



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:48 AM UTC

PDB ID : 2FAF / pdb_00002faf
Title : The structure of chicken mitochondrial PEPCK.
Authors : Holyoak, T.; Sullivan, S.M.; Nowak, T.
Deposited on : 2005-12-07
Resolution : 1.70 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
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

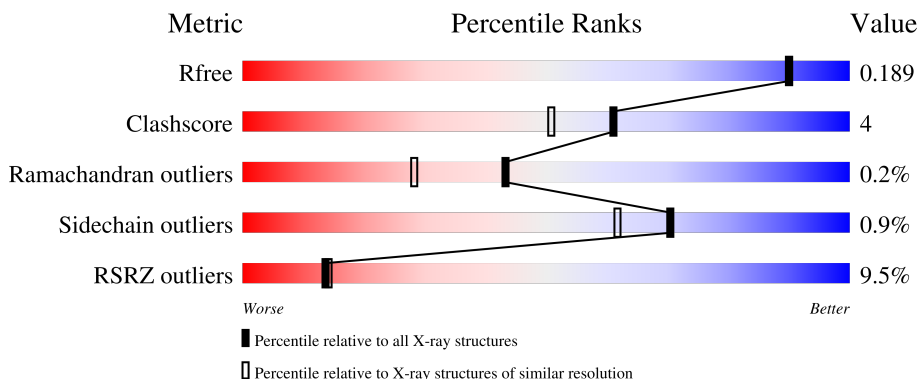
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	608	 7% 91% 7%
1	B	608	 12% 88% 10%
2	C	2	 100%

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
4	1PE	A	1262[B]	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10569 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 Phosphoenolpyruvate carboxykinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	596	4741	3016	842	849	34	0	17	0
1	B	596	4767	3033	854	847	33	0	20	0

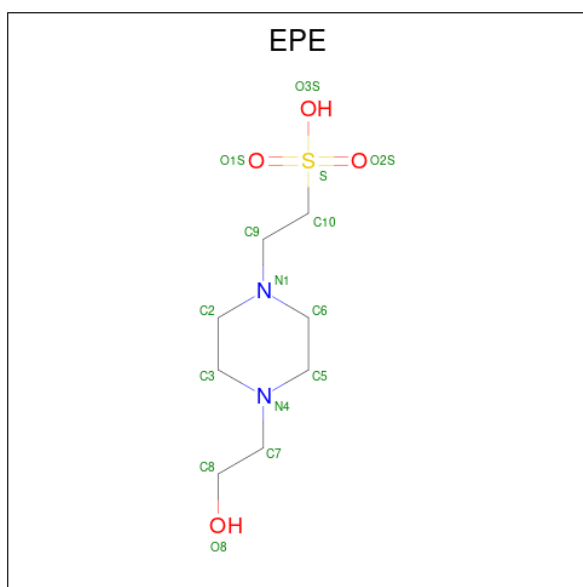
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	GLY	-	insertion	UNP P21642
A	130	PRO	SER	SEE REMARK 999	UNP P21642
A	233	PRO	ARG	SEE REMARK 999	UNP P21642
A	268	ARG	ALA	SEE REMARK 999	UNP P21642
A	339	GLU	ARG	SEE REMARK 999	UNP P21642
A	502	ARG	SER	SEE REMARK 999	UNP P21642
B	129	GLY	-	insertion	UNP P21642
B	130	PRO	SER	SEE REMARK 999	UNP P21642
B	233	PRO	ARG	SEE REMARK 999	UNP P21642
B	268	ARG	ALA	SEE REMARK 999	UNP P21642
B	339	GLU	ARG	SEE REMARK 999	UNP P21642
B	502	ARG	SER	SEE REMARK 999	UNP P21642

- Molecule 2 is an oligosaccharide called beta-D-fructofuranose-(2-1)-6-O-octanoyl-alpha-D-glucopyranose.

