



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:26 AM UTC

PDB ID : 4WI4 / pdb_00004wi4
Title : Structural mapping of the human IgG1 binding site for FcRn: hu3S193 Fc mutation S254A
Authors : Farrugia, W.; Burvenich, I.J.G.; Scott, A.M.; Ramsland, P.A.
Deposited on : 2014-09-25
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)
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

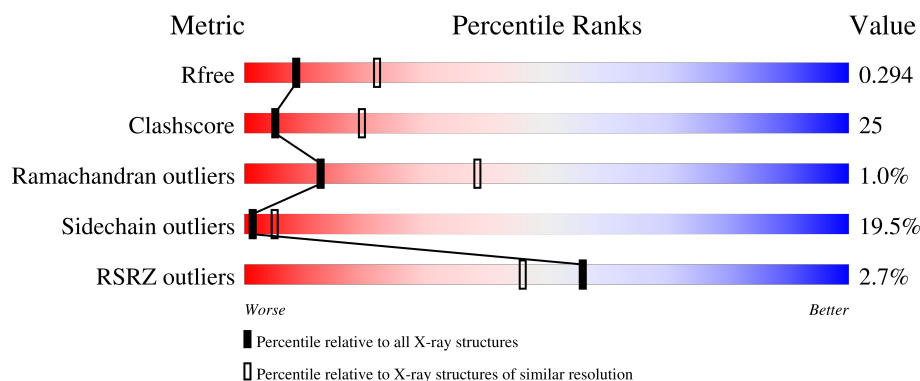
1 Overall quality at a glance

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	207	2% 52% 34% 13% ..
1	B	207	3% 49% 35% 14% .
2	C	8	12% 50% 38%
2	D	8	25% 62% 12%

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
2	NAG	D	1	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3548 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.

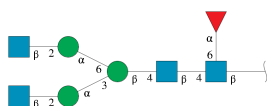
- Molecule 1 is a protein called Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1646	1049	277	314	6			
1	B	207	Total	C	N	O	S	0	0	0
			1659	1057	279	317	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	254	ALA	SER	engineered mutation	UNP P01857
B	254	ALA	SER	engineered mutation	UNP P01857

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	0	0	0
			99	56	4	39			
2	D	8	Total	C	N	O	0	0	0
			99	56	4	39			

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

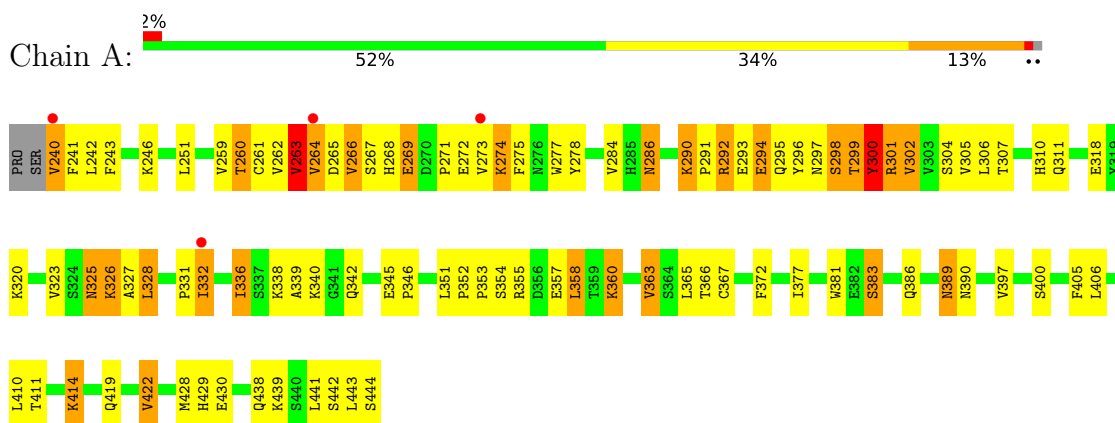
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total	O	0	0
			16	16		
4	B	17	Total	O	0	0
			17	17		

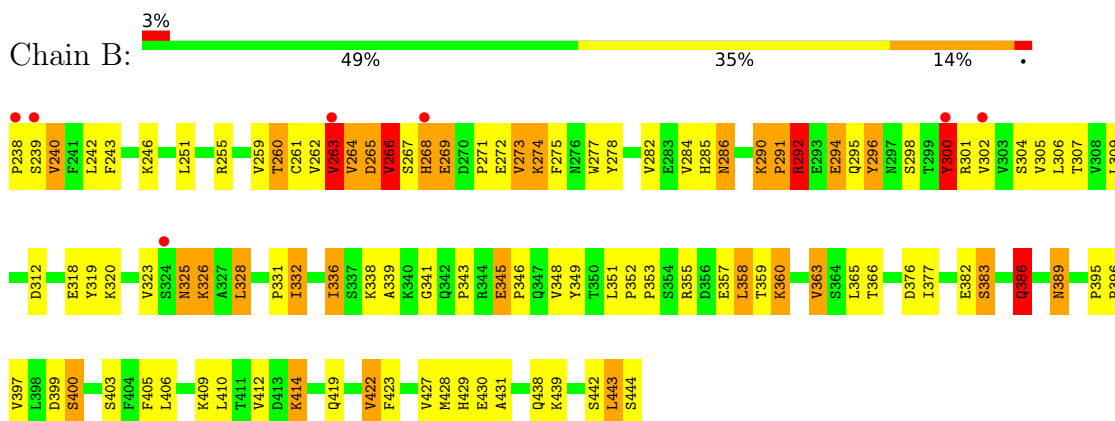
3 Residue-property plots [i](#)

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.

