



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 3S8Z / pdb_00003s8z
Title : Crystal structure of LRP6-E3E4
Authors : Cheng, Z.; Xu, W.
Deposited on : 2011-05-31
Resolution : 2.80 Å(reported)

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

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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

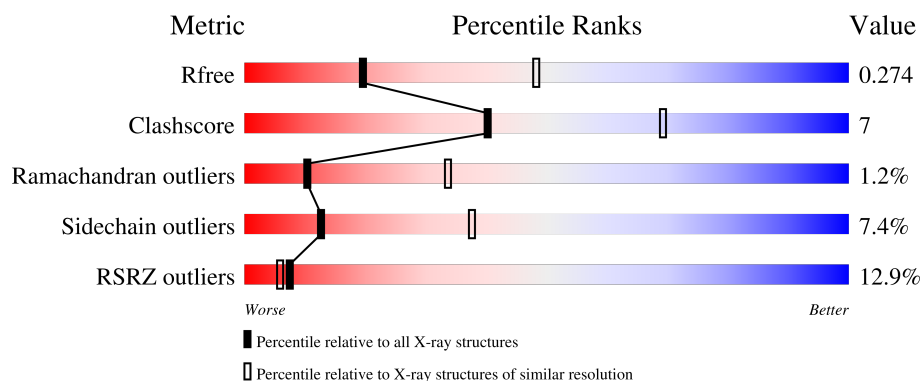
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	623	
2	B	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	1244	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4903 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 Low-density lipoprotein receptor-related protein 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	606	4833	3035	856	917	25	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

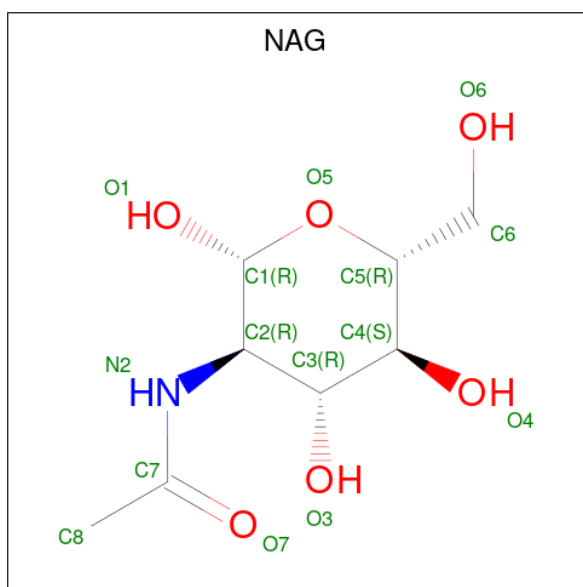
Chain	Residue	Modelled	Actual	Comment	Reference
A	621	HIS	-	expression tag	UNP O75581
A	622	HIS	-	expression tag	UNP O75581
A	623	HIS	-	expression tag	UNP O75581
A	624	HIS	-	expression tag	UNP O75581
A	625	HIS	-	expression tag	UNP O75581
A	626	HIS	-	expression tag	UNP O75581
A	627	HIS	-	expression tag	UNP O75581
A	628	HIS	-	expression tag	UNP O75581
A	1062	ILE	VAL	variant	UNP O75581

- Molecule 2 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			
2	B	2	28	16	2	10	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