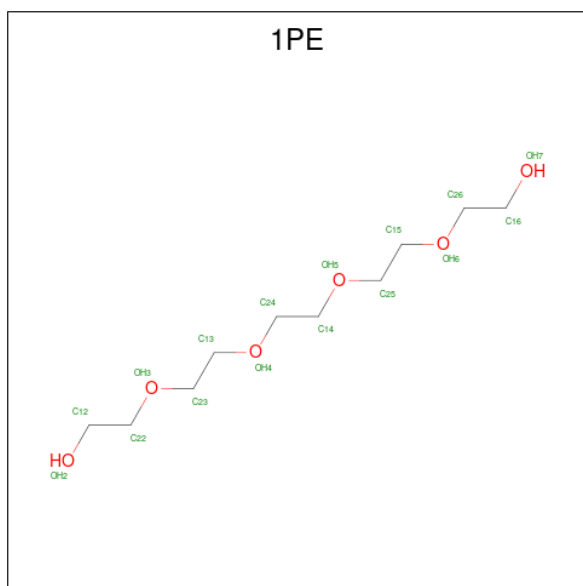
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	C	2	32	20	12	0	0	0

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



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

- Molecule 4 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	32	20	12	0	1

- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Mn 1	0	0
5	B	1	Total 1	Mn 1	0	0

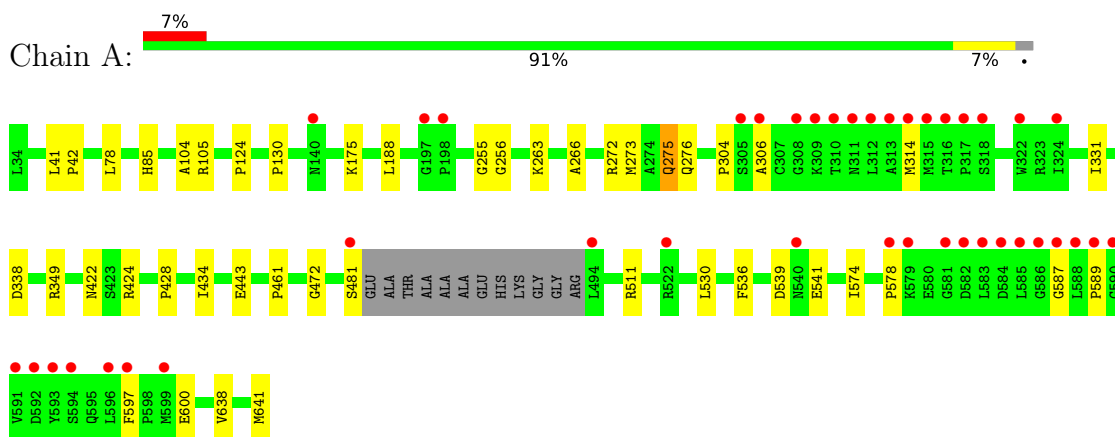
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	572	Total 572	O 572	0	0
6	B	408	Total 408	O 408	0	0

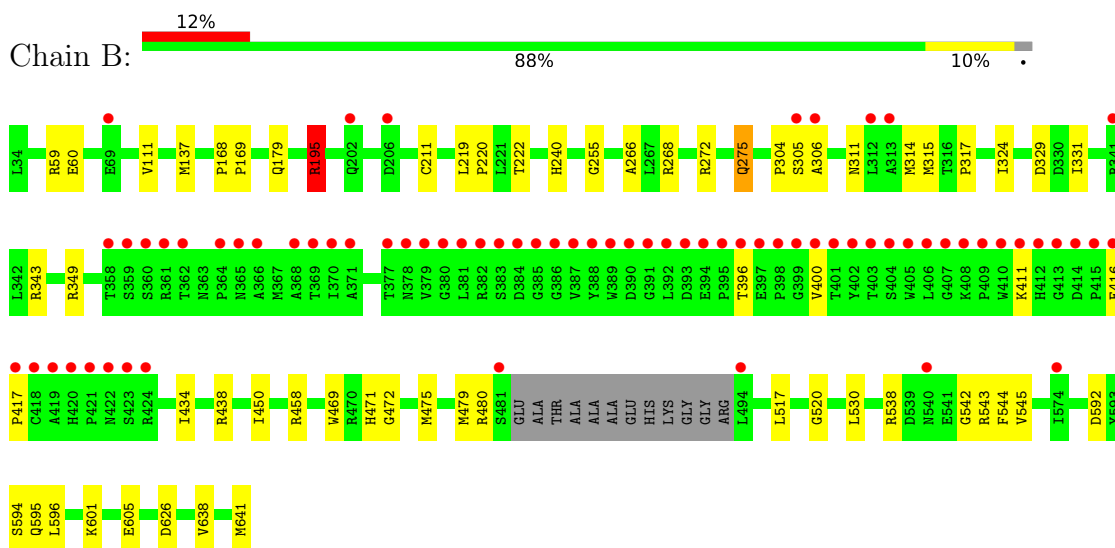
3 Residue-property plots

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.

