



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 11:25 AM UTC

PDB ID : 3H9Z / pdb_00003h9z
Title : Crystal structure of the IgE-Fc3-4 domains
Authors : Wurzburg, B.A.
Deposited on : 2009-04-30
Resolution : 2.45 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:

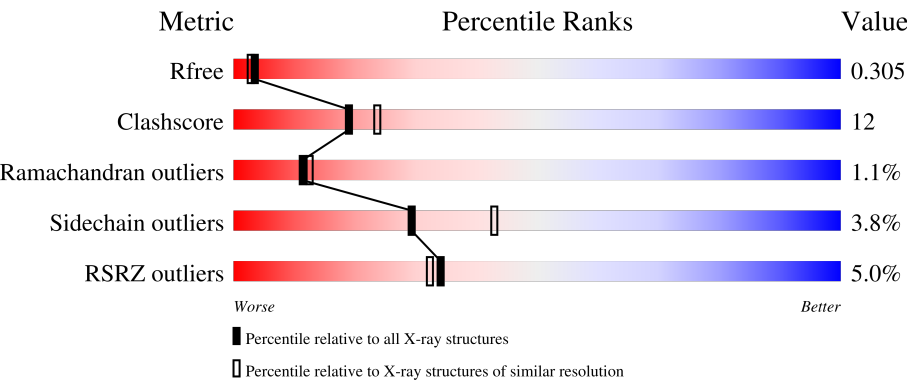
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	223	6% 75%17%6%
1	B	223	6% 71%19%6%
1	C	223	4% 75%17%6%
1	D	223	8% 74%19%6%
2	E	5	100%

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Mol	Chain	Length	Quality of chain
2	F	5	20%20%60%
2	G	5	20%80%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6954 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 Ig epsilon chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1656	1037	305	308	6			
1	B	209	Total	C	N	O	S	0	0	0
			1656	1037	305	308	6			
1	C	209	Total	C	N	O	S	0	0	0
			1656	1037	305	308	6			
1	D	209	Total	C	N	O	S	0	0	0
			1656	1037	305	308	6			

There are 20 discrepancies between the modelled and reference sequences:

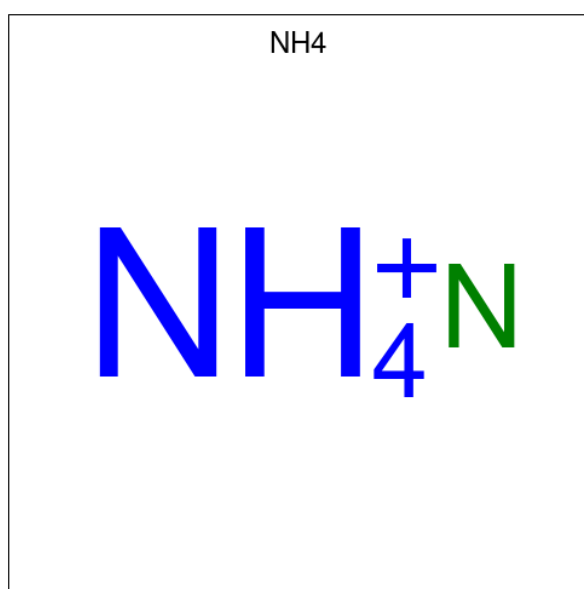
Chain	Residue	Modelled	Actual	Comment	Reference
A	325	ALA	-	expression tag	UNP P01854
A	326	ASP	-	expression tag	UNP P01854
A	327	PRO	-	expression tag	UNP P01854
A	371	GLN	ASN	engineered mutation	UNP P01854
A	383	GLN	ASN	engineered mutation	UNP P01854
B	325	ALA	-	expression tag	UNP P01854
B	326	ASP	-	expression tag	UNP P01854
B	327	PRO	-	expression tag	UNP P01854
B	371	GLN	ASN	engineered mutation	UNP P01854
B	383	GLN	ASN	engineered mutation	UNP P01854
C	325	ALA	-	expression tag	UNP P01854
C	326	ASP	-	expression tag	UNP P01854
C	327	PRO	-	expression tag	UNP P01854
C	371	GLN	ASN	engineered mutation	UNP P01854
C	383	GLN	ASN	engineered mutation	UNP P01854
D	325	ALA	-	expression tag	UNP P01854
D	326	ASP	-	expression tag	UNP P01854
D	327	PRO	-	expression tag	UNP P01854
D	371	GLN	ASN	engineered mutation	UNP P01854
D	383	GLN	ASN	engineered mutation	UNP P01854

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(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
2	E	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	F	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	G	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 3 is AMMONIUM ION (CCD ID: NH4) (formula: H₄N).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	N	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	31	Total	O	0	0
			31	31		
4	B	38	Total	O	0	0
			38	38		

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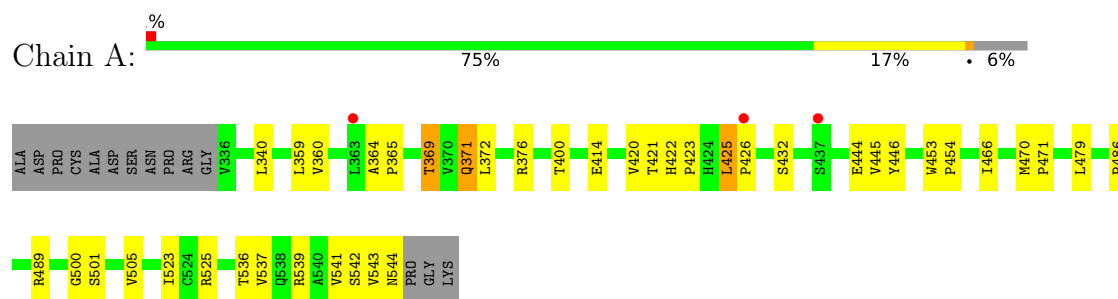
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	47	Total	O	0	0
			47	47		
4	D	30	Total	O	0	0
			30	30		

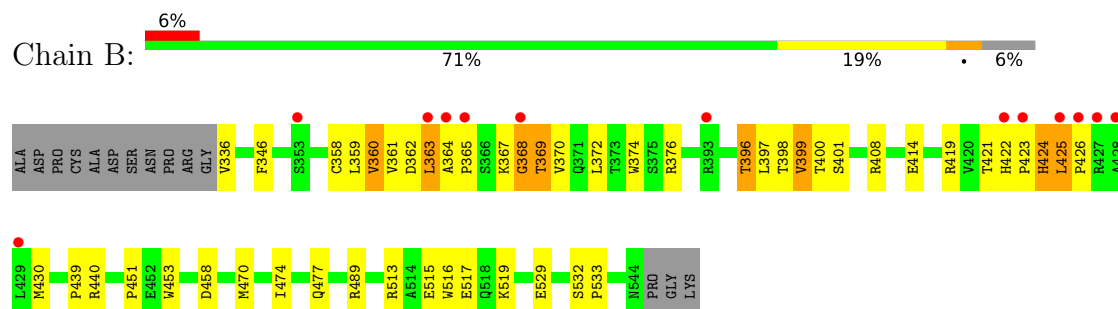
3 Residue-property plots

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.

