



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:20 AM UTC

PDB ID : 2QZY / pdb_00002qzy
Title : The structure of chicken mitochondrial PEPCK in complex with PEP
Authors : Holyoak, T.; Sullivan, S.M.; Nowak, T.
Deposited on : 2007-08-17
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
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

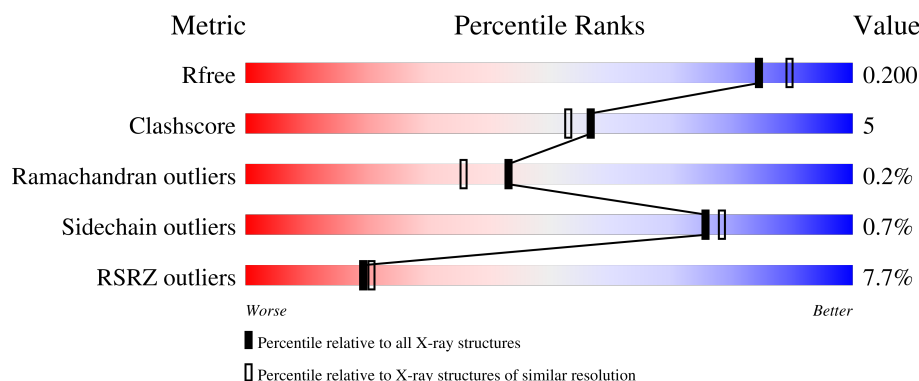
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	608	5% 89% 8% ..
1	B	608	10% 88% 10% .
2	C	2	50% 50%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10506 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 [GTP].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	15	0
			4746	3019	853	841	33			
1	B	597	Total	C	N	O	S	0	6	0
			4695	2981	841	840	33			

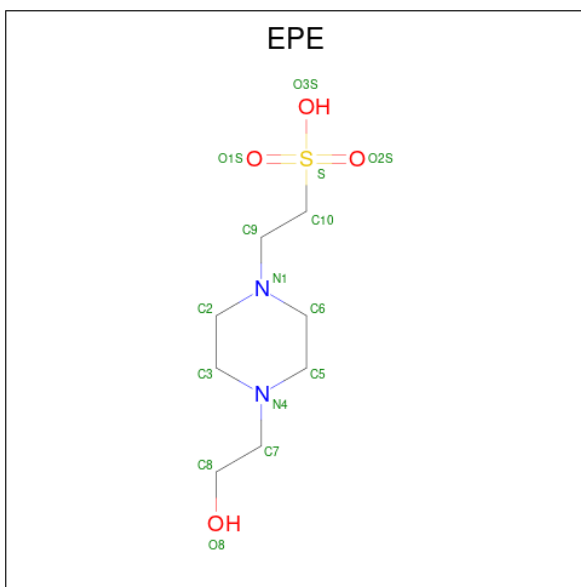
There are 12 discrepancies between the modelled and reference sequences:

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	131	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
2	C	2	Total	C	O	0	0	0
			32	20	12			

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

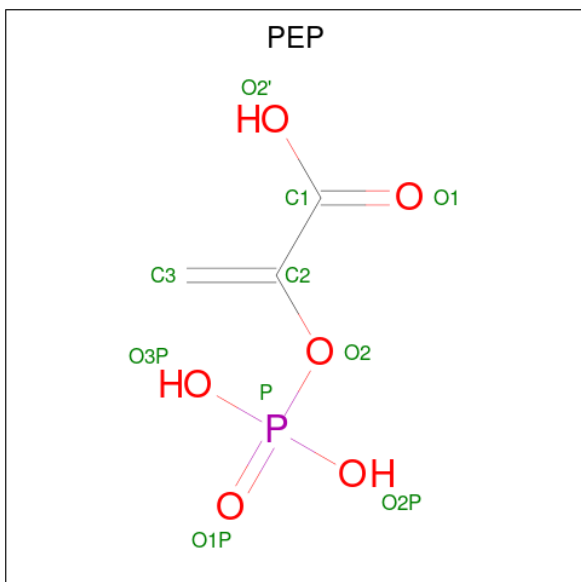


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 5 is PHOSPHOENOLPYRUVATE (CCD ID: PEP) (formula: C₃H₅O₆P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			10	3	6	1		
5	B	1	Total	C	O	P	0	0
			10	3	6	1		

