WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Nov 28, 2023 – 04:28 PM EST

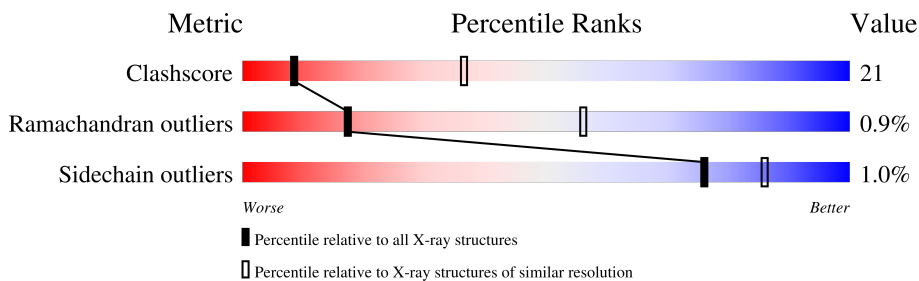|		
PDB ID	:	2GJ7
Title	:	Crystal Structure of a gE-gI/Fc complex
Authors	:	Sprague, E.R.; Wang, C.; Baker, D.; Bjorkman, P.J.
Deposited on	:	2006-03-30
Resolution	:	5.00 Å(reported)

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	Percentile Ranks	Value
Clashscore		21
Ramachandran outliers		0.9%
Sidechain outliers		1.0%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1000 (6.16-3.82)
Ramachandran outliers	138981	1146 (6.20-3.80)
Sidechain outliers	138945	1122 (6.20-3.80)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	227	73% 18% 9%
1	B	227	72% 19% • 9%
2	E	401	34% 8% 57%
2	F	401	33% 8% 57%
3	C	8	62% 25% 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 1659	C 1056	N 279	O 317	S 7	19	0	0
1	B	207	Total 1659	C 1056	N 279	O 317	S 7	11	0	0

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 1319	C 829	N 229	O 250	S 11	0	0	0
2	E	171	Total 1319	C 829	N 229	O 250	S 11	0	0	0

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-b
  eta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]be
  ta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucop
  yranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.
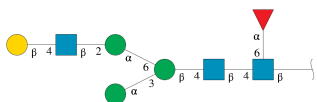
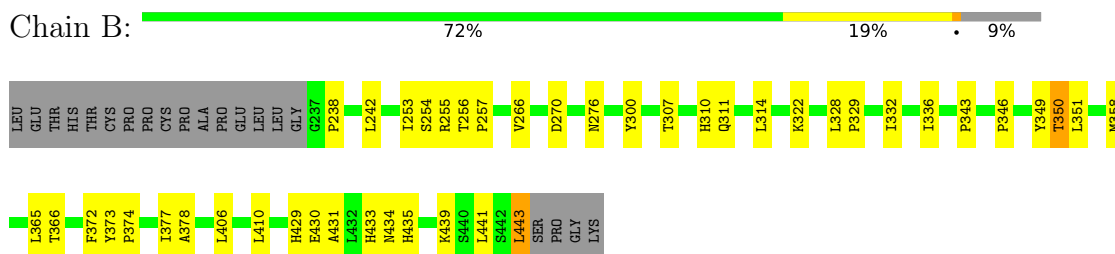| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	8	Total 96	C 54	N 3	O 39	0	0	0
3	D	8	Total 96	C 54	N 3	O 39	0	0	0