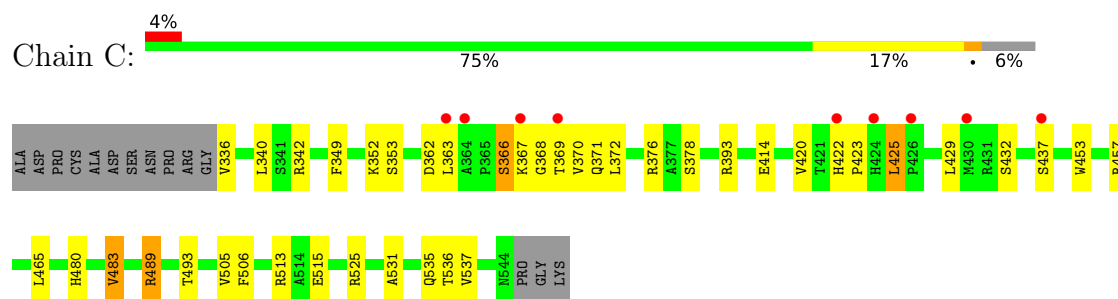
- Molecule 1: Ig epsilon chain C region



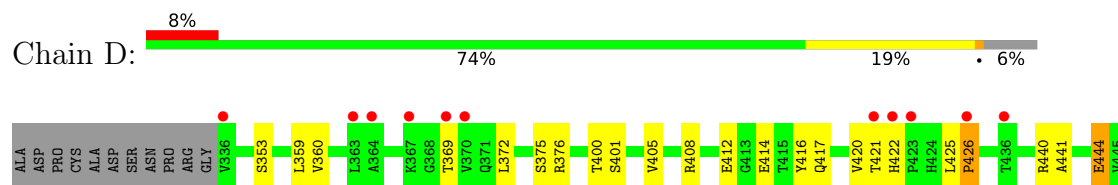
- Molecule 1: Ig epsilon chain C region

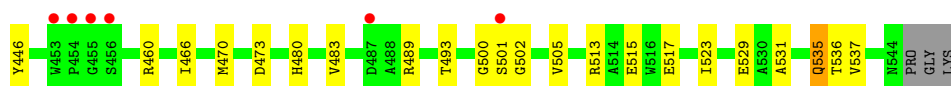


- Molecule 1: Ig epsilon chain C region



- Molecule 1: Ig epsilon chain C region



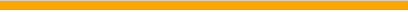


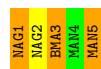
- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%



- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  20%  20%  60%



- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  20%  80%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.66Å 99.35Å 77.64Å 90.00° 97.40° 90.00°	Depositor
Resolution (Å)	28.71 – 2.45 28.71 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.8 (28.71-2.45) 98.7 (28.71-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.45Å)	Xtriage
Refinement program	REFMAC, CNS	Depositor
R, R_{free}	0.229 , 0.277 (Not available) , 0.305	Depositor DCC
R_{free} test set	1824 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6954	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.21 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.3678e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NH4, NAG, BMA, MAN

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	0.63	0/1698	0.89	2/2311 (0.1%)
1	B	0.62	0/1698	0.92	0/2311
1	C	0.59	0/1698	0.89	0/2311
1	D	0.64	0/1698	0.91	0/2311
All	All	0.62	0/6792	0.90	2/9244 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	364	ALA	CA-C-N	5.39	126.58	119.84
1	A	364	ALA	C-N-CA	5.39	126.58	119.84

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	1656	0	1642	37	0
1	B	1656	0	1641	50	0
1	C	1656	0	1641	36	0
1	D	1656	0	1641	42	0
2	E	61	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	61	0	52	3	0
2	G	61	0	52	0	0
3	C	1	0	0	1	0
4	A	31	0	0	1	0
4	B	38	0	0	0	0
4	C	47	0	0	1	0
4	D	30	0	0	4	0
All	All	6954	0	6721	159	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 12.