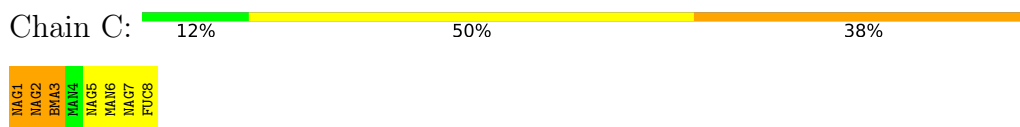
- Molecule 1: Ig gamma-1 chain C region



- Molecule 1: Ig gamma-1 chain C region



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



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

Chain D:  25% 62% 12%

NAG1	NAG2	BR43	MAN4	NAG5	NAG6	NAG7	FUC8
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.16Å 79.11Å 141.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.67 – 2.80 28.67 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.8 (28.67-2.80) 96.7 (28.67-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.80Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.240 , 0.308 0.229 , 0.294	Depositor DCC
R_{free} test set	1372 reflections (9.67%)	wwPDB-VP
Wilson B-factor (Å ²)	61.1	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 70.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3548	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.24% 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: EDO, FUC, MAN, NAG, BMA

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	0.93	6/1691 (0.4%)	1.21	14/2304 (0.6%)
1	B	0.99	10/1705 (0.6%)	1.24	16/2323 (0.7%)
All	All	0.96	16/3396 (0.5%)	1.23	30/4627 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	266	VAL	C-O	9.37	1.35	1.23
1	A	386	GLN	CD-OE1	-8.74	1.06	1.23
1	B	386	GLN	CD-OE1	-7.80	1.08	1.23
1	B	266	VAL	N-CA	6.58	1.53	1.46
1	B	386	GLN	CD-NE2	-5.75	1.21	1.33
1	A	419	GLN	CB-CG	-5.75	1.35	1.52
1	A	311	GLN	CA-C	-5.73	1.45	1.52
1	B	268	HIS	CE1-NE2	5.54	1.38	1.32
1	B	266	VAL	CA-C	5.49	1.59	1.52
1	A	386	GLN	CD-NE2	-5.42	1.21	1.33
1	B	419	GLN	CB-CG	-5.40	1.36	1.52
1	B	325	ASN	CG-ND2	-5.33	1.22	1.33
1	B	265	ASP	C-O	5.28	1.30	1.24
1	A	325	ASN	CG-ND2	-5.20	1.22	1.33
1	B	300	TYR	CA-C	-5.05	1.46	1.53
1	A	300	TYR	CA-C	-5.02	1.47	1.53

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	291	PRO	CA-C-O	-10.67	109.19	121.56
1	A	291	PRO	CA-C-N	9.42	134.95	122.42
1	A	291	PRO	C-N-CA	9.42	134.95	122.42
1	B	263	VAL	CB-CA-C	-9.10	102.04	111.23
1	A	291	PRO	O-C-N	8.78	133.53	122.91
1	A	263	VAL	CB-CA-C	-7.77	101.92	111.32
1	B	266	VAL	N-CA-C	-7.61	97.12	108.99
1	B	352	PRO	CA-C-N	7.50	127.55	119.90
1	B	352	PRO	C-N-CA	7.50	127.55	119.90
1	B	291	PRO	CA-C-N	7.11	134.50	121.70
1	B	291	PRO	C-N-CA	7.11	134.50	121.70
1	A	310	HIS	CA-C-N	7.08	129.65	120.44
1	A	310	HIS	C-N-CA	7.08	129.65	120.44
1	A	352	PRO	CA-C-N	6.74	128.26	119.84
1	A	352	PRO	C-N-CA	6.74	128.26	119.84
1	B	291	PRO	O-C-N	-6.23	115.29	123.01
1	B	292	ARG	NE-CZ-NH1	-6.13	115.37	121.50
1	B	332	ILE	CB-CG1-CD1	6.05	126.50	113.80
1	B	265	ASP	CA-C-N	-5.90	112.83	122.57
1	B	265	ASP	C-N-CA	-5.90	112.83	122.57
1	A	292	ARG	CB-CA-C	-5.58	101.60	110.81
1	B	273	VAL	N-CA-C	5.43	116.10	108.17
1	A	419	GLN	N-CA-CB	-5.36	101.89	110.19
1	A	263	VAL	CG1-CB-CG2	-5.35	99.03	110.80
1	B	419	GLN	CB-CA-C	-5.34	102.06	110.86
1	A	327	ALA	N-CA-C	-5.14	106.51	112.89
1	B	345	GLU	CA-C-N	5.09	125.33	119.83
1	B	345	GLU	C-N-CA	5.09	125.33	119.83
1	A	300	TYR	N-CA-CB	5.03	117.19	109.94
1	A	266	VAL	CG1-CB-CG2	5.03	121.86	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	291	PRO	Peptide

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	1646	0	1615	92	0
1	B	1659	0	1628	82	1
2	C	99	0	85	7	0
2	D	99	0	85	1	0
3	A	4	0	6	0	0
3	B	8	0	12	1	0
4	A	16	0	0	7	0
4	B	17	0	0	1	0
All	All	3548	0	3431	172	1

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 25.

