



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:19 AM UTC

PDB ID : 3RSJ / pdb_00003rsj
Title : Structure of HCRF in complex with Ganglioside GD1a
Authors : Fu, Z.; Benson, M.A.; Barbieri, J.T.; Kim, J.-J.P.; Baldwin, M.R.
Deposited on : 2011-05-02
Resolution : 2.00 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:

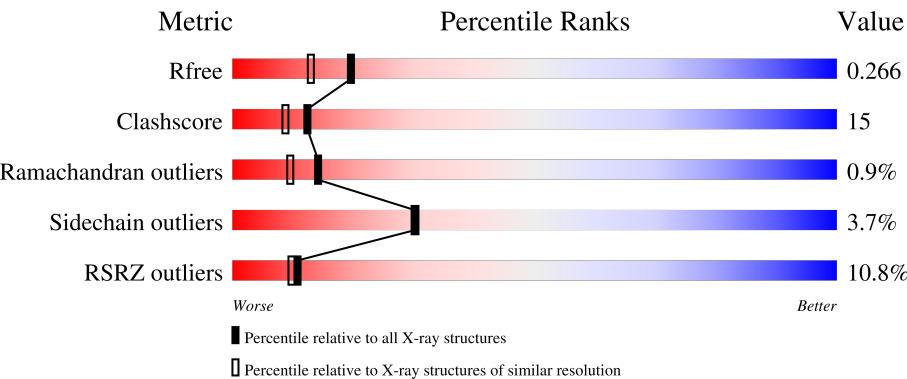
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.00 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.



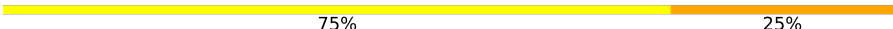
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	413	11% 63% 32% ..
1	B	413	12% 66% 28% ..
1	C	413	11% 65% 30% ..
1	D	413	9% 71% 24% ..
2	E	3	67% 33%

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Mol	Chain	Length	Quality of chain	
2	H	3		
3	F	5		
4	G	4		

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13922 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 BoNT/F.

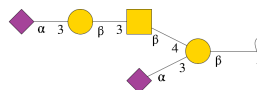
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	0	0	0
			3334	2114	577	635	8			
1	B	402	Total	C	N	O	S	0	0	0
			3307	2097	572	630	8			
1	C	402	Total	C	N	O	S	0	0	0
			3307	2097	572	630	8			
1	D	404	Total	C	N	O	S	0	0	0
			3324	2109	575	632	8			

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			46	25	2	19			
2	H	3	Total	C	N	O	0	0	0
			46	25	2	19			

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	5	Total	C	N	O	0	0	0
			77	42	3	32			

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			57	31	2	24			

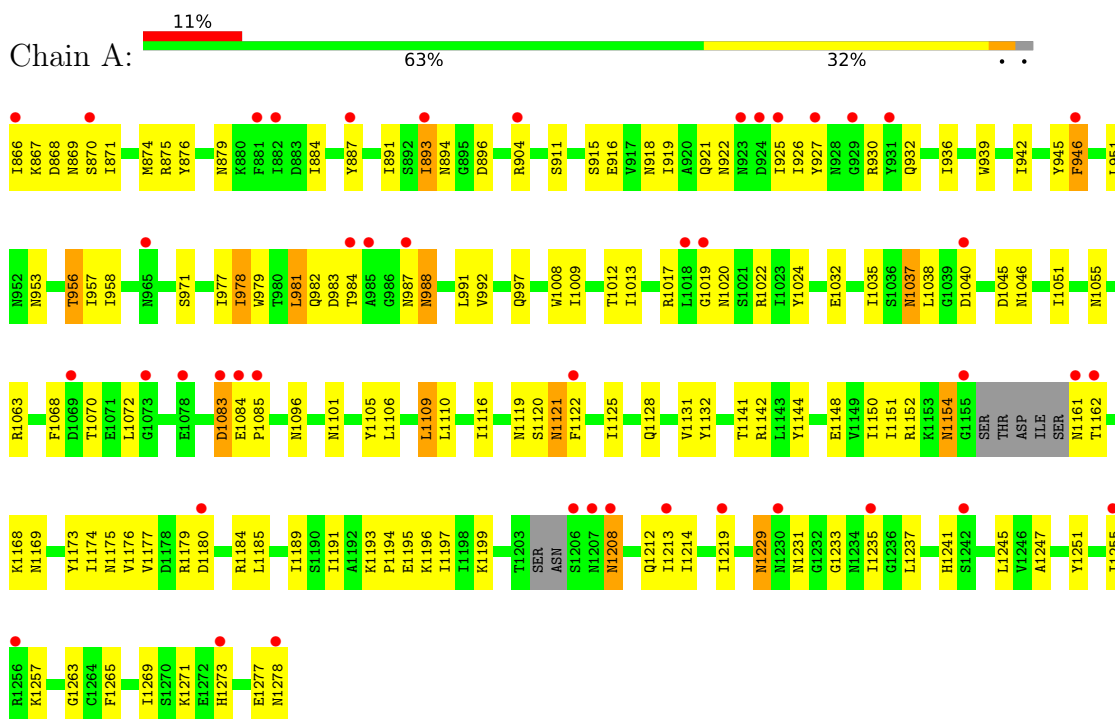
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	117	Total	O	0	0
			117	117		
5	B	98	Total	O	0	0
			98	98		
5	C	96	Total	O	0	0
			96	96		
5	D	113	Total	O	0	0
			113	113		

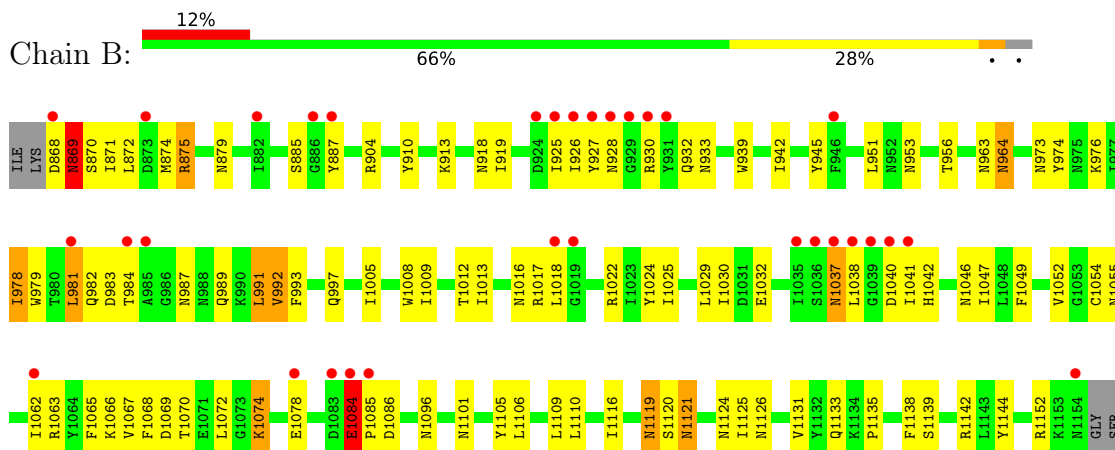
3 Residue-property plots [i](#)

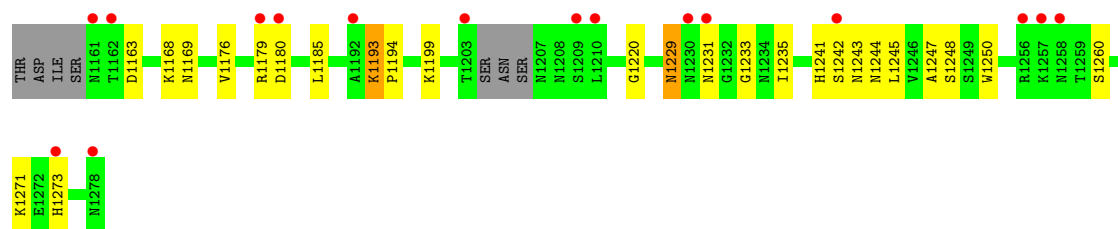
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: BoNT/F

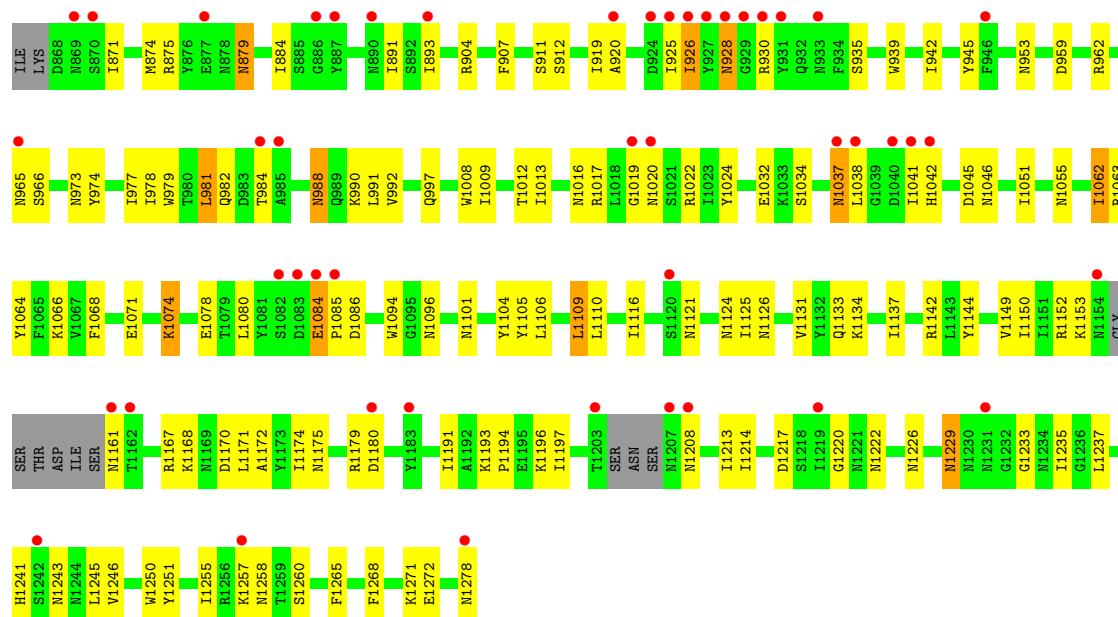


• Molecule 1: BoNT/F

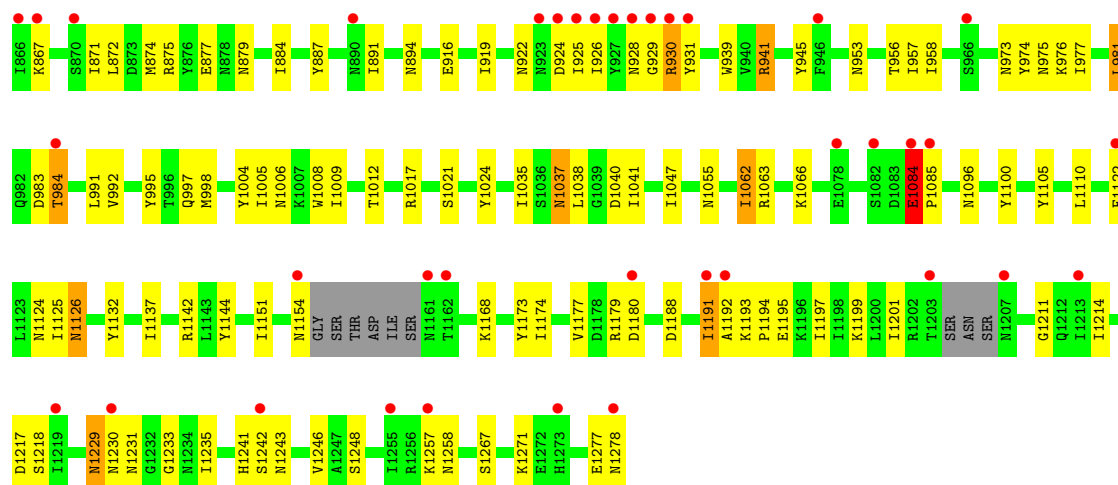




• Molecule 1: BoNT/F



• Molecule 1: BoNT/F



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose

Chain E:  67% 33%

NGA1
GAL2
SIA3

- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose

Chain H:  67% 33%

NGA1
GAL2
SIA3

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose

Chain F:  40% 60%

GAL1
NGA2
GAL3
SIA4
SIA5

- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain G:  75% 25%

GAL1
NGA2
GAL3
SIA4

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.47Å 84.27Å 117.60Å 72.55° 87.01° 67.13°	Depositor
Resolution (Å)	29.86 – 2.00 29.86 – 2.00	Depositor EDS
% Data completeness (in resolution range)	87.0 (29.86-2.00) 87.0 (29.86-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.00Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.232 , 0.263 0.235 , 0.266	Depositor DCC
R_{free} test set	12918 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13922	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.34% 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: GAL, SIA, NGA