All (159) 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:425:LEU:HD12	1:A:425:LEU:O	1.31	1.30
1:B:425:LEU:HD12	1:B:425:LEU:O	1.50	1.09
1:A:369:THR:HG21	1:D:369:THR:HG21	1.46	0.97
1:C:425:LEU:HD12	1:C:425:LEU:O	1.66	0.94
1:B:369:THR:HG22	1:B:369:THR:O	1.71	0.91
1:B:363:LEU:HD11	1:B:422:HIS:CE1	2.11	0.85
1:D:372:LEU:HD22	1:D:420:VAL:HG22	1.57	0.84
1:A:425:LEU:O	1:A:425:LEU:CD1	2.24	0.84
1:A:425:LEU:HD12	1:A:425:LEU:C	2.05	0.81
1:B:359:LEU:HD13	1:B:400:THR:HG22	1.64	0.78
1:B:425:LEU:HD12	1:B:425:LEU:C	2.08	0.78
1:D:372:LEU:CD2	1:D:420:VAL:HG22	2.14	0.77
1:D:531:ALA:HB1	1:D:537:VAL:HG23	1.69	0.74
1:D:422:HIS:HB3	1:D:425:LEU:HB2	1.70	0.73
1:B:364:ALA:HB3	1:B:365:PRO:HD3	1.71	0.73
1:A:369:THR:CG2	1:D:369:THR:HG21	2.18	0.72
1:C:489:ARG:NH2	1:C:515:GLU:OE1	2.22	0.71
1:A:445:VAL:HG22	1:A:466:ILE:HD12	1.72	0.70
1:A:369:THR:HG21	1:D:369:THR:CG2	2.22	0.70
1:A:376:ARG:HD2	1:A:414:GLU:OE2	1.91	0.70
1:C:457:ARG:O	1:C:513:ARG:NH1	2.25	0.69
1:D:489:ARG:NH2	1:D:515:GLU:OE1	2.25	0.69
1:B:422:HIS:CG	1:B:423:PRO:HD2	2.30	0.66
1:D:425:LEU:HD12	1:D:426:PRO:HD2	1.79	0.65
1:D:473:ASP:CG	4:D:18:HOH:O	2.37	0.65
1:C:363:LEU:CD2	2:F:1:NAG:H83	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:LEU:C	1:B:425:LEU:CD1	2.69	0.65
1:C:480:HIS:O	1:C:483:VAL:CG1	2.45	0.64
1:C:342:ARG:O	3:C:548:NH4:N	2.31	0.64
1:D:531:ALA:O	1:D:535:GLN:HA	1.97	0.64
1:B:376:ARG:HD2	1:B:414:GLU:OE2	1.98	0.63
1:B:424:HIS:CD2	1:B:424:HIS:O	2.51	0.63
1:D:513:ARG:O	1:D:517:GLU:HB2	1.99	0.63
1:C:493:THR:O	1:C:505:VAL:HG23	1.99	0.62
1:A:444:GLU:HG2	1:B:453:TRP:CE2	2.35	0.61
1:A:371:GLN:HB2	1:A:421:THR:HB	1.82	0.60
1:C:369:THR:HG23	1:C:369:THR:O	2.01	0.60
1:B:422:HIS:ND1	1:B:423:PRO:HD2	2.18	0.59
1:B:359:LEU:HD13	1:B:400:THR:CG2	2.31	0.59
1:C:480:HIS:O	1:C:483:VAL:HG13	2.02	0.59
1:C:531:ALA:O	1:C:535:GLN:HA	2.01	0.59
1:A:425:LEU:CD1	1:A:425:LEU:C	2.72	0.59
1:A:445:VAL:HG13	1:A:466:ILE:CD1	2.33	0.59
1:B:419:ARG:HG3	1:B:430:MET:HG2	1.83	0.59
1:B:369:THR:O	1:B:369:THR:CG2	2.43	0.59
1:A:422:HIS:CG	1:A:423:PRO:HD2	2.38	0.58
1:A:466:ILE:HB	1:A:505:VAL:HG12	1.85	0.58
1:B:346:PHE:HE1	1:B:477:GLN:HE22	1.50	0.58
1:D:470:MET:HE2	1:D:502:GLY:HA2	1.86	0.58
1:B:424:HIS:O	1:B:424:HIS:HD2	1.87	0.57
1:D:470:MET:HE1	1:D:501:SER:HB3	1.86	0.57
1:C:425:LEU:HD12	1:C:425:LEU:C	2.30	0.57
1:A:372:LEU:HD22	1:A:420:VAL:HG22	1.86	0.57
1:B:513:ARG:HG3	1:B:517:GLU:HG3	1.86	0.57
1:A:445:VAL:HG13	1:A:466:ILE:HD11	1.85	0.57
1:B:346:PHE:CE1	1:B:477:GLN:NE2	2.73	0.57
1:B:361:VAL:HG12	1:B:362:ASP:N	2.20	0.57
1:B:363:LEU:HD21	1:B:422:HIS:ND1	2.21	0.56
1:D:359:LEU:HD13	1:D:400:THR:HG22	1.87	0.55
1:A:359:LEU:CD1	1:A:400:THR:HG22	2.36	0.55
1:D:537:VAL:HG22	4:D:179:HOH:O	2.07	0.54
1:D:470:MET:HE1	1:D:501:SER:C	2.32	0.54
1:B:489:ARG:NH2	1:B:515:GLU:OE1	2.39	0.54
1:B:359:LEU:CD1	1:B:400:THR:HG22	2.36	0.54
1:A:470:MET:HE1	1:A:501:SER:HB3	1.90	0.54
1:A:359:LEU:HD13	1:A:400:THR:HG22	1.91	0.53
1:C:372:LEU:HD22	1:C:420:VAL:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:HIS:CE1	1:B:423:PRO:HD2	2.44	0.53
1:A:360:VAL:HG21	1:A:372:LEU:HD21	1.91	0.53
1:B:364:ALA:HB3	1:B:365:PRO:CD	2.39	0.52
1:C:340:LEU:HD23	1:C:432:SER:C	2.34	0.52
1:C:525:ARG:HD2	1:C:536:THR:CG2	2.39	0.52
1:A:421:THR:HG23	1:A:425:LEU:CD2	2.40	0.51
1:B:396:THR:HG23	1:B:397:LEU:N	2.26	0.51
1:C:336:VAL:HG22	1:C:362:ASP:OD1	2.10	0.51
1:C:480:HIS:O	1:C:483:VAL:HG12	2.09	0.51
1:B:372:LEU:HD23	1:B:401:SER:CB	2.40	0.51
1:D:360:VAL:HG21	1:D:372:LEU:HD21	1.91	0.51
1:C:393:ARG:HG3	4:C:235:HOH:O	2.10	0.51
1:C:349:PHE:HB3	1:C:535:GLN:HG3	1.92	0.51
1:D:470:MET:CE	1:D:501:SER:C	2.84	0.50
1:A:479:LEU:HD21	1:A:525:ARG:NH2	2.27	0.50
1:B:372:LEU:HD23	1:B:401:SER:HB2	1.92	0.50
1:D:359:LEU:CD1	1:D:400:THR:HG22	2.41	0.50
1:C:493:THR:O	1:C:505:VAL:CG2	2.60	0.50
1:B:424:HIS:CD2	1:B:424:HIS:C	2.91	0.49
1:A:421:THR:HG23	1:A:425:LEU:HD21	1.92	0.49
1:D:441:ALA:HB3	1:D:470:MET:HG2	1.95	0.49
1:A:453:TRP:O	1:A:454:PRO:C	2.57	0.48
1:D:375:SER:OG	1:D:417:GLN:HG3	2.14	0.48
1:B:439:PRO:HB2	1:B:470:MET:HE2	1.94	0.48
1:C:366:SER:O	1:C:368:GLY:N	2.46	0.48
1:C:363:LEU:HD21	2:F:1:NAG:H83	1.95	0.48
1:C:453:TRP:CE2	1:D:444:GLU:HB3	2.49	0.48
1:B:422:HIS:HD2	1:B:424:HIS:CD2	2.31	0.48
1:A:444:GLU:O	1:A:466:ILE:HA	2.15	0.47
1:D:376:ARG:HD2	1:D:414:GLU:OE2	2.14	0.47
1:B:513:ARG:HA	1:B:516:TRP:CD2	2.50	0.47
1:C:370:VAL:HG22	1:C:422:HIS:CD2	2.50	0.47
1:C:368:GLY:HA3	1:C:423:PRO:HG2	1.97	0.47
1:C:378:SER:OG	1:C:414:GLU:OE2	2.26	0.47
1:C:425:LEU:C	1:C:425:LEU:CD1	2.87	0.47
1:C:493:THR:HG21	1:D:493:THR:HG21	1.96	0.47
1:D:473:ASP:HB2	4:D:18:HOH:O	2.14	0.47
1:D:470:MET:HE1	1:D:501:SER:CB	2.45	0.47
1:D:493:THR:O	1:D:505:VAL:CG2	2.64	0.46
1:A:422:HIS:N	1:A:425:LEU:HD23	2.31	0.46
1:B:440:ARG:NH1	1:B:529:GLU:OE2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:408:ARG:NE	1:D:412:GLU:OE2	2.48	0.46
1:C:525:ARG:HD2	1:C:536:THR:HG21	1.97	0.46
1:D:493:THR:O	1:D:505:VAL:HG23	2.15	0.46
1:B:367:LYS:HB3	1:B:423:PRO:HG2	1.98	0.46
2:F:3:BMA:H61	2:F:5:MAN:H2	1.53	0.46
1:C:531:ALA:HB1	1:C:537:VAL:HG23	1.97	0.45
1:D:473:ASP:CB	4:D:18:HOH:O	2.63	0.45
1:B:361:VAL:CG1	1:B:362:ASP:N	2.79	0.45
1:D:359:LEU:HD13	1:D:400:THR:CG2	2.46	0.45
1:A:466:ILE:HB	1:A:505:VAL:CG1	2.47	0.45
1:C:420:VAL:HB	1:C:429:LEU:HB2	1.99	0.45
1:A:523:ILE:HD12	4:A:181:HOH:O	2.16	0.45
1:C:370:VAL:HG22	1:C:422:HIS:HD2	1.81	0.44
1:D:372:LEU:HD12	1:D:401:SER:HB2	1.98	0.44
1:D:531:ALA:CB	1:D:537:VAL:HG23	2.43	0.44
1:A:525:ARG:HD2	1:A:536:THR:HG23	1.98	0.44
1:D:440:ARG:NH1	1:D:529:GLU:OE2	2.51	0.44
1:A:340:LEU:HD23	1:A:432:SER:C	2.43	0.44
1:A:486:PRO:O	1:A:489:ARG:HB2	2.18	0.44
1:D:444:GLU:OE1	1:D:446:TYR:OH	2.28	0.43
1:B:422:HIS:CD2	1:B:424:HIS:CD2	3.06	0.43
1:B:363:LEU:HD23	1:B:370:VAL:HG21	2.01	0.43
1:B:422:HIS:CG	1:B:423:PRO:CD	2.99	0.43
1:B:358:CYS:HB2	1:B:374:TRP:CH2	2.53	0.43
1:D:480:HIS:O	1:D:483:VAL:HG12	2.19	0.43
1:C:425:LEU:O	1:C:425:LEU:CD1	2.52	0.43
1:A:446:TYR:CD2	1:B:451:PRO:HD2	2.53	0.43
1:B:368:GLY:O	1:B:369:THR:OG1	2.31	0.43
1:B:513:ARG:CG	1:B:517:GLU:HG3	2.49	0.43
1:C:376:ARG:HD2	1:C:414:GLU:OE2	2.18	0.43
1:B:513:ARG:HA	1:B:516:TRP:CE2	2.53	0.43
1:A:422:HIS:HB3	1:A:425:LEU:HB3	2.01	0.42
1:B:532:SER:HA	1:B:533:PRO:HA	1.85	0.42
1:C:349:PHE:O	1:C:352:LYS:NZ	2.53	0.42
1:A:371:GLN:HE21	1:A:371:GLN:HA	1.85	0.42
1:B:376:ARG:HD3	1:B:414:GLU:HG2	2.01	0.41
1:B:360:VAL:HG13	1:B:399:VAL:HG13	2.02	0.41
1:B:458:ASP:OD1	1:B:513:ARG:NH1	2.53	0.41
1:C:371:GLN:C	1:C:372:LEU:HD23	2.45	0.41
1:D:470:MET:CE	1:D:502:GLY:HA2	2.49	0.41
1:A:543:VAL:O	1:A:544:ASN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:PRO:CB	1:B:470:MET:HE2	2.51	0.41
1:A:470:MET:HA	1:A:471:PRO:C	2.46	0.41
1:B:336:VAL:HG22	1:B:363:LEU:HD13	2.01	0.41
1:D:422:HIS:HB3	1:D:425:LEU:CB	2.46	0.41
1:D:466:ILE:HB	1:D:505:VAL:HG12	2.03	0.41
1:A:541:VAL:HG22	1:A:542:SER:N	2.36	0.40
1:D:405:VAL:HG12	1:D:416:TYR:CE2	2.55	0.40
1:B:421:THR:HA	1:B:425:LEU:HD23	2.04	0.40
1:D:408:ARG:HG2	1:D:412:GLU:CD	2.46	0.40
1:C:465:LEU:HD13	1:C:506:PHE:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	207/223 (93%)	197 (95%)	7 (3%)	3 (1%)	9	8
1	B	207/223 (93%)	193 (93%)	11 (5%)	3 (1%)	9	8
1	C	207/223 (93%)	199 (96%)	7 (3%)	1 (0%)	24	32
1	D	207/223 (93%)	197 (95%)	8 (4%)	2 (1%)	12	14
All	All	828/892 (93%)	786 (95%)	33 (4%)	9 (1%)	11	12