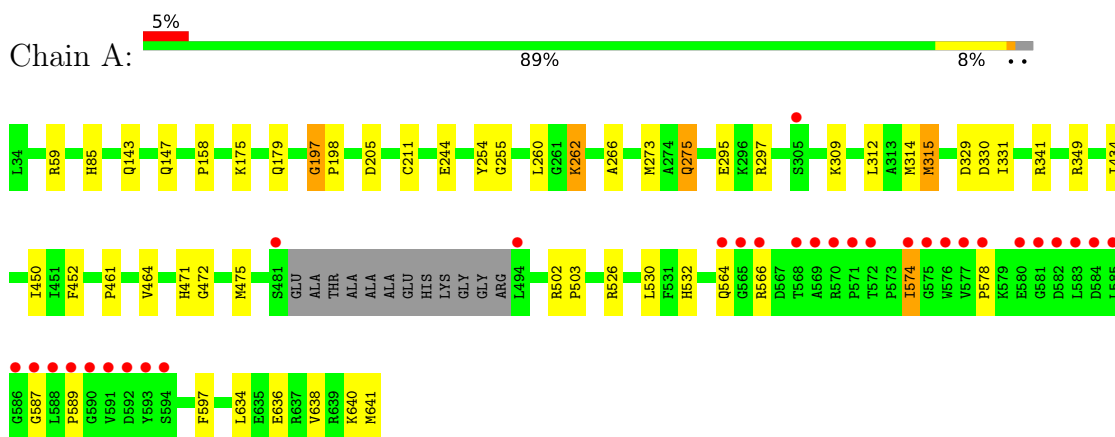
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	584	Total	O	0	0
			584	584		
6	B	412	Total	O	0	0
			412	412		

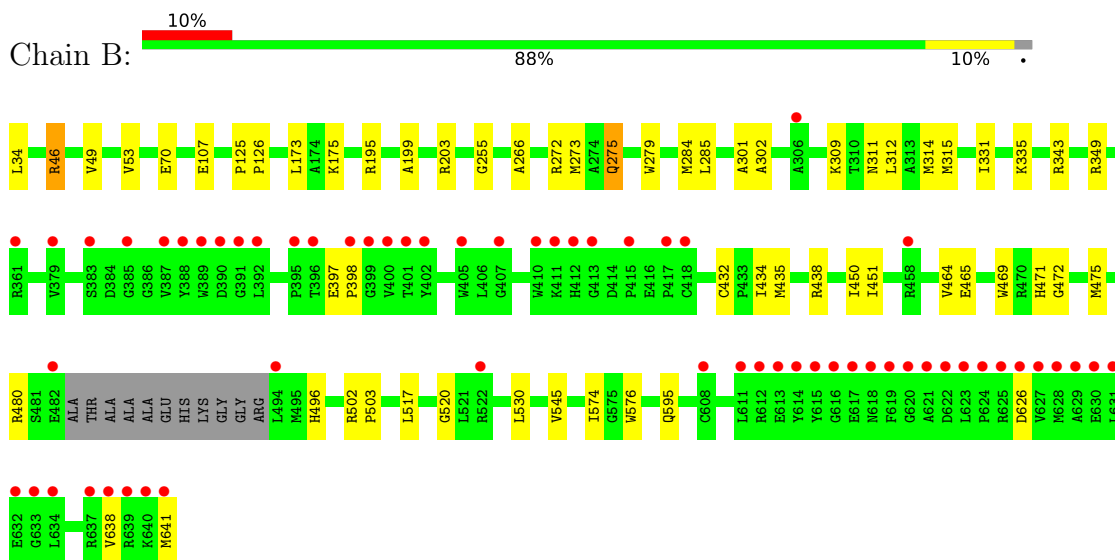
3 Residue-property plots

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 [GTP]



- Molecule 1: Phosphoenolpyruvate carboxykinase [GTP]



- 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	110.35Å 48.02Å 126.32Å 90.00° 111.39° 90.00°	Depositor
Resolution (Å)	35.09 – 1.90 35.09 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.8 (35.09-1.90) 97.8 (35.09-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 1.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.161 , 0.200 0.161 , 0.200	Depositor DCC
R_{free} test set	4789 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	18.6	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10506	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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: PEP, MN, EPE, FRU, TQY

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	0.61	0/4933	0.79	3/6708 (0.0%)
1	B	0.54	0/4854	0.77	1/6603 (0.0%)
All	All	0.58	0/9787	0.78	4/13311 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	GLY	CA-C-N	7.34	129.02	119.84
1	A	197	GLY	C-N-CA	7.34	129.02	119.84
1	B	398	PRO	CA-C-O	5.34	127.75	121.56
1	A	262	LYS	N-CA-C	5.16	116.60	111.07

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	4746	0	4683	48	0
1	B	4695	0	4595	38	0
2	C	32	0	11	0	0
3	A	15	0	17	0	0
4	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	A	10	0	2	0	0
5	B	10	0	2	0	0
6	A	584	0	0	9	0
6	B	412	0	0	1	0
All	All	10506	0	9310	86	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 5.