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	0/3401	0.95	12/4603 (0.3%)
1	B	0.38	0/3374	0.92	14/4568 (0.3%)
1	C	0.39	0/3374	0.94	13/4568 (0.3%)
1	D	0.41	0/3391	0.94	13/4590 (0.3%)
All	All	0.40	0/13540	0.93	52/18329 (0.3%)

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1235	ILE	N-CA-C	-9.03	104.49	111.62
1	C	1121	ASN	N-CA-C	-8.29	102.47	112.59
1	A	951	LEU	N-CA-C	8.03	120.74	111.11
1	D	928	ASN	N-CA-C	-7.20	106.42	114.62
1	A	1235	ILE	N-CA-C	-7.11	106.14	111.90
1	B	1235	ILE	N-CA-C	-7.08	105.47	111.56
1	C	928	ASN	N-CA-C	-6.81	104.87	113.72
1	B	992	VAL	N-CA-C	6.59	117.79	108.17
1	C	978	ILE	N-CA-C	6.58	117.33	108.11
1	A	1121	ASN	N-CA-C	-6.42	104.75	112.59
1	C	977	ILE	N-CA-C	-6.35	98.48	107.75
1	C	942	ILE	N-CA-C	6.24	114.28	107.60
1	A	978	ILE	N-CA-C	6.20	116.79	108.11
1	B	978	ILE	N-CA-C	6.20	117.52	108.53
1	B	942	ILE	N-CA-C	6.07	114.09	107.60
1	B	1247	ALA	N-CA-C	-6.00	98.74	108.52
1	D	1105	TYR	N-CA-C	-6.00	100.51	110.17
1	D	992	VAL	N-CA-C	5.98	117.30	108.45
1	D	1235	ILE	N-CA-C	-5.97	107.07	111.90
1	A	977	ILE	N-CA-C	-5.96	98.96	107.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	977	ILE	N-CA-C	-5.95	99.06	107.75
1	B	1105	TYR	N-CA-C	-5.92	101.24	110.42
1	C	1105	TYR	N-CA-C	-5.84	101.37	110.42
1	A	942	ILE	N-CA-C	5.80	113.81	107.60
1	B	1084	GLU	CA-C-N	-5.71	113.90	119.90
1	B	1084	GLU	C-N-CA	-5.71	113.90	119.90
1	C	1172	ALA	N-CA-C	5.64	116.52	108.74
1	A	1105	TYR	N-CA-C	-5.63	101.70	110.42
1	B	1121	ASN	N-CA-C	-5.50	105.00	112.26
1	D	1137	ILE	N-CA-C	5.50	116.29	111.56
1	C	959	ASP	N-CA-C	5.47	117.44	108.52
1	A	1269	ILE	N-CA-C	5.45	115.44	107.37
1	A	1247	ALA	N-CA-C	-5.43	99.67	108.52
1	D	1084	GLU	CA-C-N	-5.42	113.98	119.83
1	D	1084	GLU	C-N-CA	-5.42	113.98	119.83
1	C	992	VAL	N-CA-C	5.38	116.48	108.46
1	B	1047	ILE	N-CA-C	-5.37	98.74	107.28
1	A	1219	ILE	N-CA-C	-5.28	99.35	106.85
1	C	1133	GLN	N-CA-C	5.28	117.10	109.07
1	C	1220	GLY	N-CA-C	-5.26	106.83	111.67
1	D	976	LYS	N-CA-C	5.26	117.38	109.23
1	B	951	LEU	N-CA-C	5.21	117.36	111.11
1	D	1021	SER	N-CA-C	-5.19	100.71	109.07
1	B	1220	GLY	N-CA-C	-5.18	103.52	111.24
1	B	1242	SER	N-CA-C	-5.18	99.77	110.80
1	A	1083	ASP	N-CA-C	5.17	119.81	112.93
1	D	1004	TYR	N-CA-C	5.17	119.94	113.43
1	D	1047	ILE	N-CA-C	-5.12	99.58	106.85
1	A	922	ASN	N-CA-C	-5.12	102.81	110.23
1	C	912	SER	N-CA-C	5.08	119.43	112.88
1	B	976	LYS	N-CA-C	5.07	116.94	108.99
1	D	1257	LYS	N-CA-C	5.06	121.57	110.80

