



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:08 PM UTC

PDB ID : 1NQE / pdb_00001nqe
Title : OUTER MEMBRANE COBALAMIN TRANSPORTER (BTUB) FROM E. COLI
Authors : Chimento, D.P.; Mohanty, A.K.; Kadner, R.J.; Wiener, M.C.
Deposited on : 2003-01-21
Resolution : 2.00 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

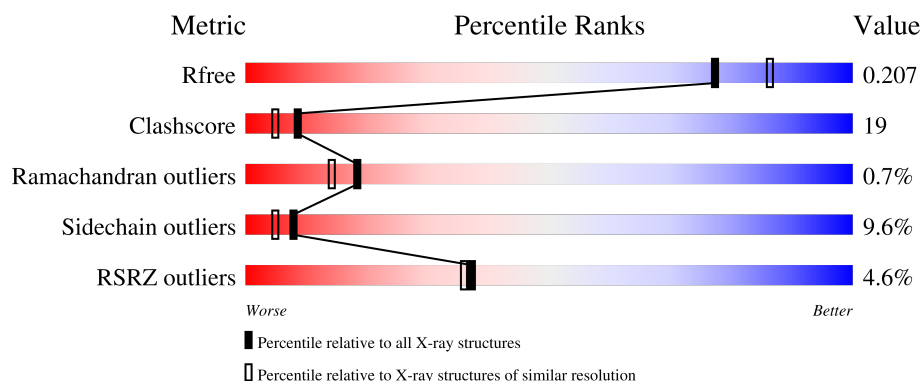
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	594	

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	C8E	A	803	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	C8E	A	805	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4733 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.

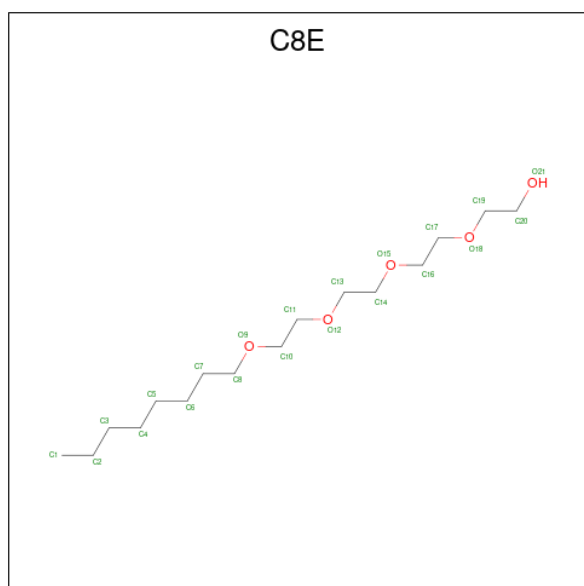
- Molecule 1 is a protein called Vitamin B12 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	0
			4350	2742	748	858	2			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- 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		

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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		

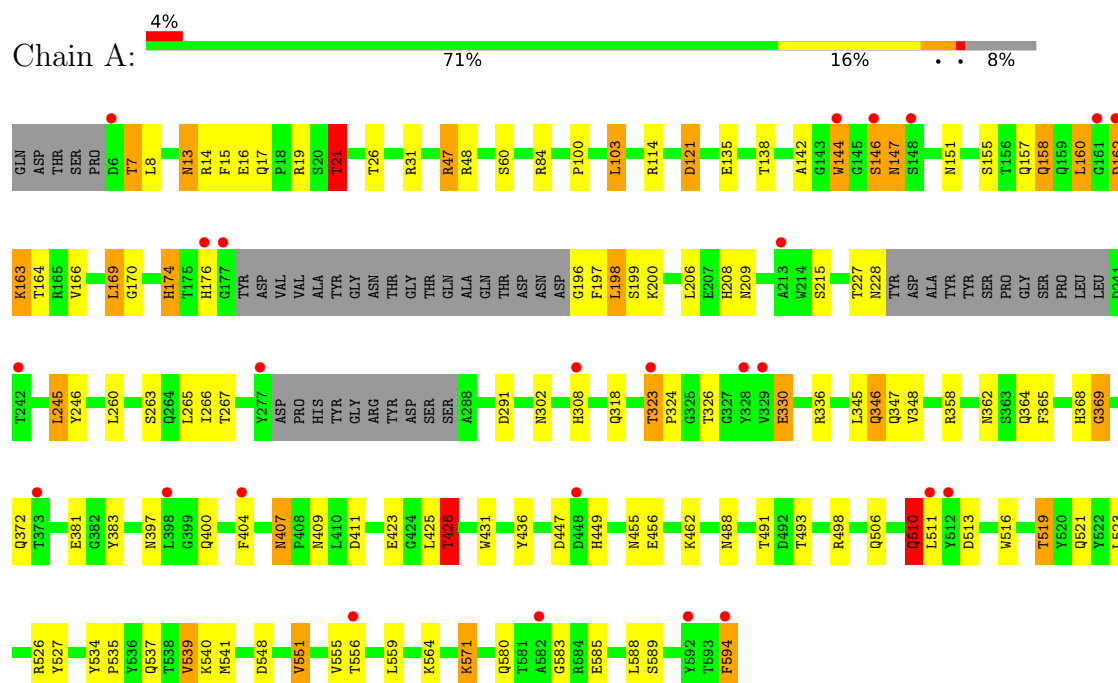
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	235	Total	O	0	0
			235	235		

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: Vitamin B12 receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	81.59Å 81.59Å 210.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.92 – 2.00 24.92 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (24.92-2.00) 99.5 (24.92-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.194 , 0.232 0.207 , 0.207	Depositor DCC
R_{free} test set	2818 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4733	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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, MG

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	1.02	8/4455 (0.2%)	1.08	4/6059 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	510	GLN	CD-NE2	12.16	1.58	1.33
1	A	541	MET	SD-CE	-9.19	1.56	1.79
1	A	571	LYS	CE-NZ	7.58	1.72	1.49
1	A	537	GLN	CD-OE1	7.55	1.37	1.23
1	A	571	LYS	CD-CE	6.19	1.71	1.52
1	A	146	SER	C-O	5.55	1.30	1.24
1	A	369	GLY	CA-C	5.28	1.56	1.52
1	A	426	THR	CB-CG2	-5.07	1.35	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	537	GLN	OE1-CD-NE2	-20.80	101.80	122.60
1	A	537	GLN	CG-CD-NE2	7.85	128.17	116.40
1	A	7	THR	N-CA-C	6.92	118.61	111.14
1	A	21	THR	N-CA-CB	-5.07	102.98	110.53

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	4350	0	4109	141	0
2	A	1	0	0	0	0
3	A	147	0	238	35	0
4	A	235	0	0	10	0
All	All	4733	0	4347	167	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 19.