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. 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. 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.
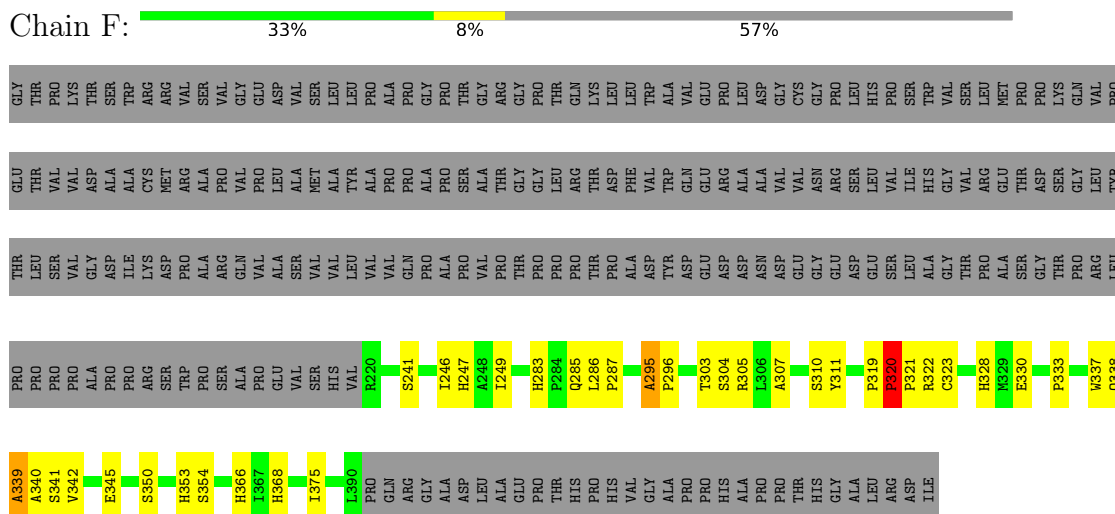
- Molecule 1: Ig gamma-1 chain C region
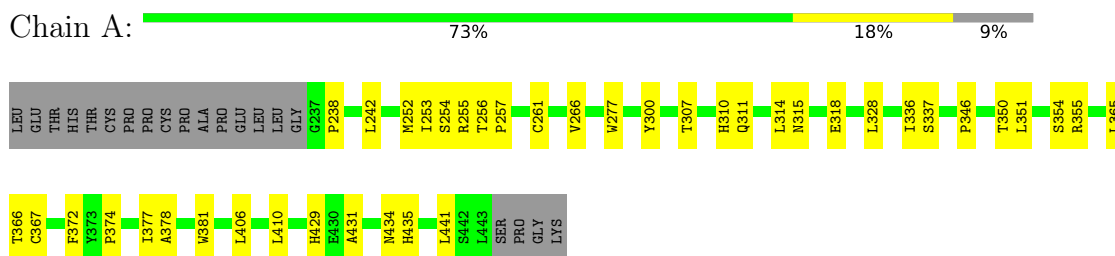
Chain A:
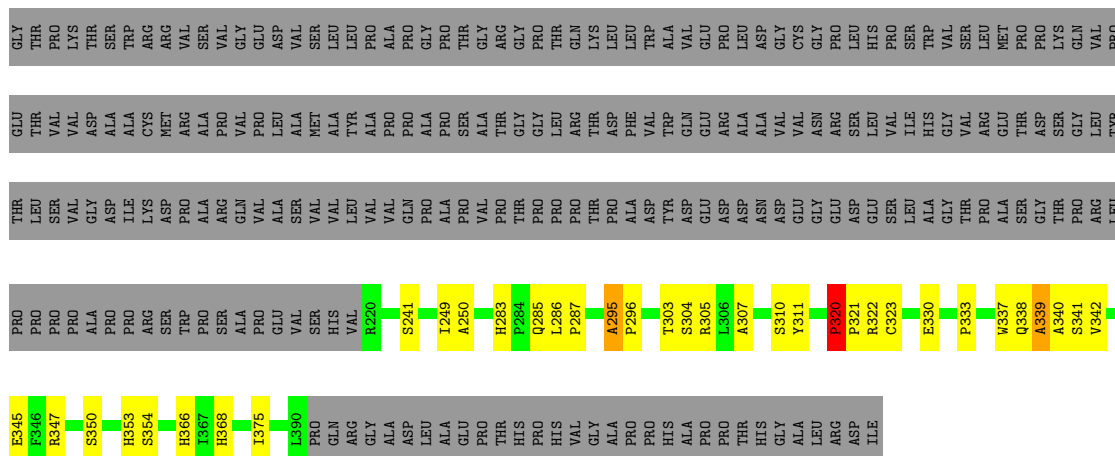