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	3334	0	3249	108	0
1	B	3307	0	3217	114	0
1	C	3307	0	3217	106	0
1	D	3324	0	3241	86	0
2	E	46	0	40	2	0
2	H	46	0	40	2	0
3	F	77	0	65	3	0
4	G	57	0	49	3	0
5	A	117	0	0	2	0
5	B	98	0	0	2	0
5	C	96	0	0	3	0
5	D	113	0	0	0	0
All	All	13922	0	13118	411	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (411) 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:D:953:ASN:HD21	1:D:1055:ASN:H	1.05	1.00
1:B:1229:ASN:HD21	1:B:1233:GLY:H	1.15	0.93
1:A:953:ASN:HD21	1:A:1055:ASN:H	1.17	0.91
1:D:945:TYR:H	1:D:997:GLN:HE22	1.18	0.90
1:C:1229:ASN:HD21	1:C:1233:GLY:H	1.22	0.88
1:D:1126:ASN:HD22	1:D:1126:ASN:H	1.17	0.88
1:A:866:ILE:HG13	1:A:868:ASP:H	1.40	0.87
1:A:945:TYR:H	1:A:997:GLN:HE22	1.24	0.85
1:D:953:ASN:ND2	1:D:1055:ASN:H	1.75	0.84
1:B:1229:ASN:C	1:B:1229:ASN:HD22	1.85	0.83
1:D:1037:ASN:H	1:D:1037:ASN:HD22	1.26	0.83
1:A:918:ASN:HD21	1:A:1046:ASN:HD22	1.25	0.82
1:A:1229:ASN:C	1:A:1229:ASN:HD22	1.86	0.82
1:A:1035:ILE:HB	1:A:1038:LEU:HD12	1.60	0.82
1:C:920:ALA:HA	1:C:1046:ASN:ND2	1.95	0.81
1:D:1229:ASN:C	1:D:1229:ASN:HD22	1.90	0.80
1:B:973:ASN:HD22	1:B:974:TYR:H	1.25	0.80
1:C:1229:ASN:ND2	1:C:1233:GLY:H	1.79	0.80
1:A:988:ASN:C	1:A:988:ASN:HD22	1.91	0.79
1:A:1101:ASN:HD22	1:A:1152:ARG:HH11	1.27	0.79
1:B:1229:ASN:ND2	1:B:1233:GLY:H	1.80	0.78
1:B:945:TYR:H	1:B:997:GLN:HE22	1.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1037:ASN:H	1:A:1037:ASN:HD22	1.34	0.76
1:B:933:ASN:ND2	1:B:1017:ARG:H	1.84	0.75
1:D:973:ASN:HD22	1:D:974:TYR:H	1.34	0.75
1:C:1012:THR:HB	1:C:1024:TYR:HB2	1.66	0.75
1:C:1229:ASN:C	1:C:1229:ASN:HD22	1.96	0.74
1:C:973:ASN:HD22	1:C:974:TYR:H	1.31	0.74
1:B:933:ASN:HD21	1:B:1017:ARG:H	1.36	0.73
1:C:871:ILE:HB	1:C:925:ILE:HD12	1.70	0.73
1:C:953:ASN:HD21	1:C:1055:ASN:H	1.34	0.73
1:A:1116:ILE:HD12	1:A:1245:LEU:HD11	1.70	0.73
1:A:1229:ASN:HD21	1:A:1233:GLY:H	1.35	0.72
1:A:1101:ASN:ND2	1:A:1152:ARG:HH11	1.87	0.72
5:A:145:HOH:O	1:D:998:MET:HE1	1.89	0.72
1:A:1273:HIS:CD2	1:B:1273:HIS:HD2	2.08	0.71
1:C:1064:TYR:HB3	1:C:1084:GLU:OE2	1.90	0.70
1:A:1037:ASN:HD22	1:A:1037:ASN:N	1.88	0.70
1:B:973:ASN:ND2	1:B:974:TYR:H	1.89	0.70
1:B:875:ARG:HH21	1:B:875:ARG:HG3	1.55	0.70
1:A:953:ASN:ND2	1:A:1055:ASN:H	1.87	0.70
1:C:1101:ASN:ND2	1:C:1152:ARG:HH11	1.89	0.70
1:A:871:ILE:HD12	1:A:925:ILE:HG23	1.74	0.69
1:C:1022:ARG:HD3	1:C:1032:GLU:OE2	1.92	0.69
1:C:871:ILE:HD12	1:C:925:ILE:HG23	1.76	0.68
1:D:953:ASN:HD21	1:D:1055:ASN:N	1.86	0.68
1:D:1008:TRP:HE1	1:D:1096:ASN:HD21	1.40	0.68
1:D:1126:ASN:HD22	1:D:1126:ASN:N	1.91	0.68
1:D:953:ASN:H	1:D:973:ASN:HD21	1.40	0.68
1:C:1037:ASN:N	1:C:1037:ASN:HD22	1.92	0.68
1:A:939:TRP:HB2	1:A:1063:ARG:HG2	1.76	0.67
1:B:874:MET:CE	1:B:1065:PHE:HB3	2.25	0.67
1:B:984:THR:HG22	1:B:1040:ASP:HB3	1.76	0.67
1:C:920:ALA:HA	1:C:1046:ASN:HD22	1.59	0.67
1:C:1142:ARG:HH11	1:C:1278:ASN:HB2	1.60	0.67
1:B:874:MET:HE3	5:B:139:HOH:O	1.95	0.67
1:C:973:ASN:ND2	1:C:974:TYR:H	1.93	0.67
1:A:1229:ASN:ND2	1:A:1233:GLY:H	1.94	0.66
1:C:1150:ILE:HD12	1:C:1150:ILE:O	1.95	0.66
1:C:875:ARG:HG3	1:C:884:ILE:HD13	1.76	0.65
1:D:941:ARG:HD3	1:D:1006:ASN:O	1.96	0.65
1:D:887:TYR:HB3	1:D:925:ILE:HD11	1.79	0.65
1:B:953:ASN:HD21	1:B:1055:ASN:H	1.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1022:ARG:HD3	1:B:1032:GLU:OE2	1.96	0.65
1:C:945:TYR:H	1:C:997:GLN:HE22	1.43	0.65
1:A:953:ASN:HD21	1:A:1055:ASN:N	1.93	0.64
1:B:973:ASN:HD22	1:B:974:TYR:N	1.95	0.64
1:C:1062:ILE:HD12	1:C:1063:ARG:N	2.13	0.64
1:B:983:ASP:OD2	1:B:987:ASN:HB2	1.99	0.63
1:D:1066:LYS:NZ	1:D:1084:GLU:OE2	2.32	0.63
1:C:1272:GLU:HB3	5:C:184:HOH:O	1.99	0.62
1:D:1197:ILE:HA	1:D:1246:VAL:HG12	1.82	0.62
1:D:922:ASN:HD22	1:D:924:ASP:H	1.46	0.62
1:C:1037:ASN:HD22	1:C:1037:ASN:H	1.46	0.62
1:B:1074:LYS:O	1:B:1078:GLU:HG2	1.99	0.62
1:B:1012:THR:HB	1:B:1024:TYR:HB2	1.81	0.61
1:D:1008:TRP:HE1	1:D:1096:ASN:ND2	1.97	0.61
1:A:1142:ARG:HH11	1:A:1278:ASN:HB2	1.64	0.61
1:C:1084:GLU:HA	1:C:1084:GLU:OE1	2.01	0.61
1:B:1068:PHE:CD2	1:B:1072:LEU:HD11	2.36	0.61
1:B:1229:ASN:C	1:B:1229:ASN:ND2	2.59	0.61
1:C:1101:ASN:HD22	1:C:1152:ARG:HH11	1.48	0.61
1:C:953:ASN:H	1:C:973:ASN:HD21	1.48	0.61
1:A:1116:ILE:HD11	1:A:1125:ILE:HD12	1.82	0.60
1:B:1241:HIS:HA	3:F:3:GAL:O4	2.01	0.60
1:C:1094:TRP:NE1	1:C:1272:GLU:HG3	2.16	0.60
1:A:982:GLN:HG3	1:A:987:ASN:O	2.02	0.60
1:D:973:ASN:ND2	1:D:974:TYR:H	1.99	0.60
1:A:1022:ARG:HD3	1:A:1032:GLU:OE2	2.01	0.60
1:D:1194:PRO:HG2	1:D:1195:GLU:OE2	2.02	0.60
1:B:964:ASN:N	1:B:964:ASN:HD22	2.00	0.60
1:B:930:ARG:HA	1:B:1017:ARG:HH22	1.68	0.59
1:C:1241:HIS:HA	4:G:3:GAL:O4	2.01	0.59
1:D:874:MET:HE3	1:D:891:ILE:HD13	1.83	0.59
3:F:1:GAL:H5	3:F:5:SIA:H92	1.84	0.59
1:C:1016:ASN:HD22	1:C:1019:GLY:HA3	1.66	0.59
1:A:879:ASN:ND2	1:B:879:ASN:ND2	2.50	0.59
1:C:953:ASN:ND2	1:C:1055:ASN:H	2.00	0.59
1:B:1116:ILE:HD11	1:B:1125:ILE:HD12	1.85	0.58
1:C:1193:LYS:HG3	1:C:1194:PRO:HD2	1.85	0.58
1:D:1142:ARG:HH12	1:D:1278:ASN:HB2	1.68	0.58
1:B:1101:ASN:ND2	1:B:1152:ARG:HH11	2.02	0.58
1:D:891:ILE:HG12	1:D:919:ILE:HG12	1.86	0.58
1:C:879:ASN:N	1:C:879:ASN:HD22	1.99	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:984:THR:CG2	1:D:1040:ASP:HB3	2.33	0.58
1:C:871:ILE:HB	1:C:925:ILE:CD1	2.32	0.57
1:D:871:ILE:HA	1:D:887:TYR:CE2	2.39	0.57
1:D:1229:ASN:HD21	1:D:1233:GLY:H	1.52	0.57
1:B:1131:VAL:O	1:B:1142:ARG:NH2	2.37	0.57
1:C:879:ASN:N	1:C:879:ASN:ND2	2.48	0.57
1:D:887:TYR:CB	1:D:925:ILE:HD11	2.34	0.57
1:B:1008:TRP:HE1	1:B:1096:ASN:HD21	1.51	0.57
1:A:879:ASN:ND2	1:B:879:ASN:HD22	2.03	0.57
1:A:927:TYR:CE1	1:A:932:GLN:HG2	2.40	0.57
1:B:871:ILE:HD11	1:B:1067:VAL:HG12	1.86	0.57
1:A:1019:GLY:C	1:A:1020:ASN:HD22	2.13	0.56
1:A:1273:HIS:CD2	1:B:1273:HIS:CD2	2.93	0.56
1:B:874:MET:HE1	1:B:1049:PHE:CZ	2.40	0.56
1:A:1161:ASN:ND2	1:A:1162:THR:H	2.04	0.56
1:A:1119:ASN:C	1:A:1119:ASN:HD22	2.12	0.56
1:A:1241:HIS:HA	2:E:2:GAL:O4	2.05	0.56
1:B:1022:ARG:NH2	1:B:1032:GLU:OE2	2.39	0.56
1:B:930:ARG:HA	1:B:1017:ARG:NH2	2.20	0.56
1:B:939:TRP:HB2	1:B:1063:ARG:HG2	1.86	0.56
1:A:875:ARG:HG3	1:A:884:ILE:HD13	1.88	0.56
1:D:1062:ILE:HD12	1:D:1063:ARG:H	1.71	0.56
1:C:973:ASN:HD22	1:C:974:TYR:N	2.02	0.56
1:B:1037:ASN:ND2	1:B:1038:LEU:HG	2.21	0.55
1:B:1231:ASN:N	1:B:1231:ASN:HD22	2.04	0.55
1:B:1069:ASP:OD1	1:B:1070:THR:HG23	2.07	0.55
1:A:1208:ASN:N	1:A:1208:ASN:HD22	2.05	0.55
1:D:1229:ASN:ND2	1:D:1231:ASN:N	2.54	0.55
1:A:918:ASN:HD21	1:A:1046:ASN:ND2	1.98	0.55
1:A:946:PHE:HD1	1:A:946:PHE:H	1.55	0.55
1:B:904:ARG:HG2	1:B:904:ARG:HH21	1.72	0.54
1:D:957:ILE:HG13	1:D:958:ILE:HG13	1.89	0.54
1:D:1179:ARG:O	1:D:1180:ASP:HB2	2.06	0.54
1:C:930:ARG:HA	1:C:1017:ARG:HH22	1.72	0.54
1:A:1101:ASN:HA	1:A:1150:ILE:HD11	1.90	0.54
1:B:869:ASN:N	1:B:869:ASN:HD22	2.05	0.54
1:B:1109:LEU:HB3	1:B:1260:SER:O	2.08	0.54
1:B:1121:ASN:ND2	1:B:1199:LYS:HE2	2.23	0.54
1:D:1191:ILE:CD1	1:D:1193:LYS:HB3	2.37	0.54
1:A:946:PHE:N	1:A:946:PHE:CD1	2.76	0.54
1:B:874:MET:HE2	1:B:1065:PHE:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1101:ASN:HD22	1:A:1152:ARG:NH1	2.03	0.53
1:B:1037:ASN:HD22	1:B:1037:ASN:N	2.05	0.53
1:B:918:ASN:HD21	1:B:1046:ASN:ND2	2.06	0.53
1:B:953:ASN:ND2	1:B:1055:ASN:H	2.06	0.53
1:B:1194:PRO:O	1:B:1248:SER:HA	2.07	0.53
1:C:1066:LYS:NZ	1:C:1084:GLU:OE2	2.41	0.53
1:C:1131:VAL:O	1:C:1142:ARG:NH2	2.41	0.53
1:C:1179:ARG:O	1:C:1180:ASP:HB2	2.08	0.53
1:C:1134:LYS:HE2	1:C:1137:ILE:HD12	1.91	0.53
1:B:925:ILE:O	1:B:927:TYR:N	2.42	0.53
1:D:1229:ASN:C	1:D:1229:ASN:ND2	2.62	0.53
1:B:953:ASN:H	1:B:973:ASN:HD21	1.57	0.53
1:A:1251:TYR:O	1:A:1255:ILE:HG13	2.09	0.53
1:B:1176:VAL:HG23	1:B:1185:LEU:HD11	1.91	0.53
1:C:1116:ILE:HD12	1:C:1245:LEU:HD11	1.91	0.52
1:D:1037:ASN:HD22	1:D:1037:ASN:N	1.97	0.52
1:A:1144:TYR:CE1	1:A:1271:LYS:HA	2.43	0.52
1:A:1175:ASN:OD1	1:A:1184:ARG:HA	2.09	0.52
1:B:964:ASN:HD22	1:B:964:ASN:H	1.57	0.52
1:B:1008:TRP:HE1	1:B:1096:ASN:ND2	2.08	0.52
1:B:933:ASN:CG	1:B:1016:ASN:HA	2.34	0.52
1:B:1084:GLU:OE1	1:B:1084:GLU:HA	2.10	0.52
1:B:1168:LYS:O	1:B:1169:ASN:HB2	2.10	0.52
1:C:1109:LEU:HD23	1:C:1265:PHE:HB3	1.92	0.52
1:D:1035:ILE:HB	1:D:1038:LEU:HD12	1.90	0.52
1:D:939:TRP:HB2	1:D:1063:ARG:HG2	1.91	0.52
1:D:1154:ASN:HA	1:D:1173:TYR:CE2	2.45	0.52
1:C:1150:ILE:HD11	1:C:1175:ASN:HB2	1.91	0.52
1:D:973:ASN:HD22	1:D:974:TYR:N	2.05	0.52
1:B:1229:ASN:ND2	1:B:1233:GLY:N	2.55	0.51
1:D:1122:PHE:CE1	1:D:1199:LYS:HE2	2.44	0.51
1:A:1179:ARG:O	1:A:1180:ASP:HB2	2.09	0.51
1:D:922:ASN:ND2	1:D:924:ASP:H	2.08	0.51
1:D:1191:ILE:HD11	1:D:1195:GLU:O	2.10	0.51
1:D:1229:ASN:ND2	1:D:1233:GLY:H	2.08	0.51
1:A:1173:TYR:HB3	1:A:1184:ARG:NE	2.25	0.51
1:C:1142:ARG:NH1	1:C:1278:ASN:HB2	2.25	0.51
1:C:979:TRP:CE2	1:C:1013:ILE:HG21	2.45	0.51
1:B:933:ASN:HD21	1:B:1017:ARG:N	2.07	0.51
1:B:956:THR:CG2	1:B:1052:VAL:HB	2.41	0.51
1:A:946:PHE:HD1	1:A:946:PHE:N	2.08	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:988:ASN:C	1:A:988:ASN:ND2	2.61	0.50
1:C:911:SER:HB3	1:C:1051:ILE:HG21	1.91	0.50
1:D:875:ARG:HG3	1:D:884:ILE:HD13	1.93	0.50
1:A:1132:TYR:CE2	1:A:1277:GLU:HA	2.47	0.50
1:C:891:ILE:HG12	1:C:919:ILE:HG12	1.92	0.50
1:C:1008:TRP:HE1	1:C:1096:ASN:HD21	1.60	0.50
1:C:1153:LYS:HZ3	1:C:1161:ASN:N	2.09	0.50
1:D:1124:ASN:HB3	1:D:1126:ASN:ND2	2.25	0.50
1:A:1037:ASN:H	1:A:1037:ASN:ND2	2.06	0.50
5:C:424:HOH:O	4:G:1:GAL:C3	2.59	0.50
1:A:894:ASN:HB2	1:A:916:GLU:HG2	1.92	0.50
1:B:979:TRP:CE2	1:B:1013:ILE:HG21	2.47	0.50
1:B:927:TYR:CD1	1:B:932:GLN:HG2	2.47	0.49
1:C:1008:TRP:HE1	1:C:1096:ASN:ND2	2.09	0.49
1:D:1177:VAL:HG13	1:D:1177:VAL:O	2.11	0.49
1:B:918:ASN:HD21	1:B:1046:ASN:HD22	1.59	0.49
1:A:1191:ILE:CD1	1:A:1197:ILE:HG22	2.43	0.49
1:D:874:MET:HE2	1:D:891:ILE:HG21	1.94	0.49
