



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:34 AM UTC

PDB ID : 2OBD / pdb_00002obd
Title : Crystal Structure of Cholesteryl Ester Transfer Protein
Authors : Qiu, X.
Deposited on : 2006-12-18
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

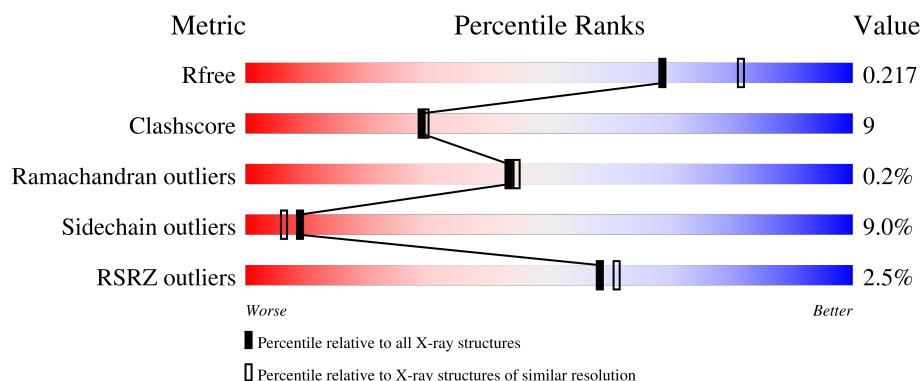
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	476	3% 79% 18% ..
2	B	3	33% 67%

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
2	NAG	B	2	X	-	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 4465 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.

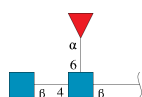
- Molecule 1 is a protein called Cholesteryl ester transfer protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	6	0
			3748	2410	613	708	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	CYS	engineered mutation	UNP P11597
A	88	ASP	ASN	engineered mutation	UNP P11597
A	131	ALA	CYS	engineered mutation	UNP P11597
A	240	ASP	ASN	engineered mutation	UNP P11597
A	341	ASP	ASN	engineered mutation	UNP P11597
A	405	ILE	VAL	engineered mutation	UNP P11597

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

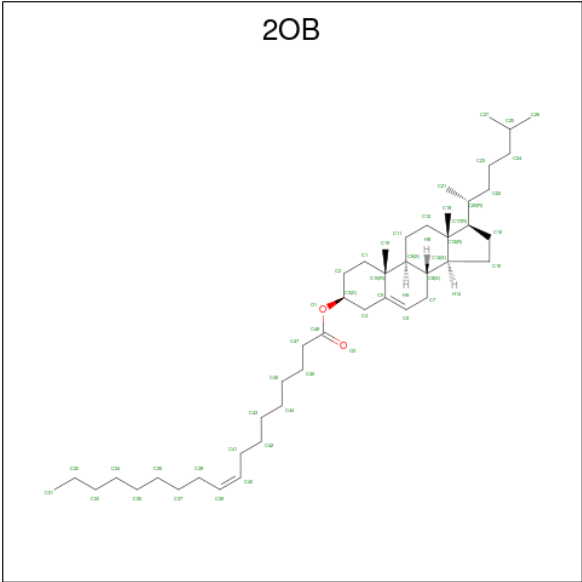


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

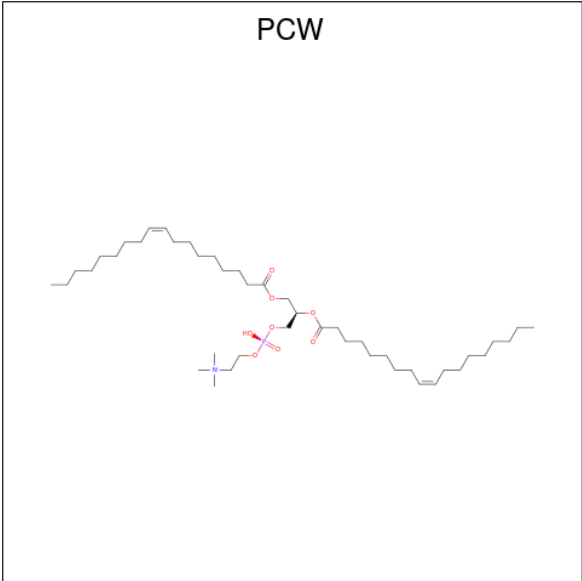
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is CHOLESTERYL OLEATE (CCD ID: 2OB) (formula: C₄₅H₇₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			47	45	2		
4	A	1	Total	C	O	0	0
			47	45	2		

- Molecule 5 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: C₄₄H₈₅NO₈P).



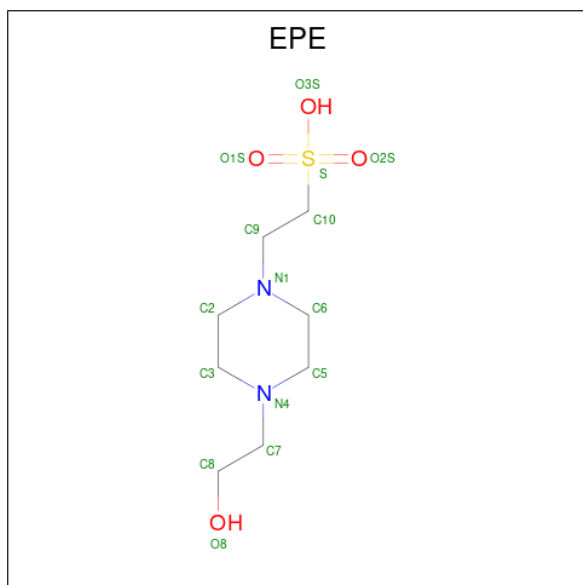
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

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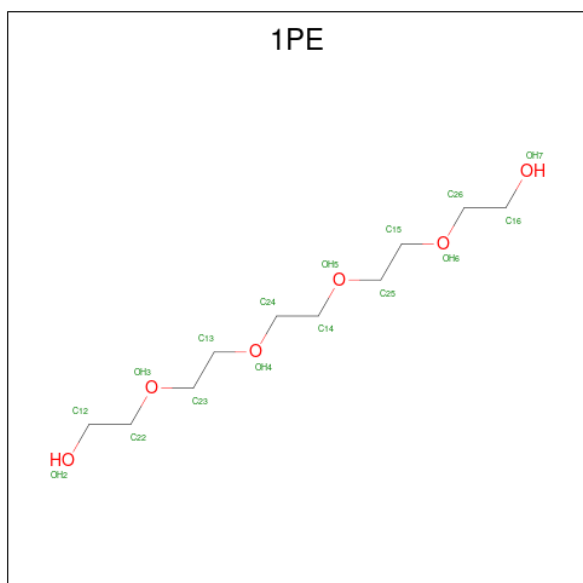
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



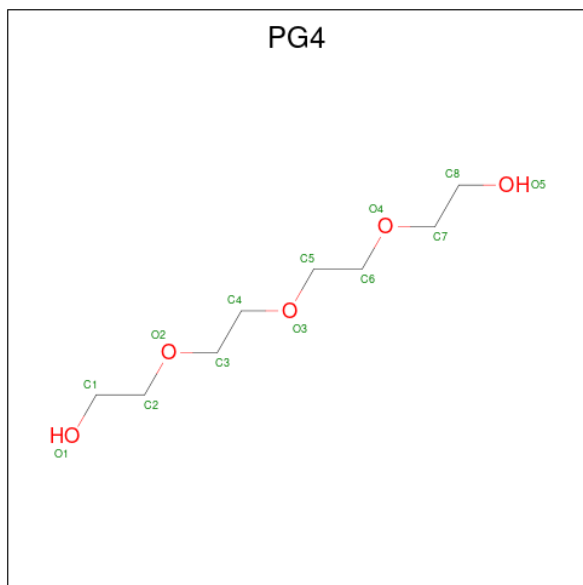
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 7 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			16	10	6		
7	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 8 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			13	8	5		