All (172) 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:B:240:VAL:HG23	1:B:263:VAL:HG13	1.41	1.02
1:A:240:VAL:HG23	1:A:263:VAL:HG12	1.44	0.98
1:B:263:VAL:HG23	1:B:302:VAL:O	1.69	0.91
1:A:294:GLU:HA	1:A:300:TYR:HB3	1.52	0.90
1:A:275:PHE:CD2	1:A:304:SER:HB2	2.10	0.87
1:B:275:PHE:CD2	1:B:304:SER:HB2	2.10	0.87
1:A:300:TYR:HD1	1:A:300:TYR:H	1.24	0.86
1:B:240:VAL:CG2	1:B:263:VAL:HG13	2.11	0.81
1:B:240:VAL:HG23	1:B:263:VAL:CG1	2.12	0.80
1:A:264:VAL:HG11	2:C:2:NAG:H2	1.62	0.79
1:A:325:ASN:H	1:A:328:LEU:HD11	1.47	0.79
1:B:383:SER:OG	1:B:422:VAL:O	2.02	0.77
1:A:240:VAL:HG23	1:A:263:VAL:CG1	2.14	0.77
1:A:293:GLU:O	1:A:295:GLN:NE2	2.17	0.77
1:B:267:SER:O	1:B:300:TYR:OH	2.03	0.76
1:B:325:ASN:H	1:B:328:LEU:HD11	1.48	0.76
1:A:383:SER:OG	1:A:422:VAL:O	2.04	0.74
1:B:295:GLN:HG3	1:B:296:TYR:H	1.51	0.74
1:B:403:SER:OG	4:B:615:HOH:O	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ASN:OD1	1:B:326:LYS:N	2.18	0.72
1:B:275:PHE:HD2	1:B:304:SER:HB2	1.56	0.71
1:A:263:VAL:HG23	1:A:302:VAL:O	1.91	0.70
1:A:278:TYR:HB2	1:A:320:LYS:HB3	1.74	0.69
1:B:292:ARG:HH22	1:B:300:TYR:HB3	1.57	0.69
1:A:275:PHE:HD2	1:A:304:SER:HB2	1.55	0.69
1:B:300:TYR:H	1:B:300:TYR:HD1	1.37	0.69
1:B:292:ARG:NH1	1:B:300:TYR:HD2	1.91	0.68
1:B:278:TYR:HB2	1:B:320:LYS:HB3	1.75	0.67
1:B:292:ARG:HG2	1:B:302:VAL:HG23	1.77	0.67
1:A:300:TYR:HD1	1:A:300:TYR:N	1.93	0.66
1:A:342:GLN:HG2	4:A:601:HOH:O	1.95	0.66
1:B:443:LEU:HG	1:B:444:SER:N	2.09	0.65
1:A:267:SER:O	1:A:300:TYR:OH	2.10	0.65
1:A:353:PRO:HD3	1:A:365:LEU:HD23	1.79	0.64
1:A:240:VAL:HG21	1:A:323:VAL:HG21	1.80	0.64
1:B:365:LEU:HD12	1:B:410:LEU:HD23	1.79	0.64
1:A:338:LYS:HZ1	1:A:430:GLU:CD	2.06	0.63
1:A:271:PRO:HA	1:A:300:TYR:OH	1.99	0.61
1:A:365:LEU:HD12	1:A:410:LEU:HD23	1.82	0.61
1:A:292:ARG:HA	1:A:302:VAL:HG23	1.83	0.60
1:B:240:VAL:HG21	1:B:323:VAL:HG21	1.83	0.59
1:B:377:ILE:HG13	1:B:429:HIS:HB2	1.83	0.59
1:B:277:TRP:HZ2	1:B:304:SER:HB3	1.67	0.59
1:A:267:SER:C	1:A:300:TYR:HE1	2.10	0.58
1:A:295:GLN:H	1:A:300:TYR:HA	1.66	0.58
1:A:360:LYS:HB3	4:A:615:HOH:O	2.05	0.57
1:B:300:TYR:HD1	1:B:300:TYR:N	2.03	0.57
1:A:240:VAL:HG11	1:A:332:ILE:HG21	1.87	0.57
1:A:277:TRP:HZ2	1:A:304:SER:HB3	1.68	0.57
1:B:292:ARG:HH12	1:B:300:TYR:HD2	1.51	0.56
1:B:300:TYR:N	1:B:300:TYR:CD1	2.72	0.56
1:A:300:TYR:N	1:A:300:TYR:CD1	2.68	0.56
1:B:338:LYS:HZ1	1:B:430:GLU:CD	2.12	0.56
1:B:353:PRO:HD3	1:B:365:LEU:HD23	1.87	0.56
1:A:263:VAL:CG2	1:A:302:VAL:O	2.54	0.56
1:B:243:PHE:HE2	1:B:262:VAL:HB	1.71	0.56
1:B:271:PRO:HA	1:B:300:TYR:OH	2.06	0.55
1:A:377:ILE:HG13	1:A:429:HIS:HB2	1.89	0.55
1:A:306:LEU:HD12	1:A:307:THR:N	2.22	0.55
1:B:306:LEU:HD12	1:B:307:THR:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:TYR:C	1:A:298:SER:H	2.15	0.54
1:B:389:ASN:N	1:B:389:ASN:OD1	2.38	0.54
1:A:243:PHE:HE2	1:A:262:VAL:HB	1.73	0.54
1:A:389:ASN:N	1:A:389:ASN:OD1	2.41	0.53
1:A:397:VAL:HB	1:A:405:PHE:CE2	2.43	0.53
1:B:341:GLY:O	1:B:343:PRO:HD3	2.08	0.53
1:B:243:PHE:CE1	2:D:6:MAN:H2	2.44	0.53
1:B:267:SER:C	1:B:300:TYR:HE1	2.16	0.53
1:B:338:LYS:NZ	1:B:430:GLU:OE1	2.43	0.52
1:B:348:VAL:HG21	1:B:427:VAL:HG21	1.91	0.52
1:A:242:LEU:HD23	1:A:336:ILE:HB	1.90	0.51
1:B:286:ASN:OD1	1:B:286:ASN:N	2.43	0.51
1:B:242:LEU:HD23	1:B:336:ILE:HB	1.93	0.51
1:A:354:SER:HB2	1:B:349:TYR:HB3	1.92	0.50
1:A:338:LYS:HG2	1:A:339:ALA:N	2.26	0.50
1:B:261:CYS:HB2	1:B:277:TRP:CH2	2.47	0.50
1:A:296:TYR:O	1:A:298:SER:N	2.36	0.50
1:B:422:VAL:HA	1:B:442:SER:HB3	1.93	0.50
1:A:275:PHE:CE1	1:A:323:VAL:HG13	2.47	0.50
1:A:338:LYS:NZ	1:A:430:GLU:OE1	2.44	0.49
1:A:355:ARG:HA	1:A:358:LEU:HD23	1.95	0.49
1:A:241:PHE:CZ	2:C:3:BMA:H2	2.48	0.49
1:B:275:PHE:CE1	1:B:323:VAL:HG13	2.47	0.49
1:A:342:GLN:NE2	4:A:601:HOH:O	1.81	0.49
1:B:271:PRO:HA	1:B:300:TYR:CZ	2.47	0.49
1:A:422:VAL:HA	1:A:442:SER:HB3	1.94	0.49