1:C:1251:TYR:O	1:C:1255:ILE:HG13	2.13	0.49
1:B:875:ARG:HG3	1:B:875:ARG:NH2	2.27	0.49
1:C:874:MET:SD	1:C:919:ILE:HD11	2.53	0.49
1:C:904:ARG:HG2	5:C:298:HOH:O	2.11	0.49
1:C:1150:ILE:HD13	1:C:1152:ARG:NE	2.28	0.49
1:D:1192:ALA:O	1:D:1193:LYS:HB2	2.13	0.49
1:A:1008:TRP:HE1	1:A:1096:ASN:HD21	1.59	0.48
1:A:1131:VAL:O	1:A:1142:ARG:NH2	2.45	0.48
1:C:1144:TYR:CE1	1:C:1271:LYS:HA	2.48	0.48
1:D:1037:ASN:H	1:D:1037:ASN:ND2	2.04	0.48
1:B:870:SER:O	1:B:885:SER:HB2	2.12	0.48
1:C:1229:ASN:ND2	1:C:1229:ASN:C	2.69	0.48
1:B:989:GLN:OE1	1:B:989:GLN:HA	2.12	0.48
1:D:984:THR:HG21	1:D:1040:ASP:HB3	1.94	0.48
1:D:1125:ILE:HG23	1:D:1125:ILE:O	2.13	0.48
1:B:868:ASP:C	1:B:870:SER:H	2.22	0.48
1:C:1250:TRP:CE3	4:G:3:GAL:H5	2.49	0.48
1:A:1148:GLU:O	1:A:1177:VAL:HG12	2.14	0.48
1:D:929:GLY:C	1:D:931:TYR:H	2.21	0.48
1:D:984:THR:HG22	1:D:1040:ASP:HB3	1.95	0.48
1:D:1144:TYR:CE1	1:D:1271:LYS:HA	2.49	0.48
1:A:930:ARG:HA	1:A:1017:ARG:NH2	2.29	0.48
1:B:993:PHE:CD1	1:B:1025:ILE:HG13	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:975:ASN:HB3	1:D:995:TYR:O	2.14	0.48
1:D:1229:ASN:ND2	1:D:1231:ASN:H	2.11	0.48
1:D:1062:ILE:HD12	1:D:1063:ARG:N	2.29	0.47
1:D:1132:TYR:CE2	1:D:1277:GLU:HA	2.49	0.47
1:A:983:ASP:HB2	1:A:1040:ASP:O	2.14	0.47
1:A:1122:PHE:HE1	1:A:1199:LYS:HE2	1.80	0.47
1:B:1193:LYS:HB2	1:B:1193:LYS:NZ	2.29	0.47
1:B:1066:LYS:NZ	1:B:1084:GLU:OE2	2.44	0.47
1:A:891:ILE:HG12	1:A:919:ILE:HG12	1.96	0.47
1:A:1068:PHE:CD2	1:A:1072:LEU:HD11	2.49	0.47
1:C:935:SER:HA	1:C:1013:ILE:O	2.14	0.47
1:C:1074:LYS:O	1:C:1078:GLU:HG2	2.15	0.47
1:D:981:LEU:CD2	1:D:1041:ILE:HD13	2.44	0.47
1:B:953:ASN:HD21	1:B:1054:CYS:HA	1.79	0.47
1:B:1193:LYS:HB2	1:B:1193:LYS:HZ2	1.79	0.47
1:C:1037:ASN:H	1:C:1037:ASN:ND2	2.12	0.47
1:D:1242:SER:OG	1:D:1243:ASN:N	2.27	0.47
1:A:1012:THR:HB	1:A:1024:TYR:HB2	1.97	0.47
1:A:1174:ILE:HG12	1:A:1214:ILE:HD12	1.97	0.47
1:B:982:GLN:HG3	1:B:987:ASN:O	2.15	0.47
1:C:879:ASN:OD1	1:D:879:ASN:ND2	2.47	0.47
1:C:1222:ASN:ND2	1:C:1260:SER:HB2	2.29	0.47
1:B:981:LEU:HD21	1:B:1041:ILE:HD13	1.97	0.47
1:B:984:THR:CG2	1:B:1040:ASP:HB3	2.43	0.47
1:A:1237:LEU:HD12	1:A:1251:TYR:HB2	1.96	0.47
1:A:1084:GLU:HB2	1:A:1085:PRO:HD3	1.97	0.47
1:A:1154:ASN:C	1:A:1154:ASN:ND2	2.72	0.47
1:B:910:TYR:CG	1:B:913:LYS:HE2	2.49	0.47
1:B:1025:ILE:HG12	1:B:1030:ILE:HG13	1.97	0.47
1:A:866:ILE:HD12	1:A:867:LYS:H	1.79	0.46
1:A:1191:ILE:CG2	1:A:1193:LYS:HE3	2.45	0.46
1:C:966:SER:HA	1:C:982:GLN:O	2.14	0.46
1:C:1116:ILE:HD11	1:C:1125:ILE:HD12	1.97	0.46
1:A:1116:ILE:CD1	1:A:1125:ILE:HD12	2.44	0.46
1:A:930:ARG:HA	1:A:1017:ARG:HH22	1.79	0.46
1:D:1211:GLY:HA2	1:D:1230:ASN:OD1	2.16	0.46
1:A:1208:ASN:N	1:A:1208:ASN:ND2	2.62	0.46
1:B:1144:TYR:CE2	1:B:1271:LYS:HG3	2.50	0.46
1:A:979:TRP:CZ2	1:A:981:LEU:HG	2.50	0.46
1:A:979:TRP:CD2	1:A:1013:ILE:HG21	2.49	0.46
1:D:1012:THR:HB	1:D:1024:TYR:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:965:ASN:ND2	1:C:984:THR:HA	2.31	0.46
1:D:930:ARG:HA	1:D:1017:ARG:HH22	1.81	0.46
1:D:1174:ILE:HG12	1:D:1214:ILE:HD12	1.97	0.46
1:C:893:ILE:O	1:C:893:ILE:HG13	2.15	0.46
1:D:894:ASN:HB3	1:D:916:GLU:HG2	1.98	0.46
1:D:981:LEU:HD21	1:D:1041:ILE:HD13	1.98	0.46
1:A:874:MET:HE3	1:A:891:ILE:HD13	1.97	0.46
1:C:979:TRP:CD2	1:C:1013:ILE:HG21	2.50	0.46
1:C:990:LYS:O	1:C:991:LEU:HD12	2.16	0.46
1:A:871:ILE:HA	1:A:887:TYR:CE2	2.51	0.45
1:C:939:TRP:HB2	1:C:1063:ARG:HG2	1.97	0.45
1:C:1191:ILE:O	1:C:1196:LYS:HE3	2.15	0.45
1:A:956:THR:HA	1:A:971:SER:HA	1.98	0.45
1:A:1109:LEU:HD23	1:A:1265:PHE:HB3	1.99	0.45
1:B:904:ARG:HG2	1:B:904:ARG:NH2	2.31	0.45
1:C:1104:TYR:CG	1:C:1268:PHE:HB3	2.51	0.45
1:C:1126:ASN:HB3	1:C:1243:ASN:HB3	1.97	0.45
1:B:1250:TRP:CE3	3:F:3:GAL:H5	2.51	0.45
1:C:988:ASN:HA	1:C:1038:LEU:HD21	1.98	0.45
1:D:1217:ASP:CG	1:D:1218:SER:H	2.25	0.45
1:D:1241:HIS:HA	2:H:2:GAL:O4	2.16	0.45
1:A:1068:PHE:CE2	1:A:1072:LEU:HD11	2.51	0.45
1:C:973:ASN:ND2	1:C:974:TYR:N	2.64	0.45
1:C:1150:ILE:HD12	1:C:1150:ILE:C	2.42	0.45
1:D:997:GLN:HA	1:D:1005:ILE:HD11	1.97	0.45
1:B:973:ASN:ND2	1:B:974:TYR:N	2.59	0.45
1:D:1142:ARG:HH22	1:D:1278:ASN:HB2	1.80	0.45
1:D:1191:ILE:HD12	1:D:1191:ILE:C	2.41	0.45
1:A:1168:LYS:O	1:A:1169:ASN:HB2	2.16	0.45
1:B:874:MET:HE3	1:B:1065:PHE:HB3	1.97	0.45
1:B:928:ASN:O	1:B:928:ASN:ND2	2.50	0.45
1:B:1163:ASP:C	1:B:1163:ASP:OD2	2.60	0.45
1:B:1037:ASN:HD22	1:B:1037:ASN:H	1.64	0.44
1:B:1144:TYR:CE1	1:B:1271:LYS:HA	2.51	0.44
1:B:1179:ARG:O	1:B:1180:ASP:HB2	2.17	0.44
1:C:871:ILE:HD12	1:C:925:ILE:HD12	2.00	0.44
1:A:1189:ILE:HA	1:A:1196:LYS:HD3	1.98	0.44
1:A:978:ILE:HG12	1:A:992:VAL:HG22	1.99	0.44
1:A:1083:ASP:O	1:A:1084:GLU:C	2.60	0.44
1:C:939:TRP:HA	1:C:1009:ILE:O	2.18	0.44
1:A:1110:LEU:HD12	1:A:1263:GLY:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1124:ASN:ND2	1:B:1244:ASN:OD1	2.50	0.44
1:C:953:ASN:H	1:C:973:ASN:ND2	2.12	0.44
1:C:1020:ASN:HD22	1:C:1034:SER:N	2.16	0.44
1:B:1119:ASN:HD22	1:B:1119:ASN:HA	1.54	0.44
1:B:1138:PHE:C	1:B:1138:PHE:CD1	2.96	0.44
1:B:871:ILE:HA	1:B:887:TYR:CE2	2.53	0.44
1:B:979:TRP:CD2	1:B:1013:ILE:HG21	2.52	0.44
1:C:907:PHE:CE1	1:C:1062:ILE:HG13	2.53	0.44
1:D:1229:ASN:HD22	1:D:1231:ASN:N	2.16	0.44
1:A:921:GLN:HB2	1:A:1045:ASP:O	2.17	0.43
1:C:1149:VAL:HG21	1:C:1174:ILE:CG2	2.47	0.43
1:C:1193:LYS:CG	1:C:1194:PRO:HD2	2.47	0.43
1:B:1116:ILE:HD12	1:B:1245:LEU:HD11	2.01	0.43
1:B:1133:GLN:HB3	1:B:1139:SER:HA	2.00	0.43
1:A:984:THR:CG2	1:A:1040:ASP:HB3	2.47	0.43
1:C:928:ASN:ND2	1:C:1042:HIS:CE1	2.87	0.43
1:C:1037:ASN:N	1:C:1037:ASN:ND2	2.63	0.43
1:C:1168:LYS:NZ	1:C:1217:ASP:OD1	2.50	0.43
1:C:1197:ILE:HA	1:C:1246:VAL:HG12	2.00	0.43
1:D:1194:PRO:O	1:D:1248:SER:HA	2.17	0.43
1:A:1008:TRP:HE1	1:A:1096:ASN:ND2	2.15	0.43
1:A:939:TRP:CG	1:A:1063:ARG:HE	2.35	0.43
1:A:1191:ILE:HG23	1:A:1193:LYS:HE3	2.00	0.43
1:C:1022:ARG:HG2	1:C:1032:GLU:HG3	2.00	0.43
1:B:1179:ARG:HB3	1:B:1179:ARG:NH2	2.34	0.43
1:C:1208:ASN:HD22	1:C:1208:ASN:N	2.16	0.43
1:A:1132:TYR:CE1	1:A:1278:ASN:ND2	2.86	0.43
1:A:1194:PRO:HG2	1:A:1195:GLU:OE2	2.19	0.43
1:B:1022:ARG:HB2	1:B:1029:LEU:HD11	2.00	0.43
1:D:871:ILE:HD12	1:D:925:ILE:HG23	2.01	0.43
1:A:1128:GLN:HG3	2:H:3:SIA:H111	2.01	0.43
1:C:1171:LEU:HB3	1:C:1213:ILE:HG12	2.01	0.43
1:B:997:GLN:HA	1:B:1005:ILE:HD11	2.01	0.43
1:C:1016:ASN:HB2	1:C:1071:GLU:CD	2.44	0.43
1:D:1126:ASN:H	1:D:1126:ASN:ND2	1.99	0.43
1:A:1241:HIS:HA	2:E:2:GAL:HO4	1.82	0.43
1:B:930:ARG:HG2	1:B:1040:ASP:HA	2.01	0.43
1:C:1022:ARG:HH11	1:C:1071:GLU:CD	2.26	0.43
1:A:936:ILE:HG12	1:A:1013:ILE:HB	2.01	0.42
1:C:926:ILE:HD13	1:C:1045:ASP:HA	2.01	0.42
1:C:1213:ILE:HG13	1:C:1214:ILE:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1176:VAL:HG23	1:A:1185:LEU:HD11	2.00	0.42
1:D:872:LEU:HD21	1:D:919:ILE:HD13	2.02	0.42
1:B:956:THR:HG23	1:B:1052:VAL:HB	2.01	0.42
1:B:1068:PHE:CE2	1:B:1072:LEU:HD11	2.53	0.42
1:B:871:ILE:HD12	1:B:925:ILE:HG23	2.02	0.42
1:C:1016:ASN:HB2	1:C:1071:GLU:OE2	2.19	0.42
1:A:911:SER:HB3	1:A:1051:ILE:HG21	2.02	0.42
1:B:939:TRP:HA	1:B:1009:ILE:O	2.20	0.42
1:C:930:ARG:HA	1:C:1017:ARG:NH2	2.34	0.42
1:A:957:ILE:HG13	1:A:958:ILE:HG13	2.00	0.42
1:C:962:ARG:NE	1:C:1042:HIS:CE1	2.88	0.42
1:C:1094:TRP:CD1	1:C:1272:GLU:HG3	2.54	0.42
1:D:939:TRP:HA	1:D:1009:ILE:O	2.19	0.42
1:C:1068:PHE:CZ	1:C:1080:LEU:HD11	2.55	0.42
1:D:953:ASN:H	1:D:973:ASN:ND2	2.12	0.42
1:B:1018:LEU:N	1:B:1018:LEU:HD12	2.35	0.41
1:A:939:TRP:HB2	1:A:1063:ARG:CG	2.45	0.41
1:A:1231:ASN:N	1:A:1231:ASN:HD22	2.16	0.41
1:B:1085:PRO:O	1:B:1086:ASP:C	2.63	0.41
1:D:874:MET:CE	1:D:891:ILE:HG21	2.49	0.41
1:A:939:TRP:HA	1:A:1009:ILE:O	2.20	0.41
1:A:1119:ASN:C	1:A:1119:ASN:ND2	2.78	0.41
1:B:1126:ASN:HB3	1:B:1243:ASN:HB3	2.02	0.41
1:A:876:TYR:CD2	1:A:904:ARG:HB3	2.56	0.41
1:A:1151:ILE:HG12	1:A:1174:ILE:CD1	2.51	0.41
1:A:1213:ILE:HG22	1:A:1214:ILE:H	1.85	0.41
1:A:1161:ASN:CG	1:A:1162:THR:H	2.28	0.41
1:B:872:LEU:HD21	1:B:919:ILE:HG21	2.02	0.41
1:B:928:ASN:HA	1:B:1041:ILE:O	2.20	0.41
1:A:896:ASP:OD2	1:A:896:ASP:C	2.64	0.41
1:A:1120:SER:OG	1:A:1121:ASN:N	2.54	0.41
1:A:1125:ILE:HG12	1:A:1125:ILE:O	2.21	0.41
1:C:1062:ILE:HD12	1:C:1063:ARG:H	1.84	0.41
1:C:1085:PRO:O	1:C:1086:ASP:C	2.64	0.41
1:C:1116:ILE:CD1	1:C:1125:ILE:HD12	2.51	0.41
1:C:1124:ASN:HB3	1:C:1126:ASN:HD22	1.84	0.41
1:C:1125:ILE:HG12	1:C:1125:ILE:O	2.21	0.41
1:C:1226:ASN:HB2	1:C:1237:LEU:HD23	2.01	0.41
1:D:1100:TYR:CD1	1:D:1151:ILE:HG22	2.56	0.41
1:D:1231:ASN:N	1:D:1231:ASN:HD22	2.17	0.41
1:A:1084:GLU:HB2	1:A:1085:PRO:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1167:ARG:O	1:C:1170:ASP:HB2	2.21	0.41
1:D:983:ASP:OD1	1:D:983:ASP:C	2.64	0.41
1:B:963:ASN:O	1:B:964:ASN:C	2.63	0.40
1:B:983:ASP:HB2	1:B:1040:ASP:O	2.21	0.40
1:D:1177:VAL:O	1:D:1177:VAL:CG1	2.69	0.40
1:A:869:ASN:HB3	1:A:1070:THR:HG23	2.03	0.40
1:A:893:ILE:HD11	5:A:186:HOH:O	2.20	0.40
1:A:1161:ASN:CG	1:A:1162:THR:N	2.80	0.40
1:B:978:ILE:HG23	1:B:992:VAL:HG22	2.04	0.40
1:B:991:LEU:HD12	1:B:991:LEU:HA	1.82	0.40
1:C:928:ASN:OD1	1:C:928:ASN:O	2.38	0.40
1:D:1168:LYS:HE2	1:D:1217:ASP:OD1	2.21	0.40
1:A:979:TRP:CE2	1:A:1013:ILE:HG21	2.56	0.40
1:B:928:ASN:ND2	1:B:1042:HIS:HB2	2.37	0.40
1:C:981:LEU:HD22	1:C:1041:ILE:HD13	2.04	0.40
1:D:1037:ASN:N	1:D:1037:ASN:ND2	2.67	0.40
1:B:991:LEU:HD21	1:B:1022:ARG:HA	2.04	0.40
1:B:1025:ILE:CG1	1:B:1030:ILE:HG13	2.51	0.40
1:B:1135:PRO:HG2	5:B:146:HOH:O	2.22	0.40
1:D:1084:GLU:CB	1:D:1085:PRO:CD	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	400/413 (97%)	360 (90%)	37 (9%)	3 (1%)	16	11
1	B	396/413 (96%)	355 (90%)	37 (9%)	4 (1%)	12	8
1	C	396/413 (96%)	360 (91%)	33 (8%)	3 (1%)	16	11
1	D	398/413 (96%)	362 (91%)	32 (8%)	4 (1%)	12	8
All	All	1590/1652 (96%)	1437 (90%)	139 (9%)	14 (1%)	14	9

