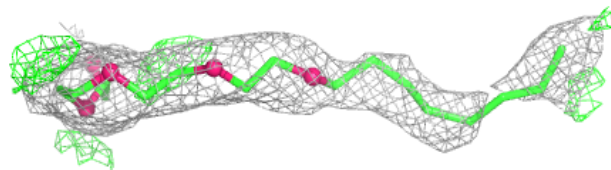
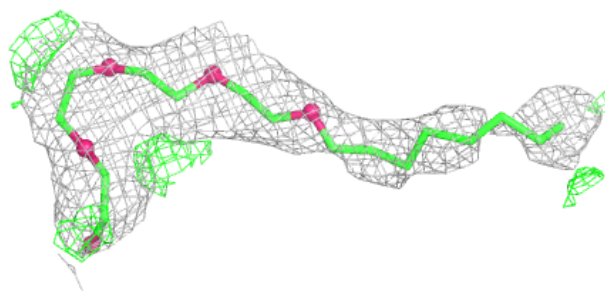
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	C8E	A	702	18/21	0.92	0.13	39,50,59,60	0
2	C8E	B	701	21/21	0.93	0.12	44,47,53,62	0

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.

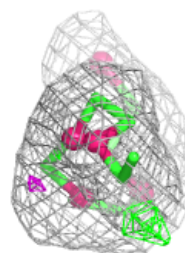
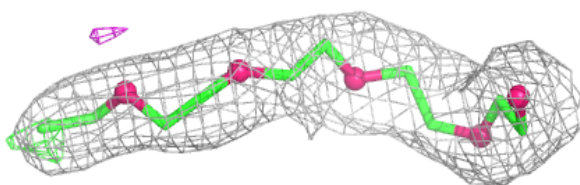
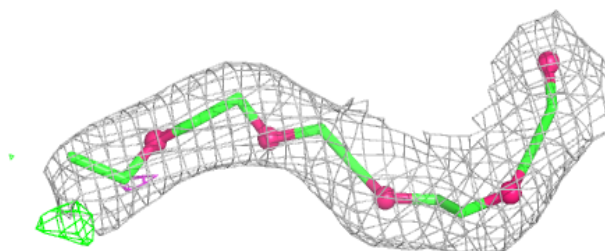
Electron density around C8E B 702:

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

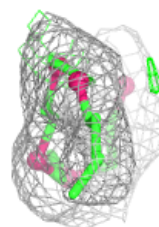
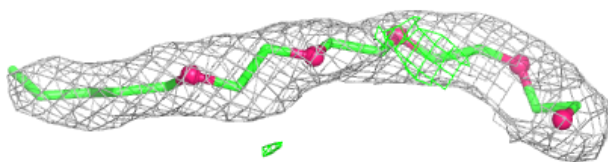
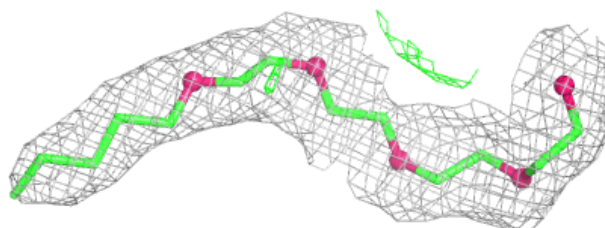


Electron density around C8E A 701:

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

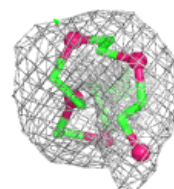
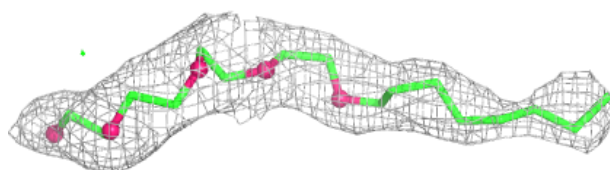
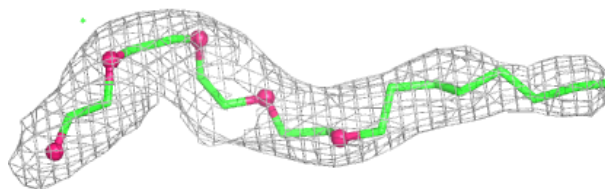
**Electron density around C8E A 702:**

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



Electron density around C8E B 701:

$2mF_o-DF_c$ (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.