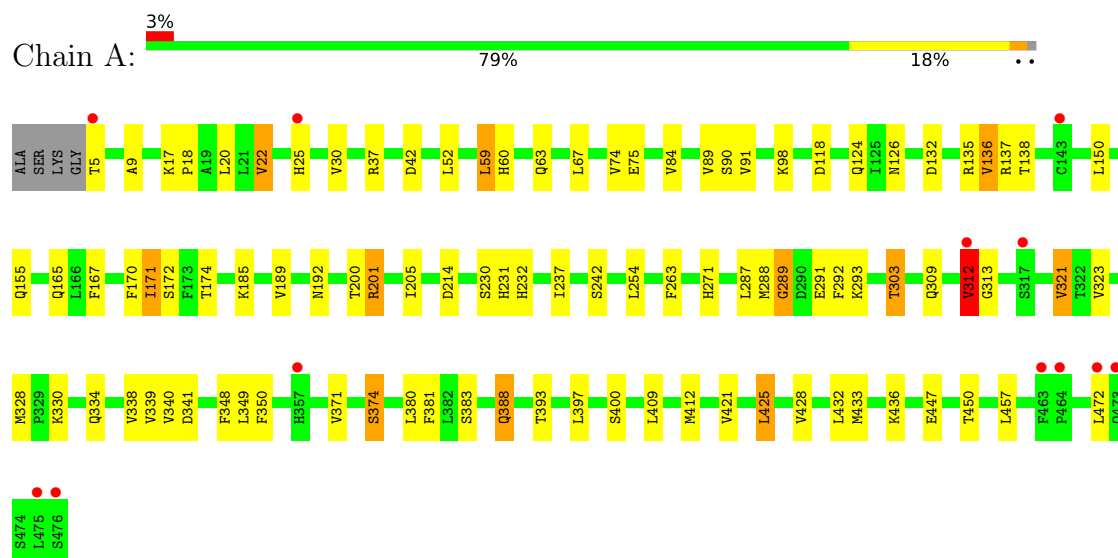
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	416	Total	O	0	0
			416	416		

3 Residue-property plots

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

- Molecule 1: Cholesteryl ester transfer protein



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.78Å 70.32Å 187.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.88 – 2.10 46.88 – 2.10	Depositor EDS
% Data completeness (in resolution range)	82.0 (46.88-2.10) 82.0 (46.88-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.217 , 0.265 0.214 , 0.217	Depositor DCC
R_{free} test set	2170 reflections (4.15%)	wwPDB-VP
Wilson B-factor (Å ²)	40.6	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4465	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: FUC, PG4, EPE, NAG, CL, 1PE, 2OB, PCW

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	0.73	1/3848 (0.0%)	0.94	4/5216 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	136	VAL	CA-CB	5.30	1.60	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	VAL	N-CA-C	10.60	120.50	110.53
1	A	170	PHE	CA-C-N	-5.83	117.20	123.08
1	A	170	PHE	C-N-CA	-5.83	117.20	123.08
1	A	171	ILE	N-CA-C	5.53	116.32	111.56

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	3748	0	3754	66	0
2	B	38	0	34	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	94	0	156	5	0
5	A	108	0	168	18	0
6	A	15	0	18	0	0
7	A	32	0	44	3	0
8	A	13	0	18	0	0
9	A	416	0	0	10	0
All	All	4465	0	4192	72	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 9.

All (72) 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:124:GLN:HE21	1:A:126:ASN:HD21	1.05	0.93
1:A:135:ARG:HH12	1:A:200[B]:THR:HG23	1.43	0.82
1:A:291[A]:GLU:HG3	9:A:751:HOH:O	1.85	0.76
1:A:201:ARG:HG2	5:A:504:PCW:H122	1.72	0.72
1:A:287:LEU:HD22	1:A:291[A]:GLU:HG2	1.73	0.71
1:A:293:LYS:HE3	1:A:303:THR:HG21	1.75	0.69
1:A:201:ARG:HG2	5:A:504:PCW:H141	1.74	0.68
5:A:504:PCW:H61	9:A:921:HOH:O	1.93	0.68
1:A:232:HIS:CE1	4:A:502:2OB:H472	2.30	0.66
1:A:124:GLN:HE21	1:A:126:ASN:ND2	1.88	0.65
1:A:132:ASP:HB3	1:A:137:ARG:HG3	1.78	0.65
1:A:447:GLU:OE1	9:A:601:HOH:O	2.14	0.64
1:A:425:LEU:HD13	5:A:505:PCW:H121	1.81	0.63
1:A:135:ARG:HH12	1:A:200[B]:THR:CG2	2.10	0.63
7:A:508:1PE:H141	9:A:889:HOH:O	2.00	0.61
1:A:312:VAL:O	1:A:350:PHE:HB3	2.00	0.60
1:A:138:THR:H	1:A:192:ASN:HD21	1.49	0.60
1:A:288:MET:H	1:A:291[B]:GLU:HG3	1.66	0.59
1:A:271[A]:HIS:CE1	1:A:328:MET:HE1	2.37	0.59
1:A:341:ASP:OD1	9:A:602:HOH:O	2.17	0.59
1:A:174:THR:HG21	9:A:760:HOH:O	2.04	0.58
1:A:201:ARG:HH21	5:A:504:PCW:H2	1.69	0.57
1:A:288:MET:N	1:A:291[B]:GLU:HG3	2.19	0.57
1:A:124:GLN:NE2	1:A:126:ASN:HD21	1.90	0.55
1:A:288:MET:H	1:A:291[B]:GLU:CG	2.19	0.55
1:A:74:VAL:HG21	5:A:504:PCW:H481	1.89	0.54
1:A:232:HIS:NE2	4:A:502:2OB:H472	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:SER:HB2	9:A:788:HOH:O	2.09	0.52
1:A:30:VAL:HG21	5:A:504:PCW:H432	1.91	0.51
1:A:138:THR:H	1:A:192:ASN:ND2	2.09	0.50
4:A:503:2OB:H183	5:A:505:PCW:H452	1.92	0.50
1:A:292:PHE:CE2	4:A:503:2OB:H312	2.48	0.49
1:A:348:PHE:CE1	1:A:412:MET:CE	2.95	0.49
1:A:388:GLN:HG3	9:A:996:HOH:O	2.13	0.48
1:A:340:VAL:HG11	5:A:505:PCW:H222	1.96	0.48
1:A:433:MET:HA	1:A:433:MET:HE2	1.95	0.48
5:A:505:PCW:H432	5:A:505:PCW:H40	1.46	0.48
1:A:201:ARG:NH2	5:A:504:PCW:H2	2.29	0.47
1:A:214:ASP:HB2	1:A:237:ILE:HD11	1.97	0.47
1:A:428:VAL:HG21	5:A:505:PCW:H11	1.95	0.47
1:A:98:LYS:NZ	7:A:507:1PE:H162	2.30	0.47
1:A:338:VAL:HG23	1:A:450:THR:HG21	1.97	0.47
1:A:17:LYS:HB3	1:A:18:PRO:HD3	1.97	0.46
1:A:167:PHE:HA	1:A:171:ILE:HB	1.98	0.46
1:A:287:LEU:CD2	1:A:291[A]:GLU:HG2	2.44	0.46
1:A:201:ARG:NH1	9:A:623:HOH:O	2.49	0.45
1:A:374:SER:HB2	9:A:885:HOH:O	2.16	0.45
1:A:42:ASP:OD2	1:A:60:HIS:HD2	2.00	0.44
1:A:348:PHE:HE1	1:A:412:MET:CE	2.30	0.44
1:A:425:LEU:CD1	5:A:505:PCW:H31	2.48	0.44
1:A:9:ALA:HB2	1:A:231:HIS:HB3	1.99	0.43
1:A:237:ILE:HG12	1:A:242:SER:HB3	2.00	0.43
1:A:421:VAL:HG21	4:A:503:2OB:H412	2.01	0.43
1:A:59:LEU:N	1:A:59:LEU:HD23	2.33	0.43
1:A:201:ARG:CG	5:A:504:PCW:H141	2.45	0.43
1:A:60:HIS:HB3	7:A:507:1PE:H152	2.00	0.43
1:A:201:ARG:CG	5:A:504:PCW:H122	2.45	0.43
1:A:59:LEU:N	1:A:59:LEU:CD2	2.82	0.42
1:A:312:VAL:HG22	1:A:313:GLY:HA2	2.02	0.42
1:A:288:MET:O	1:A:289:GLY:C	2.61	0.42
1:A:263:PHE:HB2	1:A:457:LEU:HB2	2.01	0.41
1:A:150:LEU:HD23	1:A:172:SER:HB2	2.02	0.41
1:A:205:ILE:HA	1:A:436:LYS:HG2	2.02	0.41
5:A:505:PCW:H151	5:A:505:PCW:H181	1.70	0.41
1:A:374:SER:HB3	1:A:381:PHE:HB2	2.02	0.41
5:A:504:PCW:H271	5:A:504:PCW:H39	2.03	0.41
1:A:432:LEU:HD13	5:A:505:PCW:H382	2.03	0.41
1:A:287:LEU:HB2	1:A:321:VAL:HG13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:VAL:HA	1:A:383:SER:O	2.21	0.40
1:A:309:GLN:O	1:A:313:GLY:HA3	2.22	0.40
1:A:348:PHE:HE1	1:A:412:MET:HE3	1.87	0.40
1:A:22:VAL:HA	1:A:25[B]:HIS:HD2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	476/476 (100%)	465 (98%)	10 (2%)	1 (0%)	43 44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	GLY