All (86) 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:464[A]:VAL:HG11	1:A:574[A]:ILE:HD12	1.31	1.11
1:A:464[A]:VAL:HG21	1:A:574[A]:ILE:HD11	1.31	1.09
1:A:464[A]:VAL:CG2	1:A:574[A]:ILE:HD11	1.93	0.97
1:A:464[A]:VAL:HG21	1:A:574[A]:ILE:CD1	1.94	0.97
1:B:173:LEU:HD21	1:B:335:LYS:HB2	1.59	0.83
1:A:464[A]:VAL:HG11	1:A:574[A]:ILE:CD1	2.09	0.82
1:B:195:ARG:HD3	1:B:349:ARG:HD3	1.61	0.81
1:B:46:ARG:HH11	1:B:46:ARG:HG3	1.47	0.78
1:B:279:TRP:HB3	1:B:335:LYS:HG2	1.67	0.77
1:B:312:LEU:HD12	1:B:315:MET:HE2	1.64	0.76
1:A:341:ARG:HD2	6:A:1282:HOH:O	1.85	0.76
1:A:314:MET:HA	1:A:434:ILE:HD11	1.73	0.69
1:A:312:LEU:HD12	1:A:315:MET:HE2	1.74	0.69
1:B:107[B]:GLU:OE2	6:B:1391:HOH:O	2.11	0.67
1:B:46:ARG:HH11	1:B:46:ARG:CG	2.06	0.67
1:B:195:ARG:HD3	1:B:349:ARG:CD	2.24	0.67
1:B:472:GLY:HA3	1:B:530:LEU:HD12	1.78	0.65
1:A:295[A]:GLU:OE2	1:A:564[A]:GLN:CD	2.39	0.65
1:B:314:MET:HA	1:B:434:ILE:HD11	1.81	0.63
1:A:295[A]:GLU:OE2	1:A:564[A]:GLN:NE2	2.33	0.62
1:B:46:ARG:HG3	1:B:46:ARG:NH1	2.09	0.61
1:B:545:VAL:HG21	1:B:595:GLN:HB3	1.84	0.59
1:A:295[A]:GLU:OE2	1:A:564[A]:GLN:OE1	2.21	0.59
1:A:638:VAL:O	1:A:641:MET:HG2	2.03	0.58
1:A:464[A]:VAL:CG1	1:A:574[A]:ILE:HD12	2.22	0.56
1:A:143[A]:GLN:HE21	1:A:147:GLN:HE21	1.55	0.55
1:B:173:LEU:HD21	1:B:335:LYS:CB	2.35	0.54
1:B:471:HIS:CE1	1:B:475:MET:HE3	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464[A]:VAL:CG1	1:A:574[A]:ILE:CD1	2.83	0.54
1:A:341:ARG:HD3	1:A:526:ARG:CZ	2.37	0.53
1:B:450:ILE:HB	1:B:530:LEU:HD22	1.89	0.53
1:B:343:ARG:HH12	1:B:438:ARG:HH22	1.57	0.52
1:B:175:LYS:HD2	1:B:273:MET:HE1	1.91	0.52
1:A:266:ALA:HB1	1:A:331:ILE:HG21	1.91	0.51
1:A:461:PRO:HG2	1:A:574[B]:ILE:HD11	1.92	0.50
1:B:480:ARG:HD2	1:B:496:HIS:CE1	2.47	0.50
1:A:636:GLU:HG3	1:A:640[B]:LYS:HE2	1.93	0.49
1:B:465:GLU:HB3	1:B:576:TRP:HB2	1.94	0.49
1:A:85:HIS:HD2	6:A:1111:HOH:O	1.96	0.49
1:A:85:HIS:HE1	6:A:1318:HOH:O	1.95	0.49
1:B:311:ASN:HD22	1:B:311:ASN:H	1.62	0.48
1:B:517:LEU:HD13	1:B:626:ASP:HB2	1.95	0.48
1:B:285:LEU:HD23	1:B:309:LYS:HG3	1.95	0.48
1:A:244:GLU:HG2	6:A:1612:HOH:O	2.14	0.48
1:B:469:TRP:CD1	1:B:520:GLY:HA3	2.49	0.48
1:A:275:GLN:HE21	1:A:275:GLN:HB3	1.56	0.47
