



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:36 AM UTC

PDB ID : 2GJ7 / pdb_00002gj7
Title : Crystal Structure of a gE-gI/Fc complex
Authors : Sprague, E.R.; Wang, C.; Baker, D.; Bjorkman, P.J.
Deposited on : 2006-03-30
Resolution : 5.00 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

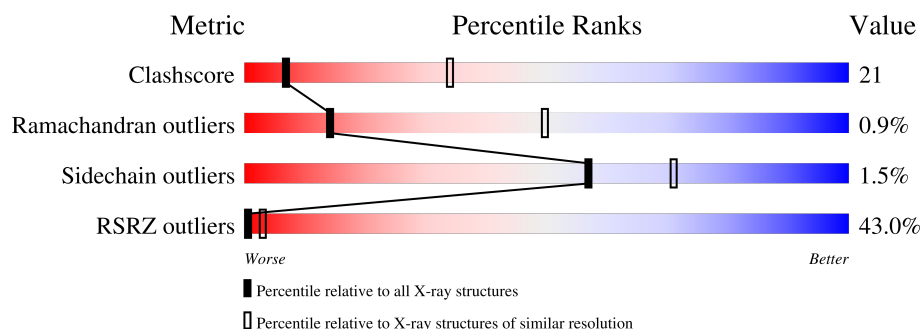
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.00 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))
Clashscore	190562	1040 (6.00-4.00)
Ramachandran outliers	187476	1015 (6.06-3.92)
Sidechain outliers	187428	1136 (6.10-3.90)
RSRZ outliers	180081	1004 (6.02-3.98)

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	227	45% 73% 18% 9%
1	B	227	43% 71% 18% 9%
2	E	401	18% 32% 10% 57%
2	F	401	13% 32% 10% 57%
3	C	8	75% 12% 12%
3	D	8	62% 38%

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	FUC	C	8	X	-	-	-
3	FUC	D	8	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6148 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	207	Total	C	N	O	S	19	0	0
			1659	1056	279	317	7			
1	B	207	Total	C	N	O	S	11	0	0
			1659	1056	279	317	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	221	LEU	-	cloning artifact	UNP P01857
A	222	GLU	-	cloning artifact	UNP P01857
A	356	GLU	ASP	conflict	UNP P01857
A	358	MET	LEU	conflict	UNP P01857
B	221	LEU	-	cloning artifact	UNP P01857
B	222	GLU	-	cloning artifact	UNP P01857
B	356	GLU	ASP	conflict	UNP P01857
B	358	MET	LEU	conflict	UNP P01857

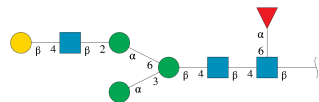
- Molecule 2 is a protein called Glycoprotein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	171	Total	C	N	O	S	0	0	0
			1319	829	229	250	11			
2	E	171	Total	C	N	O	S	0	0	0
			1319	829	229	250	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	420	ASP	-	cloning artifact	UNP P04488
F	421	ILE	-	cloning artifact	UNP P04488
E	420	ASP	-	cloning artifact	UNP P04488
E	421	ILE	-	cloning artifact	UNP P04488

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

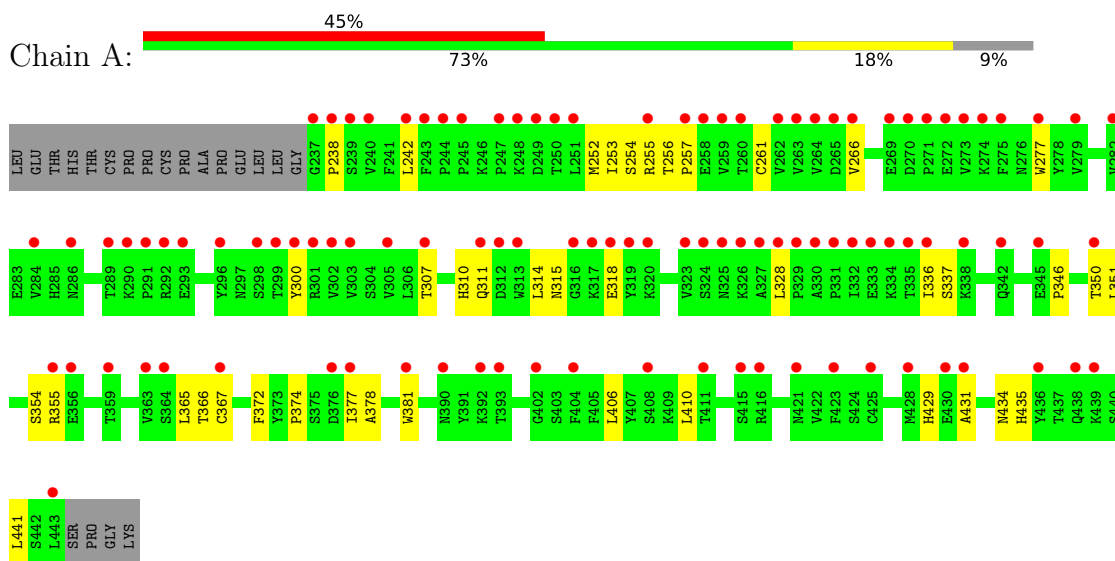


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	0	0	0
			96	54	3	39			
3	D	8	Total	C	N	O	0	0	0
			96	54	3	39			

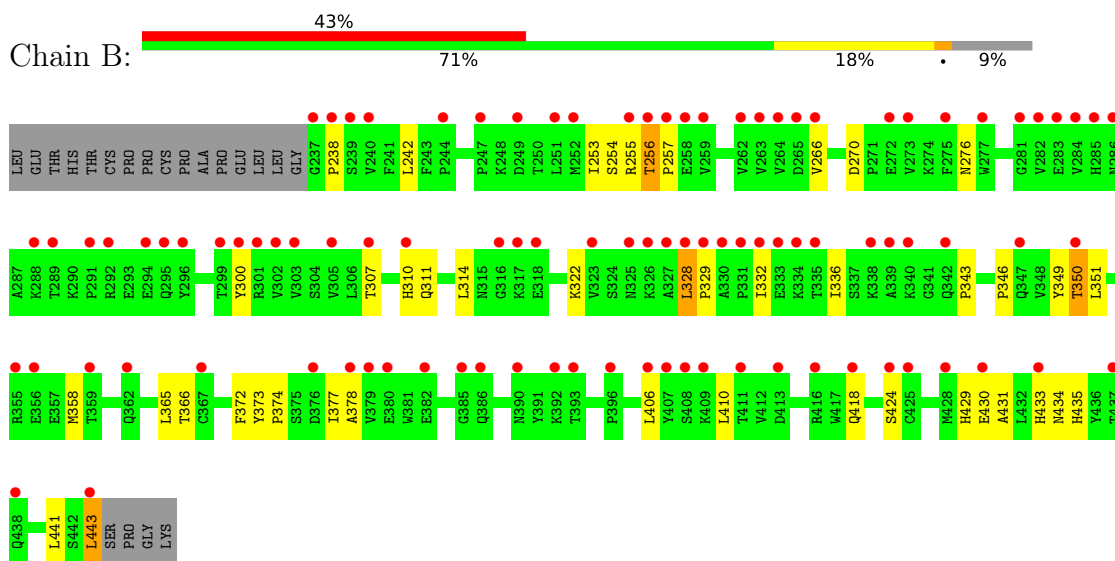
3 Residue-property plots

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.