- Molecule 1: Ig gamma-1 chain C region

Chain B:

- Molecule 2: Glycoprotein E

Chain F:

- Molecule 2: Glycoprotein E

Chain E:

34% 8% 57%

GLY THR PRO LYS THR SER TRP ARG ARG VAL VAL GLY GLU ASP VAL SER LEU LEU PRO ALA PRO GLY PRO THR GLY ARG GLY PRO THR GLN LYS LEU LEU LEU TRP ALA VAL GLU PRO LEU ASP GLY CYS GLY PRO LEU HIS PRO SER TRP VAL SER LEU MET PRO PRO LYS GLN VAL PRO

GLU THR VAL VAL ASP ALA ALA CYS MET ARG ALA PRO VAL PRO LEU ALA MET ALA TYR ALA PRO PRO ALA PRO SER ALA THR GLY LEU ARG THR ASP PHE VAL TRP GLN GLU ARG ALA ALA VAL VAL VAL ASN ARG SER LEU VAL ILE HIS GLY VAL ARG GLU THR ASP SER GLY LEU TYR

THR LEU SER VAL GLY ASP ILE LYS ASP PRO ALA ARG GLN VAL ALA SER VAL VAL LEU VAL VAL GLN PRO ALA PRO VAL PRO THR PRO PRO THR PRO ALA ASP TYR GLU ASP ASP ASN ASP GLU GLU GLU ASP GLU SER LEU ALA GLY THR PRO ALA SER GLY THR PRO ARG LEU

PRO PRO PRO PRO ALA PRO PRO ARG SER TRP PRO SER ALA PRO GLU VAL SER HIS VAL **R220** S241 I249 A250 H283 P284 Q285 L286 P287 A295 P296 T303 S304 R305 L306 A307 S310 Y311 **P320** P321 R322 C323 E330 P333 W337 Q338 A339 A340 S341 V342

E345 F346 R347 S350 H353 S354 H366 I367 H368 I375 L390 PRO GLN ARG GLY ALA ASP LEU ALA GLU PRO THR HIS PRO HIS VAL GLY ALA PRO PRO HIS ALA PRO PRO THR HIS GLY ALA LEU ARG ASP ILE

- 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:

62% 25% 12%
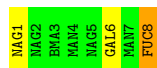
NAG1 NAG2 BMA3 MAN4 NAG5 GAL6 MAN7 FUC8

- 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 BMA3 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 35.68 – 4.99	Depositor EDS
% Data completeness (in resolution range)	(Not available) (36.00-5.00) 99.5 (35.68-4.99)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.70 (at 5.08Å)	Xtriage
Refinement program		Depositor
R, R_{free}	(Not available) , (Not available) 0.497 , (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)	0.34 , 62.8	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	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.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, BMA, FUC, GAL, 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	0.40	0/1705	0.61	0/2322
1	B	0.40	0/1705	0.61	0/2322
2	E	0.32	0/1359	0.64	0/1866
2	F	0.32	0/1359	0.64	0/1866
All	All	0.37	0/6128	0.62	0/8376

There are no bond length outliers.

There are no bond angle outliers.