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	368	GLY
1	C	367	LYS
1	A	500	GLY
1	B	369	THR
1	D	500	GLY

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Mol	Chain	Res	Type
1	B	426	PRO
1	A	426	PRO
1	A	365	PRO
1	D	426	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	185/195 (95%)	180 (97%)	5 (3%)	39	54
1	B	185/195 (95%)	175 (95%)	10 (5%)	20	29
1	C	185/195 (95%)	179 (97%)	6 (3%)	34	49
1	D	185/195 (95%)	178 (96%)	7 (4%)	29	43
All	All	740/780 (95%)	712 (96%)	28 (4%)	29	43

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	369	THR
1	A	371	GLN
1	A	425	LEU
1	A	537	VAL
1	A	539	ARG
1	B	360	VAL
1	B	363	LEU
1	B	396	THR
1	B	398	THR
1	B	399	VAL
1	B	408	ARG
1	B	424	HIS
1	B	425	LEU
1	B	474	ILE
1	B	519	LYS
1	C	353	SER
1	C	366	SER

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Mol	Chain	Res	Type
1	C	425	LEU
1	C	437	SER
1	C	483	VAL
1	C	489	ARG
1	D	353	SER
1	D	421	THR
1	D	444	GLU
1	D	460	ARG
1	D	523	ILE
1	D	535	GLN
1	D	536	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	371	GLN
1	A	481	ASN
1	A	484	GLN
1	A	490	HIS
1	A	518	GLN
1	A	535	GLN
1	B	422	HIS
1	B	424	HIS
1	B	490	HIS
1	B	538	GLN
1	B	544	ASN
1	C	417	GLN
1	C	468	ASN
1	C	484	GLN
1	D	371	GLN
1	D	384	HIS
1	D	392	GLN
1	D	484	GLN
1	D	535	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 ⓘ

15 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	E	1	1,2	14,14,15	0.50	0	17,19,21	1.33	2 (11%)
2	NAG	E	2	2	14,14,15	0.56	0	17,19,21	1.37	2 (11%)
2	BMA	E	3	2	11,11,12	0.69	0	15,15,17	1.86	3 (20%)
2	MAN	E	4	2	11,11,12	0.58	0	15,15,17	1.40	3 (20%)
2	MAN	E	5	2	11,11,12	0.63	0	15,15,17	1.39	3 (20%)
2	NAG	F	1	1,2	14,14,15	0.50	0	17,19,21	1.13	1 (5%)
2	NAG	F	2	2	14,14,15	0.45	0	17,19,21	1.28	1 (5%)
2	BMA	F	3	2	11,11,12	0.58	0	15,15,17	1.83	3 (20%)
2	MAN	F	4	2	11,11,12	0.58	0	15,15,17	1.04	0
2	MAN	F	5	2	11,11,12	0.73	0	15,15,17	1.36	2 (13%)
2	NAG	G	1	1,2	14,14,15	0.51	0	17,19,21	1.23	2 (11%)
2	NAG	G	2	2	14,14,15	0.55	0	17,19,21	0.75	0
2	BMA	G	3	2	11,11,12	0.62	0	15,15,17	1.22	2 (13%)
2	MAN	G	4	2	11,11,12	0.58	0	15,15,17	1.09	1 (6%)
2	MAN	G	5	2	11,11,12	0.57	0	15,15,17	1.11	2 (13%)