1:A:263:VAL:HG21	1:A:302:VAL:HG12	1.94	0.48
1:A:325:ASN:CG	1:A:326:LYS:H	2.21	0.48
1:B:332:ILE:HD12	3:B:510:EDO:O2	2.12	0.48
1:B:264:VAL:HG23	1:B:265:ASP:OD1	2.13	0.48
1:B:397:VAL:HB	1:B:405:PHE:CE2	2.49	0.48
1:A:301:ARG:HG2	1:A:301:ARG:NH1	2.29	0.48
1:A:286:ASN:OD1	1:A:286:ASN:N	2.47	0.47
1:A:260:THR:HG23	1:A:305:VAL:HG22	1.97	0.47
1:B:348:VAL:CG2	1:B:427:VAL:HG21	2.45	0.46
1:B:238:PRO:HA	1:B:265:ASP:O	2.14	0.46
1:A:275:PHE:HE1	1:A:323:VAL:HG13	1.81	0.46
1:A:274:LYS:HE3	1:A:274:LYS:HB3	1.68	0.46
1:B:274:LYS:HB3	1:B:274:LYS:HE3	1.70	0.46
1:A:241:PHE:HE2	2:C:2:NAG:H4	1.81	0.46
1:B:338:LYS:HG2	1:B:339:ALA:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:ARG:HA	1:B:358:LEU:HD23	1.98	0.46
1:A:271:PRO:HA	1:A:300:TYR:CZ	2.51	0.46
1:A:340:LYS:N	4:A:609:HOH:O	2.39	0.45
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.52	0.45
1:B:292:ARG:HH11	1:B:292:ARG:HD2	1.51	0.45
1:A:345:GLU:HA	1:A:346:PRO:HD2	1.75	0.45
1:B:444:SER:O	1:B:444:SER:OG	2.34	0.45
1:A:295:GLN:HB2	1:A:299:THR:O	2.16	0.45
1:B:290:LYS:HE2	1:B:290:LYS:HB3	1.58	0.45
1:A:301:ARG:HG2	1:A:301:ARG:HH11	1.82	0.45
1:A:354:SER:CB	1:B:349:TYR:HB3	2.45	0.45
1:A:353:PRO:HG3	1:A:363:VAL:HG13	1.98	0.45
1:B:269:GLU:OE1	1:B:269:GLU:N	2.49	0.45
1:A:351:LEU:HB2	1:A:366:THR:HB	1.97	0.45
1:A:357:GLU:O	1:A:360:LYS:HG2	2.17	0.45
1:B:358:LEU:HD12	1:B:414:LYS:HE3	1.99	0.45
1:A:290:LYS:HB3	1:A:290:LYS:HE2	1.53	0.44
1:A:390:ASN:OD1	1:A:411:THR:HB	2.17	0.44
1:A:261:CYS:HB2	1:A:277:TRP:CH2	2.51	0.44
1:A:264:VAL:HG23	1:A:265:ASP:OD1	2.16	0.44
1:A:300:TYR:HB2	1:A:301:ARG:H	1.60	0.44
1:B:266:VAL:O	1:B:300:TYR:CD1	2.70	0.44
1:B:295:GLN:HG3	1:B:296:TYR:N	2.25	0.44
1:B:357:GLU:O	1:B:360:LYS:HG2	2.18	0.44
1:A:263:VAL:CG2	1:A:302:VAL:HG12	2.47	0.44
1:B:267:SER:C	1:B:300:TYR:CE1	2.94	0.44
1:B:328:LEU:HD13	1:B:331:PRO:HA	1.98	0.44
1:B:382:GLU:HB2	1:B:386:GLN:O	2.18	0.44
1:A:240:VAL:HG11	1:A:332:ILE:CG2	2.47	0.43
1:A:268:HIS:NE2	1:A:298:SER:HA	2.33	0.43
1:A:428:MET:HE3	1:A:428:MET:HB2	1.62	0.43
1:A:328:LEU:HD13	1:A:331:PRO:HA	2.01	0.43
1:A:439:LYS:HD3	1:A:439:LYS:HA	1.84	0.43
1:A:240:VAL:CG1	1:A:332:ILE:HG21	2.48	0.43
1:A:296:TYR:C	1:A:298:SER:N	2.76	0.43
1:A:301:ARG:HD2	2:C:2:NAG:H82	2.01	0.43
1:A:444:SER:O	1:A:444:SER:OG	2.36	0.43
1:B:428:MET:HE3	1:B:428:MET:HB2	1.73	0.43
1:A:358:LEU:HD12	1:A:414:LYS:HE3	2.01	0.43
1:B:376:ASP:O	1:B:429:HIS:HD2	2.01	0.43
1:B:260:THR:HG23	1:B:305:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ASN:CG	1:A:326:LYS:N	2.78	0.42
1:A:441:LEU:HA	4:A:607:HOH:O	2.19	0.42
1:A:301:ARG:HD2	2:C:2:NAG:C8	2.49	0.42
1:A:430:GLU:N	4:A:606:HOH:O	2.27	0.42
1:A:265:ASP:OD1	2:C:1:NAG:H3	2.19	0.42
1:B:275:PHE:HE1	1:B:323:VAL:HG13	1.83	0.42
1:B:353:PRO:HG3	1:B:363:VAL:HG13	2.02	0.42
1:A:271:PRO:CA	1:A:300:TYR:OH	2.66	0.41
1:A:264:VAL:CG1	2:C:2:NAG:H2	2.40	0.41
1:A:342:GLN:CG	4:A:601:HOH:O	2.58	0.41
1:B:351:LEU:HB2	1:B:366:THR:HB	2.02	0.41
1:A:301:ARG:HH11	1:A:301:ARG:CG	2.33	0.41
1:B:255:ARG:HE	1:B:255:ARG:HB3	1.63	0.41
1:B:345:GLU:HA	1:B:346:PRO:HD2	1.70	0.41
1:B:292:ARG:HE	1:B:292:ARG:HB3	1.52	0.41
1:A:269:GLU:OE1	1:A:269:GLU:N	2.48	0.41
1:B:325:ASN:CG	1:B:326:LYS:N	2.77	0.41
1:B:439:LYS:HD3	1:B:439:LYS:HA	1.83	0.41
1:A:266:VAL:H	1:A:266:VAL:HG23	1.73	0.41
1:A:397:VAL:HB	1:A:405:PHE:CZ	2.56	0.41
1:B:399:ASP:OD1	1:B:400:SER:N	2.48	0.41
1:A:267:SER:C	1:A:300:TYR:CE1	2.96	0.40
1:B:275:PHE:CE2	1:B:304:SER:HB2	2.54	0.40
1:A:346:PRO:HB3	1:A:372:PHE:HB3	2.03	0.40
1:B:312:ASP:HB3	1:B:319:TYR:OH	2.22	0.40
1:B:345:GLU:HG3	1:B:431:ALA:O	2.21	0.40
1:B:395:PRO:HA	1:B:396:PRO:HD3	1.94	0.40
1:B:359:THR:OG1	1:B:360:LYS:HD3	2.21	0.40
1:B:412:VAL:HG11	1:B:423:PHE:CE2	2.57	0.40
1:B:309:LEU:HA	1:B:309:LEU:HD23	1.84	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:HIS:ND1	1:B:285:HIS:O[4_555]	1.99	0.21