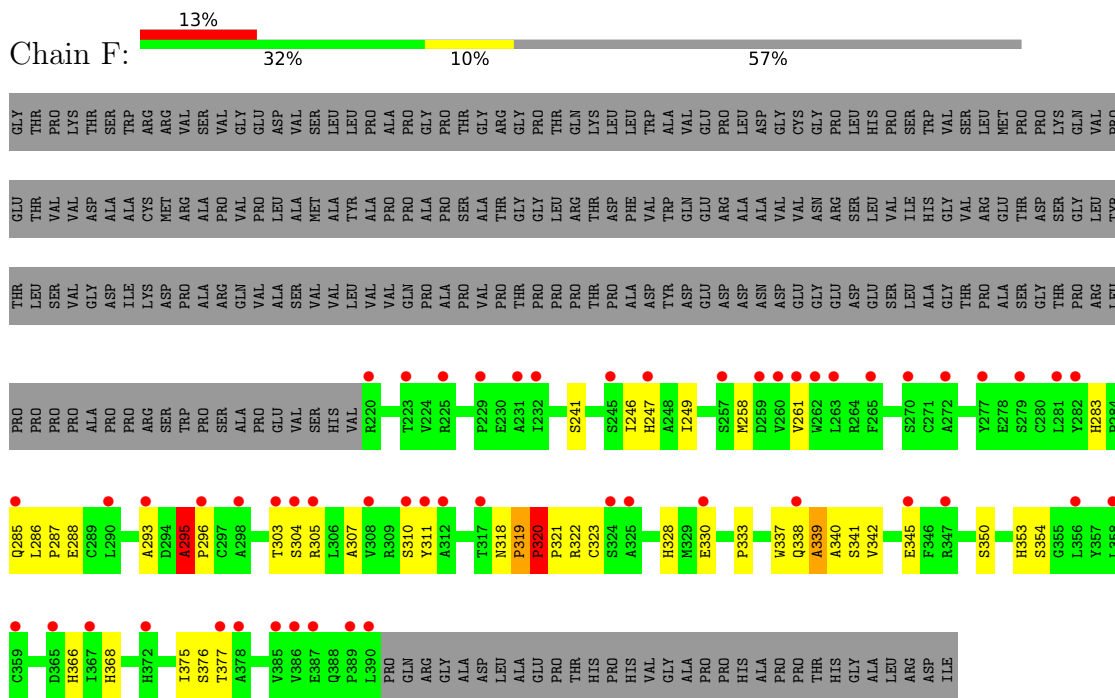
- Molecule 1: Ig gamma-1 chain C region



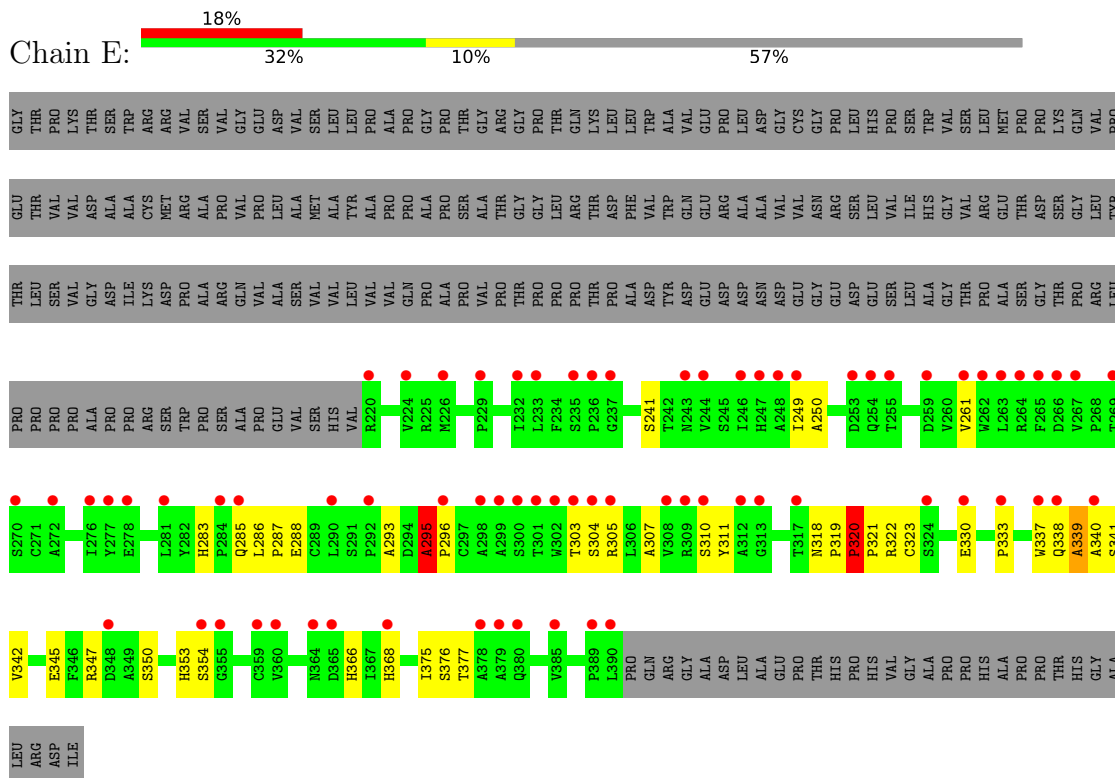
- Molecule 1: Ig gamma-1 chain C region



- Molecule 2: Glycoprotein E



- Molecule 2: Glycoprotein E



- Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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 C:  75% 12% 12%

NAG1	NAG2	MAN3	MAN4	NAG5	GAL6	MAN7	FUC8
------	------	------	------	------	------	------	------

● Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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:  62% 38%

NAG1	NAG2	MAN3	MAN4	NAG5	GAL6	MAN7	FUC8
------	------	------	------	------	------	------	------

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	174.73Å 174.73Å 316.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.00 – 5.00 36.00 – 5.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (36.00-5.00) 99.1 (36.00-5.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.70 (at 5.08Å)	Xtriage
Refinement program		Depositor
R, R_{free}	(Not available) , (Not available) 0.499 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	210.3	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 72.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.63	EDS
Total number of atoms	6148	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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, GAL, MAN, FUC, 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	0.47	0/1705	0.87	0/2322
1	B	0.48	0/1705	0.87	3/2322 (0.1%)
2	E	0.38	0/1359	1.03	12/1866 (0.6%)
2	F	0.38	0/1359	1.02	12/1866 (0.6%)
All	All	0.43	0/6128	0.94	27/8376 (0.3%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	319	PRO	CA-C-N	11.73	132.46	120.38
2	F	319	PRO	C-N-CA	11.73	132.46	120.38
2	E	319	PRO	CA-C-N	11.72	132.45	120.38
2	E	319	PRO	C-N-CA	11.72	132.45	120.38
2	E	318	ASN	CA-C-N	7.03	127.62	120.38
2	E	318	ASN	C-N-CA	7.03	127.62	120.38
2	F	318	ASN	CA-C-N	6.97	127.56	120.38
2	F	318	ASN	C-N-CA	6.97	127.56	120.38
2	F	320	PRO	N-CA-C	6.93	119.16	110.70
2	E	320	PRO	N-CA-C	6.93	119.15	110.70
2	F	295	ALA	N-CA-C	5.57	122.11	109.81
2	E	295	ALA	N-CA-C	5.55	122.07	109.81
2	E	320	PRO	CA-C-N	-5.52	112.94	119.84
2	E	320	PRO	C-N-CA	-5.52	112.94	119.84
2	F	320	PRO	CA-C-N	-5.48	112.98	119.84
2	F	320	PRO	C-N-CA	-5.48	112.98	119.84
2	E	319	PRO	N-CA-C	5.27	117.13	110.70
2	E	376	SER	N-CA-C	5.27	115.31	107.88
2	F	319	PRO	N-CA-C	5.26	117.12	110.70
2	F	376	SER	N-CA-C	5.24	115.27	107.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	377	THR	N-CA-C	-5.21	103.52	110.55
2	F	377	THR	N-CA-C	-5.16	103.58	110.55
2	F	261	VAL	N-CA-C	5.11	115.33	108.17
1	B	424	SER	N-CA-C	5.09	117.11	109.23
1	B	256	THR	CA-C-N	5.07	124.97	119.85
1	B	256	THR	C-N-CA	5.07	124.97	119.85
2	E	261	VAL	N-CA-C	5.06	115.26	108.17

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	1659	0	1622	137	0
1	B	1659	0	1623	82	0
2	E	1319	0	1239	77	30
2	F	1319	0	1238	138	30
3	C	96	0	82	1	0
3	D	96	0	82	0	0
All	All	6148	0	5886	255	30

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 21.

All (255) 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:310:HIS:CD2	2:F:321:PRO:HB3	1.12	1.60
1:A:310:HIS:CG	2:F:321:PRO:CB	1.85	1.60
1:A:310:HIS:CG	2:F:321:PRO:HB3	1.07	1.56
1:A:314:LEU:HB2	2:F:322:ARG:NH1	1.36	1.38
1:A:310:HIS:CD2	2:F:321:PRO:CB	2.01	1.34
1:A:254:SER:O	2:F:342:VAL:HG22	1.28	1.34
1:A:311:GLN:O	2:F:322:ARG:NH2	1.61	1.32