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	926	ILE
1	C	1257	LYS
1	D	1084	GLU
1	A	1257	LYS
1	D	926	ILE
1	C	1258	ASN
1	A	915	SER
1	A	926	ILE
1	B	869	ASN
1	B	1120	SER
1	C	926	ILE
1	D	930	ARG
1	D	1188	ASP
1	B	1084	GLU

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	375/382 (98%)	360 (96%)	15 (4%)	28	27
1	B	372/382 (97%)	359 (96%)	13 (4%)	32	32
1	C	372/382 (97%)	361 (97%)	11 (3%)	36	38
1	D	374/382 (98%)	358 (96%)	16 (4%)	26	25
All	All	1493/1528 (98%)	1438 (96%)	55 (4%)	30	30

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	870	SER
1	A	893	ILE
1	A	946	PHE
1	A	956	THR
1	A	981	LEU
1	A	988	ASN

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Mol	Chain	Res	Type
1	A	991	LEU
1	A	1037	ASN
1	A	1106	LEU
1	A	1109	LEU
1	A	1141	THR
1	A	1154	ASN
1	A	1208	ASN
1	A	1212	GLN
1	A	1229	ASN
1	B	869	ASN
1	B	875	ARG
1	B	964	ASN
1	B	981	LEU
1	B	991	LEU
1	B	1037	ASN
1	B	1062	ILE
1	B	1074	LYS
1	B	1106	LEU
1	B	1110	LEU
1	B	1119	ASN
1	B	1193	LYS
1	B	1229	ASN
1	C	879	ASN
1	C	981	LEU
1	C	988	ASN
1	C	1037	ASN
1	C	1062	ILE
1	C	1074	LYS
1	C	1084	GLU
1	C	1106	LEU
1	C	1109	LEU
1	C	1110	LEU
1	C	1229	ASN
1	D	867	LYS
1	D	877	GLU
1	D	941	ARG
1	D	956	THR
1	D	981	LEU
1	D	984	THR
1	D	991	LEU
1	D	1037	ASN
1	D	1062	ILE

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Mol	Chain	Res	Type
1	D	1110	LEU
1	D	1126	ASN
1	D	1191	ILE
1	D	1201	ILE
1	D	1229	ASN
1	D	1258	ASN
1	D	1267	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	879	ASN
1	A	928	ASN
1	A	950	ASN
1	A	952	ASN
1	A	953	ASN
1	A	964	ASN
1	A	988	ASN
1	A	997	GLN
1	A	1006	ASN
1	A	1020	ASN
1	A	1028	ASN
1	A	1037	ASN
1	A	1046	ASN
1	A	1055	ASN
1	A	1096	ASN
1	A	1101	ASN
1	A	1119	ASN
1	A	1124	ASN
1	A	1133	GLN
1	A	1154	ASN
1	A	1161	ASN
1	A	1208	ASN
1	A	1222	ASN
1	A	1229	ASN
1	A	1231	ASN
1	A	1241	HIS
1	A	1273	HIS
1	A	1278	ASN
1	B	869	ASN
1	B	878	ASN
1	B	923	ASN

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Mol	Chain	Res	Type
1	B	928	ASN
1	B	933	ASN
1	B	950	ASN
1	B	953	ASN
1	B	964	ASN
1	B	973	ASN
1	B	994	ASN
1	B	997	GLN
1	B	1006	ASN
1	B	1020	ASN
1	B	1028	ASN
1	B	1037	ASN
1	B	1046	ASN
1	B	1055	ASN
1	B	1096	ASN
1	B	1101	ASN
1	B	1124	ASN
1	B	1126	ASN
1	B	1128	GLN
1	B	1229	ASN
1	B	1230	ASN
1	B	1231	ASN
1	B	1244	ASN
1	B	1276	GLN
1	C	879	ASN
1	C	928	ASN
1	C	950	ASN
1	C	953	ASN
1	C	964	ASN
1	C	965	ASN
1	C	973	ASN
1	C	982	GLN
1	C	988	ASN
1	C	989	GLN
1	C	997	GLN
1	C	1006	ASN
1	C	1016	ASN
1	C	1020	ASN
1	C	1037	ASN
1	C	1046	ASN
1	C	1055	ASN
1	C	1096	ASN

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Mol	Chain	Res	Type
1	C	1101	ASN
1	C	1119	ASN
1	C	1126	ASN
1	C	1127	GLN
1	C	1133	GLN
1	C	1136	ASN
1	C	1169	ASN
1	C	1208	ASN
1	C	1222	ASN
1	C	1228	GLN
1	C	1229	ASN
1	C	1276	GLN
1	C	1278	ASN
1	D	869	ASN
1	D	879	ASN
1	D	894	ASN
1	D	921	GLN
1	D	922	ASN
1	D	928	ASN
1	D	932	GLN
1	D	953	ASN
1	D	963	ASN
1	D	964	ASN
1	D	973	ASN
1	D	994	ASN
1	D	997	GLN
1	D	1006	ASN
1	D	1028	ASN
1	D	1037	ASN
1	D	1046	ASN
1	D	1055	ASN
1	D	1096	ASN
1	D	1101	ASN
1	D	1119	ASN
1	D	1124	ASN
1	D	1126	ASN
1	D	1127	GLN
1	D	1128	GLN
1	D	1221	ASN
1	D	1229	ASN
1	D	1231	ASN
1	D	1243	ASN

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Mol	Chain	Res	Type
1	D	1254	ASN
1	D	1273	HIS
1	D	1278	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 ⓘ

15 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NGA	E	1	2	15,15,15	0.88	0	21,21,21	1.20	2 (9%)
2	GAL	E	2	2	11,11,12	0.80	1 (9%)	15,15,17	1.06	0
2	SIA	E	3	2	20,20,21	2.50	4 (20%)	21,28,31	1.42	2 (9%)
3	GAL	F	1	3	12,12,12	0.93	1 (8%)	17,17,17	0.98	1 (5%)
3	NGA	F	2	3	14,14,15	0.86	0	17,19,21	1.43	2 (11%)
3	GAL	F	3	3	11,11,12	0.82	1 (9%)	15,15,17	1.16	1 (6%)
3	SIA	F	4	3	20,20,21	2.44	4 (20%)	21,28,31	1.43	4 (19%)
3	SIA	F	5	3	20,20,21	1.62	4 (20%)	21,28,31	1.41	2 (9%)
4	GAL	G	1	4	12,12,12	0.64	0	17,17,17	0.80	0
4	NGA	G	2	4	14,14,15	0.90	1 (7%)	17,19,21	1.44	3 (17%)
4	GAL	G	3	4	11,11,12	0.84	1 (9%)	15,15,17	1.12	1 (6%)
4	SIA	G	4	4	20,20,21	2.48	5 (25%)	21,28,31	1.43	2 (9%)
2	NGA	H	1	2	15,15,15	0.98	2 (13%)	21,21,21	1.23	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GAL	H	2	2	11,11,12	0.78	0	15,15,17	1.05	0
2	SIA	H	3	2	20,20,21	2.47	3 (15%)	21,28,31	1.43	4 (19%)