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	203/207 (98%)	181 (89%)	20 (10%)	2 (1%)	12	38
1	B	205/207 (99%)	181 (88%)	22 (11%)	2 (1%)	12	38
All	All	408/414 (99%)	362 (89%)	42 (10%)	4 (1%)	12	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	GLU
1	B	292	ARG
1	A	297	ASN
1	B	294	GLU

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	191/193 (99%)	156 (82%)	35 (18%)	2	6
1	B	193/193 (100%)	153 (79%)	40 (21%)	1	4
All	All	384/386 (100%)	309 (80%)	75 (20%)	1	5

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	240	VAL
1	A	246	LYS

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Mol	Chain	Res	Type
1	A	251	LEU
1	A	259	VAL
1	A	260	THR
1	A	263	VAL
1	A	264	VAL
1	A	269	GLU
1	A	272	GLU
1	A	273	VAL
1	A	274	LYS
1	A	284	VAL
1	A	286	ASN
1	A	290	LYS
1	A	298	SER
1	A	299	THR
1	A	300	TYR
1	A	301	ARG
1	A	302	VAL
1	A	318	GLU
1	A	326	LYS
1	A	328	LEU
1	A	332	ILE
1	A	336	ILE
1	A	358	LEU
1	A	360	LYS
1	A	363	VAL
1	A	383	SER
1	A	389	ASN
1	A	400	SER
1	A	406	LEU
1	A	414	LYS
1	A	422	VAL
1	A	438	GLN
1	A	443	LEU
1	B	239	SER
1	B	240	VAL
1	B	246	LYS
1	B	251	LEU
1	B	259	VAL
1	B	260	THR
1	B	263	VAL
1	B	264	VAL
1	B	266	VAL

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Mol	Chain	Res	Type
1	B	269	GLU
1	B	272	GLU
1	B	273	VAL
1	B	274	LYS
1	B	282	VAL
1	B	284	VAL
1	B	286	ASN
1	B	290	LYS
1	B	292	ARG
1	B	294	GLU
1	B	296	TYR
1	B	298	SER
1	B	300	TYR
1	B	301	ARG
1	B	318	GLU
1	B	326	LYS
1	B	328	LEU
1	B	336	ILE
1	B	358	LEU
1	B	360	LYS
1	B	363	VAL
1	B	383	SER
1	B	386	GLN
1	B	389	ASN
1	B	400	SER
1	B	406	LEU
1	B	409	LYS
1	B	414	LYS
1	B	422	VAL
1	B	438	GLN
1	B	443	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	419	GLN
1	A	429	HIS
1	B	311	GLN
1	B	347	GLN
1	B	429	HIS

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 ⓘ

16 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	C	1	1,2	14,14,15	0.68	0	17,19,21	1.73	3 (17%)
2	NAG	C	2	2	14,14,15	0.69	0	17,19,21	1.59	1 (5%)
2	BMA	C	3	2	11,11,12	0.54	0	15,15,17	1.55	3 (20%)
2	MAN	C	4	2	11,11,12	0.59	0	15,15,17	0.96	0
2	NAG	C	5	2	14,14,15	0.54	0	17,19,21	0.92	2 (11%)
2	MAN	C	6	2	11,11,12	0.61	0	15,15,17	1.23	2 (13%)
2	NAG	C	7	2	14,14,15	0.55	0	17,19,21	1.56	2 (11%)
2	FUC	C	8	2	10,10,11	0.71	0	14,14,16	1.32	1 (7%)
2	NAG	D	1	1,2	14,14,15	0.36	0	17,19,21	2.01	2 (11%)
2	NAG	D	2	2	14,14,15	0.43	0	17,19,21	1.05	2 (11%)
2	BMA	D	3	2	11,11,12	0.65	0	15,15,17	1.46	1 (6%)
2	MAN	D	4	2	11,11,12	0.52	0	15,15,17	1.26	2 (13%)
2	NAG	D	5	2	14,14,15	0.62	0	17,19,21	0.78	0
2	MAN	D	6	2	11,11,12	0.77	0	15,15,17	1.28	2 (13%)
2	NAG	D	7	2	14,14,15	0.58	0	17,19,21	1.29	2 (11%)
2	FUC	D	8	2	10,10,11	0.64	0	14,14,16	0.71	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	NAG	C	5	2	-	4/6/23/26	0/1/1/1
2	MAN	C	6	2	-	2/2/19/22	0/1/1/1
2	NAG	C	7	2	-	4/6/23/26	0/1/1/1
2	FUC	C	8	2	-	-	0/1/1/1
2	NAG	D	1	1,2	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
2	MAN	D	4	2	-	2/2/19/22	0/1/1/1
2	NAG	D	5	2	-	4/6/23/26	0/1/1/1
2	MAN	D	6	2	-	2/2/19/22	0/1/1/1
2	NAG	D	7	2	-	4/6/23/26	0/1/1/1
2	FUC	D	8	2	-	-	0/1/1/1