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:HIS:CB	2:F:321:PRO:CB	2.11	1.27
1:A:256:THR:CG2	2:F:340:ALA:HB3	1.59	1.26
1:A:256:THR:HG23	2:F:340:ALA:CB	1.21	1.25
1:B:434:ASN:ND2	2:E:249:ILE:HA	1.52	1.23
1:B:314:LEU:HB2	2:E:322:ARG:NH1	1.53	1.22
1:A:310:HIS:CB	2:F:321:PRO:HB2	1.67	1.22
1:A:311:GLN:O	2:F:322:ARG:CZ	1.91	1.18
1:B:433:HIS:NE2	2:E:250:ALA:O	1.76	1.17
1:A:435:HIS:NE2	2:F:319:PRO:HG3	1.57	1.17
1:B:434:ASN:HD21	2:E:250:ALA:N	1.39	1.16
1:B:253:ILE:HD13	2:E:321:PRO:CA	1.75	1.15
1:A:253:ILE:HB	2:F:320:PRO:HB2	1.23	1.15
1:B:307:THR:CG2	2:E:339:ALA:HB1	1.76	1.15
1:B:253:ILE:CD1	2:E:321:PRO:HA	1.77	1.15
1:A:253:ILE:HB	2:F:320:PRO:CB	1.77	1.14
1:A:253:ILE:CD1	2:F:321:PRO:HA	1.78	1.13
1:B:434:ASN:ND2	2:E:250:ALA:H	1.46	1.13
1:A:307:THR:OG1	2:F:339:ALA:HB1	1.45	1.12
1:A:253:ILE:HD12	2:F:321:PRO:HA	1.29	1.12
1:A:311:GLN:HB2	2:F:322:ARG:CA	1.80	1.11
1:A:310:HIS:HB2	2:F:321:PRO:C	1.74	1.09
1:A:311:GLN:HA	2:F:322:ARG:HG2	1.27	1.09
1:A:310:HIS:HB3	2:F:321:PRO:HB2	1.07	1.07
1:B:307:THR:HG21	2:E:339:ALA:HB1	1.10	1.07
1:B:255:ARG:O	2:E:340:ALA:O	1.74	1.06
1:A:253:ILE:CD1	2:F:321:PRO:CA	2.33	1.05
1:A:314:LEU:CB	2:F:322:ARG:NH1	2.20	1.04
1:A:254:SER:HB3	2:F:246:ILE:HB	1.41	1.00
1:A:256:THR:HG23	2:F:340:ALA:HB3	1.20	1.00
1:A:253:ILE:CB	2:F:320:PRO:CB	2.40	1.00
1:B:254:SER:HA	2:E:342:VAL:HG22	1.43	1.00
1:B:434:ASN:HD22	2:E:249:ILE:HA	1.11	1.00
1:A:314:LEU:CB	2:F:322:ARG:HH11	1.74	0.99
1:A:311:GLN:HB2	2:F:322:ARG:HA	1.45	0.98
1:A:253:ILE:CB	2:F:320:PRO:HB3	1.95	0.97
1:A:257:PRO:HD2	2:F:340:ALA:HB1	1.45	0.97
1:A:311:GLN:CA	2:F:322:ARG:HG2	1.94	0.96
1:B:314:LEU:CB	2:E:322:ARG:NH1	2.28	0.96
1:A:256:THR:HG22	2:F:340:ALA:HB3	1.46	0.96
1:A:253:ILE:HD11	2:F:311:TYR:CE2	2.01	0.96
1:B:314:LEU:HB2	2:E:322:ARG:HH12	1.29	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:LEU:HB2	2:F:322:ARG:HH11	0.85	0.95
1:B:434:ASN:ND2	2:E:249:ILE:CA	2.29	0.94
1:A:253:ILE:CG1	2:F:311:TYR:CE2	2.50	0.94
1:A:310:HIS:HB3	2:F:321:PRO:CB	1.88	0.94
1:A:311:GLN:O	2:F:322:ARG:NH1	2.01	0.93
1:A:253:ILE:HD11	2:F:311:TYR:HE2	1.35	0.91
1:A:254:SER:O	2:F:342:VAL:CG2	2.16	0.91
1:A:311:GLN:HA	2:F:322:ARG:CG	2.01	0.90
1:A:253:ILE:HG21	2:F:320:PRO:HB3	1.54	0.90
1:B:314:LEU:HB2	2:E:322:ARG:HH11	1.37	0.89
1:B:256:THR:OG1	2:E:341:SER:CB	2.21	0.89
1:A:252:MET:CE	2:F:247:HIS:CE1	2.55	0.88
1:A:311:GLN:HA	2:F:322:ARG:CZ	2.03	0.88
1:A:311:GLN:HB2	2:F:322:ARG:CB	2.04	0.87
1:A:435:HIS:NE2	2:F:319:PRO:CG	2.37	0.87
1:A:238:PRO:HD2	1:A:328:LEU:HD13	1.56	0.87
1:A:253:ILE:HG13	2:F:311:TYR:CE2	2.10	0.86
1:A:253:ILE:CG2	2:F:320:PRO:HB3	2.05	0.86
1:A:252:MET:HE3	2:F:247:HIS:CE1	2.11	0.85
1:A:252:MET:HE3	2:F:247:HIS:NE2	1.91	0.85
1:B:434:ASN:ND2	2:E:250:ALA:N	2.13	0.84
1:A:252:MET:HE3	2:F:247:HIS:CD2	2.12	0.84
1:B:256:THR:HG21	2:E:339:ALA:HB3	1.57	0.84
1:B:307:THR:HG21	2:E:339:ALA:CB	2.04	0.83
1:A:253:ILE:CD1	2:F:311:TYR:CE2	2.62	0.83
1:A:253:ILE:HG21	2:F:258:MET:HE1	1.60	0.83
1:A:253:ILE:CD1	2:F:311:TYR:HE2	1.90	0.83
1:B:242:LEU:HG	1:B:336:ILE:HG12	1.59	0.82
1:B:256:THR:OG1	2:E:341:SER:HB2	1.78	0.82
1:A:310:HIS:CD2	2:F:321:PRO:CG	2.64	0.81
1:A:242:LEU:HG	1:A:336:ILE:HG12	1.62	0.81
1:A:310:HIS:CG	2:F:321:PRO:CA	2.62	0.81
1:B:433:HIS:HE2	2:E:250:ALA:C	1.89	0.81
1:B:256:THR:HG21	2:E:339:ALA:CB	2.10	0.80
1:A:254:SER:CB	2:F:246:ILE:HB	2.11	0.80
1:A:311:GLN:HA	2:F:322:ARG:NH1	1.97	0.80
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.64	0.80
1:B:254:SER:CA	2:E:342:VAL:HG22	2.11	0.78
1:B:253:ILE:HD13	2:E:321:PRO:HA	0.85	0.78
1:A:311:GLN:C	2:F:322:ARG:CZ	2.57	0.77
1:A:252:MET:HE1	2:F:247:HIS:CE1	2.20	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:PRO:HB3	1:B:372:PHE:HB3	1.65	0.76
1:A:311:GLN:CA	2:F:322:ARG:CZ	2.63	0.76
1:A:253:ILE:CB	2:F:320:PRO:HB2	2.09	0.76
1:B:434:ASN:HD21	2:E:250:ALA:H	0.78	0.75
1:A:310:HIS:CB	2:F:321:PRO:C	2.58	0.75
1:B:253:ILE:HG12	2:E:311:TYR:CE2	2.21	0.74
1:A:254:SER:C	2:F:342:VAL:HG22	2.11	0.74
1:A:253:ILE:CG1	2:F:320:PRO:HB3	2.16	0.74
1:A:311:GLN:CB	2:F:322:ARG:HB3	2.18	0.74
2:E:338:GLN:HG3	2:E:341:SER:HB3	1.70	0.74
1:B:256:THR:OG1	2:E:341:SER:N	2.21	0.74
2:F:338:GLN:HG3	2:F:341:SER:HB3	1.70	0.73
1:A:311:GLN:CB	2:F:322:ARG:CB	2.67	0.73
1:A:311:GLN:C	2:F:322:ARG:NH1	2.46	0.73
1:A:256:THR:CG2	2:F:340:ALA:CB	2.05	0.72
1:A:435:HIS:CE1	2:F:319:PRO:CG	2.73	0.71
1:B:433:HIS:CE1	2:E:250:ALA:HB3	2.24	0.71
1:A:253:ILE:HG12	2:F:320:PRO:HB3	1.70	0.71
1:A:253:ILE:HD12	2:F:321:PRO:CA	2.08	0.71
1:B:256:THR:HG21	2:E:338:GLN:O	1.91	0.70
1:A:311:GLN:HB2	2:F:322:ARG:HB3	1.73	0.69
1:B:238:PRO:HD2	1:B:328:LEU:HD13	1.73	0.69
1:A:307:THR:OG1	2:F:339:ALA:CB	2.34	0.69
1:A:350:THR:HB	1:A:441:LEU:HD13	1.74	0.69
1:B:314:LEU:CB	2:E:322:ARG:HH12	2.02	0.68
1:A:307:THR:HG1	2:F:339:ALA:HB1	1.58	0.67
1:A:311:GLN:CB	2:F:322:ARG:HA	2.22	0.67
1:A:314:LEU:CA	2:F:322:ARG:NH1	2.58	0.66
1:A:311:GLN:HB2	2:F:322:ARG:C	2.20	0.66
1:B:256:THR:OG1	2:E:340:ALA:C	2.39	0.65
1:A:311:GLN:N	2:F:322:ARG:HA	2.11	0.65
1:A:254:SER:HB2	2:F:342:VAL:HG21	1.78	0.65
1:B:434:ASN:HD22	2:E:249:ILE:CA	1.95	0.64
1:A:311:GLN:CA	2:F:322:ARG:NH1	2.61	0.63
1:A:310:HIS:CB	2:F:321:PRO:CA	2.75	0.63
1:B:310:HIS:HE1	2:E:340:ALA:O	1.82	0.63
1:B:311:GLN:HB2	2:E:322:ARG:HA	1.81	0.62
1:A:253:ILE:CG2	2:F:320:PRO:CB	2.74	0.62
1:B:257:PRO:HD2	2:E:340:ALA:CB	2.29	0.62
1:A:252:MET:CE	2:F:247:HIS:NE2	2.60	0.61
1:A:253:ILE:CG1	2:F:320:PRO:CB	2.77	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:LEU:CB	2:E:322:ARG:HH11	2.04	0.61
1:B:434:ASN:ND2	2:E:249:ILE:C	2.58	0.61
1:A:307:THR:HG23	2:F:340:ALA:HB2	1.81	0.61
1:B:433:HIS:CE1	2:E:250:ALA:O	2.52	0.60
1:B:443:LEU:N	1:B:443:LEU:HD12	2.15	0.60
1:B:254:SER:HA	2:E:342:VAL:CG2	2.27	0.60
2:E:350:SER:H	2:E:353:HIS:HD2	1.50	0.59
1:A:311:GLN:CA	2:F:322:ARG:CG	2.73	0.59
1:B:257:PRO:HD2	2:E:340:ALA:HB3	1.83	0.59
1:B:350:THR:HB	1:B:441:LEU:HD13	1.85	0.59
1:A:311:GLN:H	2:F:322:ARG:HA	1.68	0.58
2:F:350:SER:H	2:F:353:HIS:HD2	1.50	0.58
2:F:241:SER:HB3	2:F:345:GLU:HG3	1.86	0.58
1:A:311:GLN:HB2	2:F:322:ARG:O	2.04	0.58
1:B:253:ILE:HG12	2:E:311:TYR:HE2	1.69	0.58
1:A:253:ILE:HD11	2:F:311:TYR:CD2	2.38	0.57
1:A:311:GLN:CB	2:F:322:ARG:CA	2.71	0.57
1:A:314:LEU:HD12	2:F:322:ARG:HG3	1.85	0.57
1:A:310:HIS:HB2	2:F:321:PRO:CA	2.34	0.57
1:A:311:GLN:N	2:F:322:ARG:HG2	2.20	0.56
2:E:241:SER:HB3	2:E:345:GLU:HG3	1.86	0.56
1:B:256:THR:HG23	2:E:340:ALA:HB3	1.87	0.56
1:A:255:ARG:O	2:F:340:ALA:O	2.20	0.56
1:A:314:LEU:HD12	2:F:322:ARG:CG	2.36	0.56
1:A:252:MET:HE3	2:F:247:HIS:CG	2.41	0.55
1:B:253:ILE:CG1	2:E:311:TYR:CE2	2.88	0.55
1:A:253:ILE:CG2	2:F:258:MET:HE1	2.32	0.55
1:B:253:ILE:CG1	2:E:311:TYR:HE2	2.19	0.55
1:A:307:THR:CG2	2:F:340:ALA:HB2	2.36	0.55
2:E:283:HIS:CD2	2:E:286:LEU:HD12	2.42	0.55
2:E:320:PRO:HA	2:E:323:CYS:SG	2.47	0.55
1:A:314:LEU:N	2:F:322:ARG:HH12	2.03	0.55
2:F:320:PRO:HA	2:F:323:CYS:SG	2.47	0.54
2:F:283:HIS:CD2	2:F:286:LEU:HD12	2.42	0.54
1:B:256:THR:CG2	2:E:339:ALA:CB	2.84	0.54
1:B:351:LEU:HB2	1:B:366:THR:HB	1.90	0.54
1:B:365:LEU:HD12	1:B:410:LEU:HD23	1.89	0.53
1:A:311:GLN:HA	2:F:322:ARG:NE	2.22	0.53
1:A:310:HIS:HB2	2:F:321:PRO:O	2.04	0.53
1:A:435:HIS:CE1	2:F:319:PRO:HG2	2.43	0.52
1:B:429:HIS:O	1:B:435:HIS:HA	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ILE:HG21	2:F:320:PRO:CB	2.33	0.52
1:A:253:ILE:HG12	2:F:320:PRO:CB	2.40	0.52
1:A:374:PRO:O	1:A:429:HIS:HE1	1.93	0.52
2:F:333:PRO:O	2:F:353:HIS:HE1	1.93	0.51
1:A:365:LEU:HD12	1:A:410:LEU:HD23	1.92	0.51
1:A:406:LEU:HD12	1:A:406:LEU:C	2.35	0.51
1:A:314:LEU:HB2	2:F:322:ARG:CZ	2.28	0.51
1:A:307:THR:HG23	2:F:340:ALA:CB	2.41	0.51
1:B:434:ASN:HD21	2:E:249:ILE:C	2.07	0.51
2:E:333:PRO:O	2:E:353:HIS:HE1	1.93	0.50
2:F:338:GLN:HB3	2:F:345:GLU:OE2	2.11	0.50
2:E:338:GLN:HB3	2:E:345:GLU:OE2	2.11	0.50
1:B:253:ILE:CD1	2:E:311:TYR:HE2	2.24	0.50
1:B:429:HIS:CD2	1:B:431:ALA:H	2.29	0.50
1:B:253:ILE:HD11	2:E:311:TYR:HE2	1.77	0.50
1:A:351:LEU:HB2	1:A:366:THR:HB	1.93	0.50
1:B:433:HIS:HE2	2:E:250:ALA:CA	2.25	0.49
2:E:304:SER:HB3	2:E:330:GLU:OE2	2.12	0.49
2:F:304:SER:HB3	2:F:330:GLU:OE2	2.12	0.49
3:C:1:NAG:O6	3:C:8:FUC:H63	2.12	0.49
1:B:256:THR:CG2	2:E:339:ALA:HB3	2.37	0.49
1:B:256:THR:OG1	2:E:341:SER:HB3	2.11	0.49
1:A:257:PRO:CD	2:F:340:ALA:HB1	2.32	0.48
1:A:253:ILE:HG13	2:F:311:TYR:CZ	2.48	0.48
2:F:366:HIS:O	2:F:368:HIS:HD2	1.97	0.48
2:E:366:HIS:O	2:E:368:HIS:HD2	1.97	0.48
1:B:256:THR:CG2	2:E:338:GLN:O	2.60	0.48
1:B:406:LEU:C	1:B:406:LEU:HD12	2.39	0.48
1:A:377:ILE:HG12	1:A:378:ALA:H	1.78	0.47
1:A:434:ASN:CB	2:F:249:ILE:HA	2.43	0.47
1:A:256:THR:CA	2:F:340:ALA:CB	2.92	0.47
1:B:307:THR:HG23	2:E:339:ALA:HB1	1.87	0.47
2:F:333:PRO:O	2:F:353:HIS:CE1	2.68	0.47
1:B:256:THR:CB	2:E:338:GLN:O	2.62	0.47
2:E:333:PRO:O	2:E:353:HIS:CE1	2.68	0.47
1:B:374:PRO:O	1:B:429:HIS:HE1	1.98	0.47
2:E:338:GLN:HG3	2:E:341:SER:CB	2.42	0.47
1:B:310:HIS:CG	2:E:321:PRO:HB3	2.50	0.46
1:A:311:GLN:HA	2:F:322:ARG:CD	2.46	0.46
1:A:318:GLU:HA	1:A:337:SER:HB3	1.98	0.46
2:F:338:GLN:HG3	2:F:341:SER:CB	2.42	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:LEU:N	2:F:322:ARG:NH1	2.64	0.45
1:B:430:GLU:HA	1:B:435:HIS:CD2	2.51	0.45
1:A:255:ARG:C	2:F:341:SER:HA	2.41	0.45
1:A:429:HIS:CD2	1:A:431:ALA:H	2.35	0.45
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.51	0.45
1:A:377:ILE:HG12	1:A:378:ALA:N	2.31	0.45
1:A:354:SER:HB2	1:B:349:TYR:HB3	1.99	0.44
1:B:256:THR:OG1	2:E:341:SER:CA	2.65	0.44
1:A:429:HIS:O	1:A:435:HIS:HA	2.18	0.44
1:A:253:ILE:HG12	2:F:311:TYR:CE2	2.47	0.44
1:B:257:PRO:HD2	2:E:340:ALA:HB1	1.99	0.44
2:E:320:PRO:HB2	2:E:321:PRO:HD3	2.00	0.44
1:A:266:VAL:HB	1:A:300:TYR:HB2	1.98	0.44
1:B:377:ILE:HG12	1:B:378:ALA:N	2.33	0.44
1:A:256:THR:HA	2:F:340:ALA:CB	2.47	0.43
2:F:295:ALA:HB3	2:F:296:PRO:CD	2.49	0.43
2:E:295:ALA:HB3	2:E:296:PRO:CD	2.48	0.43
1:B:377:ILE:HG12	1:B:378:ALA:H	1.82	0.43
2:F:307:ALA:HB1	2:F:337:TRP:CZ2	2.54	0.43
1:A:314:LEU:CA	2:F:322:ARG:HH12	2.28	0.43
1:B:238:PRO:HD2	1:B:328:LEU:CD1	2.45	0.43
2:F:320:PRO:HB2	2:F:321:PRO:HD3	2.00	0.42
1:A:253:ILE:HA	2:F:321:PRO:HG3	2.02	0.42
2:F:319:PRO:HA	2:F:320:PRO:HD3	1.94	0.42
2:E:307:ALA:HB1	2:E:337:TRP:CZ2	2.54	0.42
1:B:254:SER:CB	2:E:342:VAL:CG2	2.97	0.42
2:F:293:ALA:C	2:F:295:ALA:H	2.28	0.42
1:B:266:VAL:HB	1:B:300:TYR:HB2	2.02	0.42
2:E:295:ALA:HB3	2:E:296:PRO:HD3	2.01	0.42
2:E:293:ALA:C	2:E:295:ALA:H	2.28	0.41
1:B:276:ASN:HB2	1:B:322:LYS:HB3	2.02	0.41
1:B:328:LEU:HD21	1:B:332:ILE:HD12	2.02	0.41
2:F:354:SER:HA	2:F:375:ILE:O	2.20	0.41
1:B:328:LEU:HA	1:B:329:PRO:HD2	1.87	0.41
2:E:345:GLU:OE1	2:E:347:ARG:NH2	2.48	0.41
2:F:295:ALA:HB3	2:F:296:PRO:HD3	2.01	0.41
1:A:256:THR:HB	2:F:341:SER:HB2	1.68	0.41
1:B:443:LEU:HD12	1:B:443:LEU:H	1.86	0.41
1:A:261:CYS:HB2	1:A:277:TRP:CH2	2.56	0.41
1:B:429:HIS:HD2	1:B:431:ALA:H	1.69	0.40
2:E:354:SER:HA	2:E:375:ILE:O	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:ASN:N	2:F:322:ARG:NH1	2.70	0.40
1:B:343:PRO:HA	1:B:373:TYR:O	2.21	0.40