All (167) 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:571:LYS:NZ	1:A:571:LYS:CE	1.72	1.49
3:A:802:C8E:H52	3:A:802:C8E:C1	1.49	1.31
1:A:169:LEU:C	1:A:169:LEU:HD13	1.75	1.09
1:A:169:LEU:HD13	1:A:170:GLY:N	1.67	1.09
3:A:802:C8E:C5	3:A:802:C8E:H13	1.79	1.09
1:A:169:LEU:C	1:A:169:LEU:CD1	2.37	0.97
3:A:802:C8E:H52	3:A:802:C8E:H13	0.97	0.96
3:A:802:C8E:C1	3:A:802:C8E:C5	2.40	0.96
3:A:803:C8E:H13	3:A:805:C8E:C14	1.97	0.95
1:A:198:LEU:HD13	1:A:199:SER:N	1.82	0.94
1:A:48:ARG:HH12	1:A:519:THR:HG21	1.37	0.90
1:A:197:PHE:HD2	1:A:227:THR:HG22	1.35	0.90
1:A:197:PHE:CD2	1:A:227:THR:HG22	2.08	0.88
1:A:411:ASP:H	1:A:455:ASN:HD21	1.18	0.88
3:A:802:C8E:H52	3:A:802:C8E:H12	1.57	0.87
1:A:527:TYR:CE1	1:A:540:LYS:HG3	2.10	0.87
1:A:160:LEU:HD23	1:A:166:VAL:HG21	1.55	0.86
1:A:198:LEU:HD13	1:A:198:LEU:C	2.00	0.85
1:A:516:TRP:CE3	1:A:551:VAL:HG13	2.11	0.85
1:A:506:GLN:HE22	1:A:519:THR:CG2	1.91	0.83
1:A:198:LEU:C	1:A:198:LEU:CD1	2.53	0.81
3:A:803:C8E:H13	3:A:805:C8E:H141	1.62	0.80
1:A:144:TRP:C	1:A:144:TRP:CD1	2.61	0.78
1:A:135:GLU:H	1:A:157:GLN:HE22	1.32	0.78
1:A:169:LEU:HD13	1:A:170:GLY:CA	2.12	0.78
1:A:539:VAL:CG2	1:A:540:LYS:N	2.48	0.77
1:A:580:GLN:HG2	4:A:953:HOH:O	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:THR:CG2	1:A:431:TRP:HE1	1.96	0.77
1:A:404:PHE:HD2	1:A:404:PHE:O	1.71	0.73
1:A:539:VAL:HG22	1:A:540:LYS:N	2.01	0.73
1:A:397:ASN:H	1:A:400:GLN:HE21	1.37	0.72
1:A:160:LEU:HD23	1:A:166:VAL:CG2	2.19	0.72
1:A:506:GLN:NE2	1:A:519:THR:HB	2.04	0.72
1:A:146:SER:O	1:A:147:ASN:HB2	1.88	0.72
1:A:100:PRO:HG2	1:A:103:LEU:HD22	1.71	0.71
1:A:358:ARG:O	3:A:800:C8E:H82	1.90	0.71
1:A:506:GLN:HE22	1:A:519:THR:HG22	1.55	0.71
1:A:369:GLY:C	3:A:800:C8E:H111	2.16	0.70
1:A:362:ASN:ND2	1:A:364:GLN:H	1.89	0.70
1:A:47:ARG:NH2	4:A:832:HOH:O	2.25	0.70
3:A:803:C8E:C1	3:A:805:C8E:C14	2.71	0.69
1:A:407:ASN:C	1:A:407:ASN:HD22	2.00	0.68
1:A:397:ASN:H	1:A:400:GLN:NE2	1.92	0.68
1:A:48:ARG:NH1	1:A:519:THR:HG21	2.10	0.66
1:A:516:TRP:CE3	1:A:551:VAL:CG1	2.78	0.66
1:A:144:TRP:C	1:A:144:TRP:HD1	2.02	0.66
3:A:803:C8E:H112	3:A:805:C8E:H82	1.78	0.66
1:A:534:TYR:CG	1:A:535:PRO:HA	2.30	0.66
1:A:13:ASN:ND2	1:A:15:PHE:H	1.95	0.65
3:A:803:C8E:H13	3:A:805:C8E:O15	1.96	0.65
1:A:174:HIS:CE1	1:A:176:HIS:CE1	2.85	0.64
1:A:383:TYR:OH	1:A:426:THR:HB	1.98	0.64
1:A:571:LYS:NZ	1:A:571:LYS:CD	2.62	0.63
1:A:491:THR:HG23	1:A:493:THR:H	1.63	0.63
1:A:411:ASP:H	1:A:455:ASN:ND2	1.93	0.63
1:A:516:TRP:CZ3	1:A:551:VAL:HG13	2.33	0.62
1:A:114:ARG:HA	1:A:372:GLN:HE22	1.64	0.62
1:A:174:HIS:CD2	1:A:174:HIS:C	2.77	0.61
1:A:144:TRP:HD1	1:A:144:TRP:O	1.83	0.61
1:A:47:ARG:NH2	1:A:548:ASP:OD2	2.26	0.61
1:A:488:ASN:CG	1:A:491:THR:HG22	2.25	0.61
3:A:802:C8E:H101	3:A:802:C8E:H141	1.82	0.60
1:A:491:THR:CG2	1:A:493:THR:OG1	2.50	0.60
3:A:803:C8E:C1	3:A:805:C8E:H141	2.31	0.59
1:A:13:ASN:HD22	1:A:13:ASN:C	2.10	0.59
1:A:19:ARG:HE	1:A:26:THR:HG23	1.68	0.59
1:A:539:VAL:CG2	1:A:540:LYS:H	2.16	0.58
1:A:323:THR:HG23	1:A:324:PRO:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:GLU:H	1:A:157:GLN:NE2	1.98	0.58
1:A:527:TYR:CZ	1:A:540:LYS:HG3	2.37	0.58
1:A:510:GLN:NE2	4:A:902:HOH:O	2.37	0.58
1:A:358:ARG:C	3:A:800:C8E:H71	2.30	0.57
1:A:426:THR:HG23	1:A:431:TRP:HE1	1.70	0.57
1:A:19:ARG:HE	1:A:26:THR:CG2	2.18	0.56
1:A:516:TRP:CZ3	1:A:551:VAL:CG1	2.88	0.56
1:A:539:VAL:HG23	1:A:540:LYS:H	1.70	0.56
1:A:245:LEU:HD23	1:A:246:TYR:N	2.22	0.55
1:A:245:LEU:CD2	1:A:245:LEU:C	2.79	0.55
1:A:245:LEU:CD2	1:A:246:TYR:N	2.69	0.55
1:A:358:ARG:O	3:A:800:C8E:C8	2.54	0.55
1:A:174:HIS:HE1	1:A:176:HIS:CE1	2.25	0.55
3:A:803:C8E:C11	3:A:805:C8E:H61	2.37	0.54
1:A:13:ASN:HD22	1:A:15:PHE:H	1.54	0.54
1:A:426:THR:HG22	1:A:431:TRP:HE1	1.73	0.54