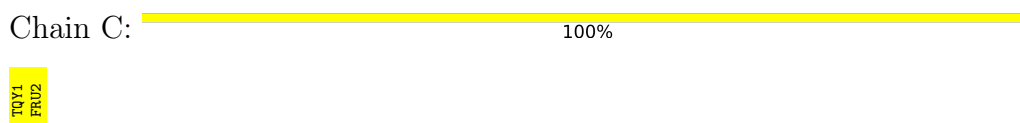
- Molecule 1: Phosphoenolpyruvate carboxykinase



- Molecule 1: Phosphoenolpyruvate carboxykinase



- Molecule 2: beta-D-fructofuranose-(2-1)-6-O-octanoyl-alpha-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	110.81Å 47.74Å 127.20Å 90.00° 111.31° 90.00°	Depositor
Resolution (Å)	34.08 – 1.70 34.08 – 1.70	Depositor EDS
% Data completeness (in resolution range)	90.6 (34.08-1.70) 90.5 (34.08-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 1.70Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.161 , 0.191 0.160 , 0.189	Depositor DCC
R_{free} test set	6219 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtrriage
Anisotropy	0.043	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10569	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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: FRU, TQY, MN, 1PE, EPE

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	0.71	1/4934 (0.0%)	0.84	2/6709 (0.0%)
1	B	0.62	0/4966	0.84	5/6751 (0.1%)
All	All	0.67	1/9900 (0.0%)	0.84	7/13460 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	124	PRO	CA-C	6.20	1.55	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	195	ARG	NE-CZ-NH2	10.48	128.63	119.20
1	B	195	ARG	NE-CZ-NH1	-9.52	111.98	121.50
1	B	195	ARG	CD-NE-CZ	6.97	134.15	124.40
1	B	195	ARG	CG-CD-NE	-6.18	98.41	112.00
1	B	306	ALA	N-CA-C	-5.89	105.95	113.02
1	A	536	PHE	N-CA-C	5.16	119.11	112.41
1	A	130	PRO	O-C-N	5.08	123.54	121.15

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	4741	0	4663	41	0
1	B	4767	0	4716	39	0
2	C	32	0	11	0	0
3	A	15	0	17	0	0
4	A	32	0	44	18	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	572	0	0	8	0
6	B	408	0	0	2	0
All	All	10569	0	9451	80	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 4.