All (30) 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)
2:F:305:ARG:NH2	2:E:285:GLN:CB[3_444]	0.59	1.61
2:F:285:GLN:CB	2:E:305:ARG:NH2[3_444]	0.81	1.39
2:F:305:ARG:NH1	2:E:285:GLN:O[3_444]	1.28	0.92
2:F:303:THR:CB	2:E:303:THR:CB[3_444]	1.37	0.83
2:F:305:ARG:NH1	2:E:285:GLN:C[3_444]	1.40	0.80
2:F:285:GLN:O	2:E:305:ARG:NH1[3_444]	1.45	0.75
2:F:285:GLN:OE1	2:E:305:ARG:NE[3_444]	1.55	0.65
2:F:305:ARG:CZ	2:E:285:GLN:CB[3_444]	1.55	0.65
2:F:305:ARG:NE	2:E:285:GLN:OE1[3_444]	1.60	0.60
2:F:305:ARG:NH1	2:E:285:GLN:CA[3_444]	1.68	0.52
2:F:305:ARG:CZ	2:E:285:GLN:CA[3_444]	1.72	0.48
2:F:285:GLN:C	2:E:305:ARG:NH1[3_444]	1.76	0.44
2:F:285:GLN:CG	2:E:305:ARG:NH2[3_444]	1.77	0.43
2:F:285:GLN:CB	2:E:305:ARG:CZ[3_444]	1.79	0.41
2:F:305:ARG:NH2	2:E:285:GLN:CG[3_444]	1.83	0.37
2:F:305:ARG:NH2	2:E:285:GLN:CA[3_444]	1.84	0.36
2:F:303:THR:CB	2:E:303:THR:CG2[3_444]	1.86	0.34
2:F:305:ARG:NE	2:E:285:GLN:CD[3_444]	1.86	0.34
2:F:285:GLN:CD	2:E:305:ARG:NE[3_444]	1.87	0.33
2:F:303:THR:CG2	2:E:303:THR:CB[3_444]	1.89	0.31
2:F:285:GLN:CA	2:E:305:ARG:NH1[3_444]	1.94	0.26
2:F:310:SER:OG	2:E:287:PRO:CD[3_444]	1.98	0.22
2:F:285:GLN:CA	2:E:305:ARG:NH2[3_444]	2.01	0.19
2:F:310:SER:OG	2:E:287:PRO:CG[3_444]	2.03	0.17
2:F:285:GLN:CA	2:E:305:ARG:CZ[3_444]	2.04	0.16
2:F:328:HIS:CD2	2:E:287:PRO:CB[3_444]	2.06	0.14
2:F:287:PRO:CG	2:E:310:SER:OG[3_444]	2.12	0.08
2:F:305:ARG:CD	2:E:285:GLN:OE1[3_444]	2.12	0.08
2:F:328:HIS:NE2	2:E:287:PRO:CB[3_444]	2.14	0.06
2:F:305:ARG:CZ	2:E:285:GLN:O[3_444]	2.17	0.03