1:A:362:ASN:HD22	1:A:365:PHE:H	1.56	0.54
1:A:407:ASN:C	1:A:407:ASN:ND2	2.65	0.54
1:A:534:TYR:CD2	1:A:535:PRO:HA	2.42	0.54
1:A:447:ASP:OD2	1:A:449:HIS:HB2	2.07	0.54
1:A:336:ARG:HD3	4:A:1010:HOH:O	2.08	0.54
1:A:510:GLN:NE2	1:A:510:GLN:N	2.56	0.54
1:A:407:ASN:ND2	1:A:409:ASN:H	2.07	0.53
1:A:491:THR:HG23	1:A:493:THR:OG1	2.09	0.53
1:A:506:GLN:NE2	1:A:519:THR:CB	2.72	0.53
1:A:368:HIS:HD2	4:A:957:HOH:O	1.92	0.52
1:A:160:LEU:CD2	1:A:166:VAL:HG21	2.34	0.52
1:A:263:SER:OG	1:A:302:ASN:ND2	2.42	0.52
1:A:198:LEU:HD11	1:A:200:LYS:HG3	1.92	0.52
1:A:521:GLN:HE21	1:A:523:LEU:HD21	1.75	0.51
1:A:491:THR:HG21	1:A:493:THR:OG1	2.11	0.51
1:A:462:LYS:HB3	3:A:804:C8E:H172	1.92	0.51
1:A:135:GLU:HA	1:A:135:GLU:OE1	2.10	0.50
1:A:527:TYR:CE1	1:A:540:LYS:CG	2.90	0.50
1:A:13:ASN:ND2	1:A:13:ASN:C	2.69	0.50
1:A:404:PHE:CD2	1:A:404:PHE:C	2.89	0.50
1:A:13:ASN:O	1:A:14:ARG:HB2	2.12	0.49
1:A:368:HIS:HE1	4:A:847:HOH:O	1.95	0.49
1:A:169:LEU:CD1	1:A:169:LEU:O	2.61	0.49
1:A:174:HIS:HB2	1:A:198:LEU:HD22	1.95	0.48
3:A:803:C8E:H82	3:A:806:C8E:H22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:GLY:O	1:A:585:GLU:HG3	2.14	0.48
1:A:162:ASP:C	1:A:163:LYS:CG	2.86	0.48
1:A:407:ASN:HD22	1:A:409:ASN:H	1.60	0.48
1:A:488:ASN:HB3	1:A:491:THR:HG22	1.96	0.48
1:A:245:LEU:C	1:A:245:LEU:HD22	2.40	0.47
1:A:404:PHE:O	1:A:404:PHE:CD2	2.58	0.47
1:A:196:GLY:N	1:A:228:ASN:HD22	2.12	0.47
1:A:516:TRP:CD2	1:A:551:VAL:CG1	2.98	0.47
1:A:519:THR:HG23	4:A:872:HOH:O	2.15	0.47
1:A:157:GLN:C	1:A:158:GLN:HG2	2.40	0.47
1:A:346:GLN:NE2	3:A:805:C8E:H202	2.30	0.47
1:A:519:THR:CG2	4:A:872:HOH:O	2.63	0.46
1:A:526:ARG:C	1:A:527:TYR:HD1	2.23	0.46
1:A:506:GLN:HE22	1:A:519:THR:CB	2.27	0.46
1:A:506:GLN:NE2	1:A:519:THR:CG2	2.70	0.46
3:A:803:C8E:H111	3:A:805:C8E:H61	1.97	0.46
1:A:17:GLN:OE1	1:A:21:THR:HG22	2.15	0.46
1:A:8:LEU:HD13	1:A:16:GLU:OE2	2.16	0.45
1:A:144:TRP:CD1	1:A:144:TRP:O	2.65	0.45
1:A:516:TRP:CH2	1:A:551:VAL:HG11	2.52	0.45
3:A:802:C8E:C10	3:A:802:C8E:C14	2.94	0.45
1:A:362:ASN:HD22	1:A:364:GLN:H	1.59	0.45
1:A:436:TYR:O	3:A:804:C8E:H202	2.17	0.45
3:A:803:C8E:H22	3:A:805:C8E:H142	1.98	0.45
1:A:372:GLN:NE2	4:A:809:HOH:O	2.49	0.45
1:A:426:THR:HG23	1:A:431:TRP:NE1	2.32	0.44
1:A:146:SER:O	1:A:147:ASN:CB	2.62	0.44
1:A:160:LEU:HD13	1:A:160:LEU:HA	1.60	0.44
1:A:369:GLY:HA3	3:A:800:C8E:C11	2.48	0.44
3:A:803:C8E:H101	3:A:803:C8E:H71	1.25	0.44
3:A:804:C8E:H112	3:A:804:C8E:H82	1.21	0.44
1:A:488:ASN:HB3	1:A:491:THR:CG2	2.47	0.44
1:A:169:LEU:O	1:A:169:LEU:HD12	2.18	0.43
3:A:801:C8E:H142	4:A:861:HOH:O	2.18	0.43
3:A:803:C8E:H172	3:A:803:C8E:H142	1.44	0.43
1:A:164:THR:OG1	1:A:208:HIS:CD2	2.72	0.43
1:A:308:HIS:HB3	1:A:347:GLN:HE21	1.83	0.43
3:A:805:C8E:H191	3:A:805:C8E:H161	1.76	0.43
1:A:555:VAL:HG12	1:A:556:THR:HG23	2.02	0.42
1:A:245:LEU:HD22	1:A:246:TYR:N	2.34	0.42
3:A:805:C8E:H52	3:A:806:C8E:H41	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LEU:CD2	1:A:166:VAL:CG2	2.95	0.42
1:A:462:LYS:HB3	3:A:804:C8E:H201	2.02	0.42
1:A:588:LEU:HD13	1:A:588:LEU:C	2.44	0.42
1:A:174:HIS:HB2	1:A:198:LEU:CD2	2.49	0.42
1:A:84:ARG:HH11	1:A:318:GLN:HE22	1.67	0.41
3:A:801:C8E:H102	3:A:801:C8E:H131	1.44	0.41
1:A:488:ASN:CB	1:A:491:THR:HG22	2.50	0.41
1:A:163:LYS:HB3	1:A:209:ASN:O	2.21	0.41
1:A:330:GLU:H	1:A:330:GLU:HG3	1.55	0.41
1:A:491:THR:OG1	1:A:493:THR:HG23	2.20	0.41
1:A:31:ARG:O	1:A:31:ARG:HD3	2.21	0.40
1:A:291:ASP:HA	1:A:326:THR:HG23	2.03	0.40
3:A:800:C8E:H112	3:A:800:C8E:H141	1.07	0.40
1:A:142:ALA:HB1	1:A:151:ASN:O	2.21	0.40
3:A:801:C8E:H171	3:A:801:C8E:H141	1.73	0.40
1:A:411:ASP:N	1:A:455:ASN:HD21	2.00	0.40
1:A:594:PHE:N	1:A:594:PHE:CD1	2.90	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	541/594 (91%)	522 (96%)	15 (3%)	4 (1%)	18	14