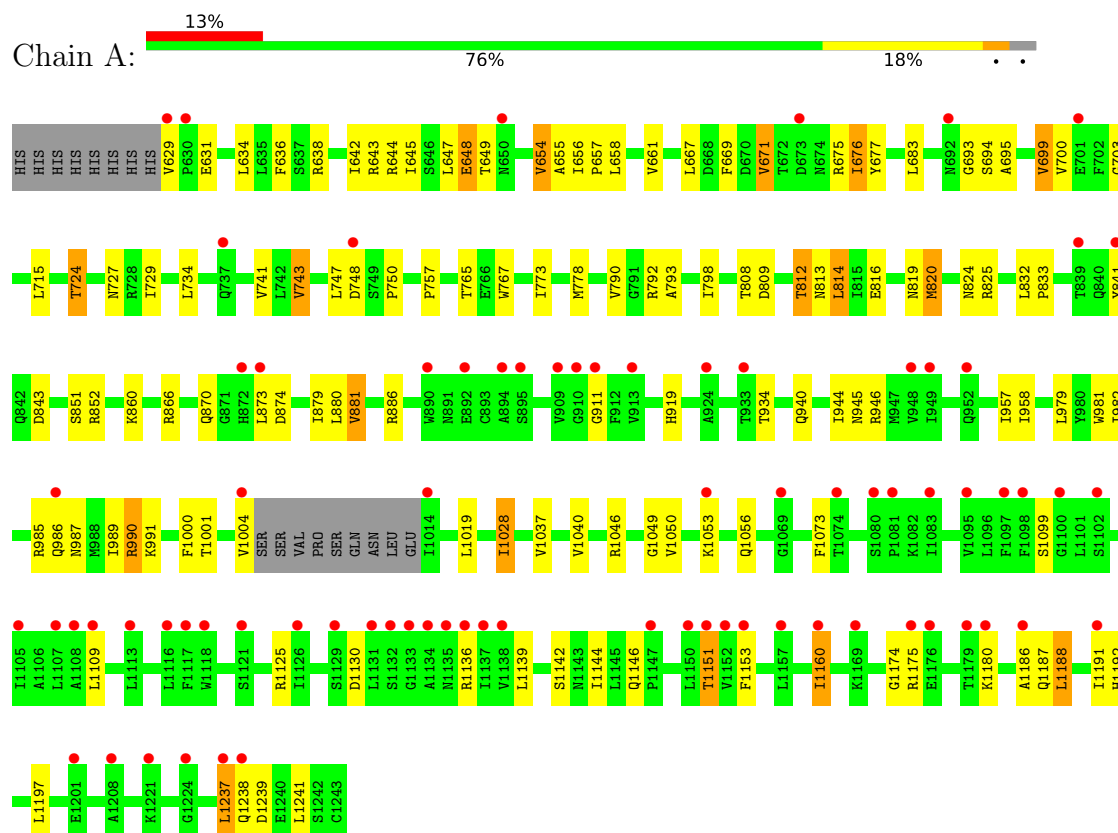


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots [i](#)

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

- Molecule 1: Low-density lipoprotein receptor-related protein 6



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-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	68.60Å 83.75Å 166.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-2.80) 99.8 (30.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.257 , 0.282 0.250 , 0.274	Depositor DCC
R_{free} test set	1309 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	69.6	Xtriage
Anisotropy	0.547	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 65.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4903	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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	0.44	0/4935	0.73	3/6696 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	694	SER	N-CA-C	7.29	120.28	108.76
1	A	695	ALA	N-CA-C	-5.84	98.37	110.80
1	A	1073	PHE	N-CA-C	5.23	116.23	108.60

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	4833	0	4717	64	0
2	B	28	0	25	1	0
3	A	42	0	39	0	0
All	All	4903	0	4781	64	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 7.