5.3.2 Protein sidechains [i](#)

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	428/424 (101%)	388 (91%)	40 (9%)	8 6

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	20	LEU
1	A	22	VAL
1	A	37[A]	ARG
1	A	37[B]	ARG
1	A	52	LEU
1	A	59	LEU
1	A	63	GLN
1	A	67	LEU
1	A	75	GLU
1	A	84	VAL
1	A	89	VAL
1	A	91	VAL
1	A	118	ASP
1	A	136	VAL
1	A	155	GLN
1	A	165[A]	GLN
1	A	165[B]	GLN
1	A	185	LYS
1	A	189	VAL
1	A	201	ARG
1	A	230	SER
1	A	254	LEU
1	A	303	THR
1	A	312	VAL
1	A	321	VAL
1	A	323	VAL
1	A	330	LYS
1	A	334	GLN
1	A	339	VAL
1	A	349	LEU
1	A	374	SER
1	A	380	LEU
1	A	388	GLN
1	A	393	THR
1	A	397	LEU
1	A	400	SER
1	A	409	LEU
1	A	425	LEU
1	A	472	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	63	GLN
1	A	73	GLN
1	A	87	GLN
1	A	126	ASN
1	A	192	ASN
1	A	279	GLN
1	A	334	GLN
1	A	356	GLN
1	A	357	HIS
1	A	406	GLN
1	A	410	GLN
1	A	458	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 ⓘ

3 monosaccharides 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	NAG	B	1	1,2	14,14,15	0.59	0	17,19,21	1.45	2 (11%)
2	NAG	B	2	2	14,14,15	0.81	1 (7%)	17,19,21	2.16	5 (29%)
2	FUC	B	3	2	10,10,11	0.32	0	14,14,16	0.65	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	NAG	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	1/1/5/7	4/6/23/26	0/1/1/1
2	FUC	B	3	2	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	C1-C2	2.73	1.56	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C1-O5-C5	6.42	120.79	112.19
2	B	1	NAG	C4-C3-C2	3.56	116.24	111.02
2	B	1	NAG	O5-C1-C2	-3.23	106.30	111.29
2	B	2	NAG	C1-C2-N2	2.99	115.14	110.43
2	B	2	NAG	C3-C4-C5	-2.33	106.00	110.23
2	B	2	NAG	C4-C3-C2	-2.26	107.71	111.02
2	B	2	NAG	O5-C1-C2	2.17	114.64	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	2	NAG	C1

All (6) torsion outliers are listed below:

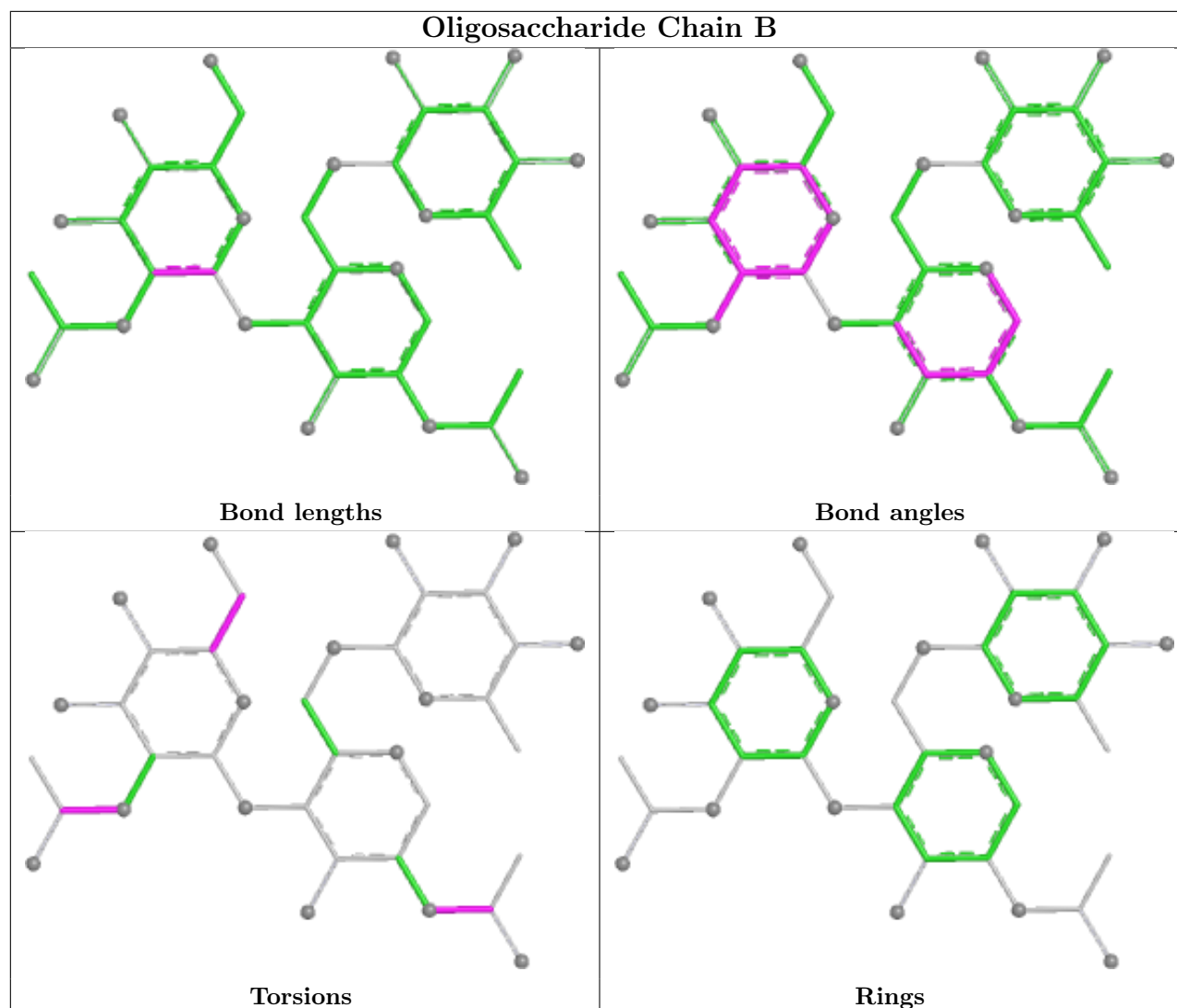
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C4-C5-C6-O6
2	B	1	NAG	C8-C7-N2-C2
2	B	2	NAG	O5-C5-C6-O6
2	B	1	NAG	O7-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	B	2	NAG	C8-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\# Z > 2$
7	1PE	A	507	-	15,15,15	0.54	0	14,14,14	0.18	0
7	1PE	A	508	-	15,15,15	0.50	0	14,14,14	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	2OB	A	502	-	50,50,50	0.79	1 (2%)	68,68,68	1.16	6 (8%)
4	2OB	A	503	-	50,50,50	0.70	1 (2%)	68,68,68	1.36	9 (13%)
6	EPE	A	506	-	15,15,15	2.04	1 (6%)	19,20,20	1.00	1 (5%)
5	PCW	A	504	-	53,53,53	1.27	4 (7%)	59,61,61	0.91	3 (5%)
5	PCW	A	505	-	53,53,53	1.27	4 (7%)	59,61,61	1.12	5 (8%)
8	PG4	A	509	-	12,12,12	0.46	0	11,11,11	0.32	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
7	1PE	A	507	-	-	6/13/13/13	-
7	1PE	A	508	-	-	9/13/13/13	-
4	2OB	A	502	-	-	9/31/89/89	0/4/4/4
4	2OB	A	503	-	-	20/31/89/89	0/4/4/4
6	EPE	A	506	-	-	2/9/19/19	0/1/1/1
5	PCW	A	504	-	-	18/57/57/57	-
5	PCW	A	505	-	-	28/57/57/57	-
8	PG4	A	509	-	-	7/10/10/10	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	506	EPE	C10-S	-7.50	1.67	1.77
5	A	505	PCW	P-O1P	5.33	1.80	1.55
5	A	504	PCW	P-O1P	5.25	1.79	1.55
5	A	505	PCW	O2-C31	4.55	1.47	1.34
5	A	504	PCW	O3-C11	4.50	1.46	1.33
5	A	504	PCW	O2-C31	4.47	1.46	1.34
5	A	505	PCW	O3-C11	4.34	1.46	1.33
4	A	502	2OB	O1-C48	4.30	1.46	1.34
4	A	503	2OB	O1-C48	3.53	1.44	1.34
5	A	505	PCW	P-O2P	2.89	1.60	1.50
5	A	504	PCW	P-O2P	2.76	1.60	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	502	2OB	O1-C48-C47	5.14	122.59	111.48
5	A	505	PCW	O3-C11-C12	3.90	123.72	111.83
4	A	503	2OB	C21-C20-C22	-3.68	104.64	110.34
4	A	503	2OB	C4-C5-C6	-3.46	115.87	120.57
5	A	505	PCW	O2-C31-C32	3.27	118.56	111.48
4	A	503	2OB	C4-C5-C10	3.05	120.32	116.42
5	A	505	PCW	O2-C2-C3	3.01	119.13	108.34
5	A	504	PCW	O2-C31-C32	2.99	117.94	111.48
4	A	503	2OB	C8-C7-C6	-2.96	108.66	112.76
5	A	504	PCW	O3-C11-C12	2.91	120.69	111.83
4	A	502	2OB	C7-C8-C9	2.77	112.93	109.72
5	A	505	PCW	O3-C11-O11	-2.62	117.07	123.63
4	A	502	2OB	C4-C5-C10	2.62	119.77	116.42
6	A	506	EPE	O2S-S-C10	2.60	110.66	106.73
4	A	503	2OB	C21-C20-C17	2.53	116.68	112.88
5	A	504	PCW	O2-C2-C3	2.32	116.67	108.34
4	A	503	2OB	O1-C48-C47	2.30	116.46	111.48
4	A	503	2OB	C45-C46-C47	-2.22	104.97	113.13
4	A	502	2OB	C1-C2-C3	2.18	113.89	110.33
5	A	505	PCW	C3-O3-C11	2.17	125.05	117.12
4	A	503	2OB	C16-C17-C13	-2.16	101.30	103.84
4	A	502	2OB	C3-O1-C48	-2.14	112.67	117.80
4	A	502	2OB	O1-C48-O2	-2.08	118.83	123.70
4	A	503	2OB	C12-C11-C9	-2.03	109.69	113.14

There are no chirality outliers.