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C1-O5-C5	7.71	122.52	112.19
2	C	2	NAG	C1-O5-C5	4.99	118.88	112.19
2	C	7	NAG	C4-C3-C2	4.45	117.53	111.02
2	C	3	BMA	C1-C2-C3	4.41	116.07	109.64
2	C	1	NAG	C1-O5-C5	4.29	117.94	112.19
2	C	1	NAG	C4-C3-C2	3.80	116.59	111.02
2	C	8	FUC	C3-C4-C5	3.32	114.86	109.81
2	D	3	BMA	C3-C4-C5	3.31	116.23	110.23
2	D	4	MAN	C2-C3-C4	-3.30	105.06	110.86
2	D	7	NAG	C4-C3-C2	3.13	115.61	111.02
2	D	4	MAN	C1-O5-C5	2.76	115.89	112.19
2	D	7	NAG	C3-C4-C5	2.48	114.73	110.23
2	D	6	MAN	C1-C2-C3	-2.36	106.21	109.64
2	C	3	BMA	C1-O5-C5	2.35	115.34	112.19
2	D	6	MAN	O5-C1-C2	-2.26	105.41	110.79
2	C	1	NAG	O5-C5-C6	-2.25	103.28	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	O5-C5-C4	2.23	116.26	110.83
2	D	2	NAG	O5-C5-C6	2.22	111.98	107.66
2	C	6	MAN	C3-C4-C5	2.17	114.17	110.23
2	D	2	NAG	O5-C1-C2	-2.14	107.98	111.29
2	C	6	MAN	C1-C2-C3	-2.14	106.53	109.64
2	C	7	NAG	O5-C1-C2	-2.12	108.01	111.29
2	C	5	NAG	O5-C1-C2	-2.09	108.06	111.29
2	C	5	NAG	C1-C2-N2	2.08	113.71	110.43
2	C	3	BMA	O5-C5-C6	2.06	111.66	107.66

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	1	NAG	C1

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	C	5	NAG	C8-C7-N2-C2
2	C	5	NAG	O7-C7-N2-C2
2	C	7	NAG	C8-C7-N2-C2
2	C	7	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	7	NAG	C8-C7-N2-C2
2	D	7	NAG	O7-C7-N2-C2
2	D	6	MAN	O5-C5-C6-O6
2	D	5	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	C	5	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	D	4	MAN	O5-C5-C6-O6
2	C	6	MAN	C4-C5-C6-O6
2	D	6	MAN	C4-C5-C6-O6
2	C	7	NAG	C4-C5-C6-O6
2	D	5	NAG	C4-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6

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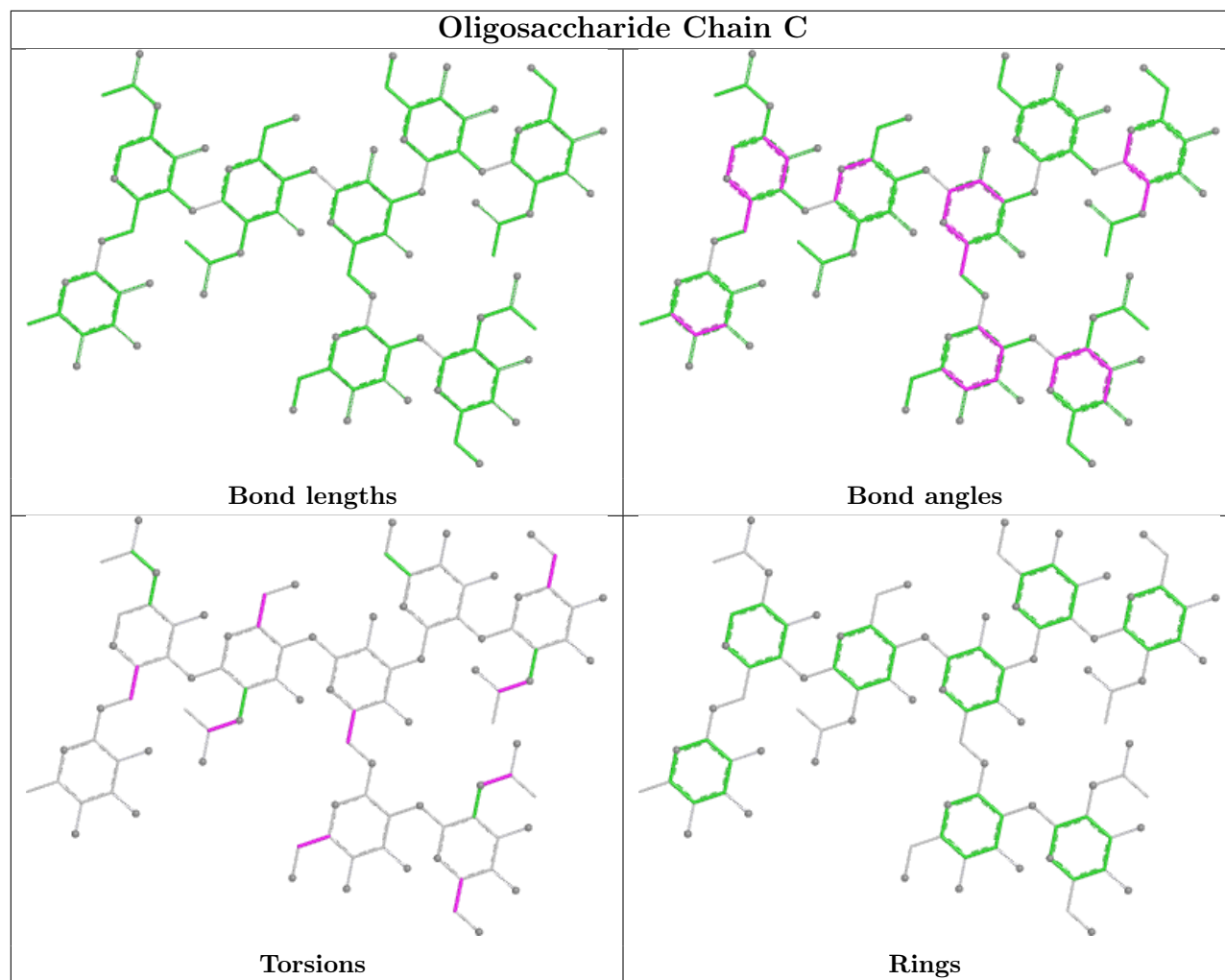
Mol	Chain	Res	Type	Atoms
2	C	6	MAN	O5-C5-C6-O6
2	D	5	NAG	C8-C7-N2-C2
2	D	5	NAG	O7-C7-N2-C2
2	C	5	NAG	C4-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
2	C	7	NAG	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	D	7	NAG	O5-C5-C6-O6
2	D	4	MAN	C4-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	D	7	NAG	C4-C5-C6-O6