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	205/227 (90%)	203 (99%)	2 (1%)	0	100	100
1	B	205/227 (90%)	199 (97%)	5 (2%)	1 (0%)	24	63
2	E	169/401 (42%)	160 (95%)	6 (4%)	3 (2%)	6	32
2	F	169/401 (42%)	160 (95%)	6 (4%)	3 (2%)	6	32
All	All	748/1256 (60%)	722 (96%)	19 (2%)	7 (1%)	14	50

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	295	ALA
2	F	320	PRO
2	F	339	ALA
2	E	295	ALA
2	E	320	PRO
2	E	339	ALA
1	B	358	MET

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	193/210 (92%)	192 (100%)	1 (0%)	81	82
1	B	193/210 (92%)	188 (97%)	5 (3%)	40	61
2	E	144/332 (43%)	142 (99%)	2 (1%)	59	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	144/332 (43%)	142 (99%)	2 (1%)	59	72
All	All	674/1084 (62%)	664 (98%)	10 (2%)	57	71

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	355	ARG
2	F	288	GLU
2	F	320	PRO
1	B	270	ASP
1	B	328	LEU
1	B	350	THR
1	B	418	GLN
1	B	443	LEU
2	E	288	GLU
2	E	320	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	347	GLN
1	A	362	GLN
1	A	390	ASN
1	A	429	HIS
1	A	438	GLN
2	F	283	HIS
2	F	338	GLN
2	F	353	HIS
2	F	368	HIS
2	F	383	ASN
1	B	310	HIS
1	B	347	GLN
1	B	361	ASN
1	B	386	GLN
1	B	429	HIS
1	B	434	ASN
2	E	283	HIS
2	E	338	GLN
2	E	353	HIS
2	E	368	HIS
2	E	383	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 ⓘ

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	$\# Z > 2$
3	NAG	C	1	1,3	14,14,15	0.48	0	17,19,21	0.75	0
3	NAG	C	2	3	14,14,15	0.46	0	17,19,21	0.76	0
3	BMA	C	3	3	11,11,12	0.63	0	15,15,17	0.54	0
3	MAN	C	4	3	11,11,12	0.51	0	15,15,17	0.56	0
3	NAG	C	5	3	14,14,15	0.49	0	17,19,21	0.78	0
3	GAL	C	6	3	11,11,12	0.74	0	15,15,17	0.70	0
3	MAN	C	7	3	11,11,12	0.60	0	15,15,17	0.74	0
3	FUC	C	8	3	10,10,11	0.73	0	14,14,16	1.08	2 (14%)
3	NAG	D	1	1,3	14,14,15	0.69	0	17,19,21	0.89	0
3	NAG	D	2	3	14,14,15	0.59	0	17,19,21	0.81	1 (5%)
3	BMA	D	3	3	11,11,12	0.78	0	15,15,17	0.47	0
3	MAN	D	4	3	11,11,12	0.56	0	15,15,17	0.85	1 (6%)
3	NAG	D	5	3	14,14,15	0.48	0	17,19,21	0.82	0
3	GAL	D	6	3	11,11,12	0.55	0	15,15,17	0.48	0
3	MAN	D	7	3	11,11,12	0.53	0	15,15,17	0.52	0
3	FUC	D	8	3	10,10,11	0.75	0	14,14,16	0.89	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '–' means no outliers of that kind were identified.