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	133	0
1	B	1659	0	1623	82	0
2	E	1319	0	1239	76	30
2	F	1319	0	1238	133	30
3	C	96	0	82	1	0
3	D	96	0	82	0	0
All	All	6148	0	5886	249	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 (249) 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:252:MET:HE3	2:F:247:HIS:CE1	1.61	1.35
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
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:311:GLN:HA	2:F:322:ARG:HG2	1.27	1.09
1:A:310:HIS:HB2	2:F:321:PRO:C	1.74	1.07
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:311:GLN:HA	2:F:322:ARG:CZ	2.03	0.88
1:A:252:MET:CE	2:F:247:HIS:CE1	2.55	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:252:MET:HE3	2:F:247:HIS:NE2	1.89	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:B:434:ASN:ND2	2:E:250:ALA:N	2.13	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:346:PRO:HB3	1:B:372:PHE:HB3	1.65	0.76
1:B:433:HIS:HE2	2:E:250:ALA:C	1.89	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:A:256:THR:CG2	2:F:340:ALA:CB	2.05	0.75
1:B:434:ASN:HD21	2:E:250:ALA:H	0.78	0.75
1:B:253:ILE:HG12	2:E:311:TYR:CE2	2.21	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:CZ	2.57	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:254:SER:C	2:F:342:VAL:HG22	2.11	0.70
1:A:310:HIS:CB	2:F:321:PRO:C	2.58	0.69
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:A:311:GLN:C	2:F:322:ARG:NH1	2.46	0.68
1:B:314:LEU:CB	2:E:322:ARG:HH12	2.02	0.68
1:A:311:GLN:CB	2:F:322:ARG:HA	2.22	0.67
1:A:307:THR:HG1	2:F:339:ALA:HB1	1.59	0.66
1:A:314:LEU:CA	2:F:322:ARG:NH1	2.58	0.66
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:314:LEU:CB	2:E:322:ARG:HH11	2.04	0.61
1:A:311:GLN:HB2	2:F:322:ARG:C	2.20	0.61
1:A:307:THR:HG23	2:F:340:ALA:HB2	1.81	0.61
1:B:256:THR:OG1	2:E:340:ALA:C	2.39	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:O	2.04	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:B:434:ASN:ND2	2:E:249:ILE:C	2.58	0.56
1:A:314:LEU:HD12	2:F:322:ARG:CG	2.36	0.56
1:B:253:ILE:CG1	2:E:311:TYR:CE2	2.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:GLN:HA	2:F:322:ARG:NE	2.22	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
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: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
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: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
1:A:406:LEU:HD12	1:A:406:LEU:C	2.35	0.47
1:A:310:HIS:HB2	2:F:322:ARG:N	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:GLU:HA	1:A:337:SER:HB3	1.98	0.46
1:B:434:ASN:HD21	2:E:249:ILE:C	2.07	0.46
2:F:338:GLN:HG3	2:F:341:SER:CB	2.42	0.46
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: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
1:B:406:LEU:C	1:B:406:LEU:HD12	2.39	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
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
1:A:255:ARG:C	2:F:341:SER:HA	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	205/227 (90%)	203 (99%)	2 (1%)	0	100	100
1	B	205/227 (90%)	199 (97%)	5 (2%)	1 (0%)	29	68
2	E	169/401 (42%)	160 (95%)	6 (4%)	3 (2%)	8	41
2	F	169/401 (42%)	160 (95%)	6 (4%)	3 (2%)	8	41
All	All	748/1256 (60%)	722 (96%)	19 (2%)	7 (1%)	17	56

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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	193/210 (92%)	192 (100%)	1 (0%)	88	93
1	B	193/210 (92%)	189 (98%)	4 (2%)	53	72
2	E	144/332 (43%)	143 (99%)	1 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	144/332 (43%)	143 (99%)	1 (1%)	84	90
All	All	674/1084 (62%)	667 (99%)	7 (1%)	76	86

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	355	ARG
2	F	320	PRO
1	B	270	ASP
1	B	350	THR
1	B	439	LYS
1	B	443	LEU
2	E	320	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	429	HIS
1	A	438	GLN
2	F	283	HIS
2	F	338	GLN
2	F	353	HIS
2	F	368	HIS
1	B	310	HIS
1	B	361	ASN
1	B	429	HIS
1	B	434	ASN
2	E	283	HIS
2	E	338	GLN
2	E	353	HIS
2	E	368	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 (i)