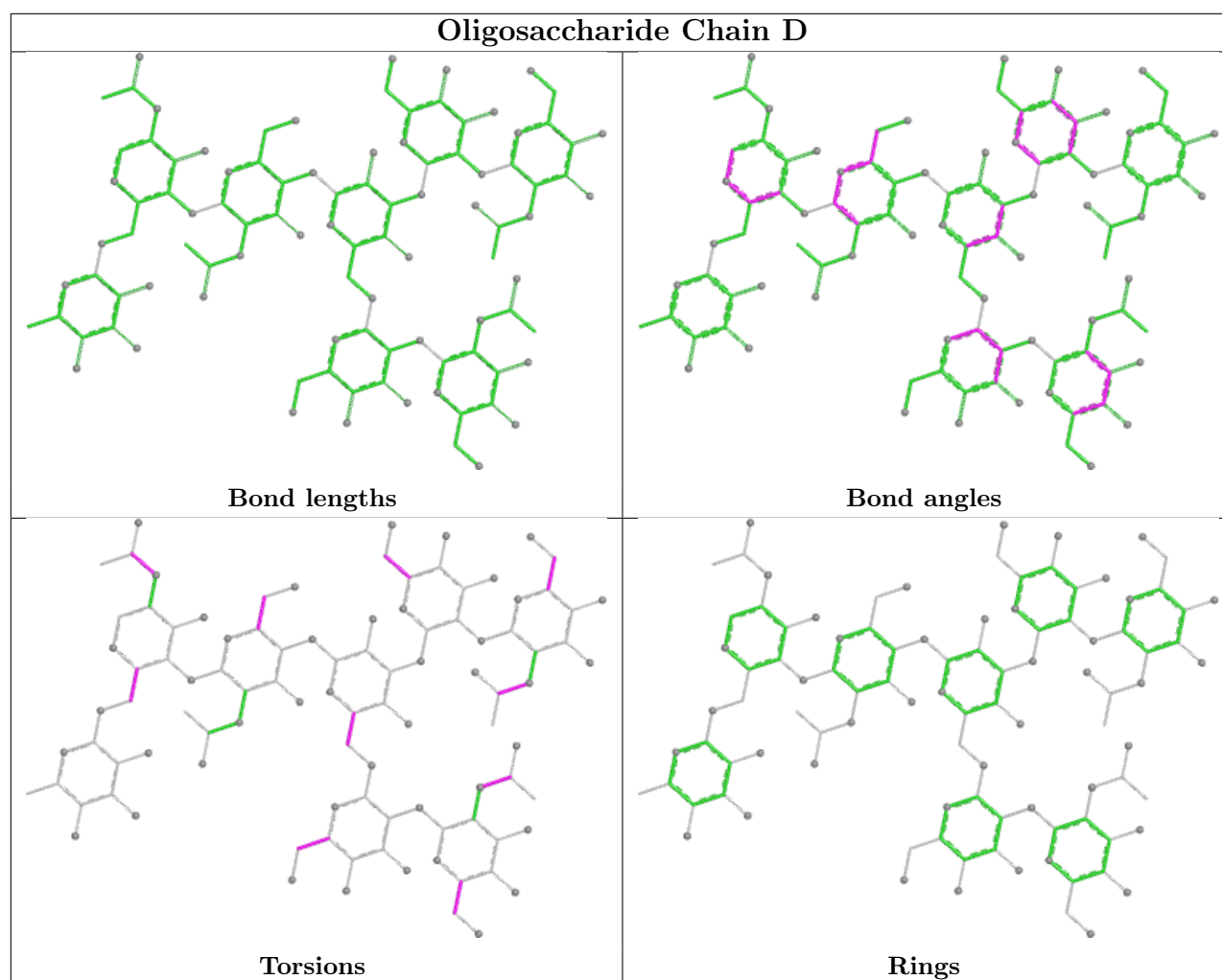
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	5	0
2	D	6	MAN	1	0
2	C	1	NAG	1	0
2	C	3	BMA	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](#)

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	EDO	B	510	-	3,3,3	0.46	0	2,2,2	0.27	0
3	EDO	A	509	-	3,3,3	0.48	0	2,2,2	0.36	0
3	EDO	B	509	-	3,3,3	0.44	0	2,2,2	0.54	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	EDO	B	510	-	-	1/1/1/1	-
3	EDO	A	509	-	-	1/1/1/1	-
3	EDO	B	509	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	509	EDO	O1-C1-C2-O2
3	B	510	EDO	O1-C1-C2-O2
3	A	509	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	510	EDO	1	0

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	205/207 (99%)	0.08	4 (1%) 65 56	39, 80, 185, 253	0
1	B	207/207 (100%)	0.16	7 (3%) 48 39	40, 82, 182, 250	0
All	All	412/414 (99%)	0.12	11 (2%) 56 46	39, 81, 183, 253	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	302	VAL	4.5
1	B	300	TYR	2.6
1	B	238	PRO	2.5
1	A	273	VAL	2.5
1	B	263	VAL	2.4
1	A	332	ILE	2.4
1	B	239	SER	2.3
1	B	268	HIS	2.2
1	A	240	VAL	2.2
1	B	324	SER	2.2
1	A	264	VAL	2.1

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](#)

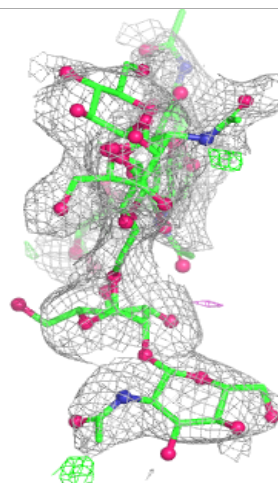
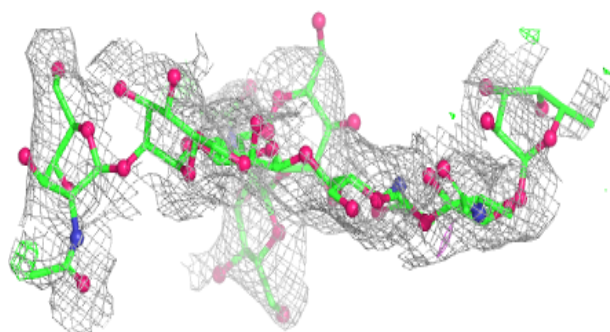
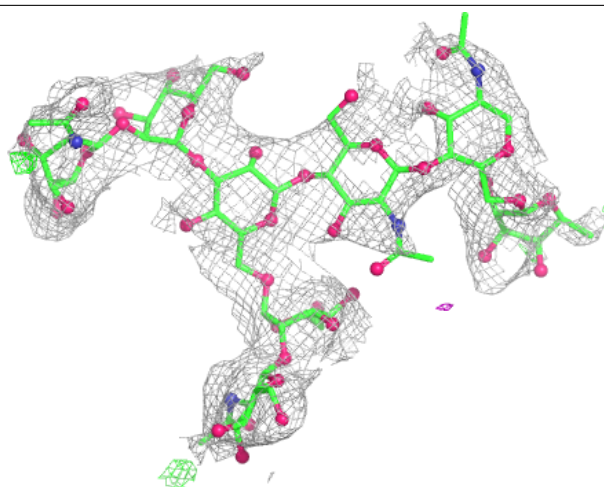
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