All (64) 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:657:PRO:HG2	1:A:693:GLY:HA2	1.43	0.98
1:A:729:ILE:HB	1:A:743:VAL:HG13	1.70	0.74
1:A:982:ILE:HG22	1:A:989:ILE:HG12	1.70	0.72
1:A:919:HIS:HD2	1:A:946:ARG:HE	1.41	0.69
1:A:1188:LEU:H	1:A:1188:LEU:HD23	1.59	0.66
1:A:812:THR:HB	1:A:814:LEU:HD22	1.80	0.62
1:A:1037:VAL:HG23	1:A:1053:LYS:HB3	1.82	0.61
1:A:1050:VAL:HG11	2:B:1:NAG:H82	1.83	0.60
1:A:647:LEU:O	1:A:648:GLU:HG2	2.03	0.58
1:A:727:ASN:ND2	1:A:748:ASP:O	2.36	0.58
1:A:990:ARG:HG2	1:A:1001:THR:HG22	1.86	0.57
1:A:1188:LEU:H	1:A:1188:LEU:CD2	2.18	0.57
1:A:852:ARG:HH22	1:A:866:ARG:HH22	1.53	0.56
1:A:1151:THR:HG21	1:A:1192:HIS:HA	1.88	0.54
1:A:1160:ILE:HD12	1:A:1191:ILE:HB	1.88	0.54
1:A:813:ASN:HB3	1:A:832:LEU:O	2.07	0.54
1:A:747:LEU:HD22	1:A:750:PRO:HG3	1.91	0.53
1:A:833:PRO:HB2	1:A:851:SER:HB3	1.89	0.52
1:A:940:GLN:HE21	1:A:945:ASN:HD21	1.57	0.52
1:A:798:ILE:O	1:A:886:ARG:NH2	2.41	0.52
1:A:647:LEU:C	1:A:649:THR:H	2.19	0.51
1:A:638:ARG:HD2	1:A:874:ASP:O	2.11	0.50
1:A:767:TRP:CE2	1:A:792:ARG:HB3	2.47	0.50
1:A:798:ILE:HG23	1:A:820:MET:HE1	1.92	0.50
1:A:944:ILE:HG21	1:A:979:LEU:HD21	1.92	0.49
1:A:703:GLY:HA2	1:A:958:ILE:HD12	1.94	0.49
1:A:991:LYS:HE3	1:A:1000:PHE:HB3	1.94	0.49
1:A:819:ASN:HD22	1:A:824:ASN:HD22	1.61	0.49
1:A:715:LEU:HD12	1:A:757:PRO:HB2	1.95	0.48
1:A:1099:SER:O	1:A:1136:ARG:NH2	2.40	0.48
1:A:793:ALA:HA	1:A:808:THR:O	2.14	0.48
1:A:985:ARG:O	1:A:986:GLN:HB2	2.13	0.48
1:A:656:ILE:HG22	1:A:658:LEU:HG	1.94	0.47
1:A:841:TYR:HB2	1:A:881:VAL:HG11	1.95	0.47
1:A:981:TRP:CZ2	1:A:990:ARG:HD2	2.50	0.47
1:A:634:LEU:HD23	1:A:645:ILE:HD11	1.97	0.47
1:A:881:VAL:HG13	1:A:886:ARG:HD2	1.97	0.47
1:A:757:PRO:HB3	1:A:778:MET:HE1	1.97	0.46
1:A:1146:GLN:HG3	1:A:1146:GLN:O	2.16	0.46
1:A:644:ARG:HG3	1:A:654:VAL:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1040:VAL:HG12	1:A:1049:GLY:O	2.17	0.45
1:A:1019:LEU:HB2	1:A:1028:ILE:HD11	1.99	0.44
1:A:676:ILE:HG12	1:A:677:TYR:N	2.33	0.43
1:A:669:PHE:CE2	1:A:671:VAL:HG13	2.53	0.43
1:A:982:ILE:CG2	1:A:989:ILE:HG12	2.45	0.43
1:A:677:TYR:OH	1:A:734:LEU:HB3	2.19	0.43
1:A:981:TRP:CE2	1:A:990:ARG:HB3	2.54	0.42
1:A:843:ASP:HA	1:A:860:LYS:HD3	2.01	0.42
1:A:870:GLN:HB3	1:A:873:LEU:HD12	2.01	0.42
1:A:1237:LEU:O	1:A:1239:ASP:N	2.49	0.41
1:A:667:LEU:HB2	1:A:880:LEU:HD23	2.02	0.41
1:A:919:HIS:CD2	1:A:946:ARG:HE	2.28	0.41
1:A:727:ASN:CG	1:A:748:ASP:O	2.64	0.41
1:A:636:PHE:HB3	1:A:879:ILE:HG22	2.02	0.41
1:A:699:VAL:HG12	1:A:700:VAL:HG23	2.02	0.41
1:A:1146:GLN:HE21	1:A:1146:GLN:HB2	1.73	0.41
1:A:669:PHE:HE2	1:A:671:VAL:HG13	1.86	0.40
1:A:809:ASP:HB3	1:A:814:LEU:HD23	2.03	0.40
1:A:765:THR:HG22	1:A:773:ILE:HG12	2.03	0.40
1:A:940:GLN:NE2	1:A:945:ASN:HD21	2.20	0.40
1:A:816:GLU:CD	1:A:825:ARG:HH21	2.28	0.40
1:A:642:ILE:HD12	1:A:658:LEU:CD1	2.51	0.40
1:A:643:ARG:NH1	1:A:655:ALA:HB2	2.36	0.40
1:A:724:THR:O	1:A:727:ASN:ND2	2.54	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	602/623 (97%)	550 (91%)	45 (8%)	7 (1%)	10 34