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	NGA	E	1	2	-	2/6/26/26	0/1/1/1
2	GAL	E	2	2	-	0/2/19/22	0/1/1/1
2	SIA	E	3	2	-	2/18/34/38	0/1/1/1
3	GAL	F	1	3	-	1/2/22/22	0/1/1/1
3	NGA	F	2	3	-	2/6/23/26	0/1/1/1
3	GAL	F	3	3	-	0/2/19/22	0/1/1/1
3	SIA	F	4	3	-	0/18/34/38	0/1/1/1
3	SIA	F	5	3	-	4/18/34/38	0/1/1/1
4	GAL	G	1	4	-	1/2/22/22	0/1/1/1
4	NGA	G	2	4	-	2/6/23/26	0/1/1/1
4	GAL	G	3	4	-	2/2/19/22	0/1/1/1
4	SIA	G	4	4	-	4/18/34/38	0/1/1/1
2	NGA	H	1	2	-	2/6/26/26	0/1/1/1
2	GAL	H	2	2	-	1/2/19/22	0/1/1/1
2	SIA	H	3	2	-	1/18/34/38	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3	SIA	C2-C1	-9.81	1.40	1.52
4	G	4	SIA	C2-C1	-9.79	1.40	1.52
3	F	4	SIA	C2-C1	-9.69	1.40	1.52
2	H	3	SIA	C2-C1	-9.68	1.40	1.52
3	F	5	SIA	O6-C2	3.86	1.51	1.43
3	F	5	SIA	C4-C5	2.96	1.55	1.53
2	H	3	SIA	O6-C2	2.61	1.48	1.43
2	E	3	SIA	O6-C2	2.57	1.48	1.43
4	G	4	SIA	O6-C2	2.54	1.48	1.43
3	F	1	GAL	O4-C4	-2.38	1.37	1.43
4	G	3	GAL	C2-C3	2.37	1.56	1.52
3	F	3	GAL	C2-C3	2.35	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	3	SIA	O6-C6	2.32	1.47	1.44
3	F	5	SIA	C3-C4	2.29	1.57	1.52
3	F	4	SIA	O6-C2	2.25	1.47	1.43
2	E	3	SIA	C7-C6	2.23	1.55	1.52
3	F	4	SIA	C7-C6	2.22	1.55	1.52
2	E	3	SIA	O6-C6	2.19	1.47	1.44
4	G	4	SIA	O6-C6	2.18	1.47	1.44
3	F	4	SIA	O6-C6	2.16	1.47	1.44
2	H	1	NGA	C1-C2	2.10	1.55	1.52
2	E	2	GAL	C2-C3	2.09	1.55	1.52
4	G	4	SIA	C7-C6	2.05	1.55	1.52
3	F	5	SIA	C2-C1	-2.05	1.49	1.52
4	G	4	SIA	O1B-C1	-2.03	1.24	1.30
4	G	2	NGA	C8-C7	-2.01	1.46	1.50
2	H	1	NGA	C8-C7	-2.00	1.46	1.50

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	5	SIA	O6-C2-C1	3.60	114.52	107.72
3	F	2	NGA	C4-C3-C2	-3.49	105.91	111.02
3	F	5	SIA	O1B-C1-C2	3.34	121.40	112.71
3	F	4	SIA	O1B-C1-C2	3.32	121.35	112.71
2	H	3	SIA	O1B-C1-C2	3.31	121.33	112.71
2	E	3	SIA	O1B-C1-C2	3.27	121.21	112.71
4	G	4	SIA	O1B-C1-C2	3.19	121.00	112.71
2	H	3	SIA	O6-C2-C1	3.13	113.62	107.72
4	G	2	NGA	C4-C3-C2	-3.12	106.45	111.02
2	E	3	SIA	O6-C2-C1	3.10	113.56	107.72
4	G	4	SIA	O6-C2-C1	3.06	113.49	107.72
2	E	1	NGA	C4-C3-C2	-2.90	106.17	110.40
3	F	4	SIA	O6-C2-C1	2.86	113.11	107.72
2	H	1	NGA	C4-C3-C2	-2.55	106.69	110.40
4	G	2	NGA	C2-N2-C7	2.48	126.22	122.90
3	F	2	NGA	O7-C7-C8	-2.46	117.67	122.05
2	H	1	NGA	O7-C7-C8	-2.41	117.76	122.05
4	G	2	NGA	O7-C7-C8	-2.40	117.78	122.05
3	F	3	GAL	O3-C3-C4	-2.31	104.94	110.38
2	E	1	NGA	O7-C7-C8	-2.30	117.97	122.05
4	G	3	GAL	O3-C3-C4	-2.19	105.21	110.38
3	F	1	GAL	C3-C4-C5	-2.13	106.37	110.23
2	H	3	SIA	C9-C8-C7	2.10	116.44	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	4	SIA	O6-C2-C3	2.06	113.32	110.56
2	H	3	SIA	O1A-C1-C2	-2.05	118.43	122.85
3	F	4	SIA	C9-C8-C7	2.01	116.27	112.17

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NGA	C8-C7-N2-C2
2	E	1	NGA	O7-C7-N2-C2
3	F	5	SIA	C6-C7-C8-C9
3	F	5	SIA	O7-C7-C8-C9
3	F	2	NGA	O5-C5-C6-O6
3	F	5	SIA	C6-C7-C8-O8
2	H	1	NGA	C8-C7-N2-C2
2	H	1	NGA	O7-C7-N2-C2
4	G	2	NGA	C8-C7-N2-C2
4	G	4	SIA	O7-C7-C8-C9
4	G	3	GAL	O5-C5-C6-O6
4	G	4	SIA	C6-C7-C8-C9
3	F	2	NGA	C4-C5-C6-O6
3	F	5	SIA	O7-C7-C8-O8
4	G	2	NGA	O7-C7-N2-C2
4	G	4	SIA	C6-C7-C8-O8
3	F	1	GAL	O5-C5-C6-O6
4	G	1	GAL	O5-C5-C6-O6
4	G	3	GAL	C4-C5-C6-O6
4	G	4	SIA	O7-C7-C8-O8
2	E	3	SIA	C7-C8-C9-O9
2	H	3	SIA	O8-C8-C9-O9
2	E	3	SIA	O8-C8-C9-O9
2	H	2	GAL	O5-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 10 short contacts:

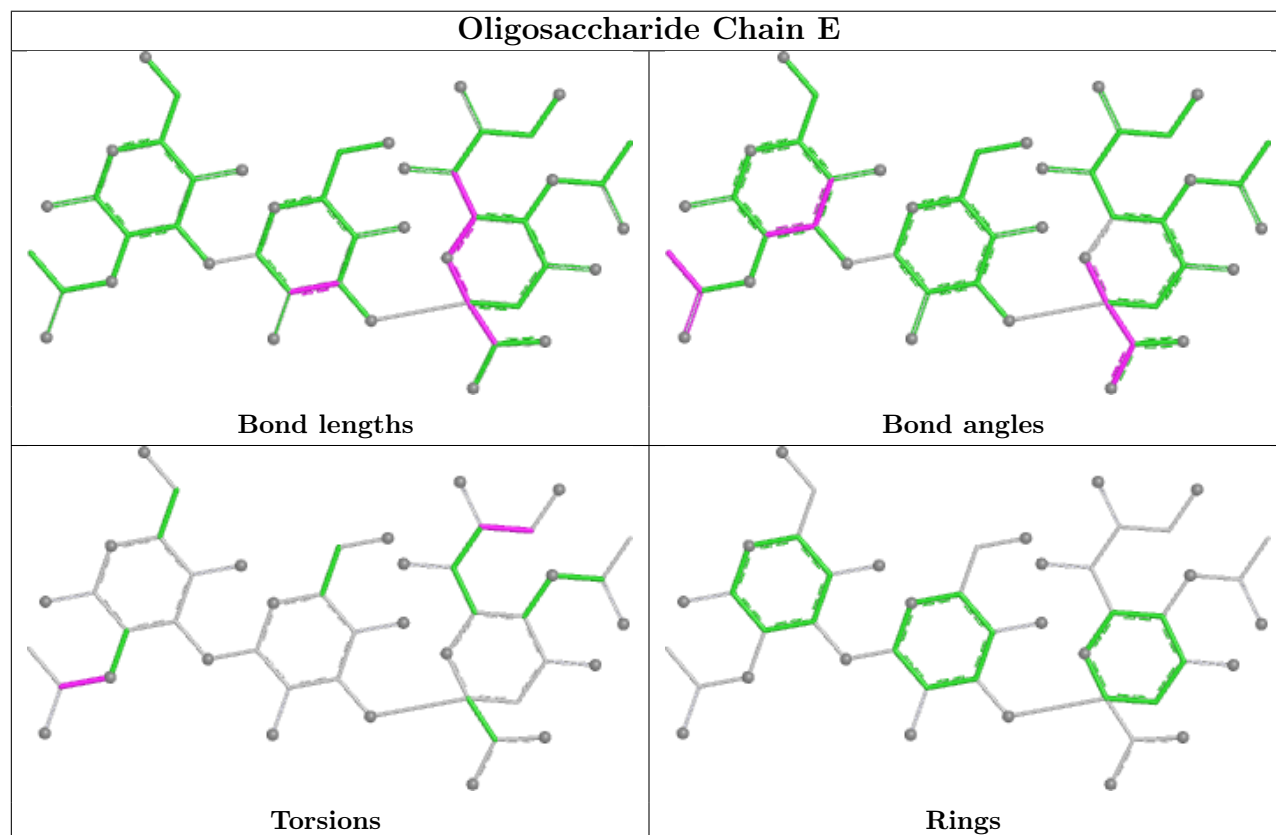
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	3	GAL	2	0
2	E	2	GAL	2	0
2	H	3	SIA	1	0
3	F	1	GAL	1	0

