



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:26 PM UTC

PDB ID : 4RT6 / pdb_00004rt6
Title : Structure of a complex between hemopexin and hemopexin binding protein
Authors : Zambolin, S.; Clantin, B.; Haouz, A.; Villeret, V.; Delepelaire, P.
Deposited on : 2014-11-13
Resolution : 2.80 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)
Xtrriage (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

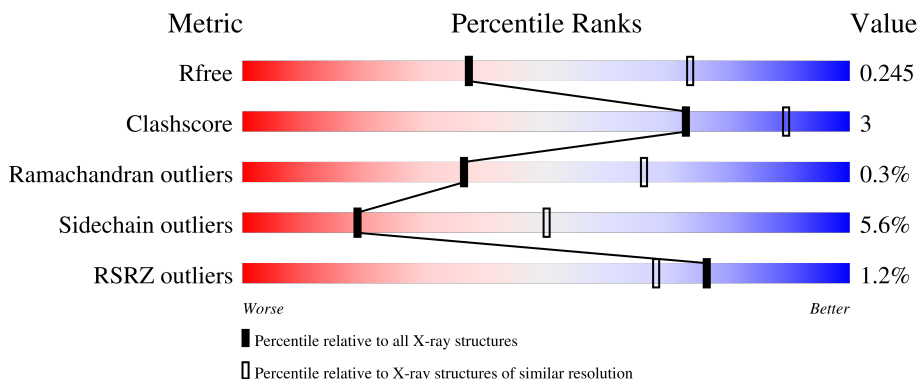
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	884	
2	B	214	
3	C	2	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7841 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 Heme/hemopexin-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	805	6204	3833	1107	1252	12	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	855	SER	CYS	engineered mutation	UNP P44602
A	861	SER	CYS	engineered mutation	UNP P44602

- Molecule 2 is a protein called Hemopexin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	172	1417	918	237	255	7	0	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	2	28	16	2	10	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	174	Total	O	0	0
			174	174		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	18	Total	O	0	0
			18	18		

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	45.06Å 348.86Å 77.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.43 – 2.80 24.43 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.0 (24.43-2.80) 96.1 (24.43-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.80Å)	Xtrriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.180 , 0.230 0.195 , 0.245	Depositor DCC
R_{free} test set	1517 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	51.7	Xtrriage
Anisotropy	0.095	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 65.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7841	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: NAG

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	0.84	2/6276 (0.0%)	1.16	27/8448 (0.3%)
2	B	0.81	0/1464	1.21	2/1984 (0.1%)
All	All	0.83	2/7740 (0.0%)	1.17	29/10432 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	629	MET	SD-CE	-6.52	1.63	1.79
1	A	662	ILE	CG1-CD1	-6.08	1.28	1.51

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	571	GLY	CA-C-N	7.84	133.24	122.19
1	A	571	GLY	C-N-CA	7.84	133.24	122.19
1	A	789	PHE	CA-C-N	7.37	132.40	120.60
1	A	789	PHE	C-N-CA	7.37	132.40	120.60
2	B	164	ASN	CA-CB-CG	6.84	119.44	112.60
1	A	225	ASP	CA-CB-CG	6.41	119.01	112.60
1	A	304	ASP	CA-CB-CG	6.39	118.99	112.60
1	A	55	ASP	CA-CB-CG	6.22	118.82	112.60
2	B	130	GLU	N-CA-C	-6.21	104.42	112.68
1	A	343	THR	N-CA-C	-6.11	102.30	110.55
1	A	740	ALA	CA-C-N	5.94	130.60	122.34
1	A	740	ALA	C-N-CA	5.94	130.60	122.34
1	A	518	ASN	CA-C-N	5.93	133.00	122.45
1	A	518	ASN	C-N-CA	5.93	133.00	122.45
1	A	551	ASP	CA-CB-CG	5.67	118.27	112.60
1	A	194	GLU	CB-CG-CD	5.54	122.02	112.60
1	A	767	GLY	CA-C-N	5.45	131.78	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	767	GLY	C-N-CA	5.45	131.78	121.97
1	A	456	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	328	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	425	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	115	GLU	CA-C-N	5.18	127.48	120.44
1	A	115	GLU	C-N-CA	5.18	127.48	120.44
1	A	708	GLY	CA-C-N	5.10	128.95	120.94
1	A	708	GLY	C-N-CA	5.10	128.95	120.94
1	A	154	ASN	CA-CB-CG	5.05	117.66	112.60
1	A	807	ALA	CA-C-N	5.04	127.00	120.44
1	A	807	ALA	C-N-CA	5.04	127.00	120.44
1	A	727	ALA	N-CA-C	-5.01	102.87	110.28

