



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:05 PM UTC

PDB ID : 4XE4 / pdb_00004xe4
Title : Coagulation Factor XII protease domain crystal structure
Authors : Pathak, M.; Wilmann, P.; Awford, J.; Li, C.; Fisher, P.M.; Dreveny, I.; Dekker, L.V.; Emsley, J.
Deposited on : 2014-12-22
Resolution : 2.40 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

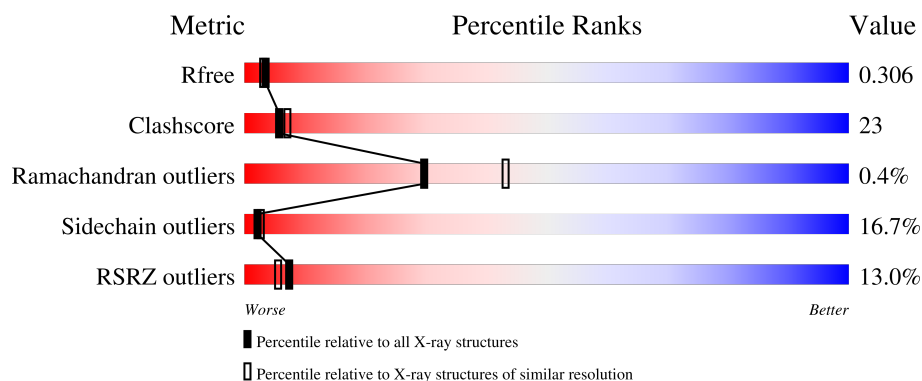
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	255	12% 48% 33% 9% 9%
2	B	3	67% 33%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1894 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.

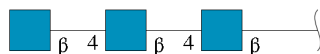
- Molecule 1 is a protein called Coagulation factor XII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	231	1768	1113	309	334	12	7	1	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	467	SER	CYS	engineered mutation	UNP P00748
A	597	HIS	-	expression tag	UNP P00748
A	598	HIS	-	expression tag	UNP P00748
A	599	THR	-	expression tag	UNP P00748
A	600	GLY	-	expression tag	UNP P00748
A	601	THR	-	expression tag	UNP P00748
A	602	ARG	-	expression tag	UNP P00748
A	603	HIS	-	expression tag	UNP P00748
A	604	HIS	-	expression tag	UNP P00748
A	605	HIS	-	expression tag	UNP P00748
A	606	HIS	-	expression tag	UNP P00748
A	607	HIS	-	expression tag	UNP P00748
A	608	HIS	-	expression tag	UNP P00748

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-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	3	42	24	3	15	0	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

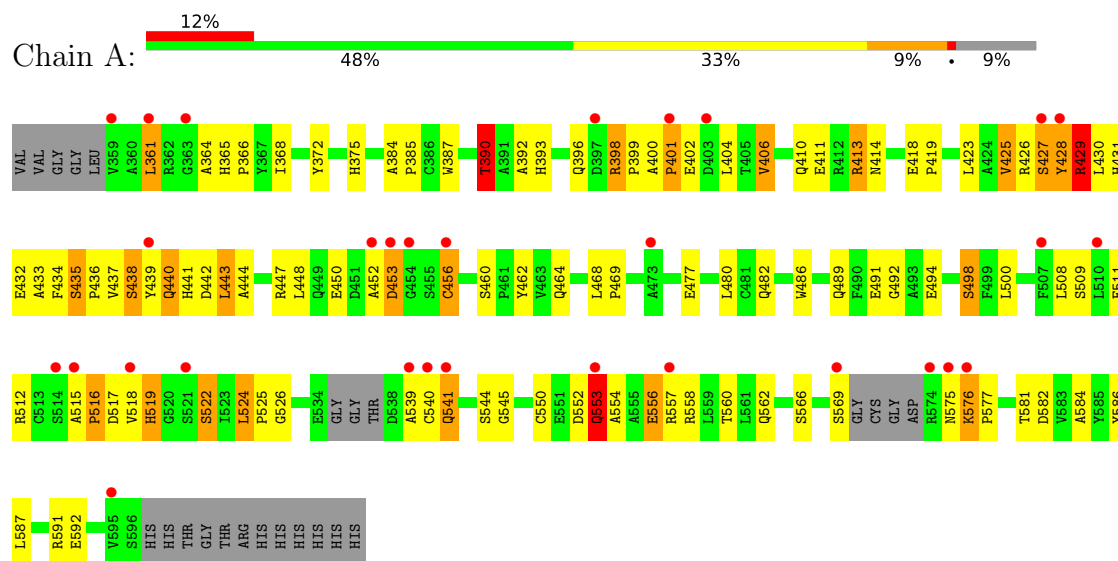
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	78	Total	O	0	0
			78	78		