All (99) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	504	PCW	C2-C1-O3P-P
5	A	505	PCW	C12-C11-O3-C3
5	A	505	PCW	O11-C11-O3-C3
5	A	505	PCW	C1-O3P-P-O1P
5	A	505	PCW	C1-O3P-P-O2P
5	A	505	PCW	C1-O3P-P-O4P
4	A	503	2OB	C13-C17-C20-C21
4	A	503	2OB	C16-C17-C20-C22
7	A	508	1PE	OH4-C13-C23-OH3
7	A	507	1PE	OH4-C13-C23-OH3
4	A	503	2OB	C17-C20-C22-C23
7	A	508	1PE	OH2-C12-C22-OH3
4	A	503	2OB	C22-C23-C24-C25
4	A	503	2OB	C21-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
5	A	504	PCW	C36-C37-C38-C39
7	A	508	1PE	OH7-C16-C26-OH6
8	A	509	PG4	O1-C1-C2-O2
8	A	509	PG4	O4-C7-C8-O5
5	A	505	PCW	C40-C41-C42-C43
7	A	507	1PE	OH2-C12-C22-OH3
4	A	502	2OB	C43-C44-C45-C46
4	A	503	2OB	C32-C33-C34-C35
5	A	505	PCW	C13-C14-C15-C16
5	A	504	PCW	C14-C15-C16-C17
5	A	505	PCW	C15-C16-C17-C18
4	A	502	2OB	C32-C33-C34-C35
5	A	505	PCW	C23-C24-C25-C26
5	A	504	PCW	C15-C16-C17-C18
5	A	505	PCW	C21-C22-C23-C24
5	A	504	PCW	C21-C22-C23-C24
5	A	504	PCW	C33-C34-C35-C36
5	A	505	PCW	C12-C13-C14-C15
5	A	504	PCW	C43-C44-C45-C46
4	A	502	2OB	C35-C36-C37-C38
5	A	505	PCW	C41-C42-C43-C44
5	A	505	PCW	C22-C23-C24-C25
7	A	508	1PE	OH5-C14-C24-OH4
5	A	505	PCW	C35-C36-C37-C38
5	A	504	PCW	C41-C42-C43-C44
5	A	505	PCW	C16-C17-C18-C19
5	A	505	PCW	C36-C37-C38-C39
4	A	503	2OB	C41-C42-C43-C44
5	A	504	PCW	O3P-C1-C2-C3
5	A	505	PCW	O3P-C1-C2-C3
4	A	503	2OB	C42-C43-C44-C45
4	A	503	2OB	C34-C35-C36-C37
4	A	503	2OB	C40-C41-C42-C43
5	A	504	PCW	C16-C17-C18-C19
5	A	505	PCW	C42-C43-C44-C45
4	A	503	2OB	C16-C17-C20-C21
4	A	503	2OB	C45-C46-C47-C48
5	A	505	PCW	C11-C12-C13-C14
4	A	503	2OB	C43-C44-C45-C46
5	A	504	PCW	C13-C14-C15-C16
5	A	505	PCW	C45-C46-C47-C48
4	A	503	2OB	C13-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
7	A	508	1PE	C16-C26-OH6-C15
5	A	504	PCW	C12-C13-C14-C15
7	A	508	1PE	OH6-C15-C25-OH5
4	A	503	2OB	C36-C37-C38-C39
4	A	503	2OB	C23-C24-C25-C27
5	A	505	PCW	C32-C33-C34-C35
4	A	502	2OB	C40-C41-C42-C43
5	A	505	PCW	C44-C45-C46-C47
5	A	505	PCW	C25-C26-C27-C28
4	A	503	2OB	C23-C24-C25-C26
8	A	509	PG4	C6-C5-O3-C4
4	A	503	2OB	C33-C34-C35-C36
8	A	509	PG4	C8-C7-O4-C6
7	A	507	1PE	C16-C26-OH6-C15
5	A	504	PCW	O3P-C1-C2-O2
5	A	505	PCW	O3P-C1-C2-O2
8	A	509	PG4	C4-C3-O2-C2
5	A	504	PCW	O4P-C4-C5-N
7	A	508	1PE	C25-C15-OH6-C26
7	A	507	1PE	C13-C23-OH3-C22
7	A	508	1PE	C14-C24-OH4-C13
5	A	504	PCW	C42-C43-C44-C45
6	A	506	EPE	C8-C7-N4-C3
5	A	504	PCW	C3-C2-O2-C31
4	A	503	2OB	C39-C40-C41-C42
8	A	509	PG4	C1-C2-O2-C3
6	A	506	EPE	C8-C7-N4-C5
5	A	504	PCW	C23-C24-C25-C26
8	A	509	PG4	C3-C4-O3-C5
4	A	503	2OB	C37-C38-C39-C40
5	A	504	PCW	C19-C20-C21-C22
5	A	505	PCW	C19-C20-C21-C22
7	A	507	1PE	C14-C24-OH4-C13
4	A	502	2OB	C46-C47-C48-O1
7	A	507	1PE	C15-C25-OH5-C14
4	A	502	2OB	C45-C46-C47-C48
5	A	505	PCW	C20-C21-C22-C23
5	A	505	PCW	C1-C2-O2-C31
5	A	505	PCW	C3-C2-O2-C31
4	A	502	2OB	C23-C24-C25-C27
4	A	502	2OB	C46-C47-C48-O2
7	A	508	1PE	C23-C13-OH4-C24

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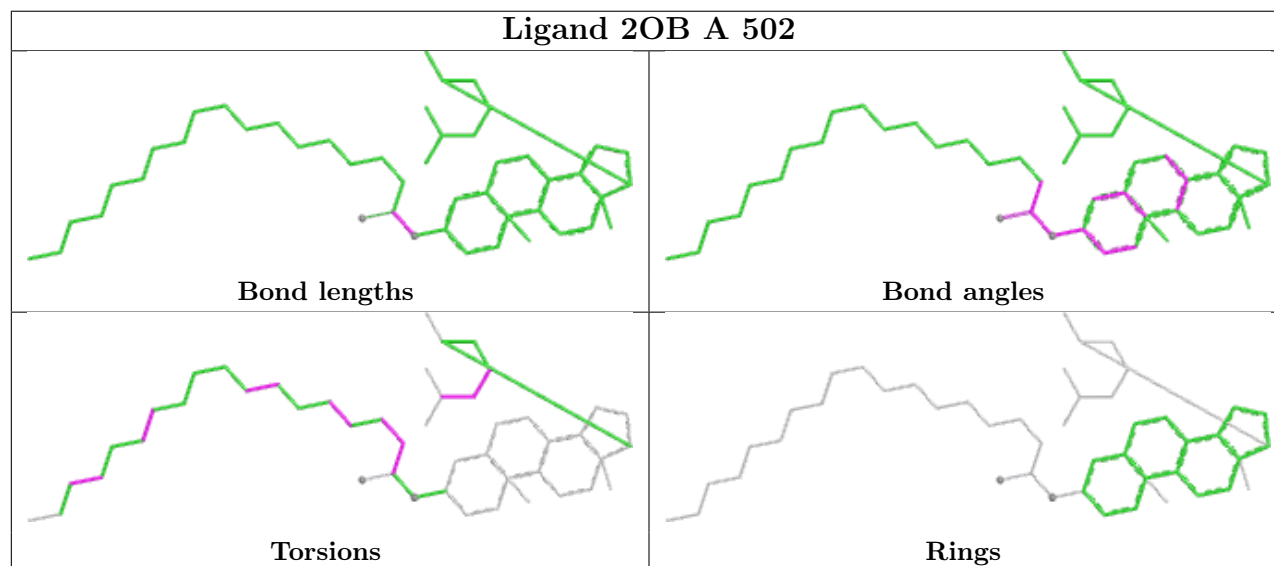
Mol	Chain	Res	Type	Atoms
4	A	502	2OB	C22-C23-C24-C25