1:B:199:ALA:O	1:B:203:ARG:HG3	2.15	0.47
1:A:464[A]:VAL:CG2	1:A:574[A]:ILE:CD1	2.72	0.46
1:A:309:LYS:HE2	1:A:329:ASP:O	2.15	0.46
1:B:311:ASN:H	1:B:311:ASN:ND2	2.14	0.46
1:A:205:ASP:HB2	6:A:1591:HOH:O	2.15	0.46
1:B:638:VAL:O	1:B:641:MET:HG2	2.15	0.46
1:B:464:VAL:HG11	1:B:574[A]:ILE:HG22	1.98	0.45
1:B:34:LEU:HG	1:B:70:GLU:HG3	1.99	0.45
1:A:450:ILE:HB	1:A:530:LEU:CD2	2.46	0.45
1:A:472:GLY:HA3	1:A:530:LEU:HD12	1.99	0.45
1:A:59:ARG:HH21	1:A:158:PRO:HG3	1.82	0.44
1:B:275:GLN:HE21	1:B:275:GLN:HB3	1.60	0.44
1:A:175:LYS:HD2	1:A:273:MET:HE1	2.00	0.44
1:A:502:ARG:HB3	1:A:503:PRO:HD3	1.98	0.44
1:A:526:ARG:HD2	6:A:1616:HOH:O	2.18	0.43
1:A:349:ARG:CZ	6:A:1440:HOH:O	2.66	0.43
1:A:634:LEU:O	1:A:638:VAL:HG23	2.19	0.43
1:A:452:PHE:O	1:A:532:HIS:HA	2.19	0.43
1:A:179:GLN:HA	1:A:211:CYS:HB2	2.01	0.42
1:A:197:GLY:HA3	1:A:198:PRO:HD2	1.83	0.42
1:A:450:ILE:HB	1:A:530:LEU:HD23	2.01	0.42
1:A:566:ARG:HD2	6:A:1604:HOH:O	2.19	0.42
1:B:266:ALA:HB1	1:B:331:ILE:HG21	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:CYS:HB3	1:B:435:MET:HG2	2.02	0.42
1:A:262:LYS:NZ	1:A:330:ASP:OD2	2.39	0.41
1:B:301:ALA:HA	1:B:451:ILE:O	2.20	0.41
1:A:578:PRO:HD2	1:A:597:PHE:CE2	2.55	0.41
1:A:143[A]:GLN:NE2	1:A:147:GLN:HE21	2.18	0.41
1:B:125:PRO:HA	1:B:126:PRO:HD3	1.94	0.41
1:A:349:ARG:NH2	6:A:1440:HOH:O	2.53	0.41
1:B:285:LEU:HD21	1:B:312:LEU:HD23	2.03	0.41
1:B:312:LEU:CD1	1:B:315:MET:HE2	2.45	0.41
1:B:502:ARG:HB3	1:B:503:PRO:HD3	2.03	0.41
1:A:587:GLY:C	1:A:589:PRO:HD3	2.46	0.40
1:B:49:VAL:O	1:B:53:VAL:HG23	2.21	0.40
1:A:297:ARG:NE	1:A:564[A]:GLN:OE1	2.54	0.40
1:A:211:CYS:HB3	1:A:260:LEU:HD12	2.03	0.40
1:B:284:MET:HG2	1:B:302:ALA:HB2	2.04	0.40
1:A:471:HIS:CE1	1:A:475:MET:HE3	2.56	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	607/608 (100%)	594 (98%)	12 (2%)	1 (0%)	43	36
1	B	599/608 (98%)	587 (98%)	11 (2%)	1 (0%)	43	36
All	All	1206/1216 (99%)	1181 (98%)	23 (2%)	2 (0%)	43	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	GLY
1	B	255	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	508/499 (102%)	504 (99%)	4 (1%)	73	75
1	B	500/499 (100%)	496 (99%)	4 (1%)	73	75
All	All	1008/998 (101%)	1000 (99%)	8 (1%)	76	75