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4	MAN	C1-O5-C5	2.63	115.71	112.19
3	C	8	FUC	C3-C4-C5	2.53	113.65	109.81
3	D	2	NAG	C2-N2-C7	-2.23	119.91	122.90
3	D	8	FUC	C1-C2-C3	2.18	112.83	109.64
3	C	8	FUC	C1-C2-C3	2.06	112.65	109.64

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	8	FUC	C1
3	D	8	FUC	C1

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	4	MAN	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

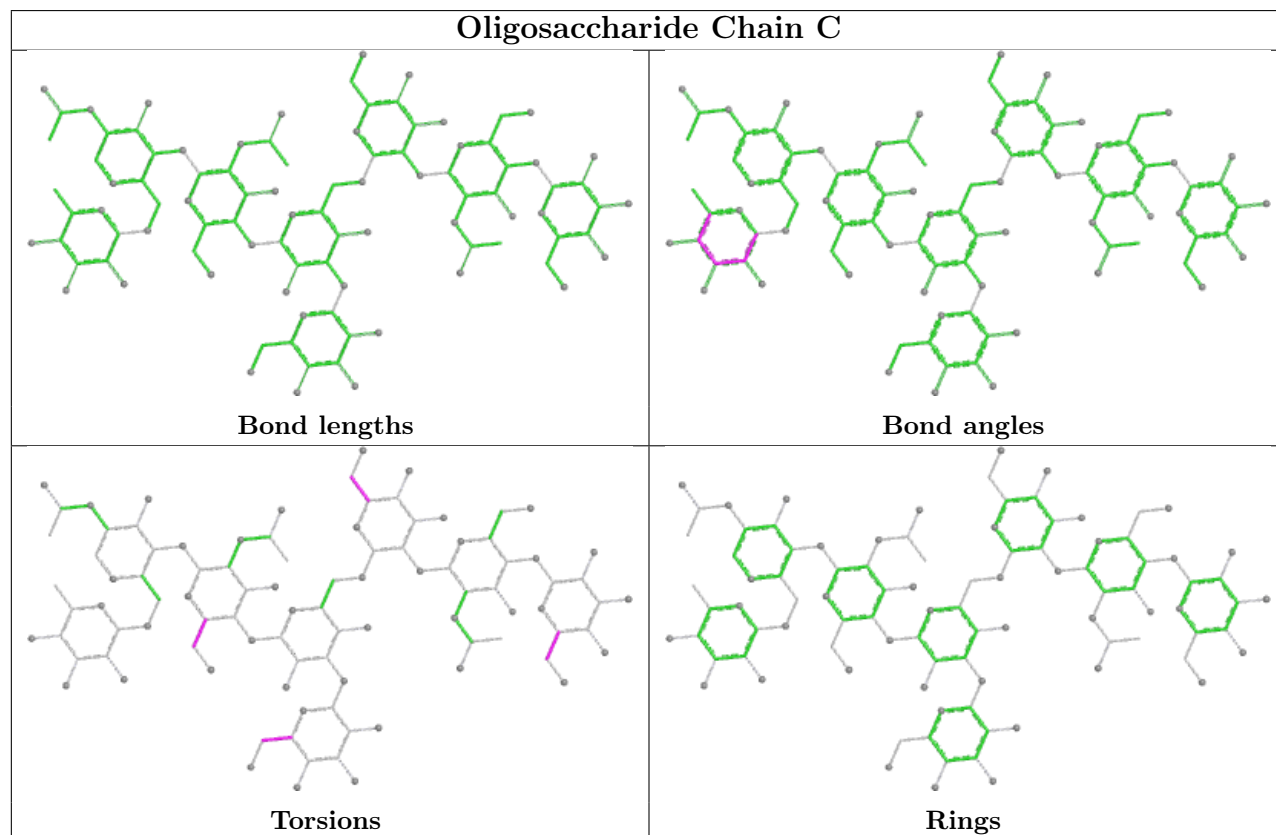
Mol	Chain	Res	Type	Atoms
3	D	4	MAN	C4-C5-C6-O6
3	C	7	MAN	C4-C5-C6-O6
3	C	7	MAN	O5-C5-C6-O6
3	C	6	GAL	O5-C5-C6-O6
3	C	4	MAN	C4-C5-C6-O6
3	C	4	MAN	O5-C5-C6-O6

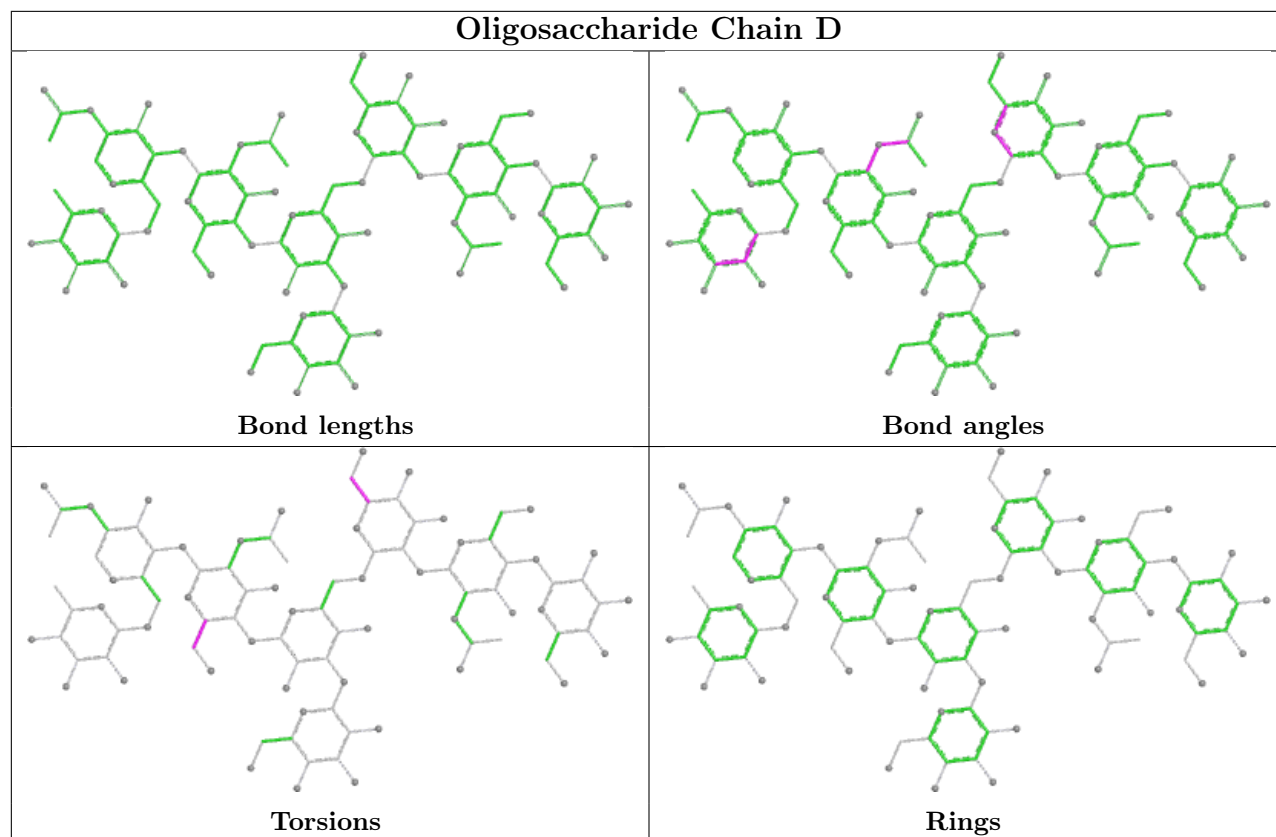
There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	8	FUC	1	0
3	C	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	207/227 (91%)	2.38	103 (49%) 0 2	9, 23, 36, 50	5 (2%)
1	B	207/227 (91%)	2.10	97 (46%) 0 2	10, 24, 45, 56	4 (1%)
2	E	171/401 (42%)	2.05	72 (42%) 0 3	11, 18, 28, 36	0
2	F	171/401 (42%)	1.67	53 (30%) 1 5	0, 0, 0, 0	0
All	All	756/1256 (60%)	2.07	325 (42%) 0 3	0, 19, 37, 56	9 (1%)