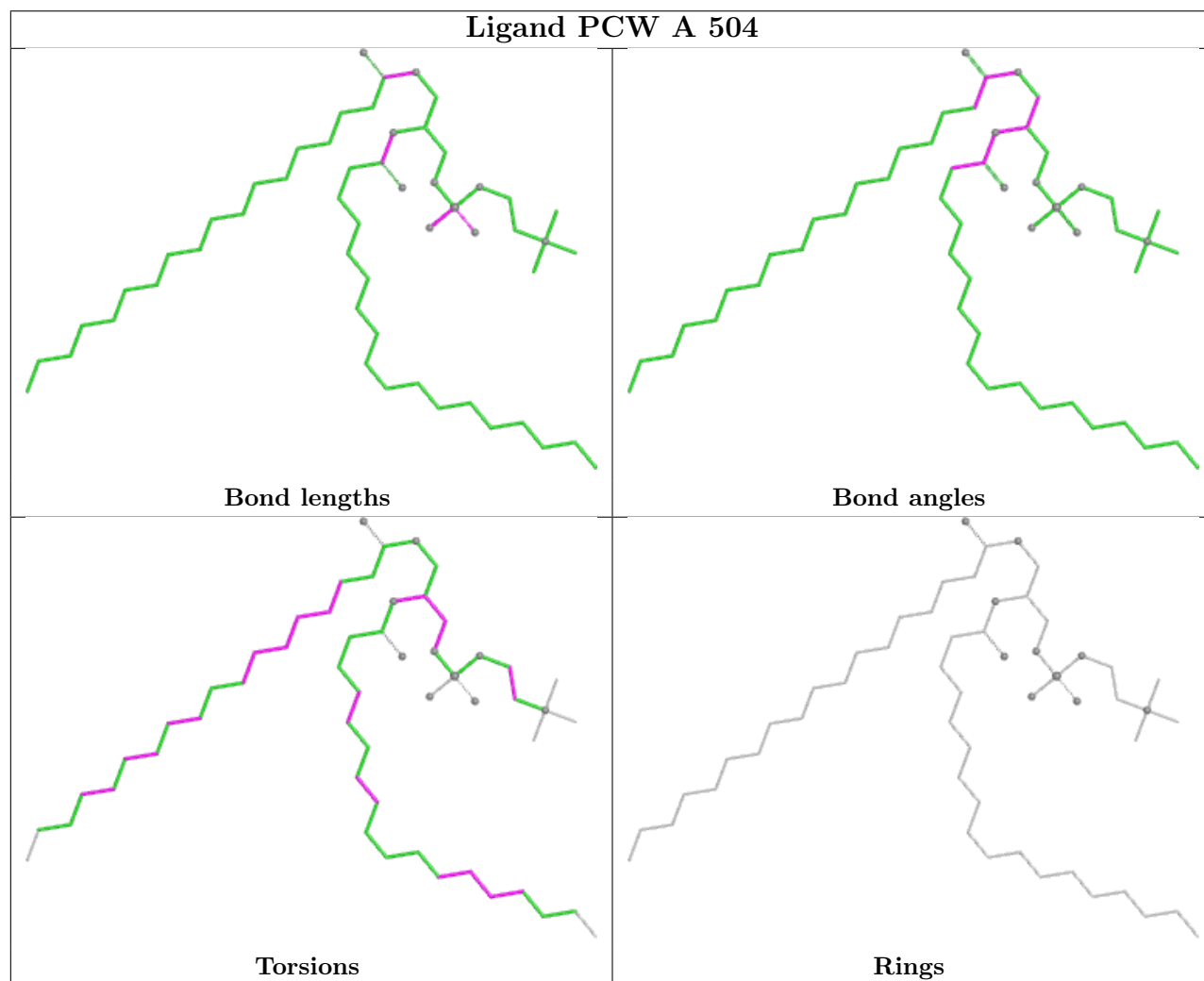
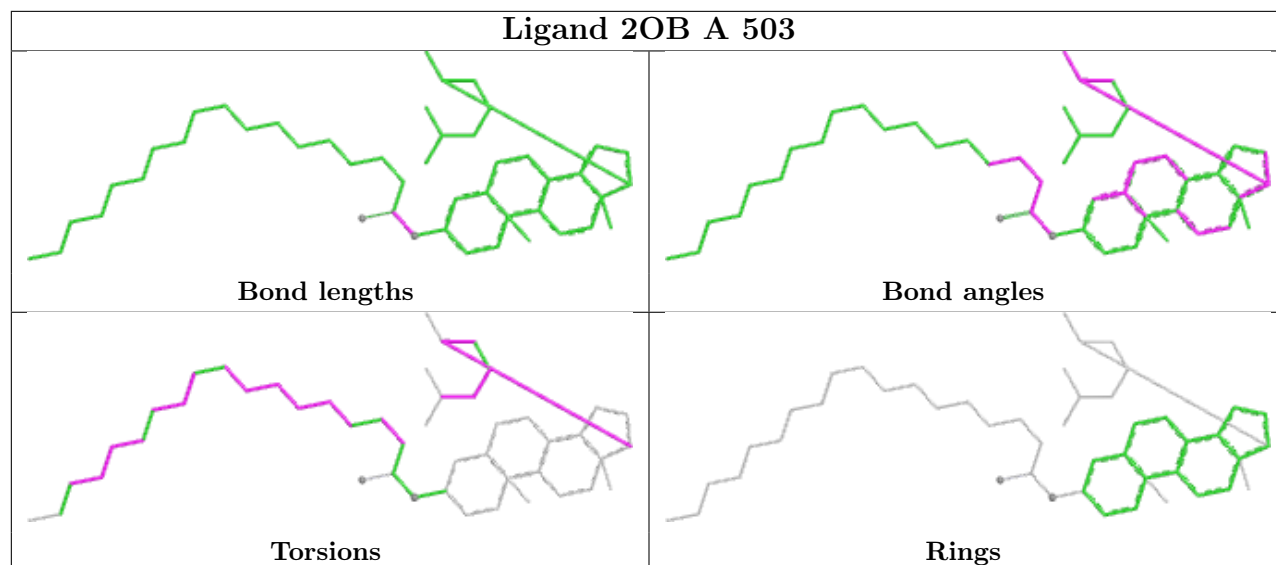
There are no ring outliers.

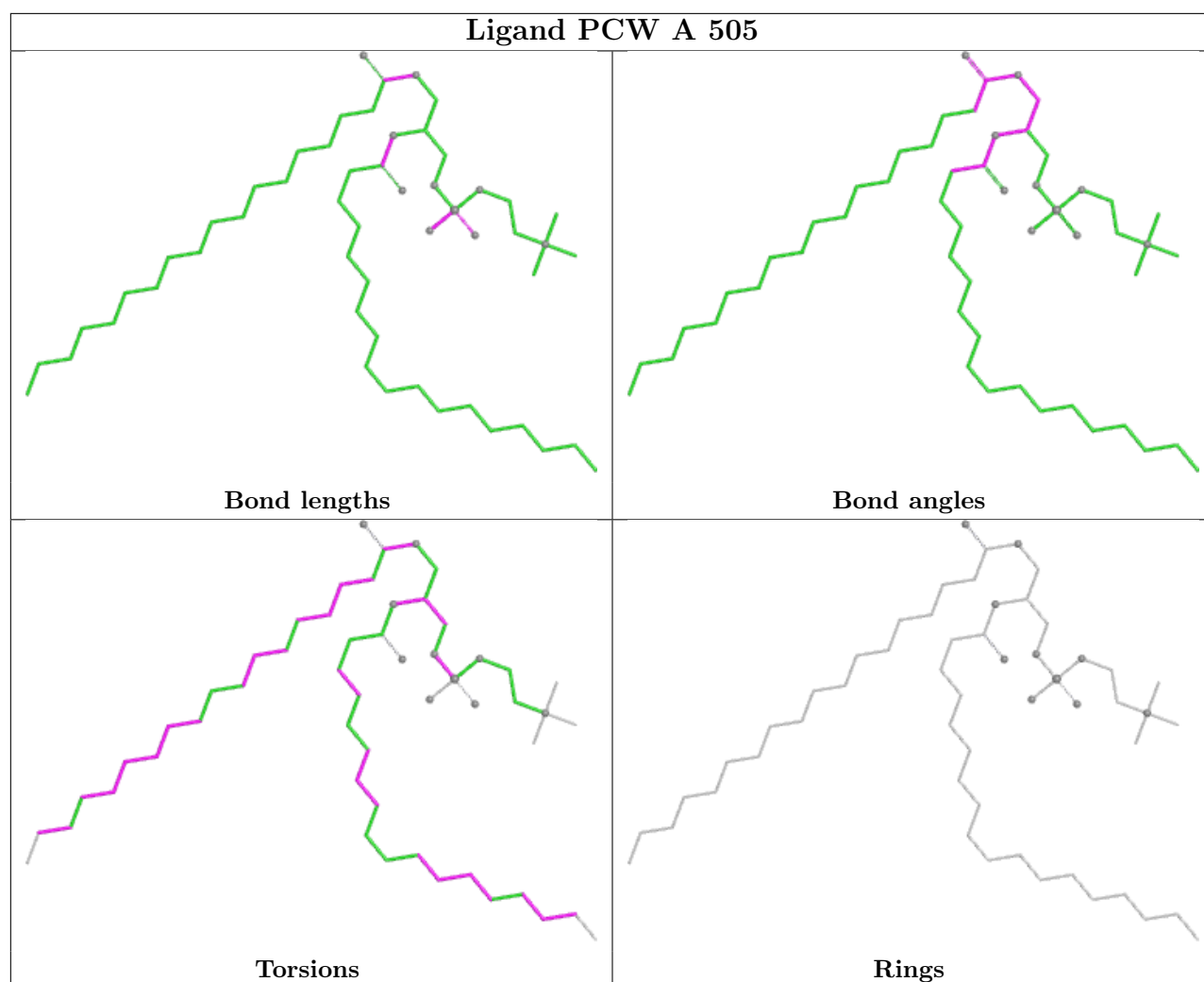
6 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	507	1PE	2	0
7	A	508	1PE	1	0
4	A	502	2OB	2	0
4	A	503	2OB	3	0
5	A	504	PCW	10	0
5	A	505	PCW	8	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	472/476 (99%)	0.31	12 (2%) 58 61	23, 41, 58, 82	6 (1%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	312	VAL	3.8
1	A	476	SER	3.6
1	A	5	THR	3.2
1	A	475	LEU	3.0
1	A	25[A]	HIS	2.9
1	A	317	SER	2.8
1	A	464	PRO	2.5
1	A	357	HIS	2.4
1	A	472	LEU	2.2
1	A	473	GLN	2.1
1	A	143	CYS	2.1
1	A	463	PHE	2.0