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	ASN
1	A	456	GLU
1	A	513	ASP
1	A	121	ASP

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	457/495 (92%)	413 (90%)	44 (10%)	8 5

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	13	ASN
1	A	21	THR
1	A	47	ARG
1	A	60	SER
1	A	103	LEU
1	A	121	ASP
1	A	138	THR
1	A	144	TRP
1	A	155	SER
1	A	158	GLN
1	A	160	LEU
1	A	162	ASP
1	A	163	LYS
1	A	169	LEU
1	A	174	HIS
1	A	198	LEU
1	A	206	LEU
1	A	215	SER
1	A	245	LEU
1	A	260	LEU
1	A	265	LEU
1	A	266	ILE
1	A	267	THR
1	A	323	THR
1	A	330	GLU
1	A	345	LEU
1	A	346	GLN
1	A	348	VAL
1	A	381	GLU

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Mol	Chain	Res	Type
1	A	407	ASN
1	A	423	GLU
1	A	425	LEU
1	A	426	THR
1	A	498	ARG
1	A	510	GLN
1	A	511	LEU
1	A	519	THR
1	A	539	VAL
1	A	551	VAL
1	A	559	LEU
1	A	564	LYS
1	A	589	SER
1	A	594	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	105	GLN
1	A	147	ASN
1	A	150	GLN
1	A	157	GLN
1	A	159	GLN
1	A	174	HIS
1	A	176	HIS
1	A	208	HIS
1	A	248	GLN
1	A	295	GLN
1	A	302	ASN
1	A	318	GLN
1	A	320	GLN
1	A	337	ASN
1	A	347	GLN
1	A	362	ASN
1	A	372	GLN
1	A	400	GLN
1	A	407	ASN
1	A	430	ASN
1	A	455	ASN
1	A	502	GLN
1	A	506	GLN

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Mol	Chain	Res	Type
1	A	510	GLN
1	A	521	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	$\# Z > 2$
3	C8E	A	801	-	20,20,20	0.59	0	19,19,19	0.85	1 (5%)
3	C8E	A	805	-	20,20,20	0.56	0	19,19,19	0.45	0
3	C8E	A	800	-	20,20,20	0.55	0	19,19,19	0.99	1 (5%)
3	C8E	A	806	-	20,20,20	0.56	0	19,19,19	0.49	0
3	C8E	A	803	-	20,20,20	0.38	0	19,19,19	0.49	0
3	C8E	A	802	-	20,20,20	0.40	0	19,19,19	0.73	0
3	C8E	A	804	-	20,20,20	0.40	0	19,19,19	0.72	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	801	-	-	11/18/18/18	-
3	C8E	A	805	-	-	9/18/18/18	-
3	C8E	A	800	-	-	11/18/18/18	-
3	C8E	A	806	-	-	14/18/18/18	-
3	C8E	A	803	-	-	13/18/18/18	-
3	C8E	A	802	-	-	12/18/18/18	-
3	C8E	A	804	-	-	14/18/18/18	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	800	C8E	O12-C11-C10	-2.19	100.38	110.35
3	A	801	C8E	C6-C7-C8	-2.07	104.45	113.47