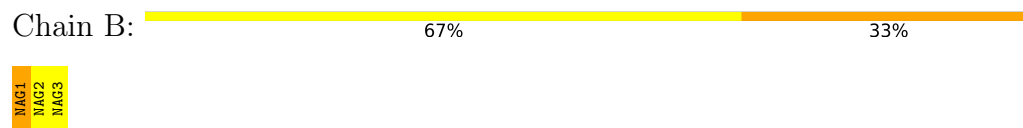
3 Residue-property plots [i](#)

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: Coagulation factor XII



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-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 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	137.06 Å 137.06 Å 37.01 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.57 – 2.40 39.57 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (39.57-2.40) 98.2 (39.57-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.39 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.218 , 0.295 0.232 , 0.306	Depositor DCC
R_{free} test set	723 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å ²)	61.7	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 66.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.052 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	1894	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.29% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, GOL

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	1.10	0/1817	1.31	22/2478 (0.9%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	456	CYS	N-CA-C	14.61	127.25	111.03
1	A	554	ALA	N-CA-C	-8.94	101.91	113.17
1	A	516	PRO	N-CA-C	8.50	124.71	113.57
1	A	541	GLN	N-CA-C	-8.10	99.18	110.35
1	A	556	GLU	CB-CA-C	7.21	122.19	110.88
1	A	518	VAL	N-CA-C	7.04	123.97	109.34
1	A	429	ARG	CB-CA-C	6.68	123.72	110.42
1	A	539	ALA	CB-CA-C	-6.42	96.97	110.45
1	A	576	LYS	CB-CA-C	6.26	122.51	110.17
1	A	515	ALA	CB-CA-C	-6.21	97.94	110.17
1	A	390	THR	CB-CA-C	-6.15	98.61	113.19
1	A	516	PRO	N-CA-CB	-6.14	97.01	103.52
1	A	553	GLN	CB-CA-C	-5.89	98.69	110.42
1	A	427	SER	O-C-N	-5.58	118.39	123.41
1	A	456	CYS	CB-CA-C	-5.34	102.67	110.95
1	A	430	LEU	N-CA-C	-5.28	101.50	109.85
1	A	519	HIS	N-CA-CB	5.10	118.60	111.15
1	A	540	CYS	N-CA-C	-5.08	107.04	113.18
1	A	384	ALA	CA-C-N	-5.07	114.60	119.87
1	A	384	ALA	C-N-CA	-5.07	114.60	119.87
1	A	375	HIS	N-CA-C	-5.05	104.03	111.81
1	A	428	TYR	N-CA-CB	5.03	118.70	110.55

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1768	0	1679	82	0
2	B	42	0	37	1	0
3	A	6	0	8	0	0
4	A	78	0	0	13	0
All	All	1894	0	1724	82	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 23.