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	6204	0	6167	29	0
2	B	1417	0	1317	20	0
3	C	28	0	25	0	0
4	A	174	0	0	4	0
4	B	18	0	0	0	0
All	All	7841	0	7509	48	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 3.

All (48) 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:239:VAL:HG22	4:A:1061:HOH:O	1.79	0.80
2:B:28:SER:HB2	2:B:31:TRP:HB2	1.79	0.64
1:A:768:VAL:HG12	1:A:768:VAL:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:HIS:CE1	2:B:125:GLU:HB2	2.35	0.61
1:A:603:LEU:HD11	1:A:629:MET:HE1	1.88	0.56
2:B:92:LYS:HB2	2:B:94:TRP:CZ3	2.41	0.56
2:B:114:PRO:HD2	2:B:147:TRP:HH2	1.70	0.55
2:B:114:PRO:HD2	2:B:147:TRP:CH2	2.43	0.54
2:B:122:ALA:HB3	2:B:139:PHE:HB2	1.91	0.53
2:B:184:LEU:HA	2:B:197:TYR:CD1	2.45	0.52
1:A:514:VAL:CG1	1:A:572:ARG:HG3	2.40	0.52
1:A:438:ASN:HA	1:A:481:ASP:O	2.10	0.52
1:A:805:GLY:HA3	4:A:1047:HOH:O	2.10	0.51
1:A:100:VAL:O	1:A:147:ALA:HA	2.11	0.51
2:B:34:ASP:HB2	2:B:47:PHE:O	2.10	0.50
1:A:586:LYS:HE2	1:A:588:ASN:HB2	1.92	0.50
1:A:183:THR:HG22	1:A:184:LEU:H	1.77	0.50
1:A:128:LEU:HD11	1:A:194:GLU:HB2	1.95	0.49
2:B:108:SER:HB3	2:B:111:ASP:HB2	1.95	0.49
2:B:34:ASP:HB3	2:B:74:VAL:O	2.13	0.48
1:A:180:PHE:CZ	1:A:189:ILE:HD12	2.50	0.47
1:A:685:ASP:OD2	1:A:737:GLY:HA3	2.13	0.47
1:A:106:THR:HA	1:A:154:ASN:O	2.15	0.47
1:A:691:ALA:HA	1:A:747:GLU:O	2.15	0.46
2:B:32:SER:HA	2:B:180:GLY:HA2	1.96	0.46
1:A:727:ALA:O	1:A:728:ASN:HB2	2.16	0.46
1:A:432:ILE:O	1:A:475:MET:HA	2.16	0.45
1:A:337:ILE:HD11	1:A:370:LEU:HD21	1.98	0.45
1:A:367:LYS:HE2	1:A:369:ASN:OD1	2.16	0.45
1:A:453:GLU:H	1:A:453:GLU:HG3	1.56	0.45
1:A:736:ILE:CD1	1:A:770:ILE:HG12	2.47	0.44
2:B:145:TRP:NE1	2:B:156:GLU:HG3	2.33	0.43
1:A:88:ASN:HA	1:A:135:LYS:HE2	2.01	0.43
1:A:764:SER:HB2	1:A:770:ILE:HG13	2.01	0.43
2:B:135:GLY:HA2	2:B:149:LEU:HG	2.01	0.42
1:A:223:ALA:O	1:A:224:LEU:HB2	2.19	0.42
1:A:596:LEU:HD12	1:A:629:MET:HE3	2.02	0.42
2:B:65:GLU:H	2:B:65:GLU:HG3	1.59	0.42
2:B:157:ARG:HH11	2:B:159:TRP:HZ2	1.67	0.42
2:B:94:TRP:CE2	2:B:106:PRO:HB3	2.55	0.41
2:B:70:PHE:HE2	2:B:74:VAL:HG22	1.85	0.41
1:A:710:THR:HG23	1:A:729:ILE:HA	2.02	0.41
1:A:233:VAL:HG23	4:A:1039:HOH:O	2.21	0.41
2:B:24:ILE:HG23	2:B:25:GLU:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:720:PRO:HB2	2:B:197:TYR:OH	2.21	0.40
1:A:625:ASN:HA	1:A:657:ALA:O	2.21	0.40
2:B:39:ASP:HB3	2:B:45:LEU:HD11	2.04	0.40
1:A:548:ASN:HB2	4:A:974:HOH:O	2.21	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	795/884 (90%)	759 (96%)	33 (4%)	3 (0%)	30	60
2	B	164/214 (77%)	149 (91%)	15 (9%)	0	100	100
All	All	959/1098 (87%)	908 (95%)	48 (5%)	3 (0%)	36	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	768	VAL
1	A	737	GLY
1	A	224	LEU