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	E	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
2	MAN	E	4	2	-	1/2/19/22	0/1/1/1
2	MAN	E	5	2	-	2/2/19/22	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	BMA	F	3	2	-	1/2/19/22	0/1/1/1
2	MAN	F	4	2	-	2/2/19/22	0/1/1/1
2	MAN	F	5	2	-	2/2/19/22	0/1/1/1
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	BMA	G	3	2	-	2/2/19/22	0/1/1/1
2	MAN	G	4	2	-	2/2/19/22	0/1/1/1
2	MAN	G	5	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	BMA	O5-C5-C6	4.95	117.29	107.66
2	F	3	BMA	O5-C5-C6	4.68	116.78	107.66
2	F	2	NAG	C1-O5-C5	3.71	117.16	112.19
2	G	1	NAG	O5-C1-C2	-3.29	106.20	111.29
2	F	3	BMA	O3-C3-C4	-3.21	102.82	110.38
2	E	3	BMA	O3-C3-C4	-3.04	103.21	110.38
2	E	5	MAN	C3-C4-C5	2.98	115.64	110.23
2	E	2	NAG	C1-O5-C5	2.87	116.03	112.19
2	E	3	BMA	C6-C5-C4	-2.85	106.01	113.02
2	E	1	NAG	O5-C5-C6	2.81	113.14	107.66
2	E	4	MAN	C3-C4-C5	-2.71	105.32	110.23
2	G	3	BMA	O5-C5-C6	2.70	112.92	107.66
2	E	5	MAN	O4-C4-C3	-2.49	104.51	110.38
2	E	1	NAG	O5-C1-C2	-2.40	107.58	111.29
2	F	3	BMA	C3-C4-C5	2.30	114.40	110.23
2	E	4	MAN	C2-C3-C4	-2.29	106.84	110.86
2	G	3	BMA	C2-C3-C4	-2.27	106.87	110.86
2	F	1	NAG	C1-O5-C5	2.25	115.21	112.19
2	G	5	MAN	O5-C1-C2	-2.19	105.56	110.79
2	F	5	MAN	C1-O5-C5	2.17	115.10	112.19
2	E	4	MAN	O5-C1-C2	-2.13	105.71	110.79
2	E	5	MAN	O5-C1-C2	-2.12	105.73	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	NAG	C6-C5-C4	-2.08	107.92	113.02
2	E	2	NAG	O7-C7-C8	-2.06	118.38	122.05
2	F	5	MAN	O4-C4-C3	-2.06	105.53	110.38
2	G	5	MAN	C1-C2-C3	-2.02	106.70	109.64
2	G	4	MAN	O5-C5-C6	2.01	111.57	107.66

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	2	NAG	O5-C5-C6-O6
2	E	5	MAN	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	F	4	MAN	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	G	3	BMA	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	E	5	MAN	C4-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6
2	G	5	MAN	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	G	5	MAN	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	F	5	MAN	O5-C5-C6-O6
2	G	3	BMA	C4-C5-C6-O6
2	G	4	MAN	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	F	4	MAN	C4-C5-C6-O6
2	F	3	BMA	O5-C5-C6-O6
2	E	3	BMA	C4-C5-C6-O6
2	F	5	MAN	C4-C5-C6-O6
2	G	4	MAN	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	E	4	MAN	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

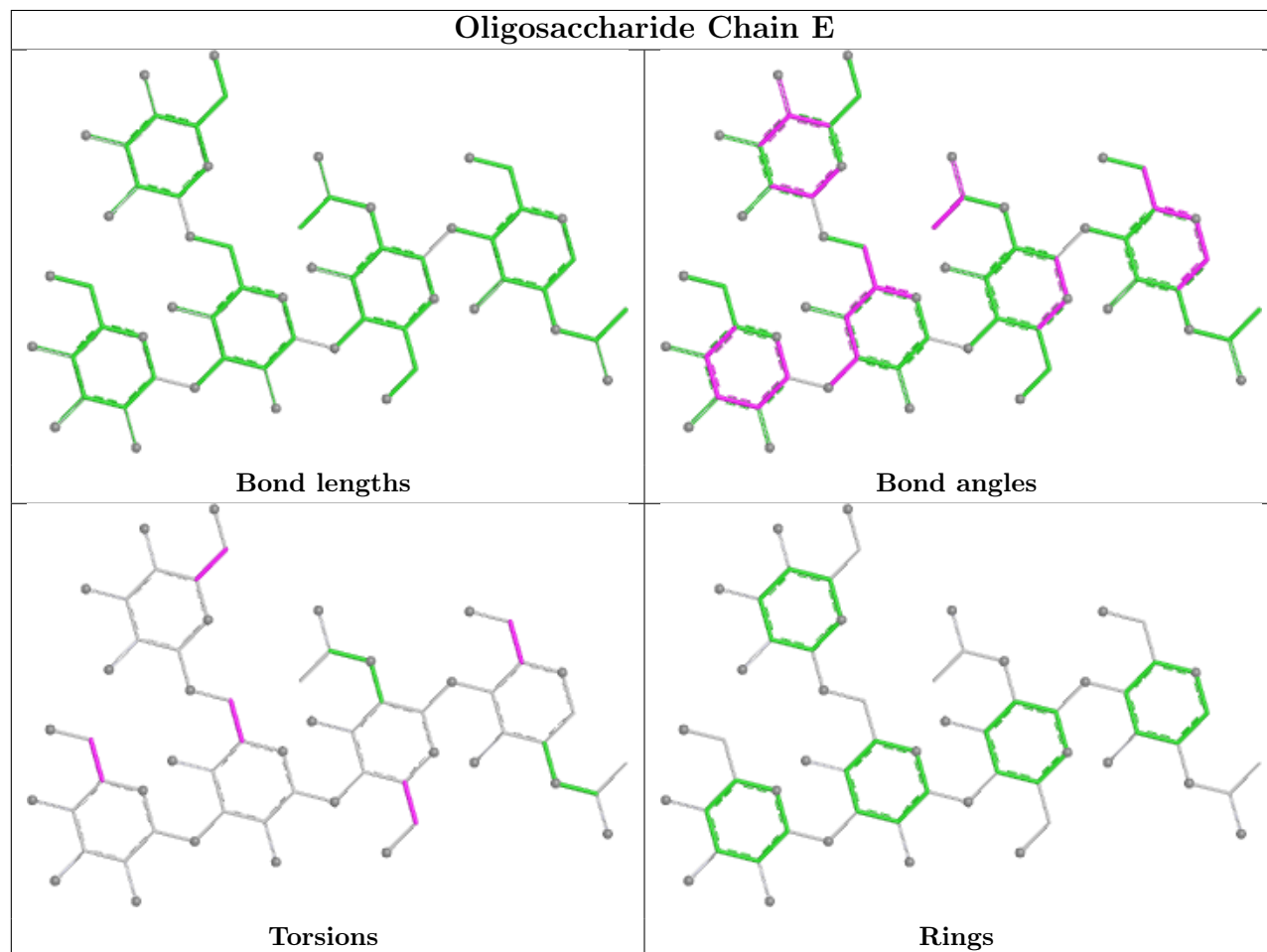
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	NAG	2	0
2	F	3	BMA	1	0