All (82) 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:423:LEU:HD11	1:A:456:CYS:O	1.44	1.16
1:A:460:SER:O	1:A:464:GLN:NE2	1.91	1.02
1:A:423:LEU:CD1	1:A:456:CYS:O	2.20	0.90
1:A:399:PRO:O	1:A:428:TYR:OH	1.93	0.84
1:A:439:TYR:HA	4:A:878:HOH:O	1.78	0.83
1:A:431:HIS:CD2	1:A:441:HIS:HB3	2.24	0.72
1:A:489:GLN:OE1	1:A:498:SER:N	2.23	0.72
1:A:398:ARG:N	1:A:399:PRO:HD3	2.05	0.72
1:A:441:HIS:CE1	4:A:875:HOH:O	2.43	0.70
1:A:434:PHE:O	1:A:436:PRO:HD3	1.92	0.70
1:A:522:SER:O	4:A:876:HOH:O	2.11	0.68
1:A:516:PRO:HD3	4:A:816:HOH:O	1.95	0.67
1:A:439:TYR:C	4:A:878:HOH:O	2.39	0.65
1:A:440:GLN:HE21	1:A:524:LEU:HB3	1.64	0.63
1:A:519:HIS:CD2	1:A:577:PRO:HG2	2.35	0.61
1:A:361:LEU:HD12	4:A:803:HOH:O	2.00	0.61
1:A:584:ALA:O	1:A:587:LEU:HB2	2.01	0.60
1:A:526:GLY:C	4:A:870:HOH:O	2.44	0.60
1:A:550:CYS:SG	1:A:562:GLN:HG3	2.42	0.60
1:A:418:GLU:HB2	1:A:419:PRO:HD3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:LEU:HB2	1:A:425:VAL:CG1	2.32	0.59
1:A:440:GLN:HG3	1:A:524:LEU:HD23	1.84	0.59
1:A:550:CYS:HB2	1:A:562:GLN:HG3	1.85	0.57
1:A:400:ALA:HB1	1:A:402:GLU:OE1	2.06	0.56
1:A:414:ASN:HA	2:B:1:NAG:O7	2.07	0.55
1:A:440:GLN:N	4:A:878:HOH:O	2.40	0.55
1:A:433:ALA:O	1:A:441:HIS:HD2	1.90	0.55
1:A:491:GLU:CD	1:A:492:GLY:N	2.66	0.54
1:A:429:ARG:O	1:A:444:ALA:HB1	2.08	0.53
1:A:575:ASN:C	1:A:575:ASN:HD22	2.17	0.53
1:A:398:ARG:N	1:A:399:PRO:CD	2.71	0.53
1:A:440:GLN:OE1	1:A:441:HIS:NE2	2.41	0.53
1:A:519:HIS:HD2	1:A:577:PRO:HG2	1.76	0.50
1:A:525:PRO:O	4:A:875:HOH:O	2.19	0.50
1:A:393:HIS:HA	1:A:396:GLN:HG2	1.93	0.50
1:A:587:LEU:O	1:A:591:ARG:HG3	2.12	0.50
1:A:477:GLU:OE2	1:A:509:SER:OG	2.17	0.48
1:A:469:PRO:HA	1:A:560:THR:OG1	2.14	0.47
1:A:393:HIS:HE1	1:A:544:SER:HB3	1.78	0.47
1:A:582:ASP:OD1	1:A:582:ASP:C	2.56	0.47
1:A:428:TYR:O	1:A:429:ARG:HB2	2.15	0.47
1:A:406:VAL:HG11	1:A:448:LEU:CD2	2.44	0.47
1:A:450:GLU:OE1	1:A:450:GLU:N	2.44	0.47
1:A:477:GLU:OE2	1:A:509:SER:N	2.41	0.47
1:A:364:ALA:O	1:A:365:HIS:C	2.58	0.46
1:A:435:SER:HG	1:A:438:SER:H	1.64	0.46
1:A:491:GLU:OE2	1:A:492:GLY:N	2.48	0.46
1:A:447:ARG:NH1	1:A:448:LEU:O	2.49	0.46
1:A:550:CYS:CB	1:A:562:GLN:HG3	2.45	0.46
1:A:434:PHE:HE1	4:A:878:HOH:O	1.93	0.46
1:A:365:HIS:O	1:A:368:ILE:HG22	2.16	0.46
1:A:434:PHE:CE1	4:A:878:HOH:O	2.56	0.45
1:A:426:ARG:O	1:A:427:SER:HB2	2.16	0.45
1:A:443:LEU:HD21	1:A:586:TYR:CB	2.47	0.44
1:A:516:PRO:CD	4:A:816:HOH:O	2.57	0.44
1:A:404:LEU:CB	1:A:425:VAL:CG1	2.96	0.44
1:A:576:LYS:HA	1:A:576:LYS:HD2	1.67	0.44
1:A:413:ARG:HG3	1:A:486:TRP:HB3	2.00	0.44
1:A:569:SER:O	1:A:569:SER:OG	2.36	0.44
1:A:418:GLU:N	1:A:419:PRO:HD2	2.34	0.43
1:A:385:PRO:O	1:A:456:CYS:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:ARG:O	1:A:592:GLU:C	2.61	0.43
1:A:404:LEU:HB2	1:A:425:VAL:HG13	2.00	0.43
1:A:372:TYR:OH	1:A:410:GLN:NE2	2.51	0.42
1:A:468:LEU:O	1:A:560:THR:OG1	2.38	0.42
1:A:392:ALA:N	1:A:442:ASP:OD1	2.51	0.42
1:A:440:GLN:HG3	1:A:524:LEU:CB	2.49	0.42
1:A:400:ALA:O	1:A:401:PRO:C	2.62	0.42
1:A:452:ALA:O	1:A:453:ASP:CB	2.68	0.42
1:A:452:ALA:C	1:A:453:ASP:CG	2.87	0.42
1:A:468:LEU:HB3	1:A:469:PRO:CD	2.50	0.42
1:A:390:THR:HG22	1:A:545:GLY:HA3	2.02	0.41
1:A:435:SER:OG	1:A:438:SER:HB3	2.20	0.41
1:A:418:GLU:N	1:A:419:PRO:CD	2.83	0.41
1:A:434:PHE:CD1	4:A:878:HOH:O	2.73	0.41
1:A:435:SER:C	1:A:437:VAL:H	2.27	0.41
1:A:442:ASP:OD2	1:A:566:SER:OG	2.34	0.41
1:A:552:ASP:O	1:A:553:GLN:HB2	2.21	0.41
1:A:442:ASP:O	1:A:581:THR:OG1	2.26	0.40
1:A:387:TRP:CH2	1:A:447:ARG:HD3	2.57	0.40
1:A:433:ALA:O	1:A:441:HIS:CD2	2.73	0.40
1:A:462:TYR:CD1	1:A:462:TYR:N	2.89	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	226/255 (89%)	187 (83%)	38 (17%)	1 (0%)	30	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	401	PRO