All (325) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	265	ASP	11.8
2	E	390	LEU	11.7
1	A	238	PRO	10.8
2	F	390	LEU	9.2
1	A	237	GLY	8.5
2	E	389	PRO	8.3
1	B	264	VAL	8.2
1	A	330	ALA	7.9
1	A	331	PRO	7.3
2	F	389	PRO	7.1
1	A	259	VAL	6.8
1	A	334	LYS	6.8
1	A	258	GLU	6.8
1	A	264	VAL	6.6
2	F	282	TYR	6.5
1	A	240	VAL	6.4
2	F	220	ARG	6.4
2	E	298	ALA	6.3
1	A	332	ILE	6.3
1	A	323	VAL	6.3
2	E	365	ASP	6.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	239	SER	6.1
1	B	333	GLU	6.0
1	B	296	TYR	6.0
1	A	345	GLU	5.9
2	E	284	PRO	5.8
1	A	319	TYR	5.8
2	E	313	GLY	5.8
1	B	266	VAL	5.7
2	E	380	GLN	5.6
1	A	242	LEU	5.6
1	B	356	GLU	5.5
1	A	430	GLU	5.4
2	E	379	ALA	5.4
1	A	247	PRO	5.3
1	B	263	VAL	5.3
2	E	220	ARG	5.2
1	B	332	ILE	5.2
1	A	327	ALA	5.1
1	A	301	ARG	5.1
2	E	301	THR	5.1
1	B	255	ARG	5.1
1	B	302	VAL	5.0
1	A	266	VAL	5.0
1	B	300	TYR	4.9
1	B	334	LYS	4.9
2	E	236	PRO	4.9
1	B	307	THR	4.8
1	B	294	GLU	4.8
1	A	355	ARG	4.8
1	A	249	ASP	4.8
2	E	337	TRP	4.7
1	B	238	PRO	4.7
1	B	331	PRO	4.7
1	A	243	PHE	4.6
1	A	260	THR	4.6
1	A	326	LYS	4.6
1	B	262	VAL	4.6
1	B	282	VAL	4.5
1	A	292	ARG	4.4
2	F	312	ALA	4.4
1	A	244	PRO	4.4
2	E	244	VAL	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	305	ARG	4.4
1	A	305	VAL	4.4
1	B	350	THR	4.3
1	A	262	VAL	4.3
1	A	329	PRO	4.3
1	A	270	ASP	4.3
2	F	298	ALA	4.3
2	E	224	VAL	4.3
2	E	285	GLN	4.3
2	E	264	ARG	4.3
1	B	258	GLU	4.2
1	B	323	VAL	4.2
1	B	330	ALA	4.2
1	A	325	ASN	4.2
1	A	423	PHE	4.2
2	E	312	ALA	4.2
2	E	368	HIS	4.2
2	F	290	LEU	4.2
2	E	276	ILE	4.2
1	A	263	VAL	4.1
2	F	265	PHE	4.1
1	A	289	THR	4.1
2	E	364	ASN	4.1
2	F	365	ASP	4.1
2	F	270	SER	4.1
2	E	299	ALA	4.1
2	F	367	ILE	4.1
1	A	255	ARG	4.1
1	A	273	VAL	4.1
1	B	316	GLY	4.0
1	A	336	ILE	4.0
2	E	302	TRP	4.0
2	E	266	ASP	4.0
2	F	378	ALA	4.0
1	A	318	GLU	4.0
1	A	239	SER	4.0
1	A	245	PRO	3.9
1	B	256	THR	3.9
1	B	443	LEU	3.9
1	A	250	THR	3.9
1	A	443	LEU	3.9
2	F	330	GLU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	327	ALA	3.8
2	F	261	VAL	3.8
1	B	340	LYS	3.8
1	B	288	LYS	3.8
1	A	274	LYS	3.8
1	B	378	ALA	3.8
1	B	240	VAL	3.8
1	A	356	GLU	3.8
1	A	279	VAL	3.7
1	B	265	ASP	3.7
2	F	305	ARG	3.7
1	B	273	VAL	3.7
1	A	299	THR	3.7
1	A	307	THR	3.7
2	E	317	THR	3.7
1	A	335	THR	3.6
2	E	254	GLN	3.6
2	F	259	ASP	3.6
2	E	333	PRO	3.6
2	F	317	THR	3.6
2	E	269	THR	3.6
1	A	272	GLU	3.6
1	A	359	THR	3.5
2	F	387	GLU	3.5
1	A	298	SER	3.5
2	F	223	THR	3.5
2	F	225	ARG	3.4
1	B	257	PRO	3.4
1	B	291	PRO	3.4
2	F	247	HIS	3.4
2	F	285	GLN	3.4
1	A	393	THR	3.4
1	B	277	TRP	3.4
2	E	272	ALA	3.4
1	A	284	VAL	3.4
1	A	381	TRP	3.4
1	B	355	ARG	3.4
2	F	257	SER	3.4
1	A	277	TRP	3.4
2	F	296	PRO	3.3
1	B	376	ASP	3.3
1	B	301	ARG	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	338	GLN	3.3
2	E	290	LEU	3.3
1	A	275	PHE	3.3
2	E	304	SER	3.3
1	A	312	ASP	3.2
1	B	430	GLU	3.2
2	F	359	CYS	3.2
1	B	299	THR	3.2
1	B	295	GLN	3.2
1	B	329	PRO	3.2
2	F	385	VAL	3.2
2	E	248	ALA	3.2
1	B	409	LYS	3.1
1	B	425	CYS	3.1
1	B	318	GLU	3.1
1	A	408	SER	3.1
1	A	286	ASN	3.1
1	B	433	HIS	3.1
1	B	292	ARG	3.1
2	F	245	SER	3.1
2	E	296	PRO	3.1
2	F	325	ALA	3.1
1	B	328	LEU	3.1
2	F	308	VAL	3.1
2	E	237	GLY	3.0
1	A	269	GLU	3.0
2	E	310	SER	3.0
1	B	380	GLU	3.0
1	B	347	GLN	3.0
1	A	313	TRP	3.0
2	F	231	ALA	3.0
1	A	416	ARG	3.0
1	B	379	VAL	3.0
1	B	286	ASN	3.0
1	A	302	VAL	3.0
1	A	317	LYS	3.0
1	B	305	VAL	2.9
2	E	308	VAL	2.9
1	A	311	GLN	2.9
2	F	279	SER	2.9
2	E	226	MET	2.9
1	B	272	GLU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	342	GLN	2.9
2	E	338	GLN	2.9
2	F	260	VAL	2.9
2	E	354	SER	2.9
1	B	408	SER	2.8
1	A	421	ASN	2.8
2	E	267	VAL	2.8
1	A	257	PRO	2.8
2	E	229	PRO	2.8
1	A	296	TYR	2.8
1	B	244	PRO	2.8
2	F	272	ALA	2.8
1	B	385	GLY	2.8
2	F	229	PRO	2.8
1	B	237	GLY	2.8
1	A	333	GLU	2.8
2	F	277	TYR	2.8
2	F	281	LEU	2.8
1	B	259	VAL	2.7
2	E	249	ILE	2.7
1	A	251	LEU	2.7
1	B	335	THR	2.7
2	F	303	THR	2.7
2	E	265	PHE	2.7
1	A	411	THR	2.7
2	F	310	SER	2.7
1	B	249	ASP	2.7
2	E	324	SER	2.7
2	E	253	ASP	2.7
2	E	348	ASP	2.7
1	B	247	PRO	2.7
2	E	255	THR	2.7
2	E	259	ASP	2.6
1	A	303	VAL	2.6
2	E	263	LEU	2.6
2	E	278	GLU	2.6
2	E	330	GLU	2.6
1	A	425	CYS	2.6
1	B	367	CYS	2.6
2	F	304	SER	2.6
1	B	317	LYS	2.6
2	E	277	TYR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	385	VAL	2.6
1	A	338	LYS	2.6
1	A	415	SER	2.6
2	F	263	LEU	2.6
2	E	359	CYS	2.6
1	B	418	GLN	2.6
2	E	292	PRO	2.6
1	A	342	GLN	2.6
1	B	326	LYS	2.6
1	B	285	HIS	2.6
1	B	281	GLY	2.6
1	A	431	ALA	2.5
1	A	439	LYS	2.5
2	F	262	TRP	2.5
1	A	316	GLY	2.5
1	A	377	ILE	2.5
1	A	402	GLY	2.5
2	F	324	SER	2.5
2	F	345	GLU	2.5
2	F	372	HIS	2.5
1	A	376	ASP	2.5
1	B	284	VAL	2.5
2	E	303	THR	2.5
1	A	438	GLN	2.5
2	E	262	TRP	2.5
2	E	281	LEU	2.4
1	B	424	SER	2.4
1	A	328	LEU	2.4
1	A	363	VAL	2.4
1	A	248	LYS	2.4
1	B	407	TYR	2.4
1	B	283	GLU	2.4
2	E	355	GLY	2.4
1	A	390	ASN	2.4
2	E	300	SER	2.4
1	A	282	VAL	2.4
1	A	350	THR	2.4
1	A	367	CYS	2.4
1	B	390	ASN	2.4
2	E	247	HIS	2.3
1	A	291	PRO	2.3
2	E	340	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	252	MET	2.3
2	F	311	TYR	2.3
2	E	233	LEU	2.3
1	A	392	LYS	2.3
2	E	261	VAL	2.3
1	A	324	SER	2.3
1	B	428	MET	2.3
1	A	271	PRO	2.3
1	B	406	LEU	2.3
2	E	309	ARG	2.3
1	A	404	PHE	2.2
2	E	360	VAL	2.2
1	A	364	SER	2.2
1	B	386	GLN	2.2
1	A	290	LYS	2.2
1	A	320	LYS	2.2
1	B	338	LYS	2.2
1	B	392	LYS	2.2
1	A	436	TYR	2.2
2	F	358	LEU	2.2
1	B	325	ASN	2.2
1	B	339	ALA	2.2
1	B	416	ARG	2.2
1	B	411	THR	2.2
1	B	251	LEU	2.2
2	F	356	LEU	2.2
1	A	428	MET	2.2
2	E	243	ASN	2.2
1	B	438	GLN	2.2
1	A	293	GLU	2.2
1	B	289	THR	2.2
1	B	437	THR	2.2
2	E	270	SER	2.2
1	B	310	HIS	2.1
1	B	382	GLU	2.1
1	B	275	PHE	2.1
2	F	347	ARG	2.1
2	E	378	ALA	2.1
2	F	377	THR	2.1
2	F	293	ALA	2.1
1	B	413	ASP	2.1
1	B	362	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	246	ILE	2.1
2	F	386	VAL	2.1
2	F	232	ILE	2.1
1	B	359	THR	2.0
2	E	232	ILE	2.0
1	B	303	VAL	2.0
2	E	235	SER	2.0
1	A	300	TYR	2.0
1	B	396	PRO	2.0
1	B	393	THR	2.0