All (80) 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:B:411[B]:LYS:NZ	1:B:411[B]:LYS:CE	1.77	1.45
1:B:272[B]:ARG:HH11	1:B:275:GLN:HE22	1.17	0.93
1:A:256:GLY:H	4:A:1262[B]:1PE:H252	1.35	0.92
1:B:315:MET:HE3	1:B:324[A]:ILE:CD1	2.00	0.92
1:B:315:MET:HE3	1:B:324[A]:ILE:HD13	1.50	0.92
1:A:105:ARG:H	4:A:1262[B]:1PE:H242	1.35	0.89
1:A:263:LYS:HE2	4:A:1262[B]:1PE:H261	1.64	0.79
1:A:314:MET:HA	1:A:434:ILE:HD11	1.66	0.78
1:A:105:ARG:H	4:A:1262[B]:1PE:C24	2.00	0.75
1:B:272[B]:ARG:HH11	1:B:275:GLN:NE2	1.84	0.74
1:A:256:GLY:H	4:A:1262[A]:1PE:H151	1.52	0.73
1:B:472:GLY:HA3	1:B:530:LEU:HD12	1.70	0.71
1:B:272[B]:ARG:NH1	1:B:275:GLN:HE22	1.87	0.71
1:B:314:MET:HA	1:B:434:ILE:HD11	1.73	0.69
1:A:104:ALA:HB1	4:A:1262[A]:1PE:H241	1.76	0.68
1:A:256:GLY:N	4:A:1262[B]:1PE:H252	2.06	0.68
1:B:545[A]:VAL:HG21	1:B:595:GLN:HB3	1.78	0.66
1:A:256:GLY:H	4:A:1262[A]:1PE:C15	2.09	0.64
1:A:263:LYS:CE	4:A:1262[B]:1PE:H261	2.31	0.61
1:A:78:LEU:CD1	1:A:188[A]:LEU:HD12	2.31	0.60
1:A:638:VAL:O	1:A:641:MET:HG2	2.03	0.59
1:B:195:ARG:HD2	6:B:1909:HOH:O	2.02	0.59
1:A:105:ARG:N	4:A:1262[B]:1PE:H242	2.14	0.58
1:B:480:ARG:HD2	6:B:1744:HOH:O	2.03	0.57
1:A:422:ASN:HD21	4:A:1262[B]:1PE:H142	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:GLY:HA3	4:A:1262[B]:1PE:H151	1.89	0.55
1:A:105:ARG:HB2	4:A:1262[B]:1PE:H231	1.89	0.55
1:B:195:ARG:HD3	1:B:349:ARG:HD3	1.89	0.54
1:B:317:PRO:HG3	1:B:324[B]:ILE:HG12	1.89	0.53
1:A:85:HIS:HE1	6:A:1904:HOH:O	1.91	0.53
1:A:105:ARG:HE	4:A:1262[A]:1PE:H262	1.74	0.53
1:B:592:ASP:OD1	1:B:594[B]:SER:OG	2.23	0.52
1:A:175:LYS:HD2	1:A:273:MET:HE1	1.92	0.52
1:A:266:ALA:HB1	1:A:331:ILE:HG21	1.91	0.52
1:B:638:VAL:O	1:B:641:MET:HG2	2.10	0.51
1:B:396[B]:THR:OG1	1:B:400:VAL:HG21	2.11	0.51
1:A:272:ARG:NH1	1:A:276[B]:GLN:HE22	2.08	0.51
1:A:256:GLY:N	4:A:1262[A]:1PE:H151	2.24	0.50
1:B:517:LEU:HD13	1:B:626:ASP:HB2	1.92	0.50
1:A:428:PRO:HB3	6:A:1970:HOH:O	2.12	0.50
1:B:59:ARG:NH2	1:B:60:GLU:OE2	2.45	0.49
1:A:424:ARG:HH22	4:A:1262[A]:1PE:H161	1.77	0.49
1:B:545[B]:VAL:HG12	1:B:596:LEU:HD23	1.94	0.49
1:B:601[A]:LYS:NZ	1:B:605:GLU:OE2	2.45	0.49
1:B:311:ASN:HD21	1:B:329:ASP:HB2	1.78	0.49
1:B:266:ALA:HB1	1:B:331:ILE:HG21	1.95	0.48
1:A:472:GLY:HA3	1:A:530:LEU:HD12	1.96	0.48
1:B:471:HIS:CE1	1:B:475:MET:HE3	2.48	0.48
1:A:256:GLY:H	4:A:1262[B]:1PE:C25	2.12	0.47
1:B:411[B]:LYS:NZ	1:B:411[B]:LYS:CD	2.71	0.47
1:B:179:GLN:HA	1:B:211:CYS:HB2	1.97	0.47
1:A:539:ASP:C	1:A:541:GLU:H	2.24	0.46
1:B:450:ILE:HB	1:B:530:LEU:HD22	1.98	0.45
1:A:600:GLU:HB3	6:A:2008:HOH:O	2.17	0.45
1:B:538:ARG:NH1	1:B:542:GLY:O	2.44	0.45
1:B:111:VAL:HG11	1:B:137:MET:HE3	1.99	0.44
1:A:587:GLY:C	1:A:589:PRO:HD3	2.42	0.44
1:A:481:SER:HA	6:A:2031:HOH:O	2.17	0.44
1:B:416:GLU:HG3	1:B:417:PRO:HD2	1.99	0.43
1:A:104:ALA:HB1	4:A:1262[B]:1PE:H241	2.00	0.43
1:B:469:TRP:CD1	1:B:520:GLY:HA3	2.53	0.43
1:A:349:ARG:CZ	6:A:1970:HOH:O	2.67	0.43
1:A:273:MET:HE3	6:A:2194:HOH:O	2.18	0.43
1:A:511:ARG:HD2	6:A:2021:HOH:O	2.20	0.42
1:B:195:ARG:HD3	1:B:349:ARG:CD	2.49	0.42
1:A:78:LEU:CD1	1:A:188[A]:LEU:CD1	2.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:LEU:HA	1:B:220:PRO:C	2.45	0.42
1:A:275:GLN:HE21	1:A:275:GLN:HB3	1.52	0.42
1:A:578:PRO:HD2	1:A:597:PHE:CE2	2.55	0.41
1:B:168:PRO:HA	1:B:169:PRO:HD3	1.94	0.41
1:B:304:PRO:HG3	1:B:479:MET:HE2	2.02	0.41
1:B:343:ARG:HH12	1:B:438:ARG:HH22	1.68	0.41
1:A:41:LEU:HA	1:A:42:PRO:HD3	1.96	0.41
1:A:85:HIS:HD2	6:A:1724:HOH:O	2.03	0.41
1:B:240:HIS:CE1	1:B:268:ARG:HD2	2.57	0.40
1:B:538:ARG:NH2	1:B:544:PHE:CZ	2.89	0.40
1:A:304:PRO:C	1:A:306:ALA:H	2.30	0.40
1:A:461:PRO:HG2	1:A:574:ILE:HD11	2.04	0.40
1:B:275:GLN:HE21	1:B:275:GLN:HB3	1.60	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	609/608 (100%)	595 (98%)	13 (2%)	1 (0%)	43	28
1	B	612/608 (101%)	599 (98%)	12 (2%)	1 (0%)	43	28
All	All	1221/1216 (100%)	1194 (98%)	25 (2%)	2 (0%)	43	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	GLY
1	B	255	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	510/499 (102%)	505 (99%)	5 (1%)	68	58
1	B	513/499 (103%)	507 (99%)	6 (1%)	63	51
All	All	1023/998 (102%)	1012 (99%)	11 (1%)	70	54