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	804	C8E	C11-C10-O9-C8
3	A	805	C8E	C14-C13-O12-C11
3	A	800	C8E	C14-C13-O12-C11
3	A	803	C8E	C17-C16-O15-C14
3	A	805	C8E	C16-C17-O18-C19
3	A	803	C8E	C14-C13-O12-C11
3	A	803	C8E	C7-C8-O9-C10
3	A	804	C8E	C4-C5-C6-C7
3	A	803	C8E	O15-C16-C17-O18
3	A	801	C8E	C6-C7-C8-O9
3	A	804	C8E	O18-C19-C20-O21
3	A	806	C8E	O15-C16-C17-O18
3	A	800	C8E	O9-C10-C11-O12
3	A	801	C8E	C11-C10-O9-C8
3	A	801	C8E	C10-C11-O12-C13
3	A	802	C8E	O18-C19-C20-O21
3	A	805	C8E	O18-C19-C20-O21
3	A	804	C8E	O15-C16-C17-O18
3	A	800	C8E	O12-C13-C14-O15
3	A	805	C8E	O12-C13-C14-O15

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Mol	Chain	Res	Type	Atoms
3	A	804	C8E	O9-C10-C11-O12
3	A	806	C8E	C6-C7-C8-O9
3	A	803	C8E	O12-C13-C14-O15
3	A	801	C8E	O18-C19-C20-O21
3	A	805	C8E	C6-C7-C8-O9
3	A	801	C8E	C4-C5-C6-C7
3	A	804	C8E	C2-C3-C4-C5
3	A	800	C8E	O15-C16-C17-O18
3	A	803	C8E	C5-C6-C7-C8
3	A	804	C8E	C5-C6-C7-C8
3	A	802	C8E	C3-C4-C5-C6
3	A	806	C8E	C5-C6-C7-C8
3	A	802	C8E	O9-C10-C11-O12
3	A	805	C8E	C13-C14-O15-C16
3	A	802	C8E	C5-C6-C7-C8
3	A	802	C8E	C2-C3-C4-C5
3	A	801	C8E	O12-C13-C14-O15
3	A	806	C8E	C4-C5-C6-C7
3	A	806	C8E	C3-C4-C5-C6
3	A	802	C8E	O15-C16-C17-O18
3	A	805	C8E	C1-C2-C3-C4
3	A	804	C8E	C1-C2-C3-C4
3	A	802	C8E	C1-C2-C3-C4
3	A	803	C8E	C4-C5-C6-C7
3	A	802	C8E	C6-C7-C8-O9
3	A	801	C8E	O15-C16-C17-O18
3	A	800	C8E	C4-C5-C6-C7
3	A	804	C8E	C3-C4-C5-C6
3	A	800	C8E	C5-C6-C7-C8
3	A	802	C8E	O12-C13-C14-O15
3	A	803	C8E	C20-C19-O18-C17
3	A	806	C8E	O12-C13-C14-O15
3	A	801	C8E	C14-C13-O12-C11
3	A	806	C8E	C14-C13-O12-C11
3	A	803	C8E	C11-C10-O9-C8
3	A	806	C8E	C16-C17-O18-C19
3	A	804	C8E	C14-C13-O12-C11
3	A	800	C8E	C3-C4-C5-C6
3	A	806	C8E	C13-C14-O15-C16
3	A	803	C8E	C16-C17-O18-C19
3	A	803	C8E	C10-C11-O12-C13
3	A	802	C8E	C16-C17-O18-C19

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Mol	Chain	Res	Type	Atoms
3	A	804	C8E	C10-C11-O12-C13
3	A	806	C8E	C20-C19-O18-C17
3	A	801	C8E	C5-C6-C7-C8
3	A	800	C8E	C10-C11-O12-C13
3	A	806	C8E	C7-C8-O9-C10
3	A	801	C8E	O9-C10-C11-O12
3	A	806	C8E	C17-C16-O15-C14
3	A	804	C8E	C6-C7-C8-O9
3	A	803	C8E	C3-C4-C5-C6
3	A	806	C8E	C2-C3-C4-C5
3	A	801	C8E	C17-C16-O15-C14
3	A	804	C8E	O12-C13-C14-O15
3	A	802	C8E	C7-C8-O9-C10
3	A	803	C8E	C1-C2-C3-C4
3	A	800	C8E	C11-C10-O9-C8
3	A	800	C8E	C17-C16-O15-C14
3	A	802	C8E	C20-C19-O18-C17
3	A	806	C8E	C10-C11-O12-C13
3	A	800	C8E	O18-C19-C20-O21
3	A	804	C8E	C20-C19-O18-C17
3	A	805	C8E	C11-C10-O9-C8
3	A	805	C8E	O15-C16-C17-O18