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	911	GLY
1	A	1186	ALA
1	A	648	GLU
1	A	1153	PHE
1	A	987	ASN
1	A	1142	SER
1	A	1174	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	529/546 (97%)	490 (93%)	39 (7%)	13	37

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	629	VAL
1	A	631	GLU
1	A	654	VAL
1	A	661	VAL
1	A	671	VAL
1	A	675	ARG
1	A	676	ILE
1	A	683	LEU
1	A	699	VAL
1	A	724	THR
1	A	741	VAL
1	A	743	VAL
1	A	790	VAL
1	A	812	THR
1	A	814	LEU
1	A	820	MET
1	A	881	VAL
1	A	934	THR

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Mol	Chain	Res	Type
1	A	957	ILE
1	A	990	ARG
1	A	1004	VAL
1	A	1028	ILE
1	A	1046	ARG
1	A	1056	GLN
1	A	1109	LEU
1	A	1125	ARG
1	A	1130	ASP
1	A	1139	LEU
1	A	1144	ILE
1	A	1151	THR
1	A	1160	ILE
1	A	1175	ARG
1	A	1180	LYS
1	A	1187	GLN
1	A	1188	LEU
1	A	1197	LEU
1	A	1237	LEU
1	A	1238	GLN
1	A	1241	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	652	ASN
1	A	727	ASN
1	A	738	HIS
1	A	824	ASN
1	A	919	HIS
1	A	940	GLN
1	A	966	ASN
1	A	987	ASN
1	A	1155	ASN
1	A	1163	GLN
1	A	1164	GLN
1	A	1182	GLN
1	A	1187	GLN
1	A	1209	GLN
1	A	1216	HIS
1	A	1238	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	NAG	B	1	1,2	14,14,15	0.53	0	17,19,21	1.32	2 (11%)
2	NAG	B	2	2	14,14,15	0.47	0	17,19,21	1.12	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
2	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C1-O5-C5	3.31	116.62	112.19
2	B	1	NAG	C1-O5-C5	3.18	116.45	112.19
2	B	1	NAG	C4-C3-C2	2.99	115.40	111.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