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	275	GLN
1	A	338[A]	ASP
1	A	338[B]	ASP
1	A	443[A]	GLU
1	A	443[B]	GLU
1	B	195	ARG
1	B	222	THR
1	B	275	GLN
1	B	305	SER
1	B	458	ARG
1	B	543	ARG

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	85	HIS
1	A	135	ASN
1	A	140	ASN
1	A	275	GLN
1	A	365	ASN
1	B	85	HIS
1	B	117	GLN
1	B	135	ASN
1	B	275	GLN
1	B	595	GLN
1	B	618	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](#)

2 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	TQY	C	1	2	20,20,21	1.80	3 (15%)	25,25,27	1.73	4 (16%)
2	FRU	C	2	2	11,12,12	0.87	1 (9%)	10,18,18	0.86	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	TQY	C	1	2	-	2/12/29/32	0/1/1/1
2	FRU	C	2	2	-	2/5/24/24	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	TQY	C11-C10	-5.12	1.26	1.51
2	C	1	TQY	C12-C11	-4.23	1.25	1.51
2	C	1	TQY	O6-C13	3.91	1.44	1.33
2	C	2	FRU	O2-C2	2.60	1.45	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	TQY	C12-C11-C10	6.82	175.05	115.25
2	C	1	TQY	C1-C2-C3	2.68	113.55	109.64
2	C	1	TQY	O6-C13-C7	2.47	119.36	111.83
2	C	1	TQY	O6-C13-O7	-2.29	117.90	123.63

There are no chirality outliers.