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	690/756 (91%)	662 (96%)	28 (4%)	27 62
2	B	151/184 (82%)	132 (87%)	19 (13%)	4 15
All	All	841/940 (90%)	794 (94%)	47 (6%)	19 50

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	28	ASP
1	A	127	LYS
1	A	184	LEU
1	A	193	LEU
1	A	222	GLN
1	A	225	ASP
1	A	277	ILE
1	A	279	ILE
1	A	316	GLU
1	A	370	LEU
1	A	453	GLU
1	A	457	ASN
1	A	484	ASP
1	A	517	ASN
1	A	556	LYS
1	A	564	MET
1	A	568	LYS
1	A	572	ARG
1	A	684	THR
1	A	716	ILE
1	A	723	ILE
1	A	735	THR
1	A	738	ASP
1	A	768	VAL
1	A	790	ASN
1	A	791	GLN
1	A	813	ILE
2	B	26	GLN
2	B	51	PHE
2	B	65	GLU
2	B	66	ARG
2	B	80	HIS
2	B	83	THR
2	B	93	VAL

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Mol	Chain	Res	Type
2	B	112	GLU
2	B	124	VAL
2	B	131	CYS
2	B	137	LEU
2	B	150	THR
2	B	154	LYS
2	B	156	GLU
2	B	169	LEU
2	B	179	GLN
2	B	184	LEU
2	B	189	VAL
2	B	199	LEU

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	17	ASN
1	A	116	ASN
1	A	122	ASN
1	A	168	ASN
1	A	241	ASN
1	A	256	ASN
1	A	275	ASN
1	A	282	GLN
1	A	300	ASN
1	A	302	ASN
1	A	584	ASN
1	A	748	ASN
1	A	757	ASN
1	A	791	GLN
2	B	41	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

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
3	NAG	C	1	3,2	14,14,15	0.31	0	17,19,21	0.98	1 (5%)
3	NAG	C	2	3	14,14,15	0.34	0	17,19,21	0.71	1 (5%)

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	NAG	C	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C1-O5-C5	3.37	116.70	112.19
3	C	2	NAG	C1-O5-C5	2.10	115.00	112.19

There are no chirality outliers.