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	0.73	0
3	NAG	C	2	3	14,14,15	0.47	0	17,19,21	0.74	0
3	BMA	C	3	3	11,11,12	0.65	0	15,15,17	0.59	0
3	MAN	C	4	3	11,11,12	0.52	0	15,15,17	0.57	0
3	NAG	C	5	3	14,14,15	0.50	0	17,19,21	0.76	0
3	GAL	C	6	3	11,11,12	0.76	0	15,15,17	0.77	1 (6%)
3	MAN	C	7	3	11,11,12	0.61	0	15,15,17	0.80	0
3	FUC	C	8	3	10,10,11	0.74	0	14,14,16	1.14	2 (14%)
3	NAG	D	1	1,3	14,14,15	0.67	0	17,19,21	0.87	0
3	NAG	D	2	3	14,14,15	0.58	0	17,19,21	0.78	1 (5%)
3	BMA	D	3	3	11,11,12	0.80	0	15,15,17	0.50	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	0.79	0
3	GAL	D	6	3	11,11,12	0.56	0	15,15,17	0.51	0
3	MAN	D	7	3	11,11,12	0.54	0	15,15,17	0.59	0
3	FUC	D	8	3	10,10,11	0.76	0	14,14,16	1.04	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	4	MAN	C1-O5-C5	2.59	115.71	112.19
3	D	8	FUC	C1-C2-C3	2.57	112.83	109.67
3	C	8	FUC	C3-C4-C5	2.49	113.65	109.77
3	C	8	FUC	C1-C2-C3	2.43	112.65	109.67
3	C	6	GAL	C1-C2-C3	2.33	112.53	109.67
3	D	2	NAG	C2-N2-C7	-2.10	119.91	122.90

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	4	MAN	C4-C5-C6-O6
3	D	2	NAG	O5-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	1	NAG	1	0
3	C	8	FUC	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.