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	275	GLN
1	A	315	MET
1	A	574[A]	ILE
1	A	574[B]	ILE
1	B	46	ARG
1	B	272	ARG
1	B	275	GLN
1	B	397	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	A	117	GLN
1	A	132	GLN
1	A	135	ASN
1	A	140	ASN
1	A	275	GLN
1	A	540	ASN
1	B	85	HIS
1	B	135	ASN
1	B	275	GLN
1	B	311	ASN
1	B	412	HIS
1	B	496	HIS
1	B	524	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	595	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 ⓘ

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	1.01	1 (5%)	25,25,27	0.95	2 (8%)
2	FRU	C	2	2	11,12,12	0.70	0	10,18,18	0.69	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	-	3/12/29/32	0/1/1/1
2	FRU	C	2	2	-	2/5/24/24	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	TQY	O6-C13	3.93	1.44	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	TQY	O6-C13-C7	2.40	119.16	111.83
2	C	1	TQY	O6-C13-O7	-2.21	118.11	123.63

There are no chirality outliers.

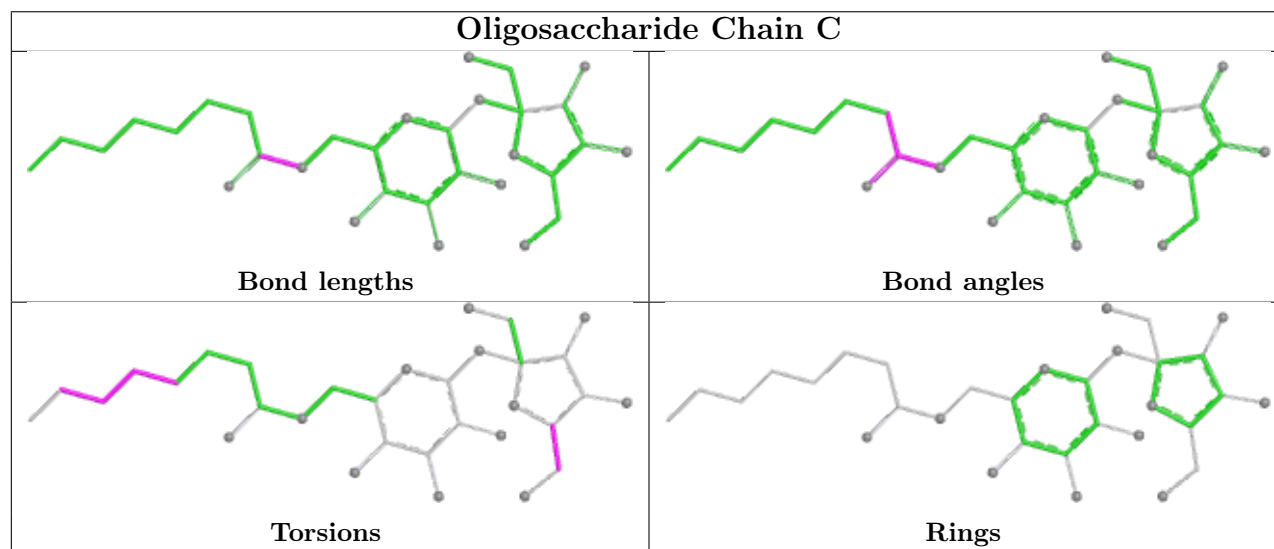
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	TQY	C9-C10-C11-C12
2	C	1	TQY	C11-C10-C9-C8
2	C	1	TQY	C10-C11-C12-C31
2	C	2	FRU	C4-C5-C6-O6
2	C	2	FRU	O5-C5-C6-O6

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
5	PEP	A	1102	-	9,9,9	1.49	2 (22%)	11,13,13	1.37	2 (18%)
3	EPE	A	1002	-	15,15,15	0.81	1 (6%)	19,20,20	1.61	3 (15%)
5	PEP	B	1202	-	9,9,9	1.55	2 (22%)	11,13,13	1.20	1 (9%)