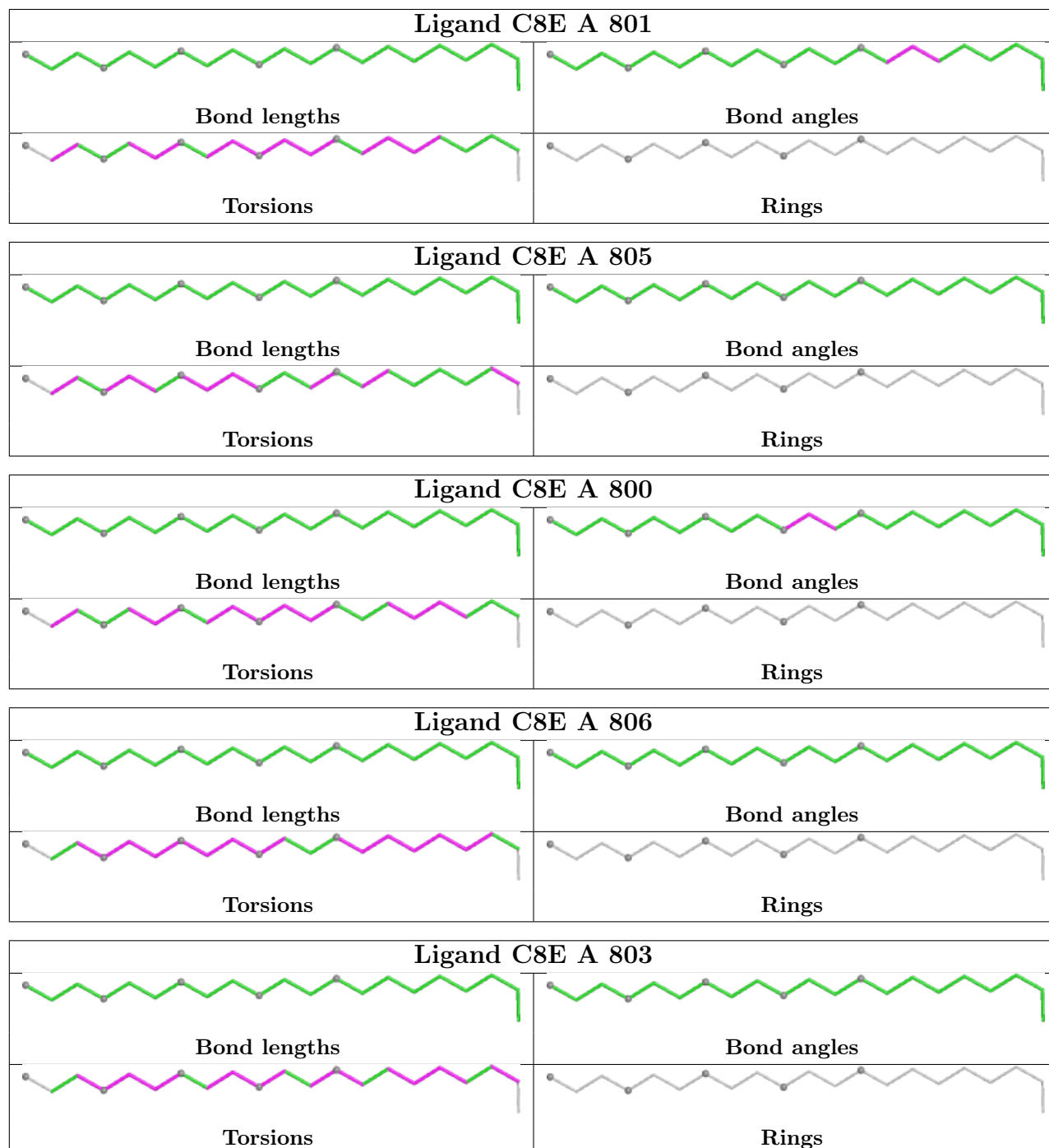
There are no ring outliers.

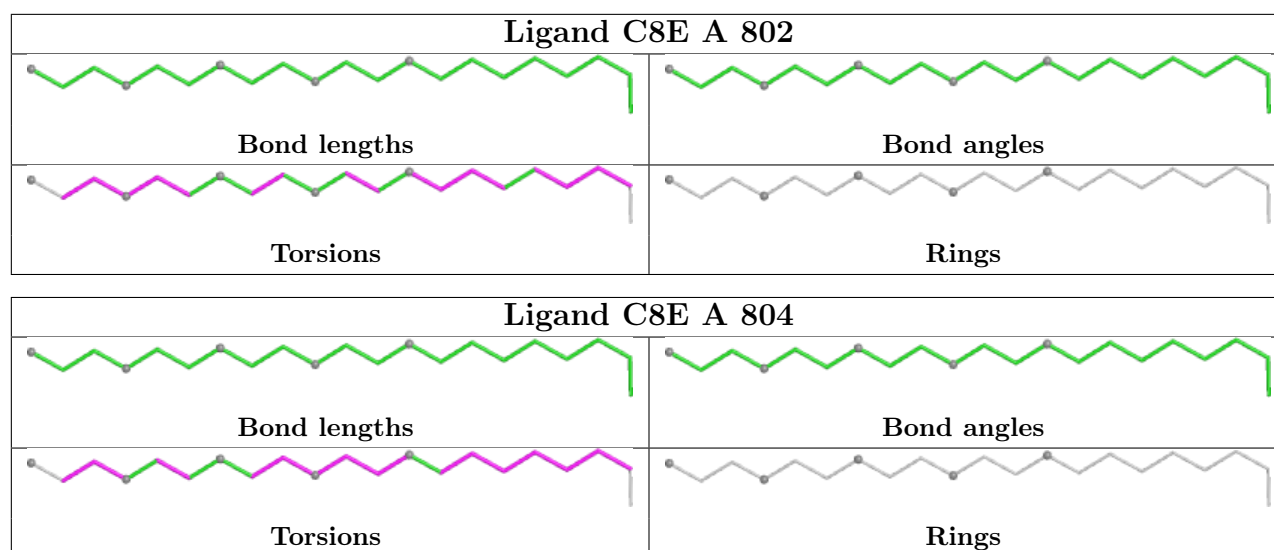
7 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	C8E	3	0
3	A	805	C8E	12	0
3	A	800	C8E	6	0
3	A	806	C8E	2	0
3	A	803	C8E	12	0
3	A	802	C8E	7	0
3	A	804	C8E	4	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	549/594 (92%)	0.31	25 (4%) 37 36	28, 40, 67, 97	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	328	TYR	3.7
1	A	6	ASP	3.6
1	A	556	THR	3.6
1	A	177	GLY	3.5
1	A	512	TYR	3.4
1	A	144	TRP	3.4
1	A	162	ASP	3.2
1	A	594	PHE	3.1
1	A	277	TYR	2.8
1	A	176	HIS	2.7
1	A	323	THR	2.6
1	A	373	THR	2.5
1	A	398	LEU	2.5
1	A	592	TYR	2.4
1	A	242	THR	2.4
1	A	404	PHE	2.3
1	A	308	HIS	2.3
1	A	161	GLY	2.3
1	A	582	ALA	2.2
1	A	146	SER	2.2
1	A	448	ASP	2.2
1	A	329	VAL	2.1
1	A	213	ALA	2.1
1	A	148	SER	2.1
1	A	511	LEU	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](#)