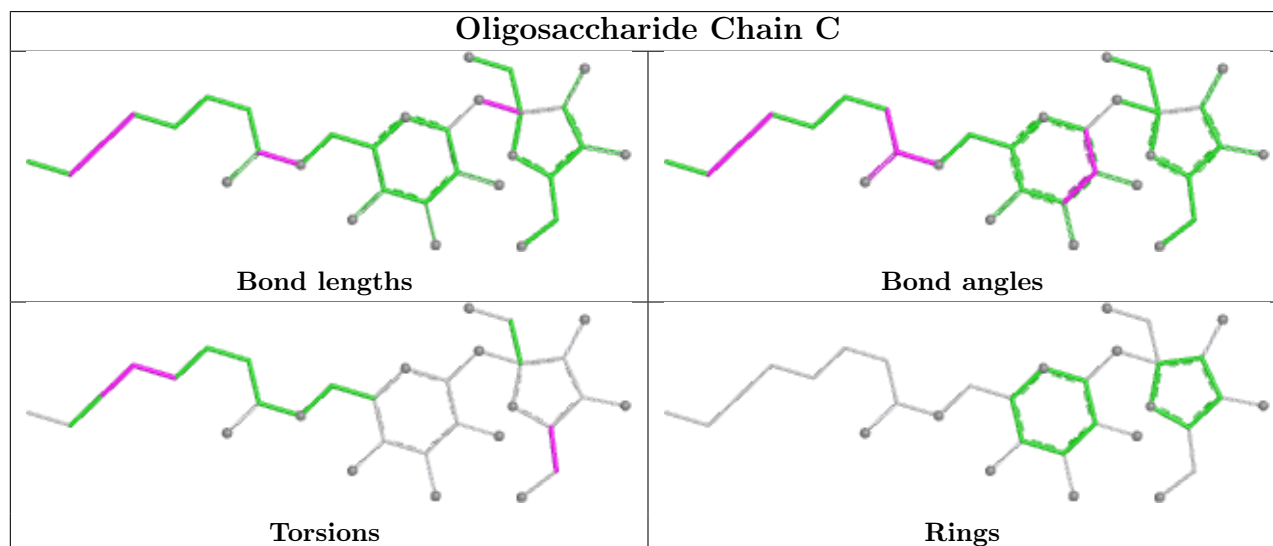
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	FRU	C4-C5-C6-O6
2	C	2	FRU	O5-C5-C6-O6
2	C	1	TQY	C9-C10-C11-C12
2	C	1	TQY	C11-C10-C9-C8

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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	EPE	A	1002	-	15,15,15	0.75	1 (6%)	19,20,20	1.78	4 (21%)
4	1PE	A	1262[A]	-	15,15,15	0.55	0	14,14,14	0.25	0
4	1PE	A	1262[B]	-	15,15,15	0.55	0	14,14,14	0.28	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	EPE	A	1002	-	-	2/9/19/19	0/1/1/1
4	1PE	A	1262[A]	-	-	11/13/13/13	-
4	1PE	A	1262[B]	-	-	9/13/13/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	EPE	C10-S	2.44	1.81	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	EPE	C5-N4-C3	4.73	119.02	108.84
3	A	1002	EPE	O2S-S-C10	3.90	112.62	106.73
3	A	1002	EPE	C7-N4-C5	2.57	118.10	111.24
3	A	1002	EPE	C7-N4-C3	2.39	117.60	111.24

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	EPE	C8-C7-N4-C3
4	A	1262[A]	1PE	OH5-C14-C24-OH4
4	A	1262[A]	1PE	OH4-C13-C23-OH3
4	A	1262[B]	1PE	OH7-C16-C26-OH6
4	A	1262[B]	1PE	OH5-C14-C24-OH4
4	A	1262[B]	1PE	OH4-C13-C23-OH3

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Mol	Chain	Res	Type	Atoms
4	A	1262[B]	1PE	OH2-C12-C22-OH3
4	A	1262[A]	1PE	OH6-C15-C25-OH5
4	A	1262[B]	1PE	C25-C15-OH6-C26
4	A	1262[A]	1PE	C13-C23-OH3-C22
4	A	1262[A]	1PE	OH2-C12-C22-OH3
4	A	1262[A]	1PE	C25-C15-OH6-C26
4	A	1262[A]	1PE	C12-C22-OH3-C23
4	A	1262[B]	1PE	C13-C23-OH3-C22
4	A	1262[A]	1PE	C14-C24-OH4-C13
4	A	1262[B]	1PE	OH6-C15-C25-OH5
4	A	1262[A]	1PE	C16-C26-OH6-C15
3	A	1002	EPE	N4-C7-C8-O8
4	A	1262[B]	1PE	C12-C22-OH3-C23
4	A	1262[A]	1PE	C23-C13-OH4-C24
4	A	1262[B]	1PE	C16-C26-OH6-C15
4	A	1262[A]	1PE	OH7-C16-C26-OH6

There are no ring outliers.