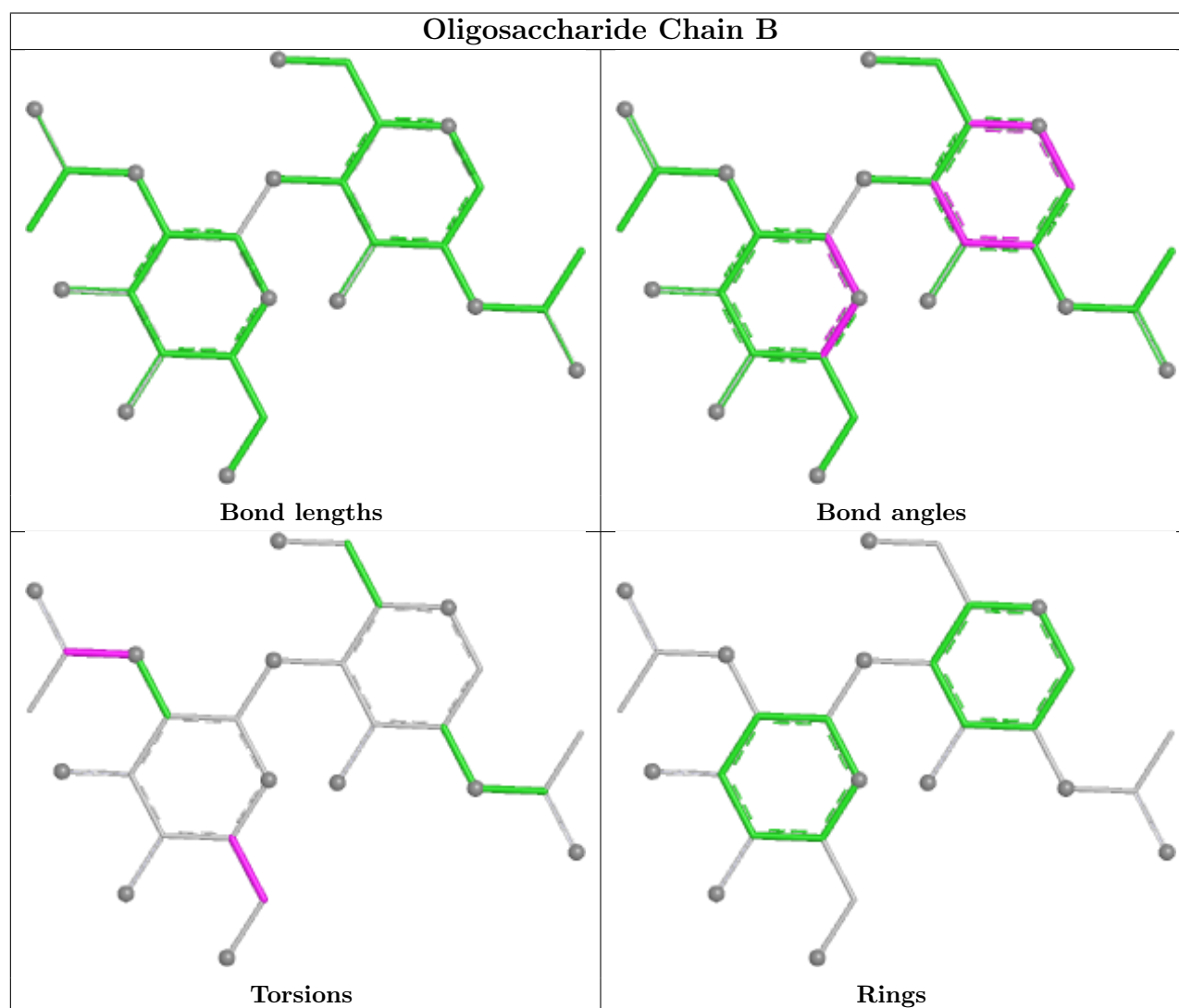
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	B	2	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	1	0

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

3 ligands 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	A	1247	1	14,14,15	0.52	0	17,19,21	1.56	2 (11%)
3	NAG	A	1244	1	14,14,15	0.66	0	17,19,21	1.00	1 (5%)
3	NAG	A	1248	1	14,14,15	0.63	0	17,19,21	1.16	3 (17%)

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	A	1247	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1244	1	1/1/5/7	1/6/23/26	0/1/1/1
3	NAG	A	1248	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1247	NAG	C1-O5-C5	5.26	119.23	112.19
3	A	1248	NAG	O5-C1-C2	-2.51	107.41	111.29
3	A	1244	NAG	C4-C3-C2	2.41	114.56	111.02
3	A	1248	NAG	C8-C7-N2	2.21	119.78	116.12
3	A	1248	NAG	C1-O5-C5	2.14	115.06	112.19
3	A	1247	NAG	C8-C7-N2	2.14	119.67	116.12