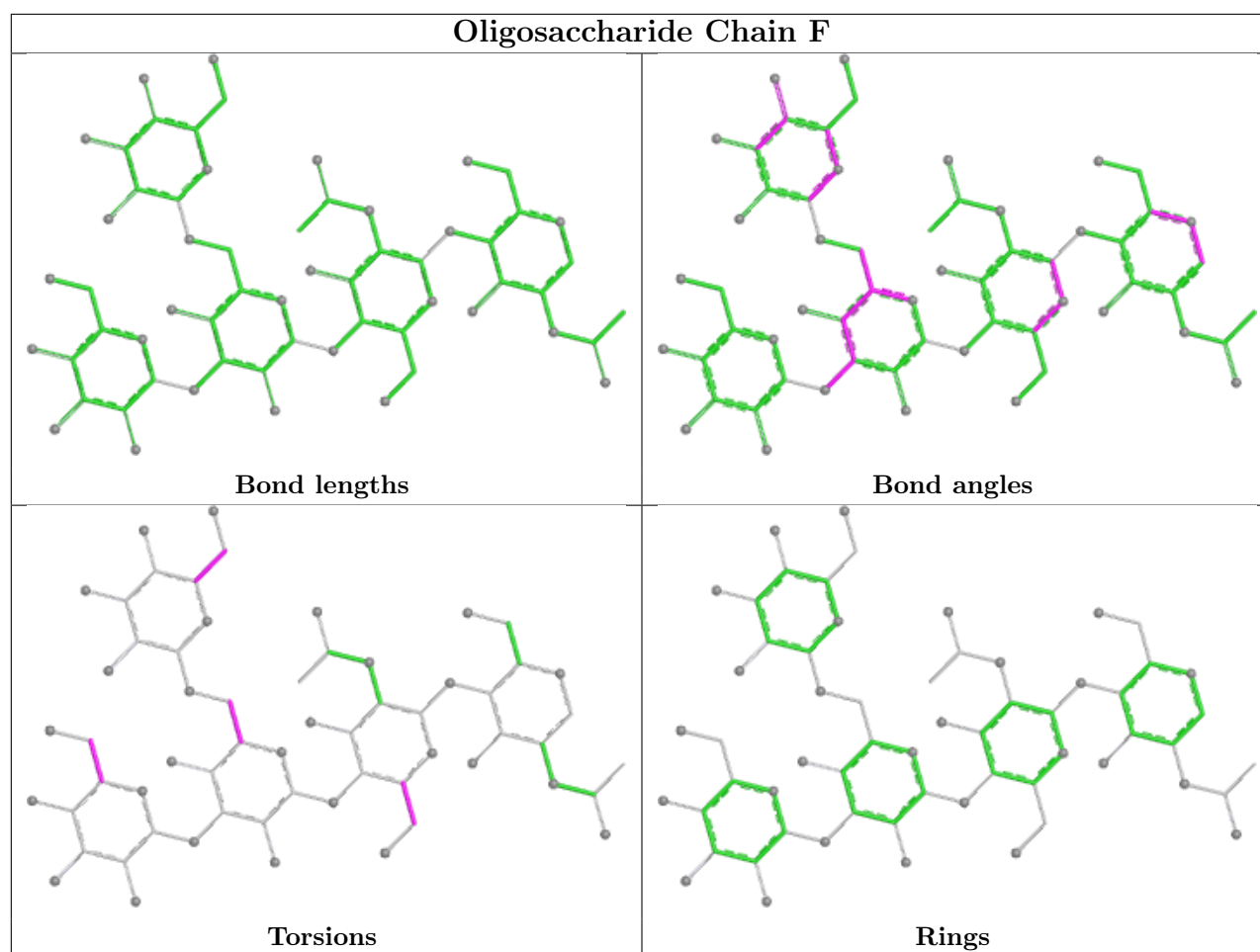
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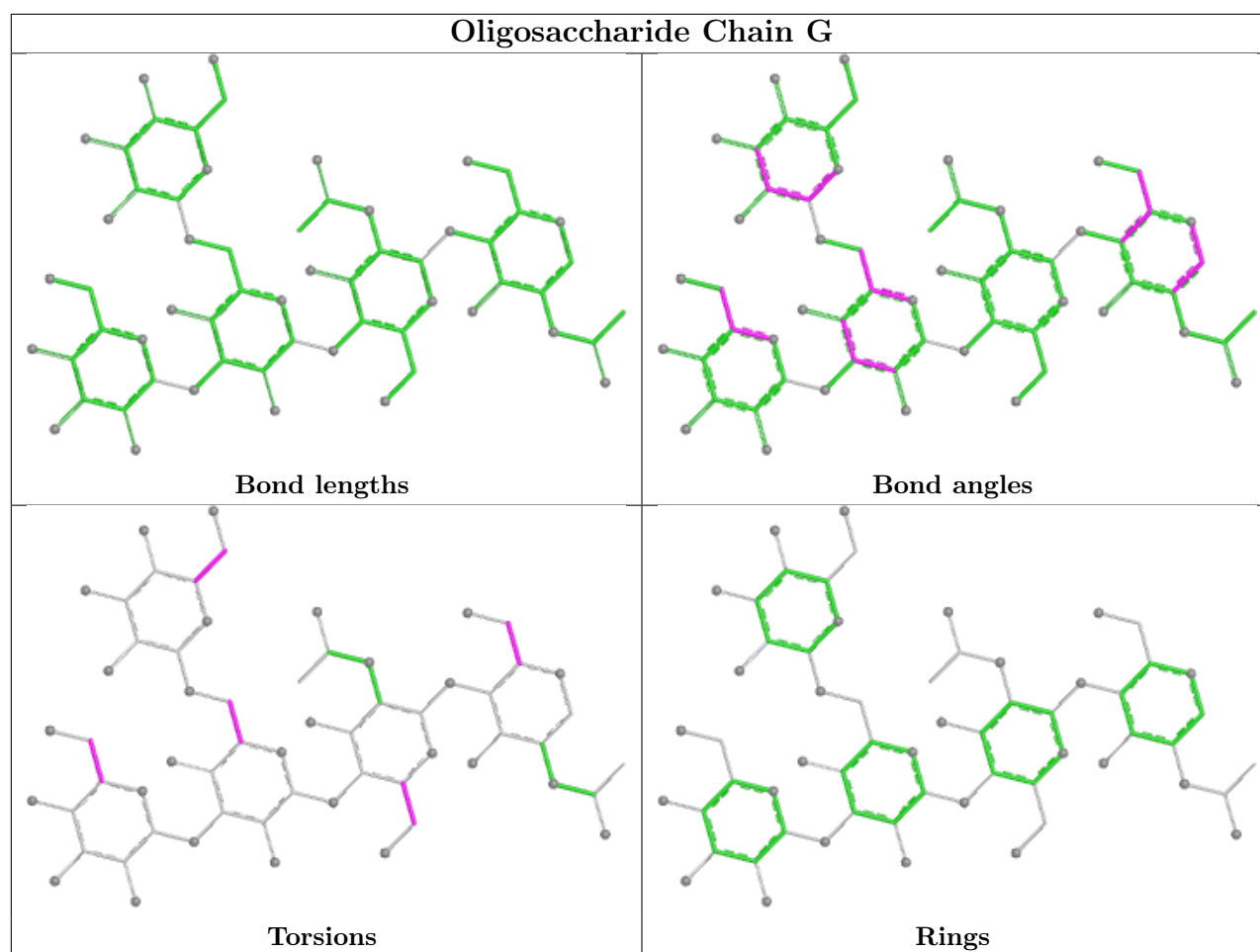
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	5	MAN	1	0