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
5	PEP	A	1102	-	-	0/9/9/9	-
3	EPE	A	1002	-	-	1/9/19/19	0/1/1/1
5	PEP	B	1202	-	-	0/9/9/9	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1202	PEP	C2-C1	-2.85	1.46	1.49
3	A	1002	EPE	C10-S	2.70	1.81	1.77
5	A	1102	PEP	C2-C1	-2.60	1.46	1.49
5	B	1202	PEP	O2-C2	2.44	1.45	1.39
5	A	1102	PEP	O2-C2	2.28	1.45	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	EPE	C5-N4-C3	4.92	119.44	108.84
5	A	1102	PEP	O3P-P-O2	-2.84	97.04	105.32
3	A	1002	EPE	C7-N4-C5	2.09	116.81	111.24
3	A	1002	EPE	O3S-S-C10	2.08	110.07	106.00
5	A	1102	PEP	O3P-P-O2P	2.07	115.57	107.80
5	B	1202	PEP	O2-P-O1P	-2.04	102.94	109.47

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	EPE	C8-C7-N4-C3

There are no ring outliers.

No monomer is involved in short contacts.

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	596/608 (98%)	0.28	31 (5%)	33 35	8, 18, 24, 31	15 (2%)
1	B	597/608 (98%)	0.64	61 (10%)	12 12	9, 18, 24, 30	6 (1%)
All	All	1193/1216 (98%)	0.46	92 (7%)	19 21	8, 18, 24, 31	21 (1%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	581	GLY	6.7
1	A	588	LEU	5.7
1	A	564[A]	GLN	5.5
1	B	629	ALA	5.4
1	A	585	LEU	5.3
1	B	638	VAL	5.1
1	B	641	MET	4.9
1	A	568	THR	4.9
1	B	627	VAL	4.9
1	B	398	PRO	4.9
1	A	586	GLY	4.8
1	B	400	VAL	4.8
1	A	583	LEU	4.6
1	B	623	LEU	4.5
1	B	389	TRP	4.5
1	A	593	TYR	4.5
1	B	631	LEU	4.4
1	A	587	GLY	4.4
1	A	584	ASP	4.4
1	A	569	ALA	4.4
1	A	590	GLY	4.3
1	A	591	VAL	4.3
1	B	616	GLY	4.3
1	A	577	VAL	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	565	GLY	4.2
1	B	388	TYR	4.1
1	B	615	TYR	4.1
1	A	481	SER	4.1
1	B	385	GLY	3.9
1	B	621	ALA	3.9
1	B	622	ASP	3.7
1	B	413	GLY	3.7
1	B	401	THR	3.6
1	B	628	MET	3.6
1	B	640	LYS	3.5
1	B	392	LEU	3.5
1	B	418	CYS	3.5
1	B	608	CYS	3.5
1	B	634	LEU	3.5
1	B	611	LEU	3.4
1	B	619	PHE	3.4
1	A	589	PRO	3.4
1	B	639	ARG	3.4
1	B	614	TYR	3.3
1	B	625	ARG	3.3
1	A	594	SER	3.3
1	B	618	ASN	3.3
1	B	402	TYR	3.3
1	A	592	ASP	3.2
1	B	624	PRO	3.2
1	B	620	GLY	3.2
1	B	405	TRP	3.1
1	A	305	SER	3.1
1	B	379	VAL	3.1
1	A	578	PRO	3.1
1	A	576	TRP	3.0
1	B	494	LEU	3.0
1	B	395	PRO	2.9
1	B	630	GLU	2.9
1	B	396	THR	2.9
1	A	571	PRO	2.9
1	A	582	ASP	2.9
1	B	632	GLU	2.8
1	A	574[A]	ILE	2.8
1	B	391	GLY	2.8
1	B	387	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	580	GLU	2.8
1	B	613	GLU	2.8
1	B	626	ASP	2.8
1	B	399	GLY	2.7
1	B	390	ASP	2.6
1	A	572	THR	2.6
1	B	633	GLY	2.6
1	A	570	ARG	2.6
1	B	306	ALA	2.6
1	B	412	HIS	2.6
1	A	566	ARG	2.6
1	B	415	PRO	2.5
1	A	494	LEU	2.4
1	B	637	ARG	2.4
1	B	411	LYS	2.4
1	B	617	GLU	2.3
1	B	361	ARG	2.3
1	B	417	PRO	2.3
1	B	407	GLY	2.2
1	B	383	SER	2.2
1	B	410	TRP	2.1
1	B	612	ARG	2.1
1	B	458	ARG	2.1
1	B	482	GLU	2.0
1	B	522	ARG	2.0
1	A	575	GLY	2.0