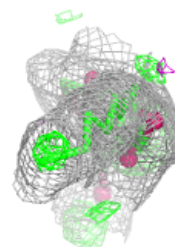
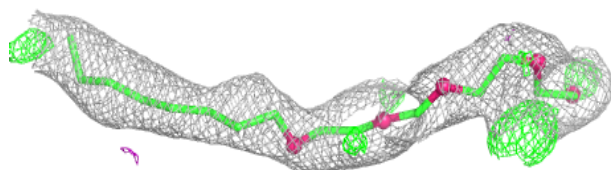
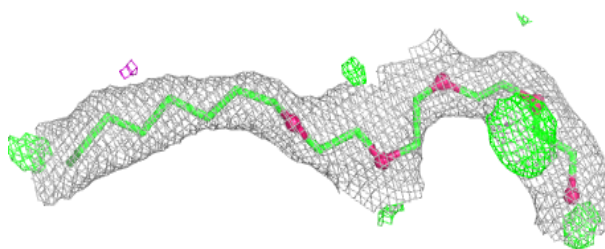
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	C8E	A	805	21/21	0.77	0.16	61,79,107,109	0
3	C8E	A	804	21/21	0.85	0.16	39,58,86,102	0
3	C8E	A	801	21/21	0.86	0.16	47,68,107,111	0
2	MG	A	595	1/1	0.88	0.12	48,48,48,48	0
3	C8E	A	803	21/21	0.88	0.14	49,89,110,117	0
3	C8E	A	802	21/21	0.89	0.13	38,57,77,86	0
3	C8E	A	800	21/21	0.89	0.15	42,58,84,96	0
3	C8E	A	806	21/21	0.90	0.15	49,100,128,136	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.

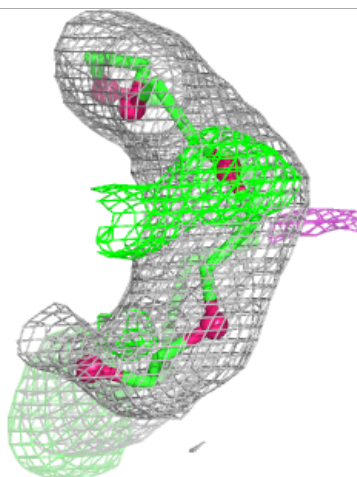
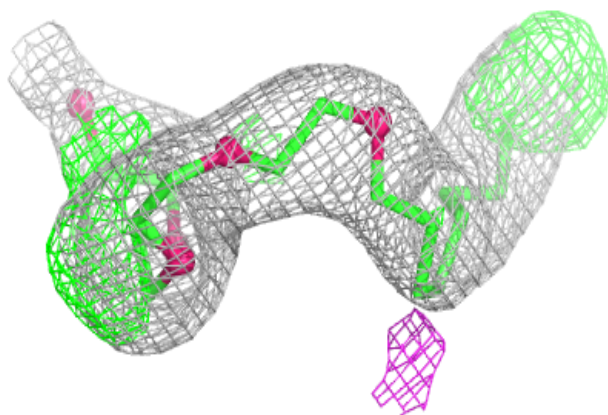
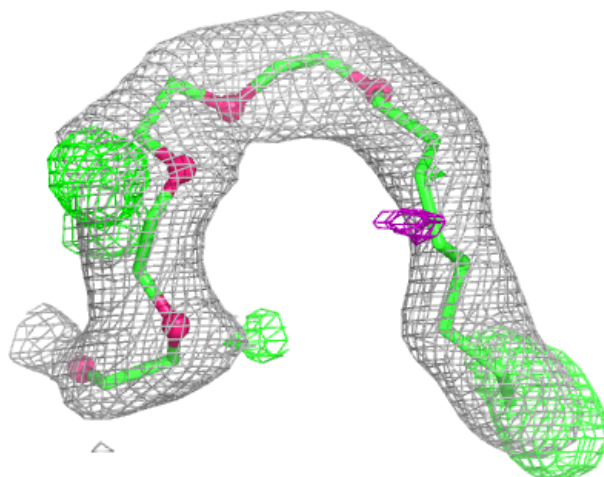
Electron density around C8E A 805:

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



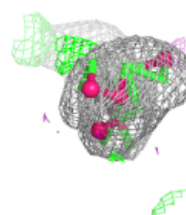
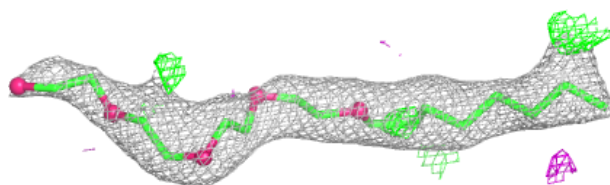
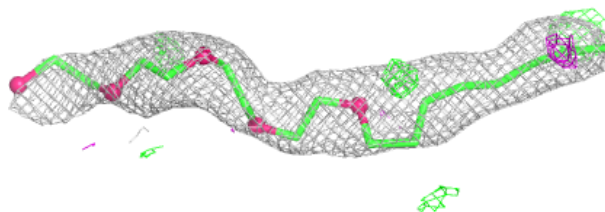
Electron density around C8E A 804:

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

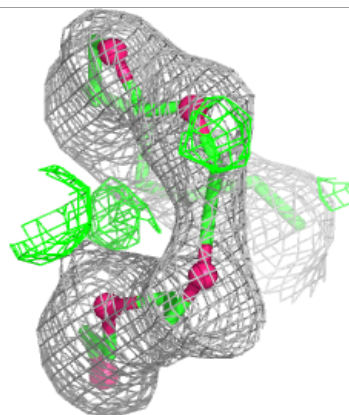
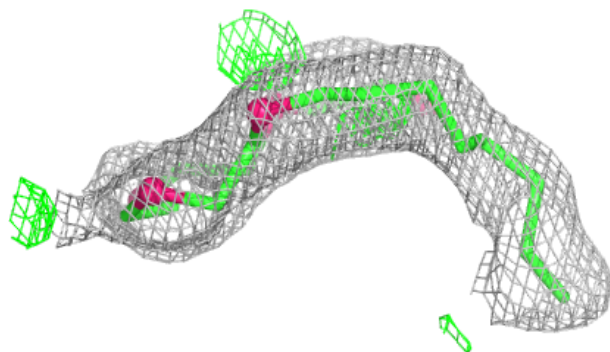
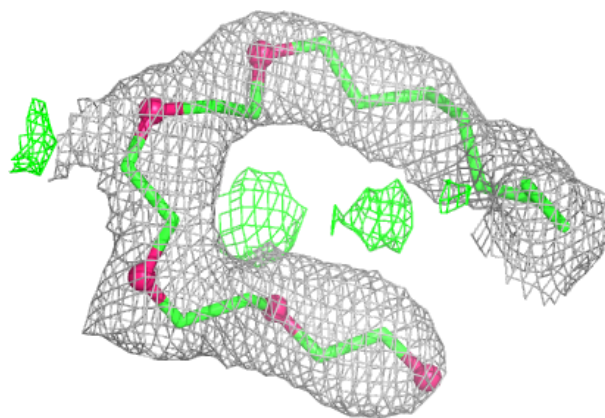


Electron density around C8E A 801:

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

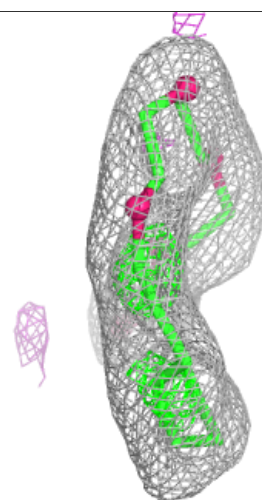
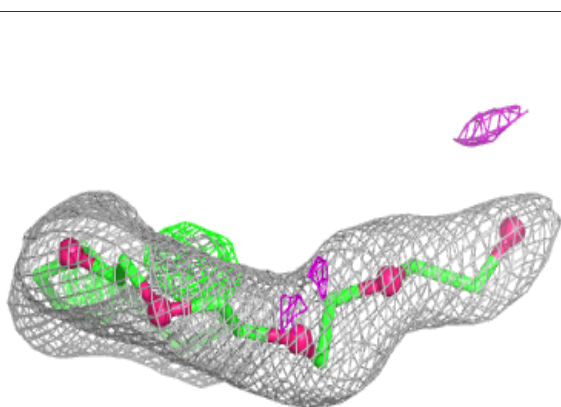
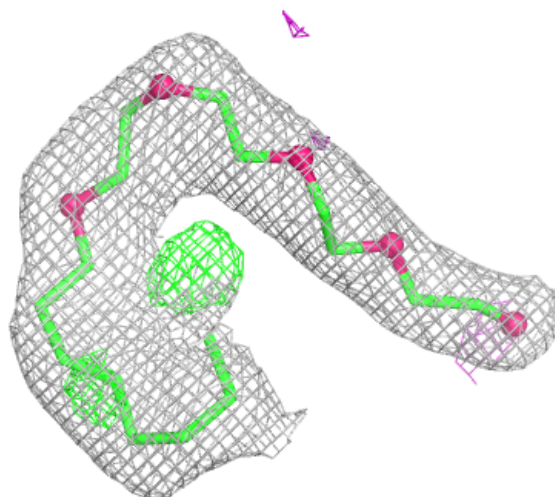
**Electron density around C8E A 803:**

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



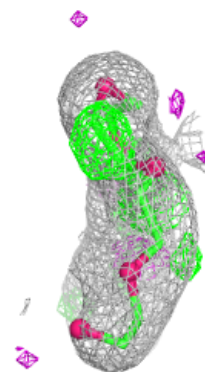
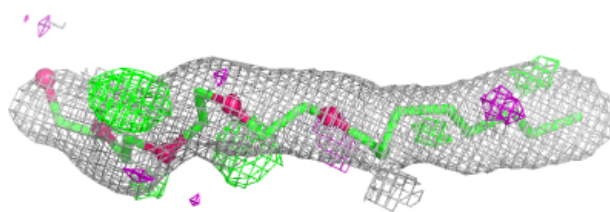
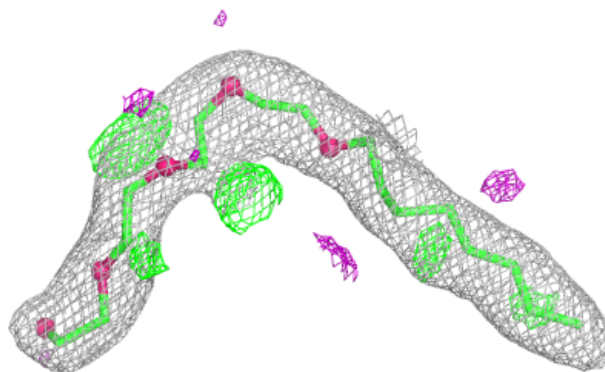
Electron density around C8E A 802:

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

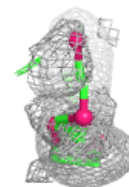
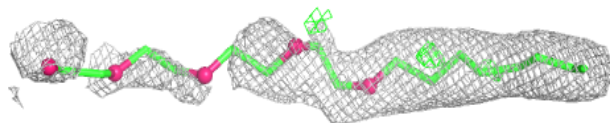
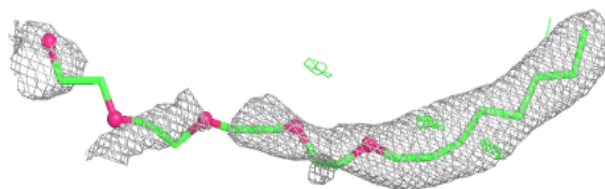


Electron density around C8E A 800:

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

**Electron density around C8E A 806:**

$2mF_o-DF_c$ (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.