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](#)

Of 1 ligands modelled in this entry, 1 is modelled with single atom - leaving 0 for Mogul analysis.

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 ⓘ

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	209/223 (93%)	0.19	3 (1%) 73 75	18, 33, 59, 70	0
1	B	209/223 (93%)	0.34	13 (6%) 26 24	18, 32, 65, 74	0
1	C	209/223 (93%)	0.25	9 (4%) 40 39	16, 33, 61, 72	0
1	D	209/223 (93%)	0.44	17 (8%) 18 16	18, 33, 66, 77	0
All	All	836/892 (93%)	0.31	42 (5%) 34 32	16, 33, 64, 77	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	364	ALA	4.3
1	B	422	HIS	4.2
1	B	365	PRO	4.0
1	C	422	HIS	3.7
1	B	368	GLY	3.7
1	B	426	PRO	3.6
1	B	363	LEU	3.6
1	B	364	ALA	3.5
1	C	363	LEU	3.5
1	D	422	HIS	3.5
1	C	424	HIS	3.1
1	D	436	THR	3.1
1	D	501	SER	3.1
1	A	363	LEU	3.0
1	D	421	THR	2.9
1	D	456	SER	2.9
1	C	430	MET	2.9
1	D	426	PRO	2.8
1	A	426	PRO	2.8
1	D	423	PRO	2.7
1	B	428	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	369	THR	2.6
1	C	426	PRO	2.6
1	D	367	LYS	2.6
1	B	429	LEU	2.5
1	C	437	SER	2.5
1	C	367	LYS	2.4
1	D	455	GLY	2.4
1	D	454	PRO	2.3
1	B	427	ARG	2.3
1	D	487	ASP	2.3
1	D	363	LEU	2.3
1	D	453	TRP	2.3
1	D	370	VAL	2.2
1	B	353	SER	2.2
1	D	369	THR	2.1
1	A	437	SER	2.1
1	B	425	LEU	2.1
1	B	393	ARG	2.0
1	D	336	VAL	2.0
1	D	364	ALA	2.0
1	B	423	PRO	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.

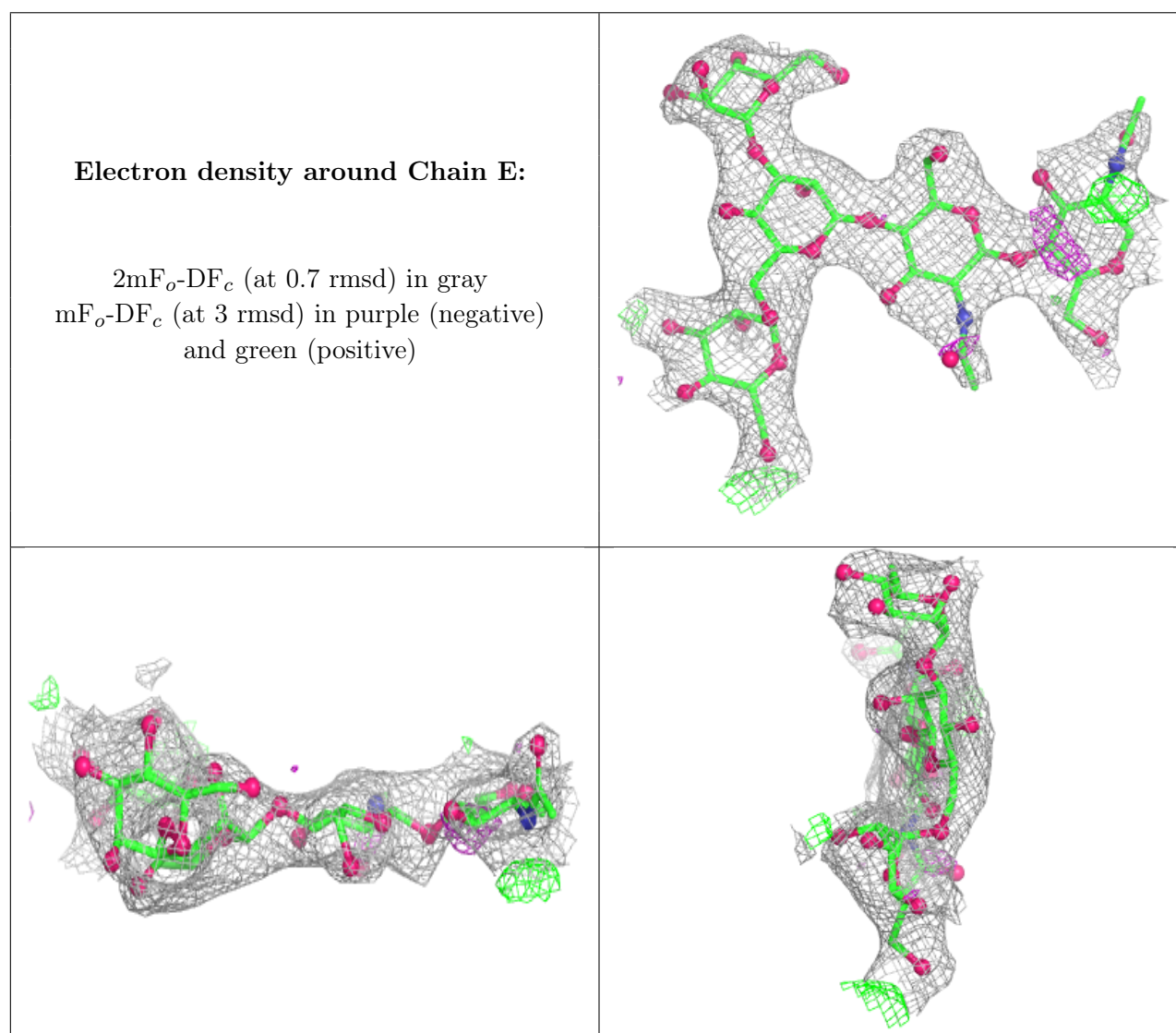
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	F	4	11/12	0.43	0.17	72,74,75,75	0
2	MAN	G	5	11/12	0.48	0.19	74,75,76,77	0
2	MAN	E	5	11/12	0.55	0.16	68,69,70,70	0
2	MAN	G	4	11/12	0.66	0.15	72,73,73,74	0
2	NAG	E	1	14/15	0.68	0.16	63,64,64,64	0
2	NAG	G	1	14/15	0.68	0.16	58,60,61,63	0
2	NAG	F	1	14/15	0.70	0.15	57,60,61,61	0