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

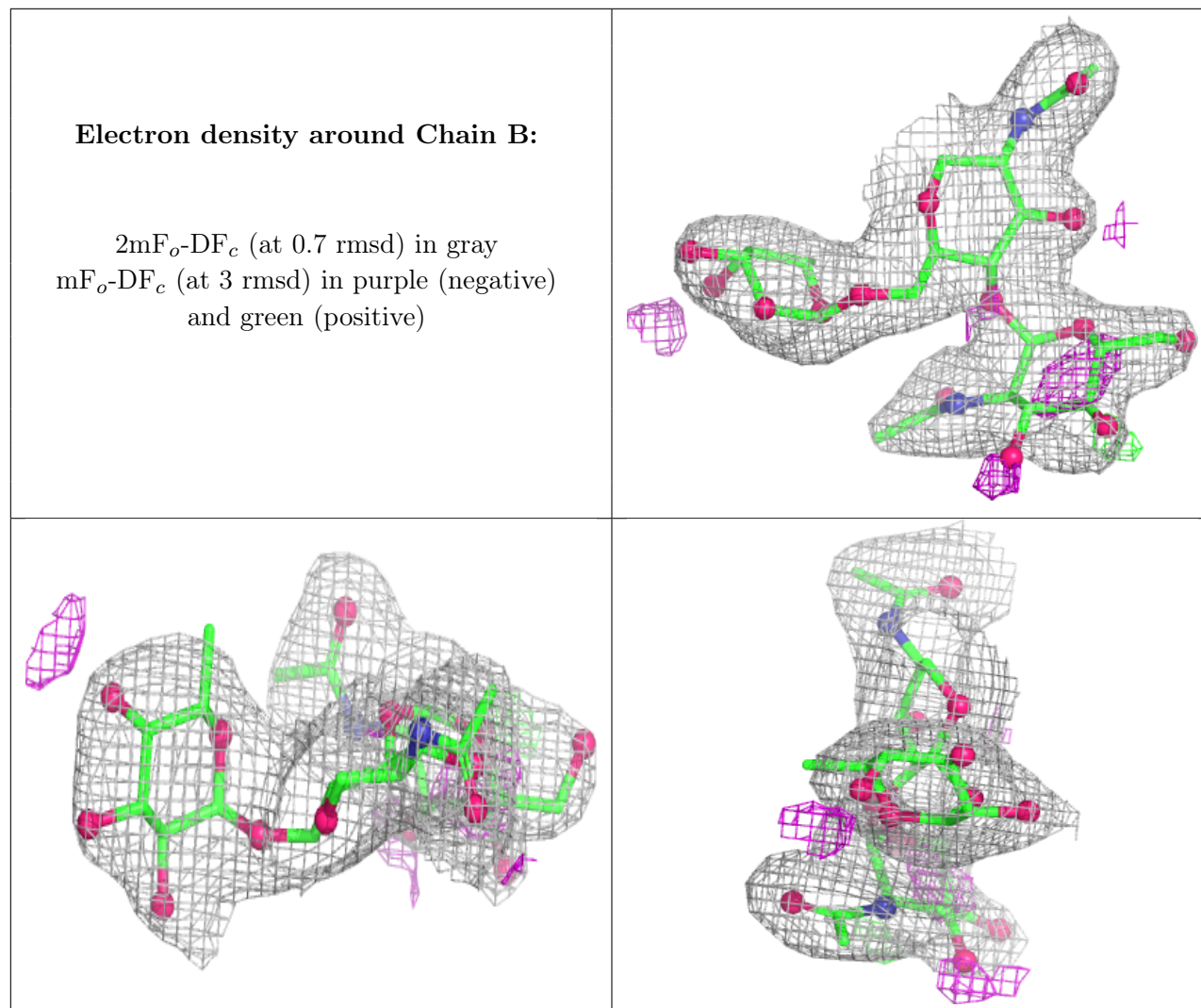
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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	NAG	B	2	14/15	0.71	0.17	72,73,75,75	0
2	NAG	B	1	14/15	0.86	0.11	58,60,65,69	0
2	FUC	B	3	10/11	0.92	0.10	60,61,63,63	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands ⓘ

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.

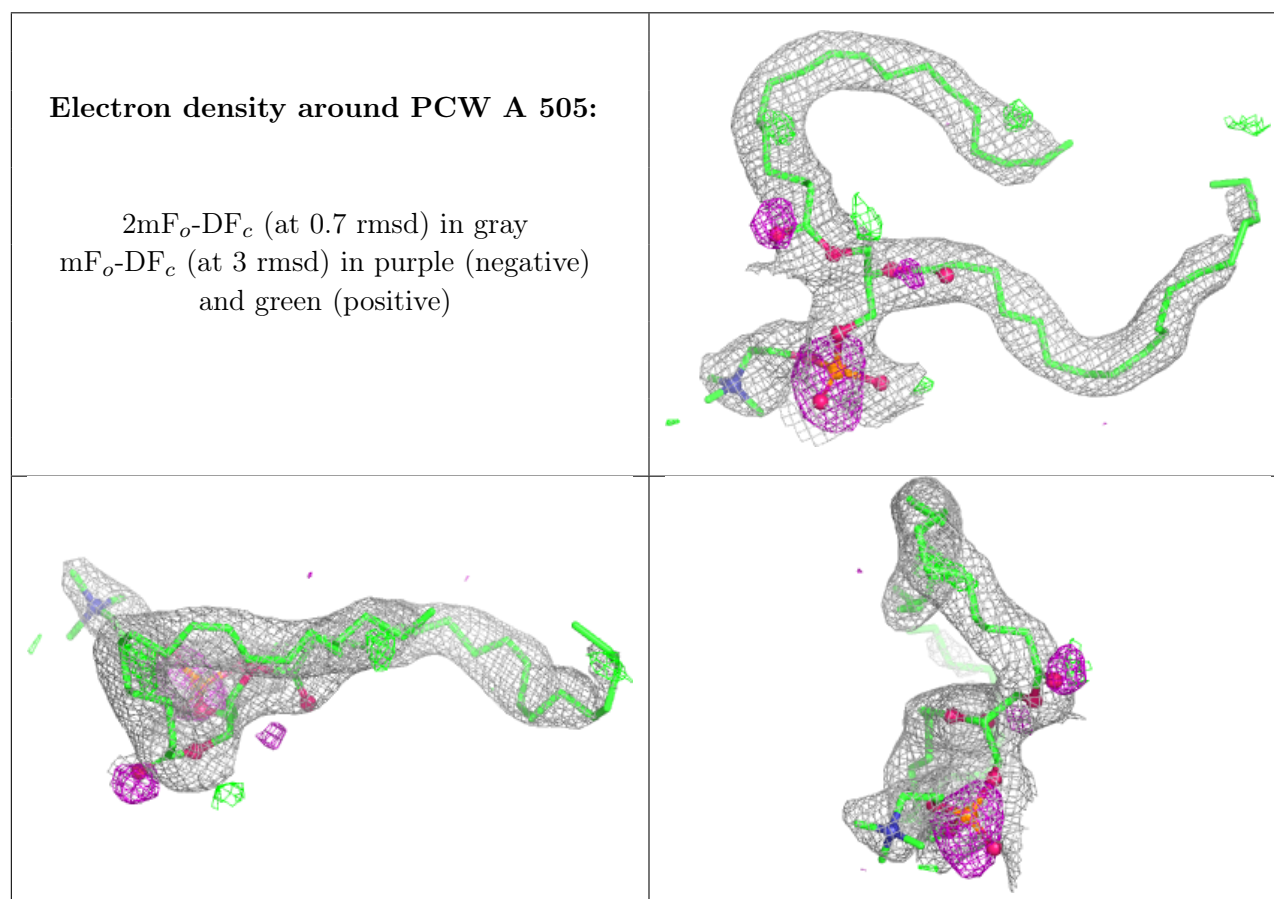
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	1PE	A	507	16/16	0.85	0.16	66,71,75,75	0