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1244	NAG	C1

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1247	NAG	C8-C7-N2-C2
3	A	1247	NAG	O7-C7-N2-C2
3	A	1248	NAG	C8-C7-N2-C2
3	A	1248	NAG	O7-C7-N2-C2
3	A	1247	NAG	O5-C5-C6-O6
3	A	1247	NAG	C4-C5-C6-O6
3	A	1244	NAG	C4-C5-C6-O6

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	606/623 (97%)	1.03	78 (12%) 7 6	74, 110, 171, 210	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1098	PHE	3.8
1	A	629	VAL	3.7
1	A	1137	ILE	3.3
1	A	952	GLN	3.3
1	A	1153	PHE	3.2
1	A	1160	ILE	3.1
1	A	1147	PRO	3.1
1	A	1014	ILE	3.1
1	A	1113	LEU	3.1
1	A	1083	ILE	3.0
1	A	630	PRO	3.0
1	A	892	GLU	3.0
1	A	1134	ALA	3.0
1	A	1131	LEU	2.9
1	A	933	THR	2.9
1	A	1117	PHE	2.9
1	A	909	VAL	2.8
1	A	1224	GLY	2.8
1	A	910	GLY	2.8
1	A	911	GLY	2.7
1	A	1180	LYS	2.7
1	A	1133	GLY	2.7
1	A	1080	SER	2.7
1	A	1157	LEU	2.7
1	A	1108	ALA	2.6
1	A	1136	ARG	2.6
1	A	1095	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	673	ASP	2.6
1	A	1097	PHE	2.6
1	A	1109	LEU	2.6
1	A	1151	THR	2.6
1	A	1074	THR	2.6
1	A	894	ALA	2.6
1	A	986	GLN	2.5
1	A	1126	ILE	2.5
1	A	1221	LYS	2.5
1	A	650	ASN	2.4
1	A	1176	GLU	2.4
1	A	1179	THR	2.4
1	A	701	GLU	2.4
1	A	1208	ALA	2.4
1	A	1150	LEU	2.3
1	A	1191	ILE	2.3
1	A	1069	GLY	2.3
1	A	1118	TRP	2.3
1	A	1138	VAL	2.3
1	A	924	ALA	2.3
1	A	1107	LEU	2.3
1	A	1053	LYS	2.3
1	A	748	ASP	2.3
1	A	1100	GLY	2.3
1	A	873	LEU	2.2
1	A	1116	LEU	2.2
1	A	949	ILE	2.2
1	A	890	TRP	2.2
1	A	1121	SER	2.2
1	A	1169	LYS	2.2
1	A	737	GLN	2.2
1	A	1105	ILE	2.2
1	A	1175	ARG	2.2
1	A	1004	VAL	2.2
1	A	1237	LEU	2.2
1	A	948	VAL	2.2
1	A	1081	PRO	2.2
1	A	1102	SER	2.2
1	A	1132	SER	2.2
1	A	913	VAL	2.2
1	A	895	SER	2.2
1	A	839	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1201	GLU	2.1
1	A	1129	SER	2.1
1	A	1238	GLN	2.1
1	A	1152	VAL	2.1
1	A	841	TYR	2.1
1	A	872	HIS	2.0
1	A	1135	ASN	2.0
1	A	1186	ALA	2.0
1	A	692	ASN	2.0