2 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1262[A]	1PE	6	0
4	A	1262[B]	1PE	12	0

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	596/608 (98%)	0.15	41 (6%) 23 25	8, 19, 33, 39	19 (3%)
1	B	596/608 (98%)	0.62	72 (12%) 8 8	11, 25, 35, 39	22 (3%)
All	All	1192/1216 (98%)	0.38	113 (9%) 14 14	8, 22, 34, 39	41 (3%)

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	407	GLY	7.5
1	B	415	PRO	6.5
1	B	405	TRP	6.5
1	B	398	PRO	6.4
1	B	385	GLY	6.3
1	B	379	VAL	6.2
1	B	387	VAL	6.1
1	B	403	THR	6.0
1	A	311[A]	ASN	5.8
1	A	310	THR	5.7
1	B	399	GLY	5.6
1	B	401	THR	5.6
1	B	381	LEU	5.4
1	B	400	VAL	5.4
1	B	409	PRO	5.3
1	B	392	LEU	5.3
1	A	309	LYS	5.1
1	B	418	CYS	4.9
1	B	419	ALA	4.9
1	B	406	LEU	4.8
1	A	305	SER	4.8
1	B	411[A]	LYS	4.7
1	B	389	TRP	4.7
1	B	380	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	402	TYR	4.6
1	A	308	GLY	4.5
1	B	377	THR	4.5
1	A	581	GLY	4.4
1	B	388	TYR	4.4
1	B	410	TRP	4.3
1	A	306	ALA	4.3
1	B	378	ASN	4.3
1	A	585	LEU	4.0
1	B	395	PRO	4.0
1	B	423	SER	4.0
1	A	312	LEU	3.9
1	B	383	SER	3.9
1	B	422	ASN	3.9
1	B	404	SER	3.9
1	B	417	PRO	3.8
1	B	305	SER	3.7
1	B	386	GLY	3.7
1	B	413	GLY	3.6
1	B	574	ILE	3.6
1	B	414	ASP	3.6
1	A	313	ALA	3.6
1	A	587	GLY	3.6
1	B	396[A]	THR	3.5
1	A	583	LEU	3.5
1	B	397[A]	GLU	3.5
1	A	481	SER	3.5
1	A	314	MET	3.4
1	A	593	TYR	3.4
1	A	588	LEU	3.4
1	A	597	PHE	3.4
1	B	494	LEU	3.4
1	A	590	GLY	3.4
1	A	578	PRO	3.3
1	B	313	ALA	3.3
1	B	368	ALA	3.3
1	B	384	ASP	3.2
1	A	596	LEU	3.2
1	A	324	ILE	3.2
1	B	366	ALA	3.2
1	A	591	VAL	3.2
1	B	420	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	316	THR	3.2
1	B	421	PRO	3.1
1	B	424	ARG	3.0
1	B	369	THR	3.0
1	A	586	GLY	3.0
1	A	589	PRO	3.0
1	B	361[A]	ARG	2.9
1	B	391	GLY	2.8
1	B	481	SER	2.8
1	B	365	ASN	2.8
1	A	584	ASP	2.8
1	B	394	GLU	2.8
1	B	382	ARG	2.7
1	A	317	PRO	2.7
1	B	390	ASP	2.7
1	A	582	ASP	2.7
1	B	370	ILE	2.7
1	A	140	ASN	2.6
1	B	341	ARG	2.6
1	B	362	THR	2.6
1	A	494	LEU	2.5
1	B	416	GLU	2.5
1	A	540	ASN	2.4
1	A	594[A]	SER	2.4
1	B	358	THR	2.4
1	B	202	GLN	2.4
1	B	364	PRO	2.4
1	A	322	TRP	2.4
1	B	393	ASP	2.4
1	A	197	GLY	2.3
1	B	306	ALA	2.3
1	B	408	LYS	2.3
1	B	371	ALA	2.3
1	B	359	SER	2.2
1	A	318	SER	2.2
1	B	206	ASP	2.2
1	B	360[A]	SER	2.2
1	B	412	HIS	2.1
1	B	540	ASN	2.1
1	A	592	ASP	2.1
1	A	579	LYS	2.1
1	A	599	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	198	PRO	2.1
1	A	522	ARG	2.1
1	B	69	GLU	2.1
1	B	312	LEU	2.0
1	A	315	MET	2.0