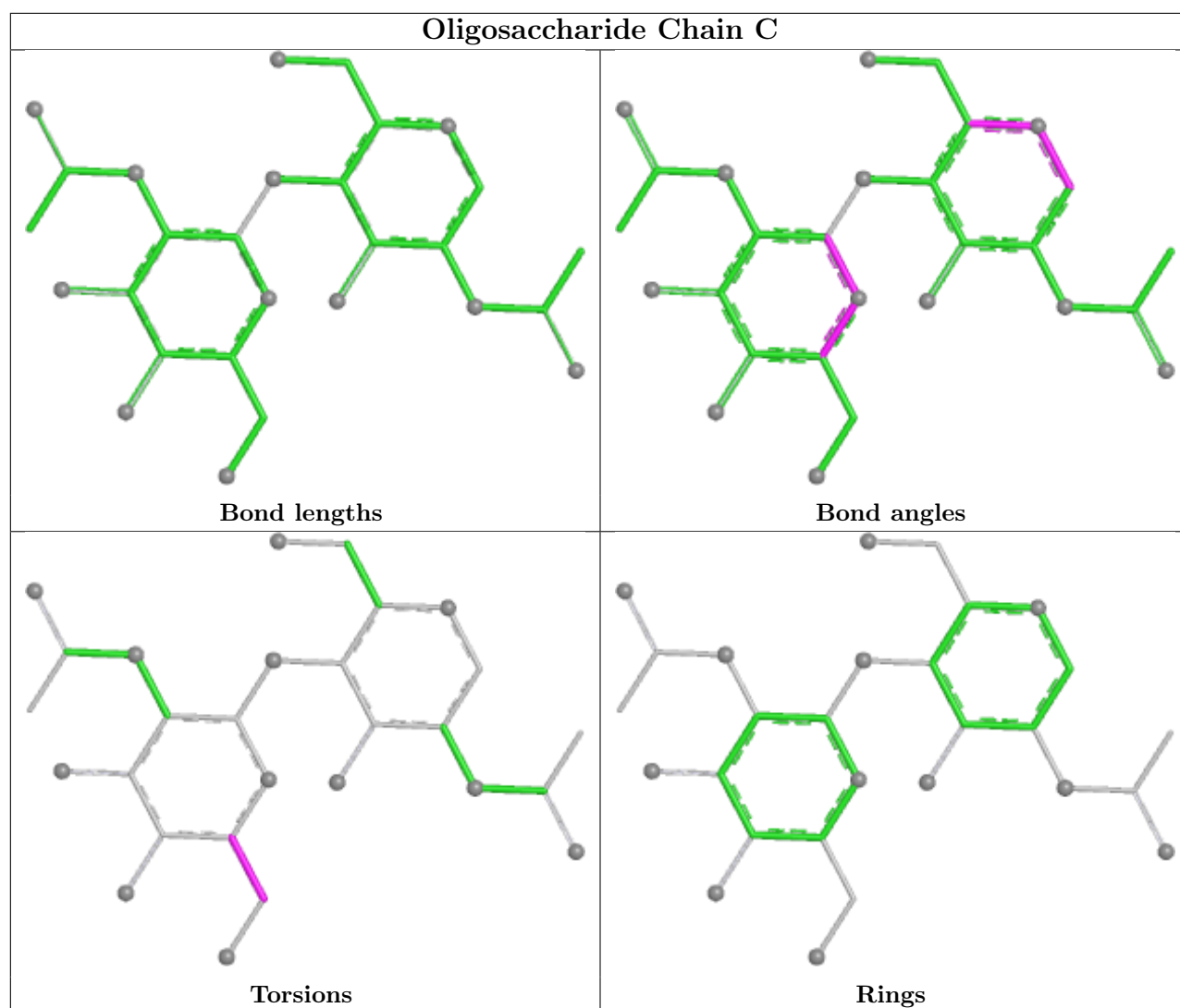
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2	NAG	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](#)

There are no ligands in this entry.

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	805/884 (91%)	-0.31	8 (0%) 79 72	21, 46, 77, 121	1 (0%)
2	B	172/214 (80%)	0.20	4 (2%) 61 51	45, 75, 115, 129	0
All	All	977/1098 (88%)	-0.22	12 (1%) 76 68	21, 50, 95, 129	1 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	208	CYS	3.6
1	A	344	GLY	3.2
1	A	219	GLY	3.1
2	B	24	ILE	3.1
1	A	118	ASN	2.8
2	B	83	THR	2.5
1	A	736	ILE	2.4
2	B	53	TRP	2.2
1	A	460	TRP	2.2
1	A	345	THR	2.2
1	A	518	ASN	2.1
1	A	688	THR	2.0