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

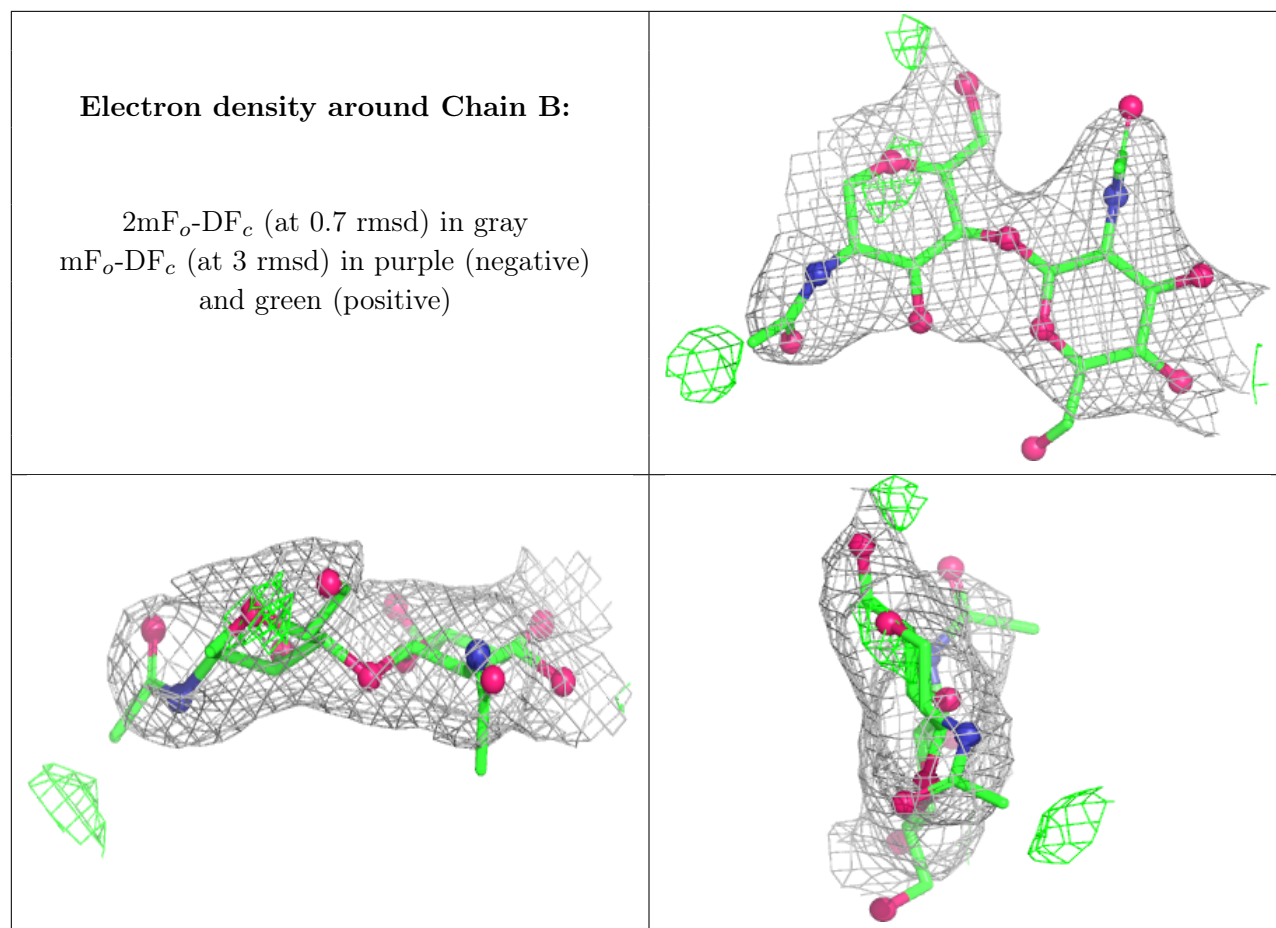
There are no non-standard protein/DNA/RNA residues in this entry.

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	NAG	B	2	14/15	0.75	0.21	163,165,166,166	0
2	NAG	B	1	14/15	0.82	0.25	147,148,149,149	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($\text{\AA}^2$)	Q<0.9
3	NAG	A	1244	14/15	0.44	0.20	170,172,175,176	0
3	NAG	A	1247	14/15	0.65	0.22	178,180,181,181	0
3	NAG	A	1248	14/15	0.71	0.25	172,173,173,174	0

6.5 Other polymers [i](#)

There are no such residues in this entry.