Oligosaccharide Chain C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D — Bond lengths, Bond angles, Torsions, Rings
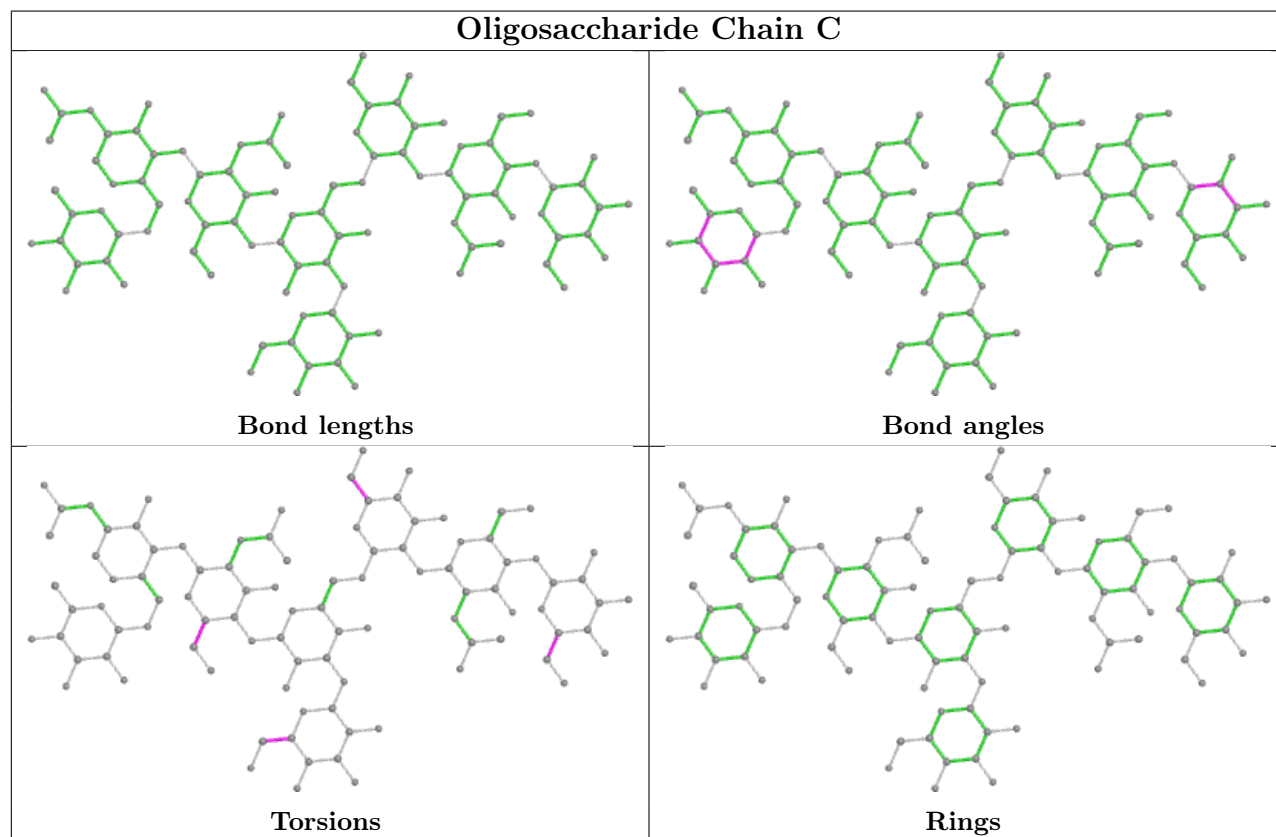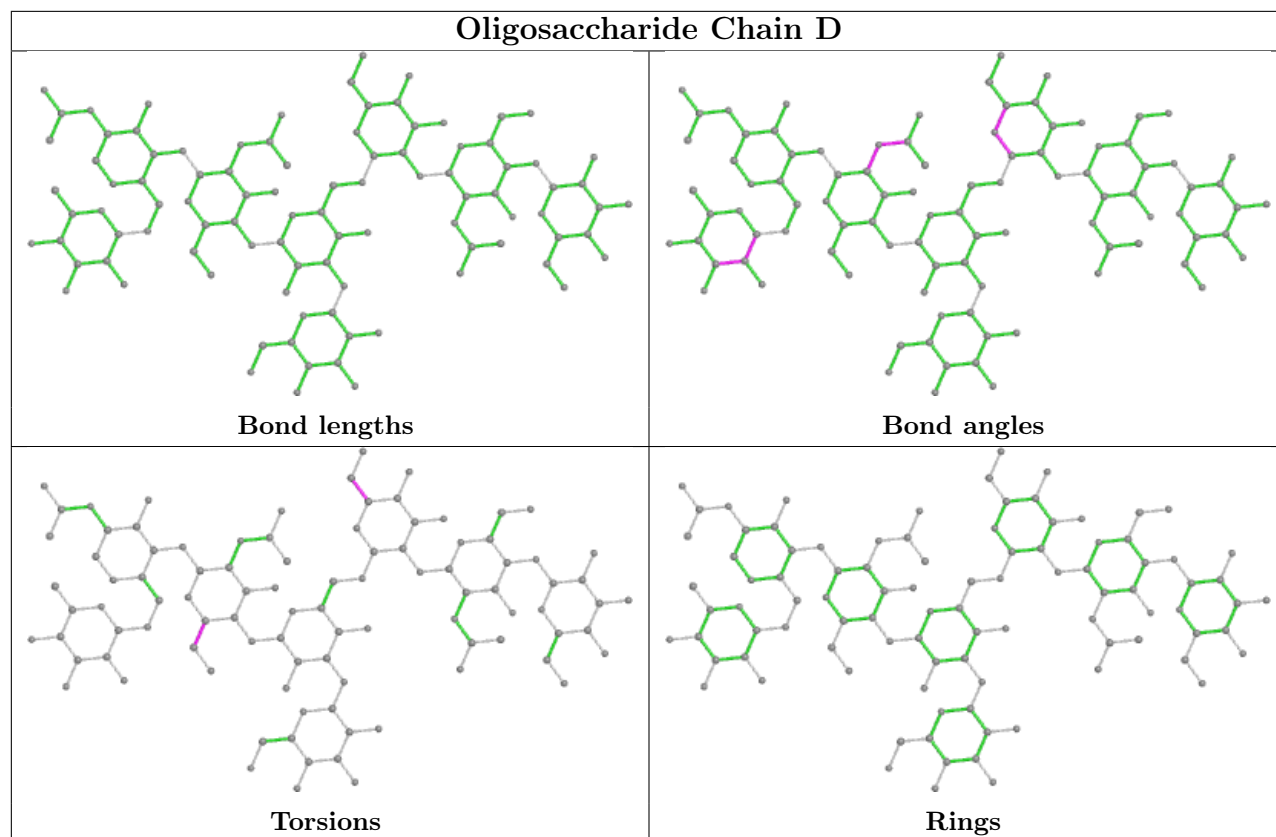
5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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 ⓘ