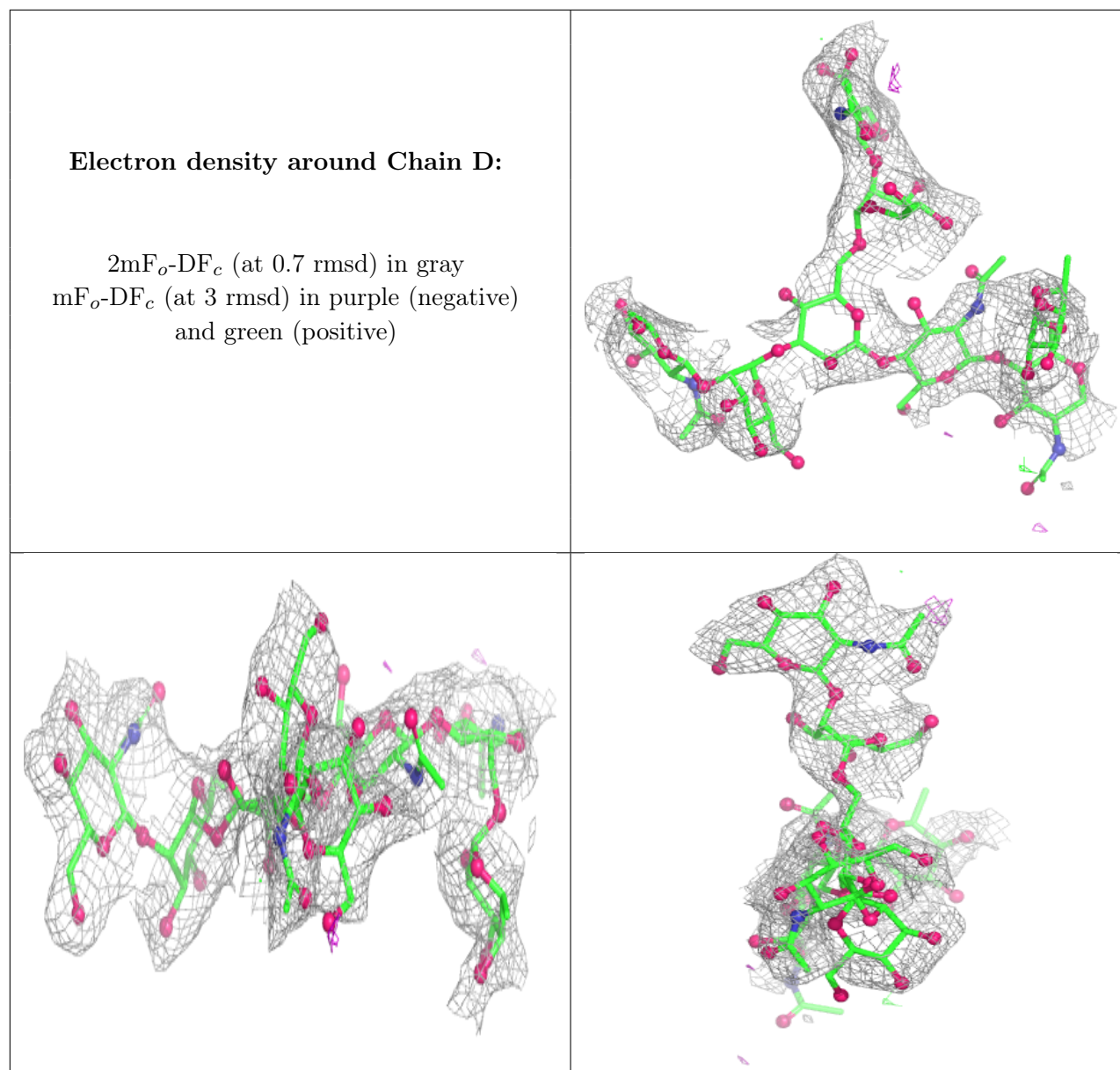
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	C	5	14/15	0.44	0.13	101,136,164,164	0
2	NAG	D	1	14/15	0.51	0.13	162,183,195,203	0
2	FUC	C	8	10/11	0.53	0.14	88,138,178,197	0
2	FUC	D	8	10/11	0.68	0.12	108,166,188,200	0
2	MAN	D	4	11/12	0.69	0.10	106,130,181,183	0
2	NAG	D	7	14/15	0.69	0.12	74,104,120,134	0
2	BMA	C	3	11/12	0.69	0.09	111,122,140,146	0
2	BMA	D	3	11/12	0.70	0.11	148,165,184,195	0
2	NAG	C	1	14/15	0.70	0.10	115,147,185,197	0
2	NAG	D	2	14/15	0.71	0.12	128,160,179,190	0
2	NAG	C	7	14/15	0.72	0.12	72,110,150,180	0
2	NAG	D	5	14/15	0.75	0.08	60,130,143,145	0
2	MAN	C	6	11/12	0.79	0.09	70,124,147,162	0
2	MAN	C	4	11/12	0.82	0.07	93,127,148,151	0
2	NAG	C	2	14/15	0.83	0.10	107,127,137,145	0
2	MAN	D	6	11/12	0.83	0.10	69,123,131,133	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 C:

$2mF_o-DF_c$ (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(Å ²)	Q<0.9
3	EDO	B	510	4/4	0.76	0.20	86,92,99,108	0
3	EDO	A	509	4/4	0.84	0.17	71,113,113,120	0
3	EDO	B	509	4/4	0.89	0.12	52,67,72,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.