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	187/203 (92%)	156 (83%)	31 (17%)	2 3

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	361	LEU
1	A	366	PRO
1	A	390	THR
1	A	398	ARG
1	A	406	VAL
1	A	411	GLU
1	A	413	ARG
1	A	425	VAL
1	A	429	ARG
1	A	432	GLU
1	A	435	SER
1	A	438	SER
1	A	440	GLN
1	A	443	LEU
1	A	453	ASP
1	A	480	LEU
1	A	482	GLN
1	A	494	GLU
1	A	498	SER
1	A	500	LEU
1	A	508	LEU
1	A	511	GLU
1	A	512	ARG
1	A	517	ASP
1	A	522	SER
1	A	524	LEU

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Mol	Chain	Res	Type
1	A	541	GLN
1	A	553	GLN
1	A	556	GLU
1	A	557	ARG
1	A	558	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	393	HIS
1	A	410	GLN
1	A	482	GLN
1	A	575	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

3 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	B	1	1,2	14,14,15	0.81	0	17,19,21	2.67	6 (35%)
2	NAG	B	2	2	14,14,15	0.97	1 (7%)	17,19,21	2.44	4 (23%)
2	NAG	B	3	2	14,14,15	0.80	0	17,19,21	2.54	8 (47%)

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	-	1/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	NAG	B	3	2	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	C1-C2	2.43	1.55	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	O4-C4-C3	6.09	124.73	110.38
2	B	1	NAG	O4-C4-C5	5.72	123.40	109.32
2	B	1	NAG	C1-C2-N2	5.24	118.69	110.43
2	B	3	NAG	C1-O5-C5	5.12	119.05	112.19
2	B	2	NAG	C1-C2-N2	4.75	117.93	110.43
2	B	1	NAG	C2-N2-C7	4.72	129.22	122.90
2	B	3	NAG	C1-C2-N2	4.17	117.00	110.43
2	B	2	NAG	O5-C1-C2	-4.15	104.87	111.29
2	B	3	NAG	C2-N2-C7	3.97	128.22	122.90
2	B	3	NAG	C8-C7-N2	3.56	122.02	116.12
2	B	3	NAG	C3-C4-C5	3.40	116.39	110.23
2	B	3	NAG	O5-C1-C2	-3.37	106.08	111.29
2	B	1	NAG	O3-C3-C4	3.34	118.24	110.38
2	B	1	NAG	C1-O5-C5	2.59	115.66	112.19
2	B	1	NAG	O5-C1-C2	-2.54	107.37	111.29
2	B	3	NAG	O7-C7-C8	-2.50	117.59	122.05
2	B	2	NAG	O7-C7-C8	-2.41	117.76	122.05
2	B	3	NAG	O5-C5-C4	2.23	116.26	110.83

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3	NAG	C4-C5-C6-O6
2	B	3	NAG	C8-C7-N2-C2