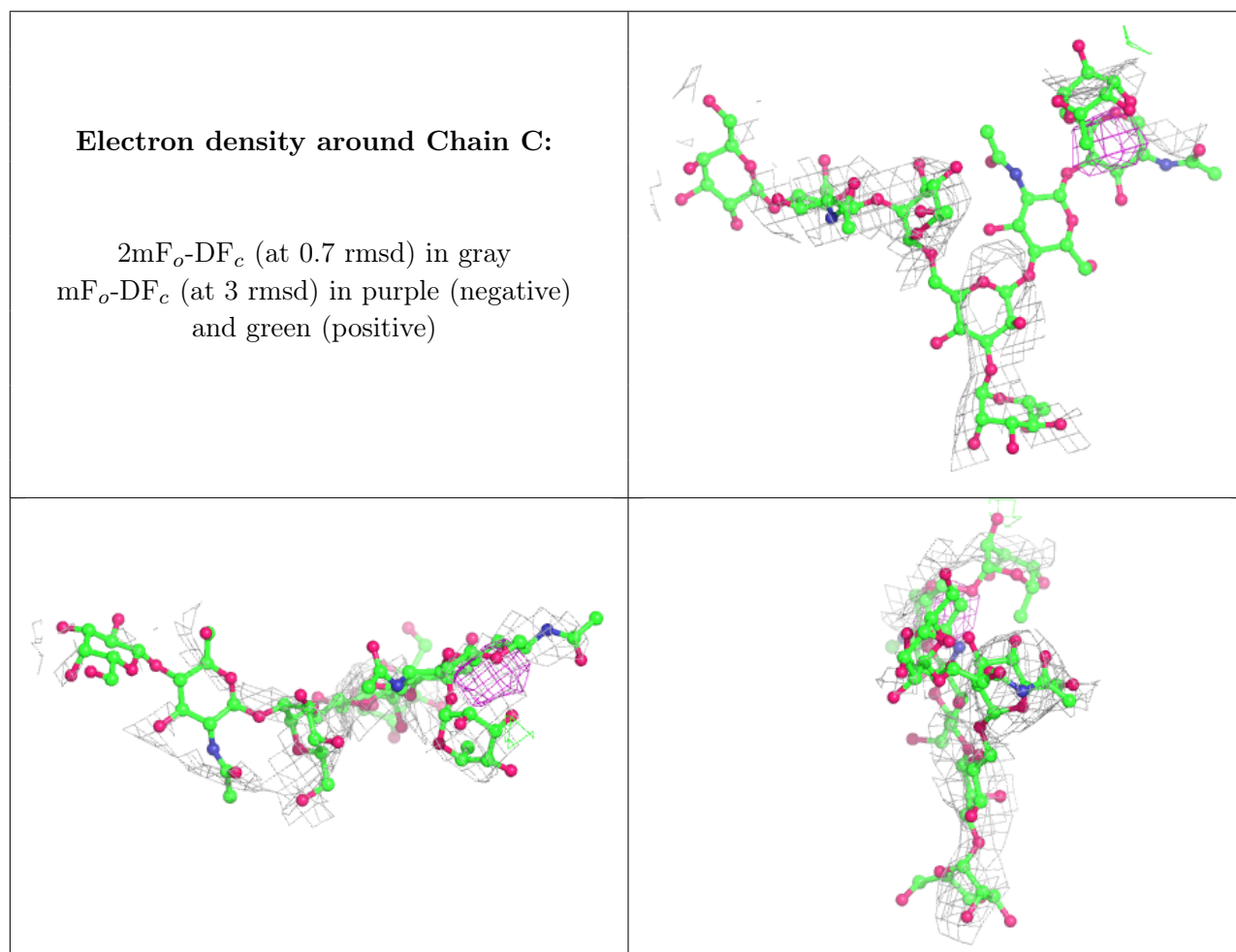Unable to reproduce the depositors R factor - this section is therefore empty.