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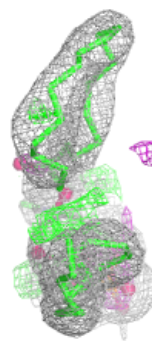
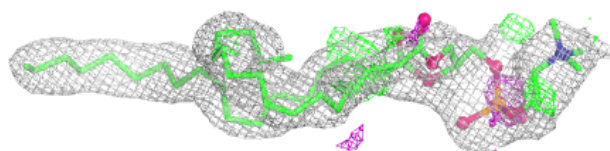
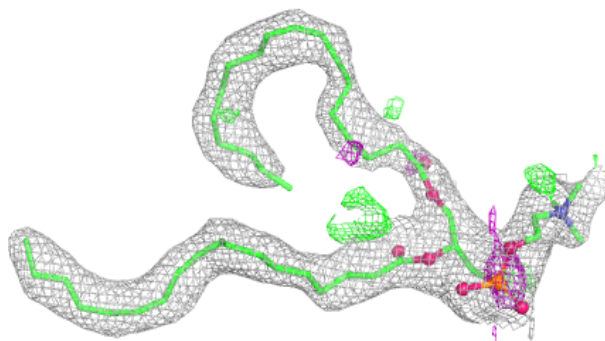
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PCW	A	505	54/54	0.87	0.20	53,62,85,86	0
6	EPE	A	506	15/15	0.87	0.14	75,79,82,82	0
5	PCW	A	504	54/54	0.87	0.19	42,70,99,99	0
7	1PE	A	508	16/16	0.87	0.18	62,75,78,79	0
8	PG4	A	509	13/13	0.88	0.12	65,68,69,69	0
4	2OB	A	502	47/47	0.94	0.13	42,51,59,63	0
4	2OB	A	503	47/47	0.94	0.12	32,41,50,55	0
3	CL	A	501	1/1	0.99	0.02	35,35,35,35	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.

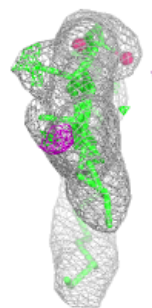
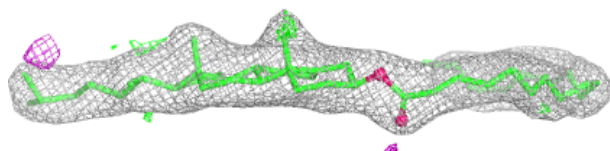
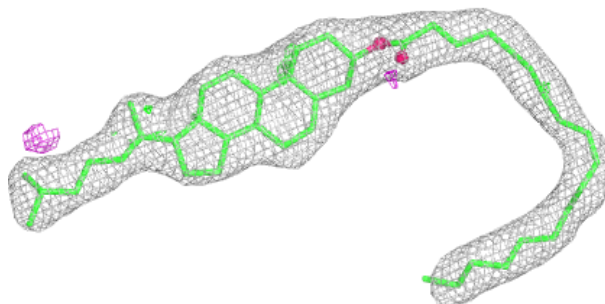


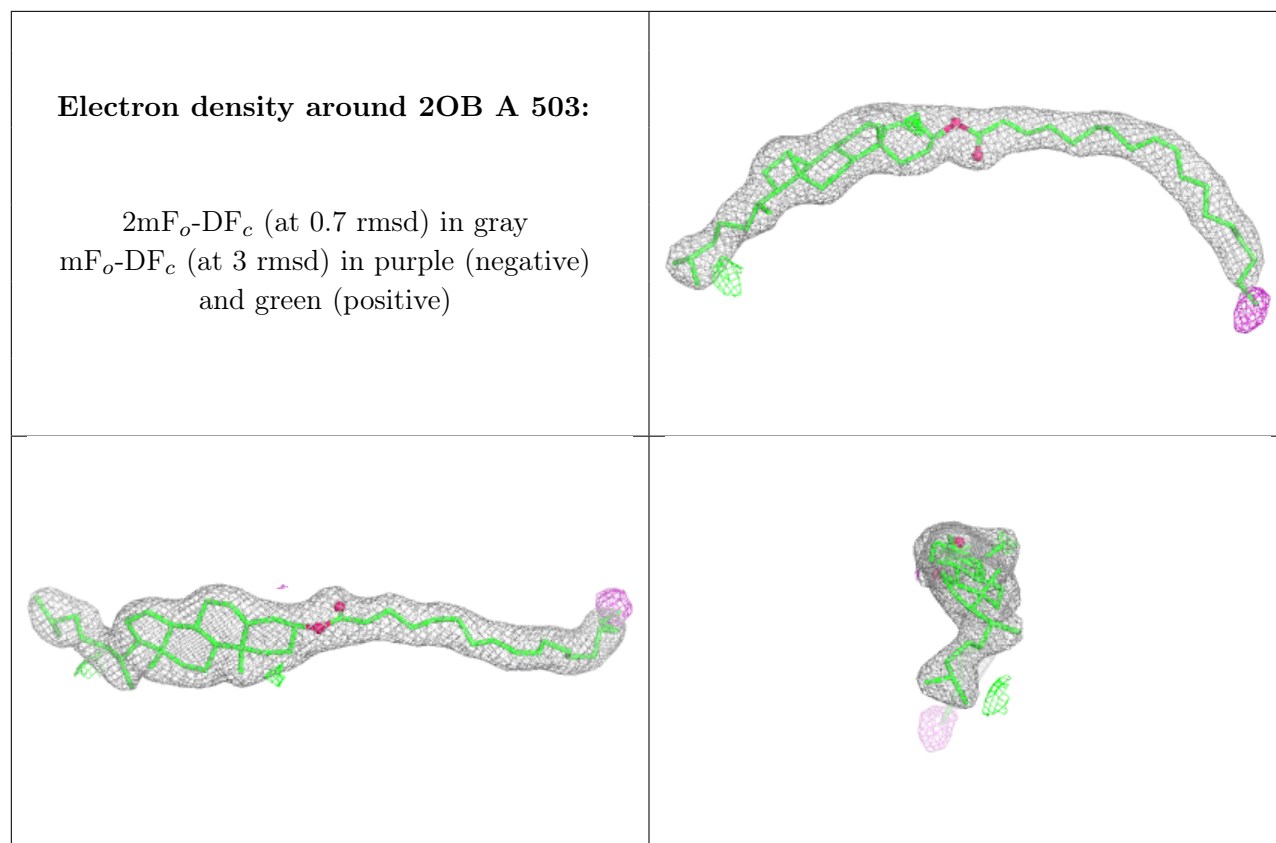
Electron density around PCW A 504:

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

**Electron density around 2OB A 502:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.