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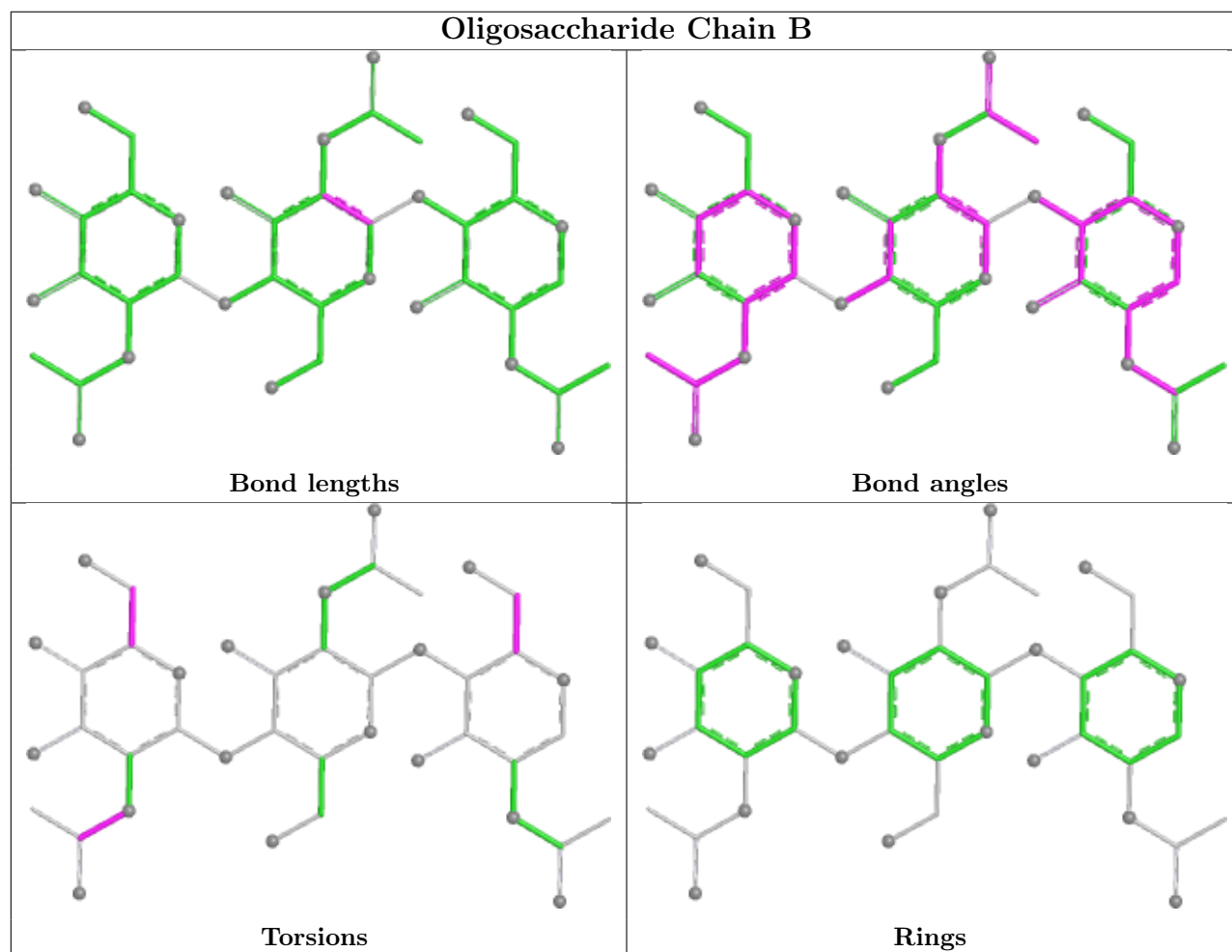
Mol	Chain	Res	Type	Atoms
2	B	3	NAG	O7-C7-N2-C2
2	B	3	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6

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 [i](#)

1 ligand is 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	GOL	A	704	-	5,5,5	0.24	0	5,5,5	0.55	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	GOL	A	704	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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	231/255 (90%)	0.78	30 (12%) 7 5	34, 67, 125, 141	8 (3%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	359	VAL	4.8
1	A	361	LEU	3.4
1	A	452	ALA	3.3
1	A	515	ALA	3.0
1	A	473	ALA	2.9
1	A	539	ALA	2.8
1	A	595	VAL	2.8
1	A	456	CYS	2.7
1	A	363	GLY	2.6
1	A	574	ARG	2.6
1	A	518	VAL	2.5
1	A	428	TYR	2.5
1	A	576	LYS	2.5
1	A	397	ASP	2.5
1	A	453	ASP	2.5
1	A	540	CYS	2.4
1	A	541	GLN	2.4
1	A	557	ARG	2.3
1	A	401	PRO	2.3
1	A	454	GLY	2.2
1	A	514	SER	2.2
1	A	521	SER	2.2
1	A	575	ASN	2.1
1	A	569	SER	2.1
1	A	553	GLN	2.1
1	A	427	SER	2.1
1	A	510	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	507	PHE	2.0
1	A	403	ASP	2.0
1	A	439	TYR	2.0