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

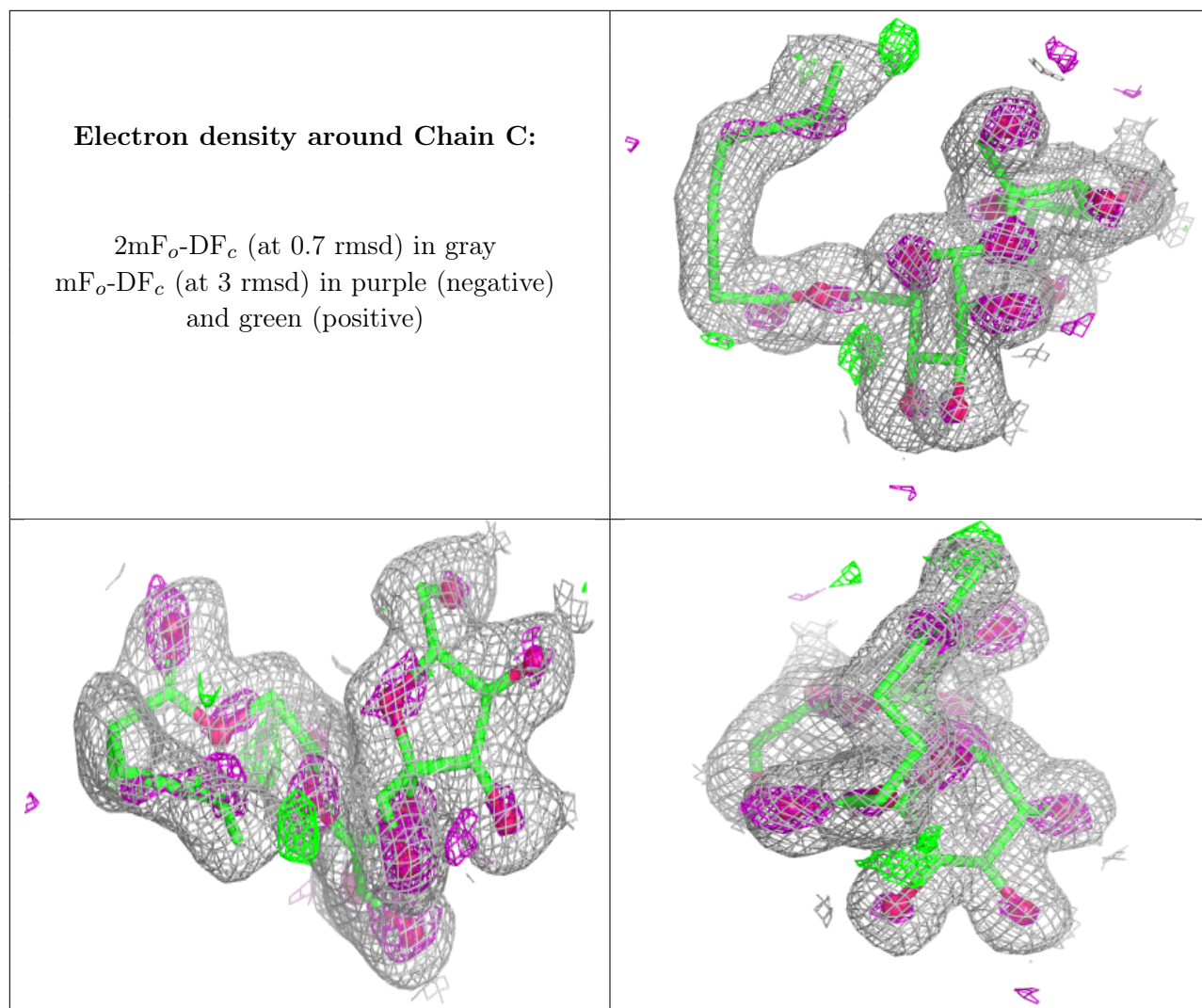
There are no non-standard protein/DNA/RNA residues in this entry.

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(Å ²)	Q<0.9
2	TQY	C	1	20/21	0.95	0.09	17,20,29,30	0
2	FRU	C	2	12/12	0.96	0.07	16,18,21,24	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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	1PE	A	1262[A]	16/16	0.61	0.23	21,28,33,34	16
4	1PE	A	1262[B]	16/16	0.61	0.23	27,30,34,34	16
3	EPE	A	1002	15/15	0.93	0.14	26,30,38,39	0
5	MN	B	1702	1/1	0.99	0.10	16,16,16,16	0
5	MN	A	1701	1/1	1.00	0.12	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.