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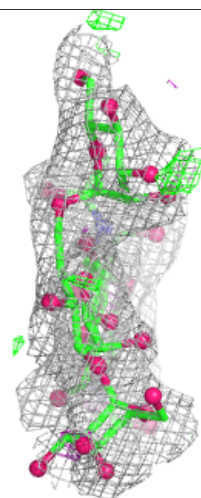
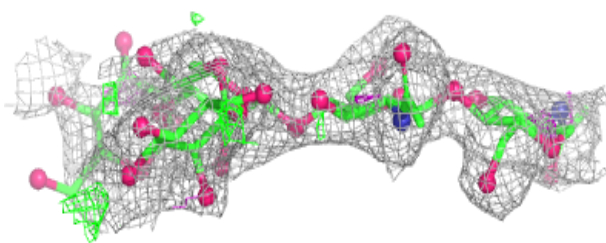
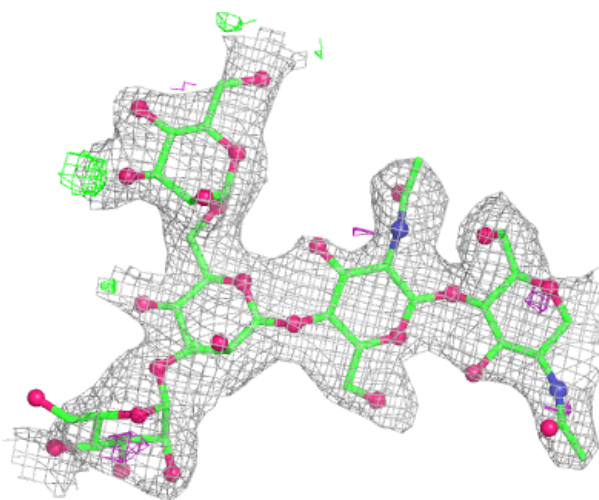
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MAN	E	4	11/12	0.71	0.13	69,69,70,70	0
2	NAG	G	2	14/15	0.74	0.14	64,65,66,67	0
2	BMA	F	3	11/12	0.77	0.12	63,64,66,69	0
2	MAN	F	5	11/12	0.78	0.12	60,61,62,62	0
2	NAG	E	2	14/15	0.80	0.13	62,65,66,67	0
2	BMA	G	3	11/12	0.80	0.12	67,69,71,72	0
2	NAG	F	2	14/15	0.81	0.13	59,61,62,63	0
2	BMA	E	3	11/12	0.82	0.11	66,67,68,69	0

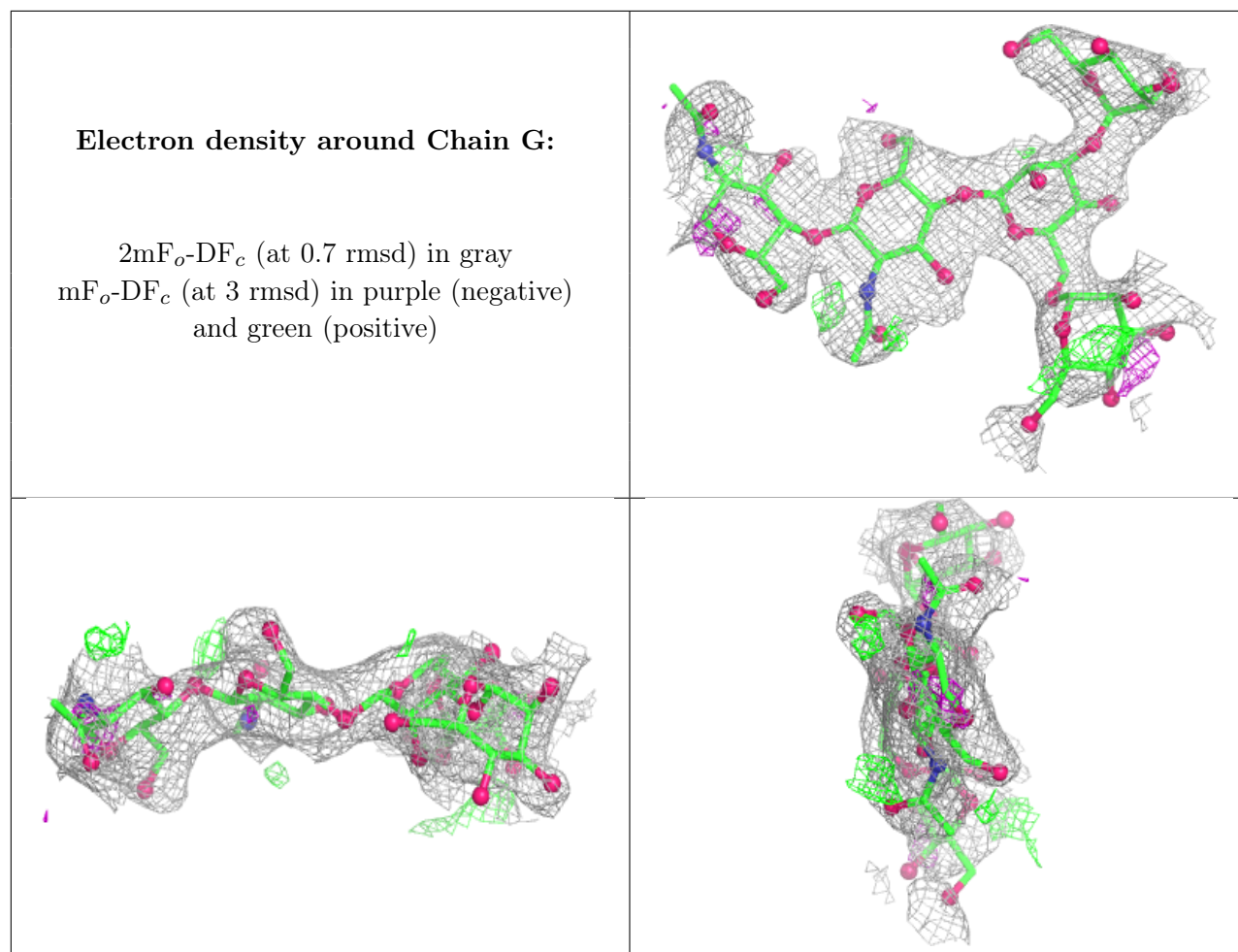
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain F:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





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	NH4	C	548	1/1	0.89	0.15	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.