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

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

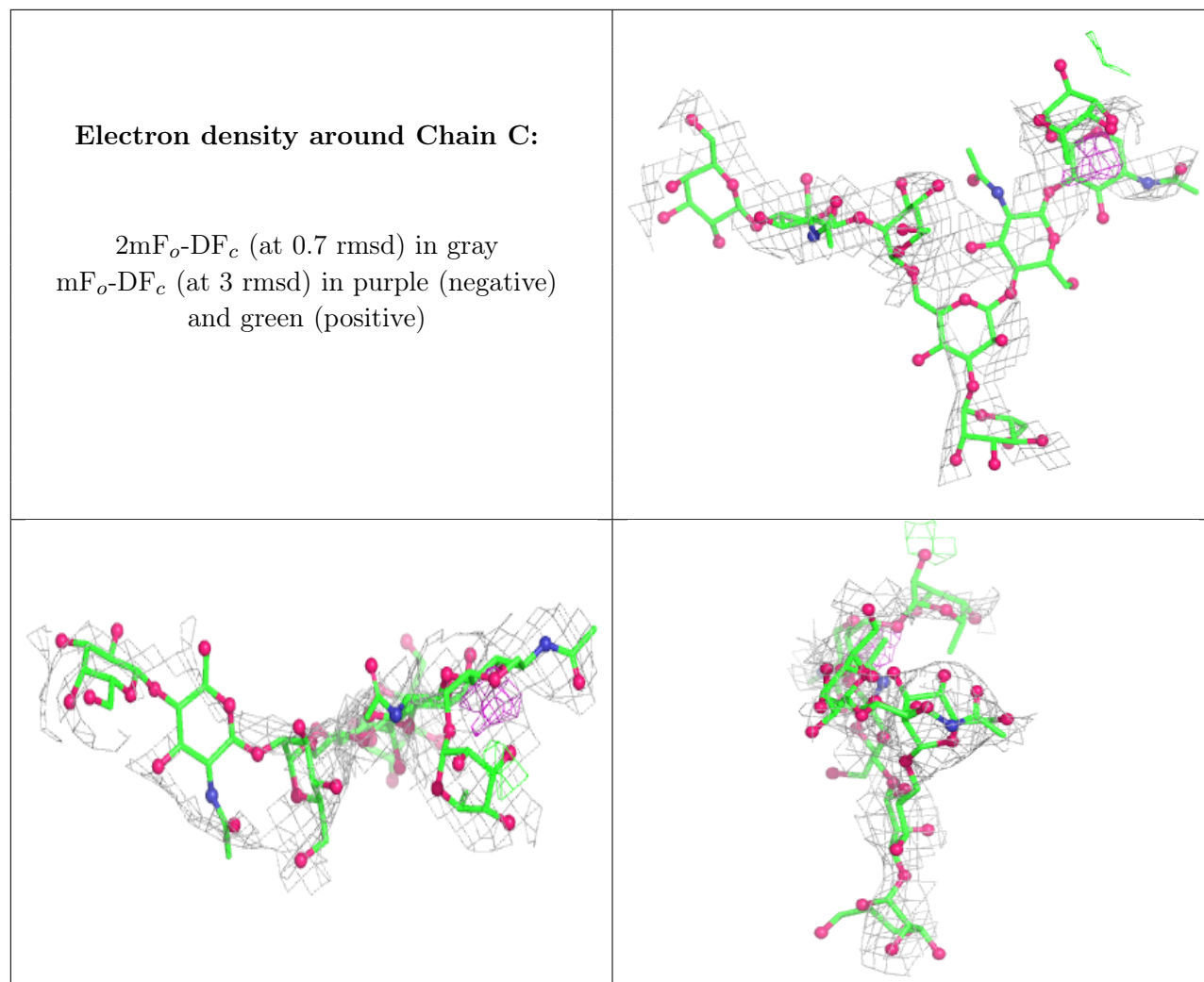
6.3 Carbohydrates [i](#)

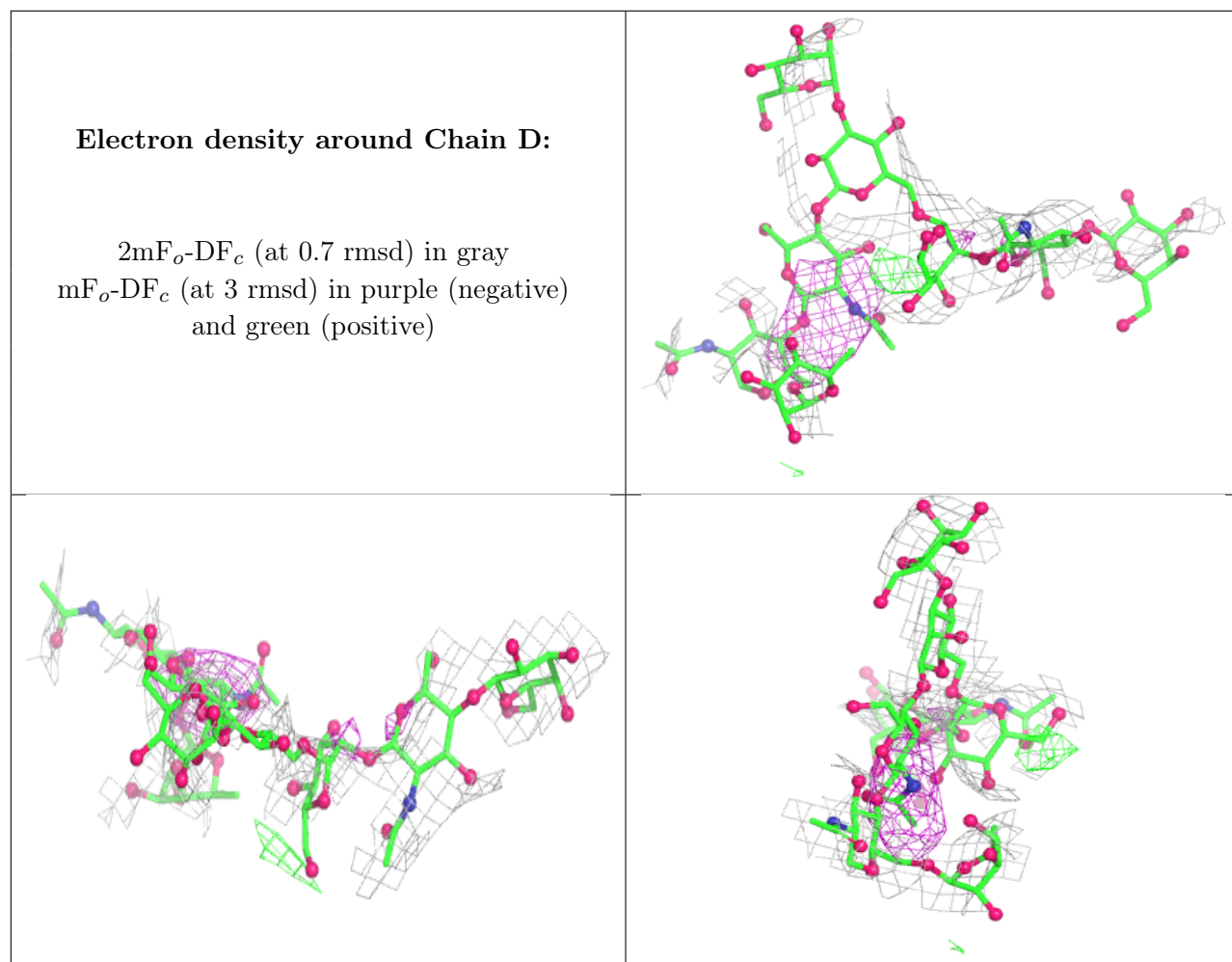
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	C	1	14/15	-	-	31,33,43,54	0
3	NAG	C	2	14/15	-	-	23,27,30,31	0
3	BMA	C	3	11/12	-	-	30,33,36,40	0
3	MAN	C	4	11/12	-	-	36,37,40,40	0
3	NAG	C	5	14/15	-	-	33,36,39,42	0
3	GAL	C	6	11/12	-	-	47,53,56,61	0
3	MAN	C	7	11/12	-	-	39,44,46,47	0
3	FUC	C	8	10/11	-	-	62,68,74,74	0
3	NAG	D	1	14/15	-	-	40,42,45,54	0
3	NAG	D	2	14/15	-	-	29,34,36,38	0
3	BMA	D	3	11/12	-	-	25,28,33,34	0
3	MAN	D	4	11/12	-	-	27,29,32,36	0
3	NAG	D	5	14/15	-	-	29,33,37,43	0
3	GAL	D	6	11/12	-	-	48,52,55,58	0
3	MAN	D	7	11/12	-	-	40,42,43,44	0
3	FUC	D	8	10/11	-	-	57,60,63,64	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.