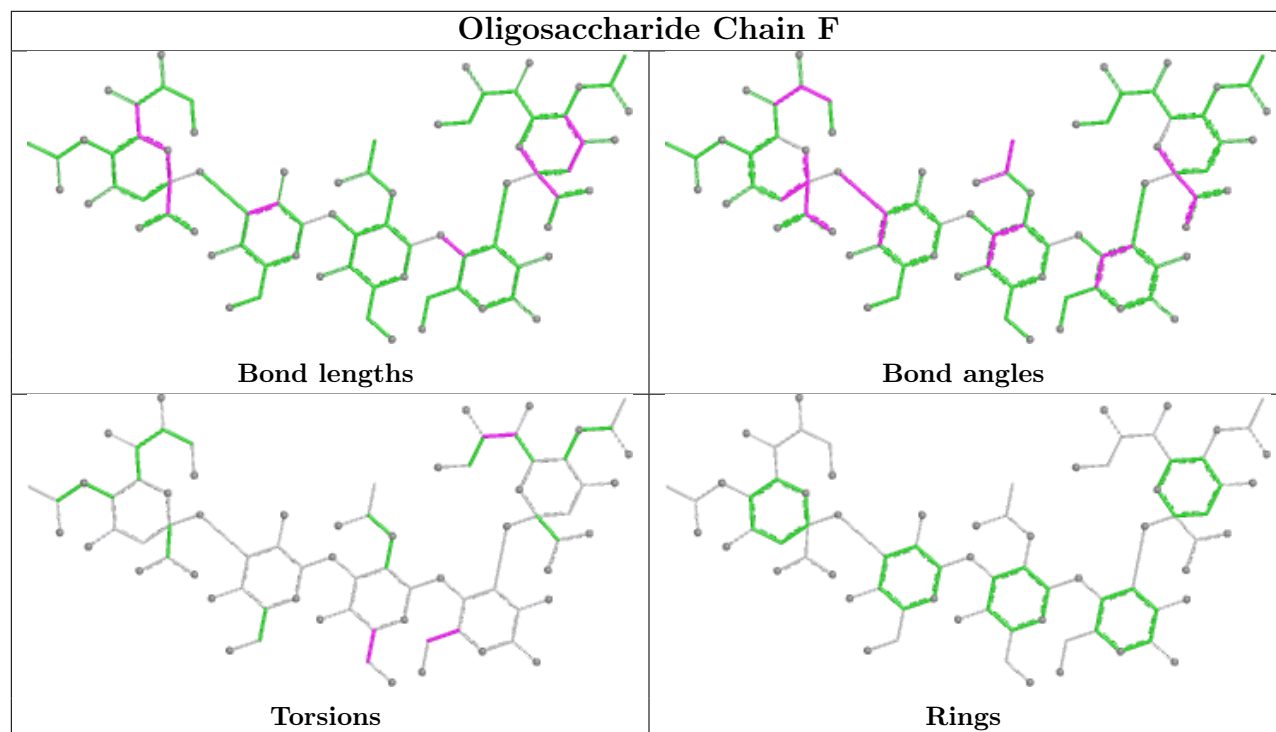
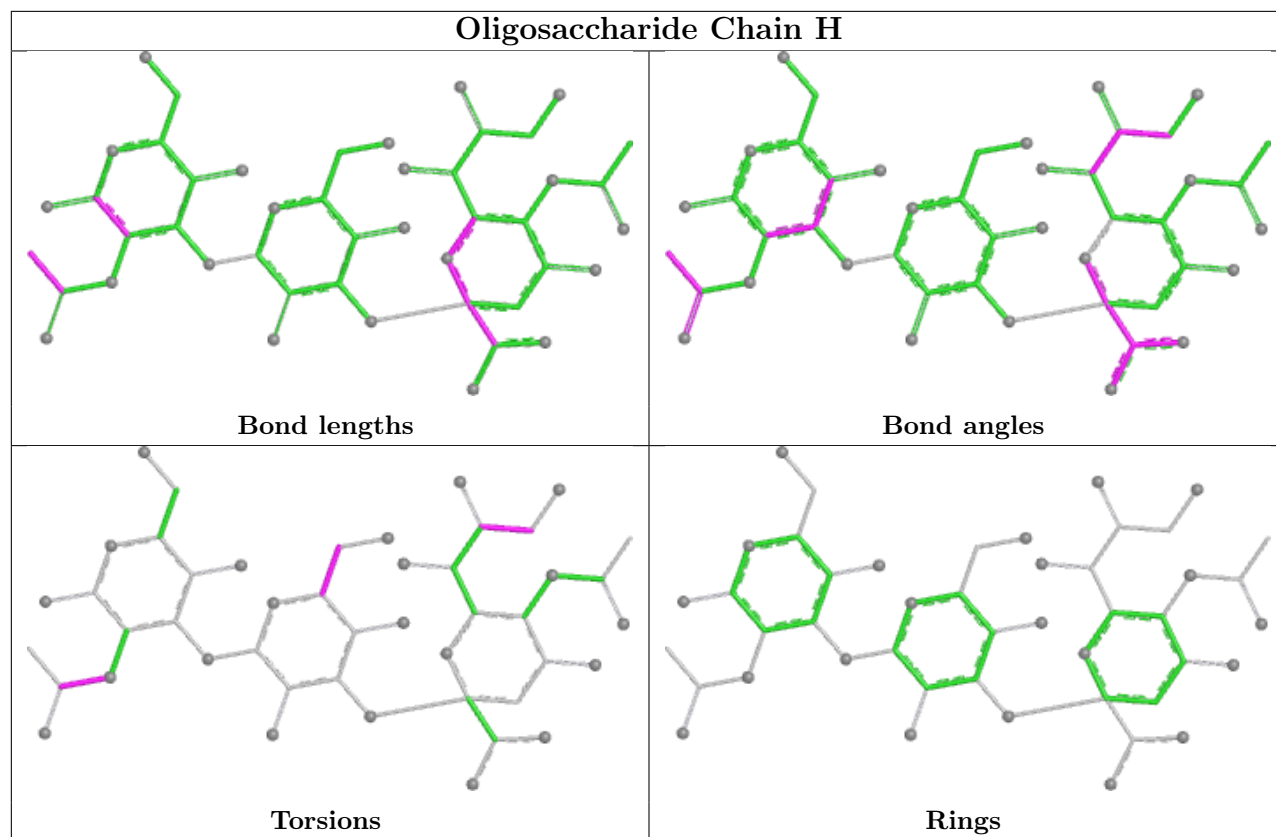
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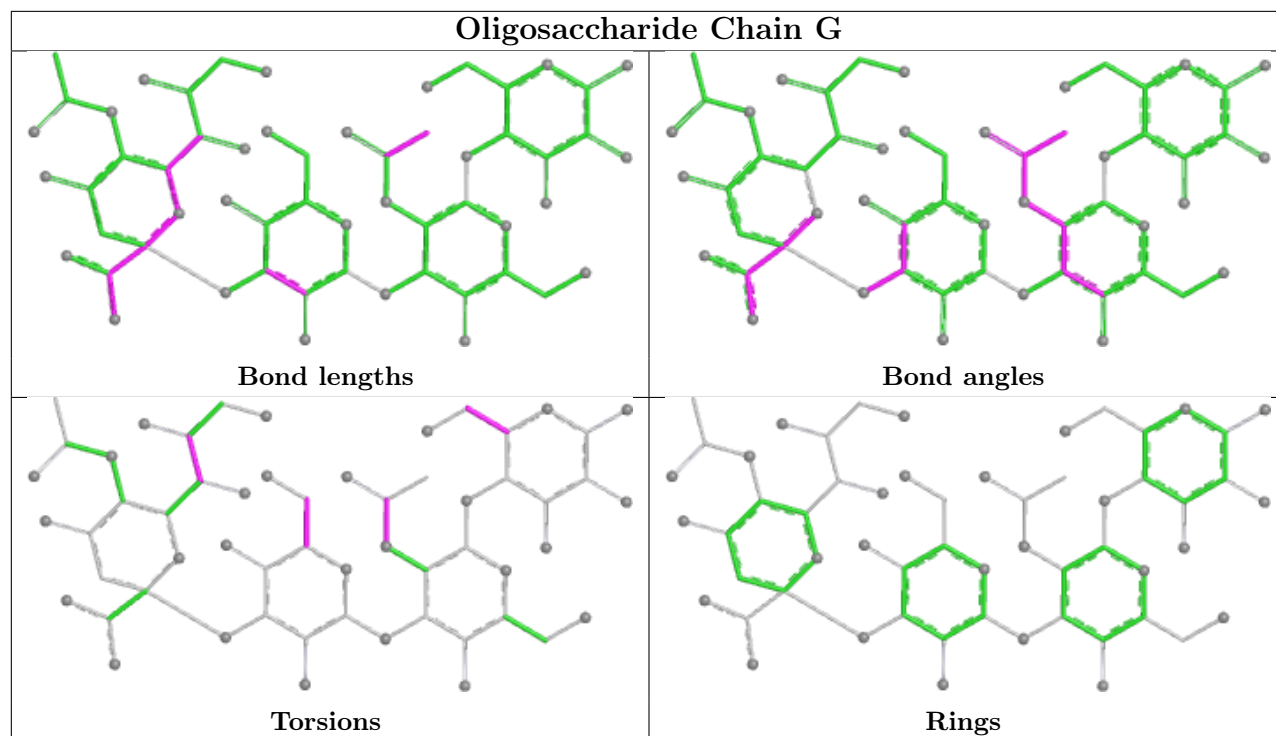
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	3	GAL	2	0
3	F	5	SIA	1	0
2	H	2	GAL	1	0
4	G	1	GAL	1	0

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	406/413 (98%)	0.69	44 (10%) 11 10	23, 39, 58, 72	0
1	B	402/413 (97%)	0.76	48 (11%) 9 8	24, 40, 62, 81	0
1	C	402/413 (97%)	0.81	46 (11%) 10 9	26, 40, 61, 76	0
1	D	404/413 (97%)	0.63	37 (9%) 14 13	24, 38, 58, 77	0
All	All	1614/1652 (97%)	0.72	175 (10%) 11 10	23, 39, 60, 81	0

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	929	GLY	6.5
1	A	866	ILE	6.0
1	D	927	TYR	5.9
1	C	929	GLY	5.0
1	C	931	TYR	4.9
1	D	866	ILE	4.7
1	A	893	ILE	4.5
1	A	1084	GLU	4.5
1	C	1162	THR	4.5
1	A	1278	ASN	4.5
1	C	925	ILE	4.4
1	A	946	PHE	4.4
1	D	1084	GLU	4.3
1	A	927	TYR	4.3
1	D	1162	THR	4.1
1	B	927	TYR	4.1
1	B	931	TYR	4.0
1	A	1122	PHE	4.0
1	A	1162	THR	3.9
1	C	1242	SER	3.8
1	C	1041	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	1084	GLU	3.8
1	C	1084	GLU	3.7
1	B	930	ARG	3.7
1	B	1085	PRO	3.7
1	C	1161	ASN	3.7
1	C	1278	ASN	3.7
1	D	923	ASN	3.7
1	B	1192	ALA	3.6
1	B	1162	THR	3.6
1	B	929	GLY	3.6
1	C	1180	ASP	3.5
1	B	1180	ASP	3.5
1	B	925	ILE	3.5
1	D	1122	PHE	3.5
1	D	1207	ASN	3.5
1	C	926	ILE	3.4
1	A	1273	HIS	3.4
1	A	1207	ASN	3.4
1	D	1278	ASN	3.4
1	B	882	ILE	3.4
1	D	931	TYR	3.4
1	D	1273	HIS	3.3
1	D	1219	ILE	3.3
1	C	1038	LEU	3.3
1	C	1085	PRO	3.2
1	D	1085	PRO	3.2
1	D	1230	ASN	3.2
1	D	1180	ASP	3.2
1	A	1206	SER	3.2
1	C	1082	SER	3.2
1	C	930	ARG	3.1
1	D	1192	ALA	3.1
1	A	1155	GLY	3.1
1	B	984	THR	3.1
1	C	1231	ASN	3.1
1	A	1069	ASP	3.1
1	D	946	PHE	3.0
1	C	924	ASP	3.0
1	B	1038	LEU	3.0
1	A	1230	ASN	3.0
1	D	1203	THR	3.0
1	B	1278	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	927	TYR	3.0
1	B	1258	ASN	2.9
1	B	946	PHE	2.9
1	C	946	PHE	2.9
1	B	1242	SER	2.9
1	A	1161	ASN	2.9
1	B	1154	ASN	2.9
1	A	1219	ILE	2.9
1	C	1203	THR	2.9
1	A	1019	GLY	2.9
1	C	887	TYR	2.9
1	B	1035	ILE	2.8
1	A	923	ASN	2.8
1	C	886	GLY	2.8
1	A	984	THR	2.8
1	C	1257	LYS	2.8
1	C	869	ASN	2.8
1	B	868	ASP	2.8
1	A	1018	LEU	2.8
1	B	1179	ARG	2.7
1	B	1083	ASP	2.7
1	D	1078	GLU	2.7
1	C	1208	ASN	2.7
1	D	925	ILE	2.7
1	B	1078	GLU	2.7
1	A	1085	PRO	2.7
1	C	1154	ASN	2.7
1	B	1230	ASN	2.6
1	A	1040	ASP	2.6
1	A	1180	ASP	2.6
1	B	887	TYR	2.6
1	B	928	ASN	2.6
1	B	1257	LYS	2.6
1	B	924	ASP	2.6
1	D	1191	ILE	2.6
1	C	1207	ASN	2.6
1	A	985	ALA	2.6
1	C	877	GLU	2.5
1	C	933	ASN	2.5
1	C	1120	SER	2.5
1	C	1040	ASP	2.5
1	B	1019	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	893	ILE	2.5
1	D	890	ASN	2.5
1	A	887	TYR	2.5
1	A	929	GLY	2.5
1	C	890	ASN	2.5
1	B	926	ILE	2.4
1	B	1041	ILE	2.4
1	A	870	SER	2.4
1	B	1037	ASN	2.4
1	C	1020	ASN	2.4
1	B	873	ASP	2.4
1	A	882	ILE	2.4
1	D	926	ILE	2.4
1	B	981	LEU	2.4
1	B	985	ALA	2.3
1	A	1208	ASN	2.3
1	C	965	ASN	2.3
1	A	904	ARG	2.3
1	A	1235	ILE	2.3
1	B	1018	LEU	2.3
1	C	1019	GLY	2.3
1	D	924	ASP	2.3
1	A	1078	GLU	2.3
1	D	1255	ILE	2.3
1	D	930	ARG	2.3
1	C	1083	ASP	2.3
1	C	1183	TYR	2.3
1	B	1209	SER	2.2
1	D	1154	ASN	2.2
1	A	1073	GLY	2.2
1	D	870	SER	2.2
1	D	966	SER	2.2
1	D	1213	ILE	2.2
1	B	1161	ASN	2.2
1	C	984	THR	2.2
1	D	984	THR	2.2
1	C	985	ALA	2.2
1	B	1231	ASN	2.2
1	B	1040	ASP	2.2
1	B	1256	ARG	2.1
1	C	870	SER	2.1
1	D	1257	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	928	ASN	2.1
1	A	1083	ASP	2.1
1	A	1213	ILE	2.1
1	B	1062	ILE	2.1
1	B	1039	GLY	2.1
1	D	1242	SER	2.1
1	C	1037	ASN	2.1
1	A	924	ASP	2.1
1	B	1203	THR	2.1
1	C	1042	HIS	2.1
1	A	1255	ILE	2.1
1	A	1256	ARG	2.1
1	C	1219	ILE	2.1
1	D	1082	SER	2.1
1	D	928	ASN	2.1
1	B	886	GLY	2.1
1	A	925	ILE	2.1
1	A	881	PHE	2.1
1	A	1242	SER	2.1
1	B	1036	SER	2.1
1	A	965	ASN	2.0
1	A	987	ASN	2.0
1	A	931	TYR	2.0
1	C	920	ALA	2.0
1	D	1161	ASN	2.0
1	B	1210	LEU	2.0
1	B	1273	HIS	2.0
1	D	867	LYS	2.0