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

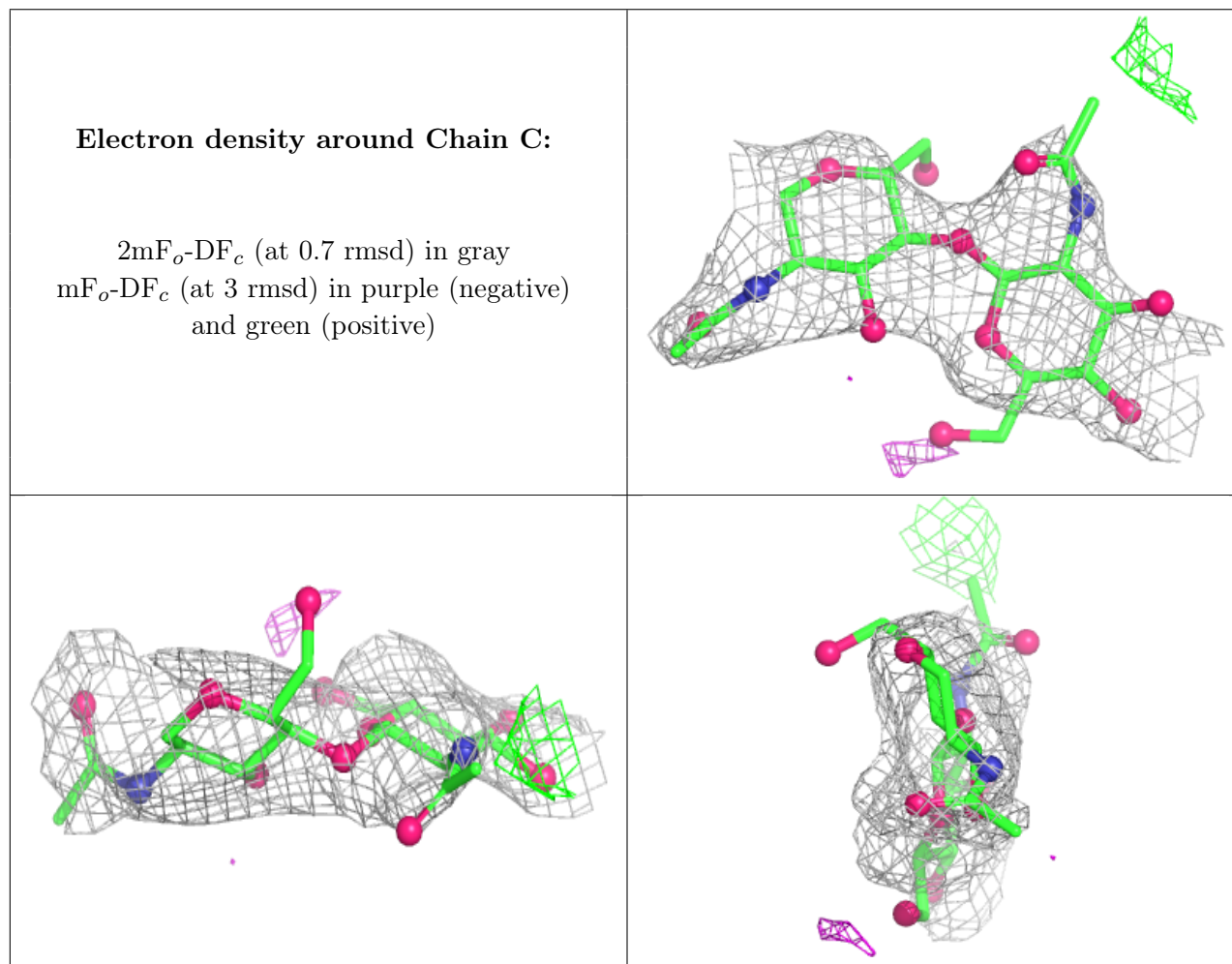
There are no non-standard protein/DNA/RNA residues in this entry.

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(\AA^2)	Q<0.9
3	NAG	C	2	14/15	0.47	0.15	118,123,129,130	0
3	NAG	C	1	14/15	0.73	0.12	110,114,120,122	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.