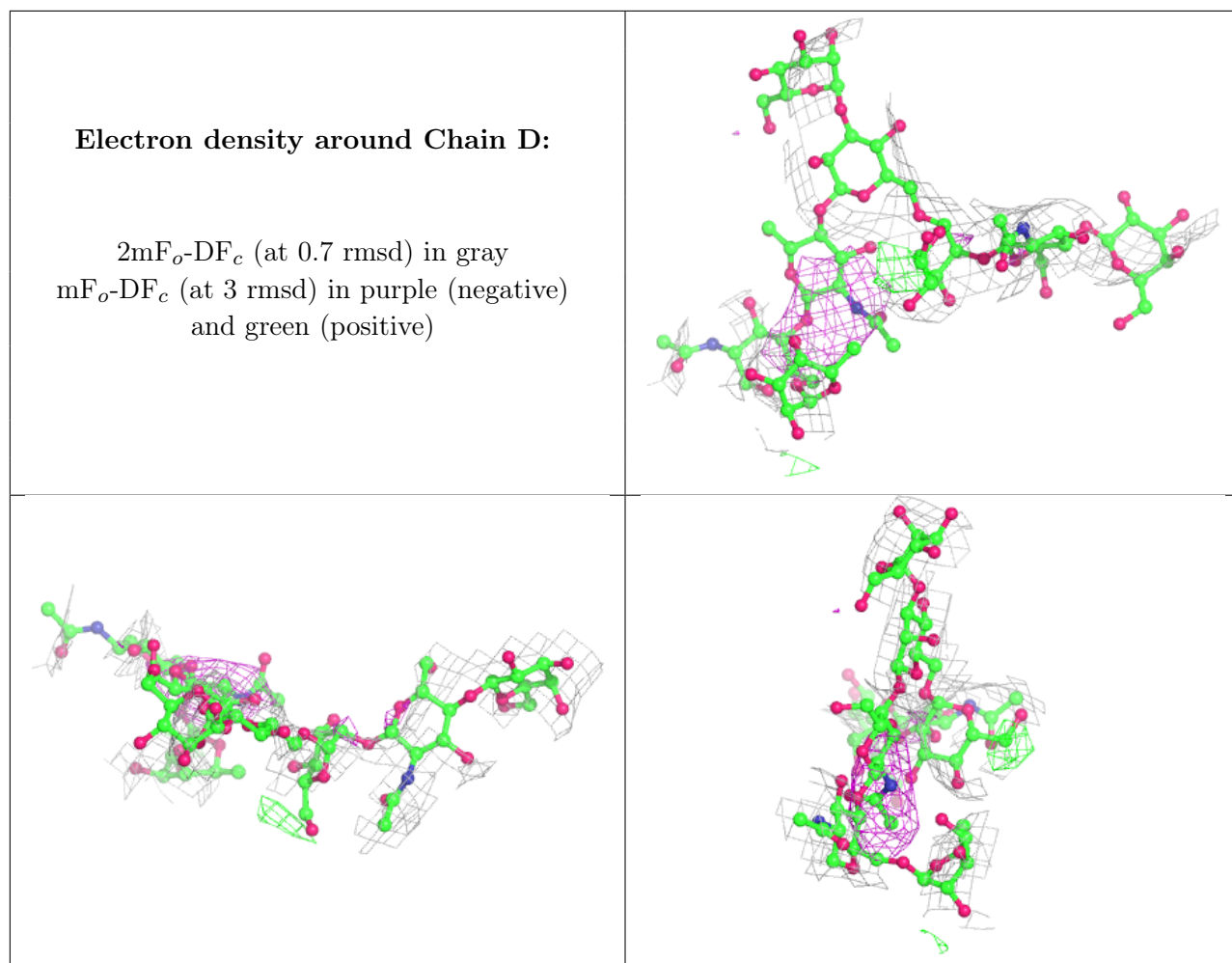## 6.2   Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3   Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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:

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

Electron density around Chain D:

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

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.