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

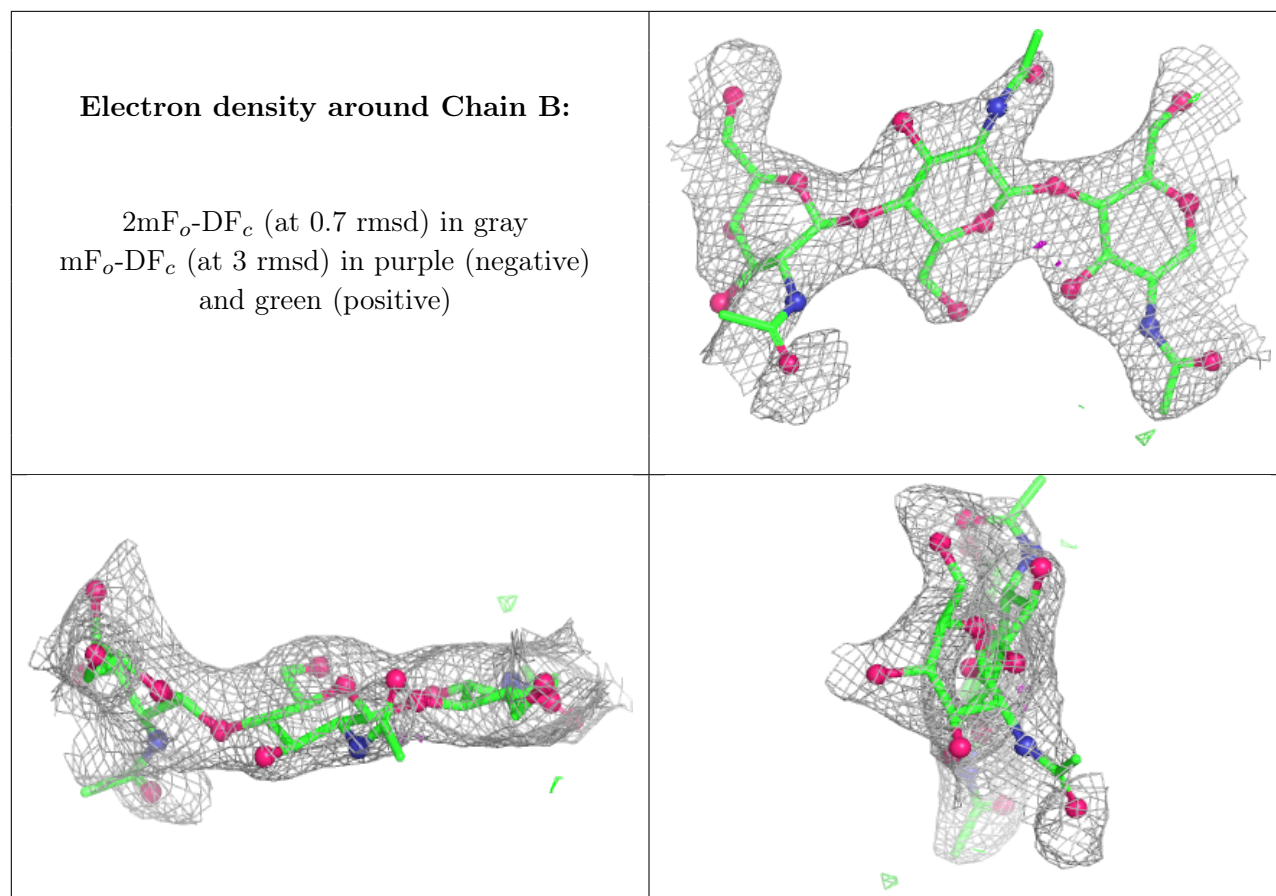
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	B	3	14/15	0.68	0.14	109,134,138,138	0
2	NAG	B	2	14/15	0.88	0.13	97,108,116,120	0
2	NAG	B	1	14/15	0.89	0.11	71,80,94,103	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	GOL	A	704	6/6	0.92	0.10	66,80,82,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.