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

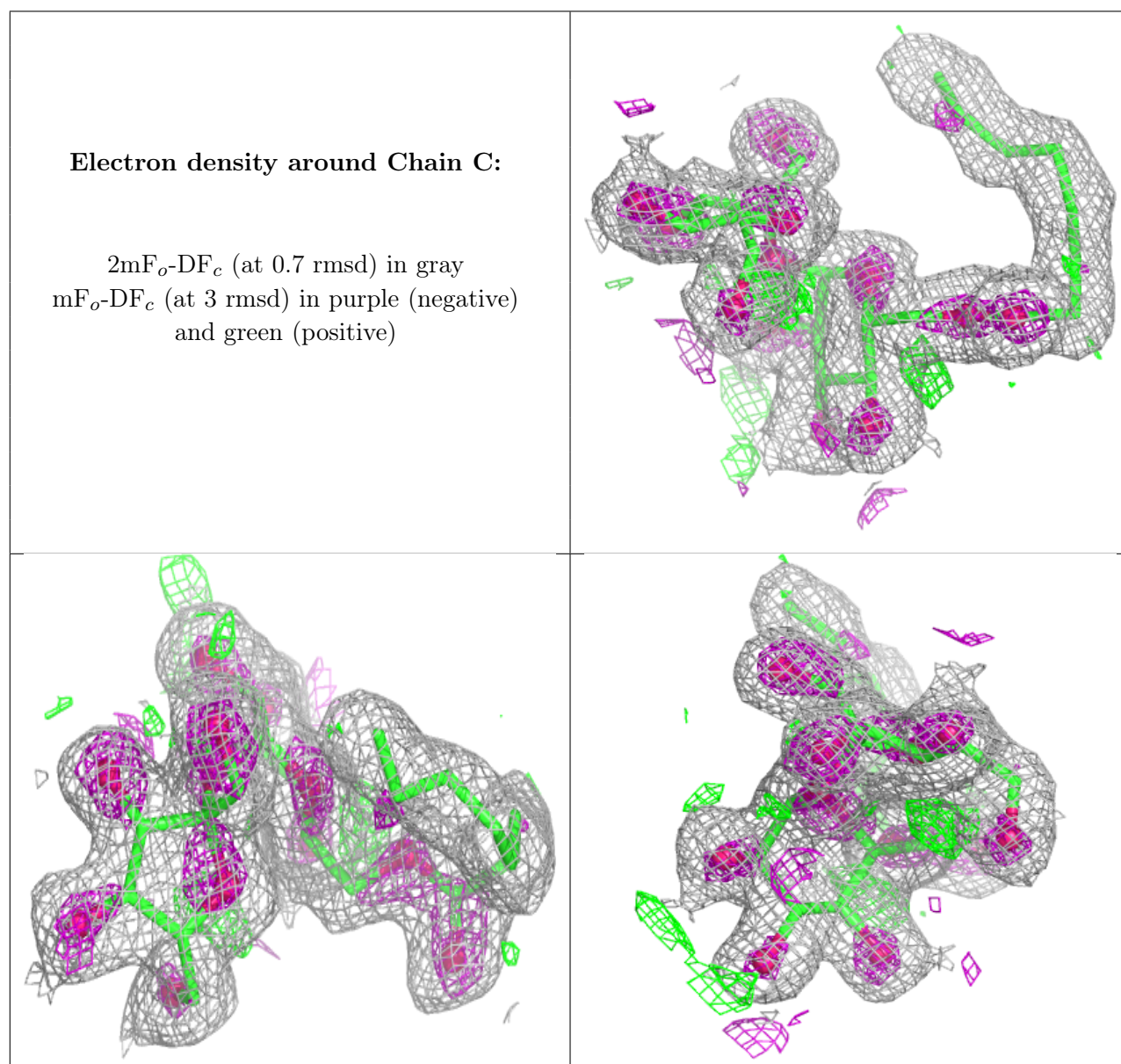
There are no non-standard protein/DNA/RNA residues in this entry.

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	0.08	9,12,22,24	0
2	FRU	C	2	12/12	0.96	0.07	10,12,16,17	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
3	EPE	A	1002	15/15	0.92	0.13	22,27,37,40	0
5	PEP	B	1202	10/10	0.94	0.13	17,21,23,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PEP	A	1102	10/10	0.95	0.12	11,13,14,14	10
4	MN	A	1101	1/1	0.99	0.17	8,8,8,8	0
4	MN	B	1201	1/1	0.99	0.16	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.