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

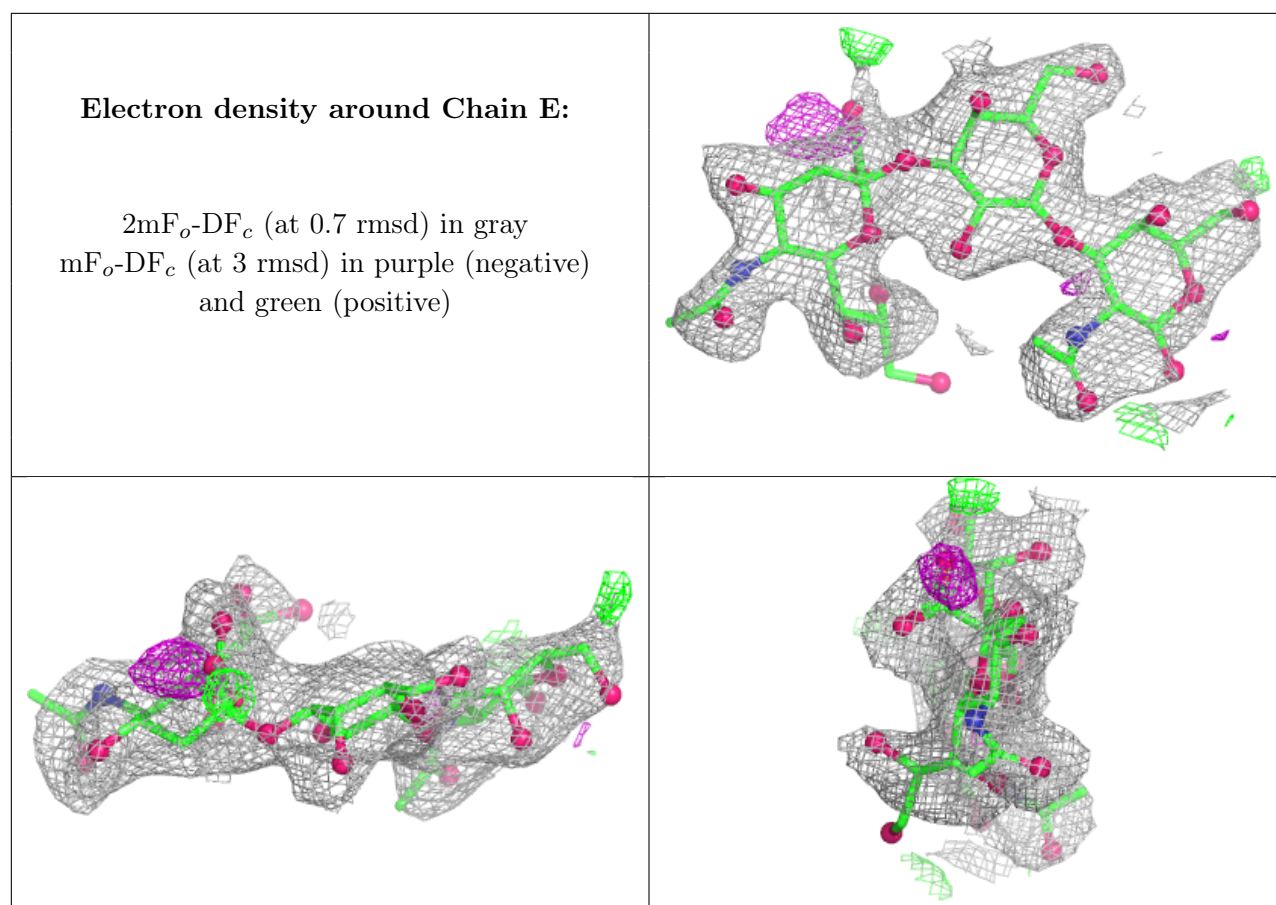
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

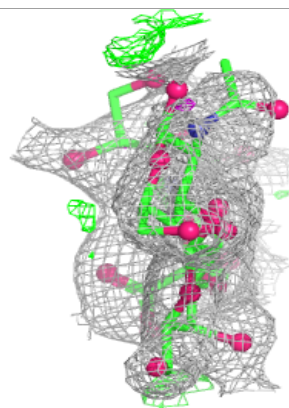
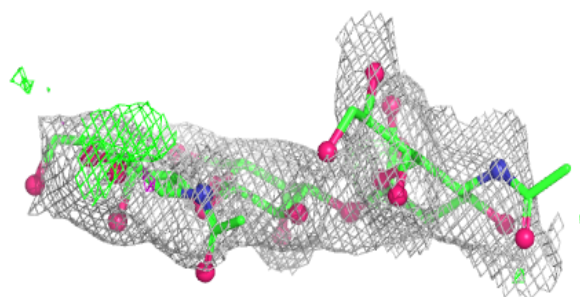
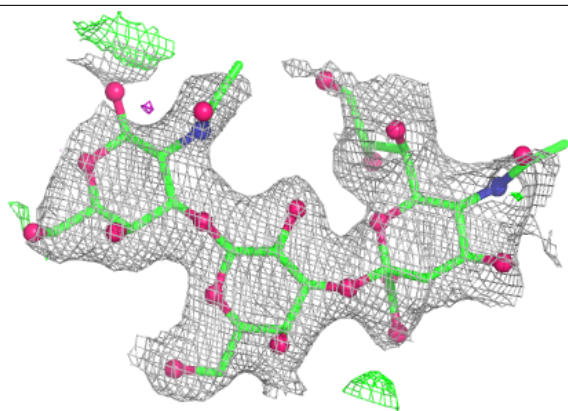
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GAL	G	1	12/12	0.56	0.18	78,83,84,86	0
3	SIA	F	5	20/21	0.64	0.20	81,83,86,86	0
2	NGA	E	1	15/15	0.70	0.17	66,68,71,72	0
2	NGA	H	1	15/15	0.71	0.18	71,75,76,77	0
2	SIA	H	3	20/21	0.74	0.17	74,76,79,79	0
4	NGA	G	2	14/15	0.76	0.17	64,69,72,73	0
3	GAL	F	1	12/12	0.77	0.14	65,74,77,81	0
2	SIA	E	3	20/21	0.80	0.13	64,66,73,74	0
4	SIA	G	4	20/21	0.83	0.14	61,63,65,67	0
2	GAL	E	2	11/12	0.86	0.12	59,63,65,65	0
2	GAL	H	2	11/12	0.87	0.13	68,71,72,73	0
3	NGA	F	2	14/15	0.87	0.12	45,55,57,58	0
3	SIA	F	4	20/21	0.89	0.12	53,57,60,61	0
4	GAL	G	3	11/12	0.90	0.12	57,60,62,63	0
3	GAL	F	3	11/12	0.91	0.11	43,46,49,49	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.

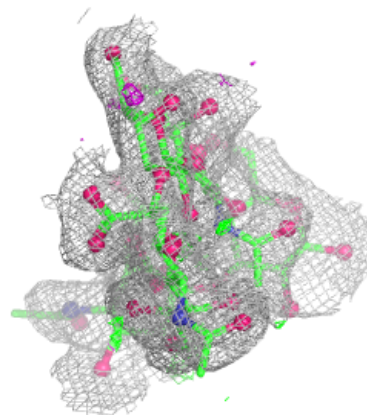
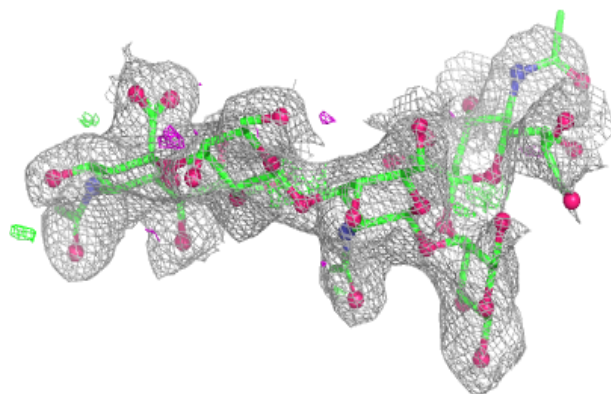
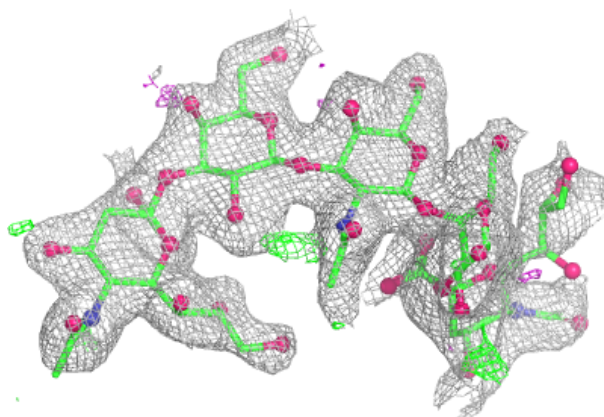


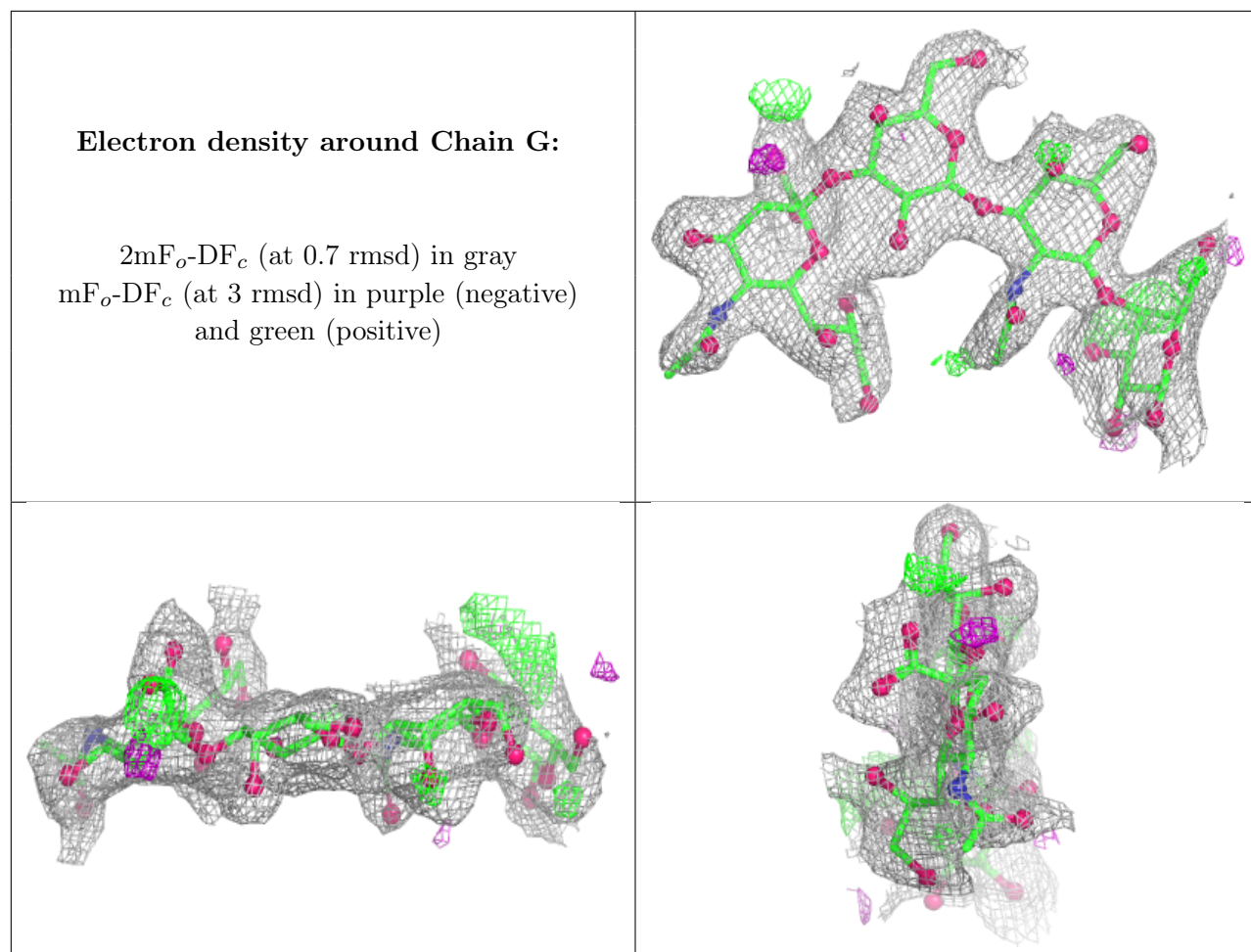
Electron density around Chain H:

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

**Electron density around Chain F:**

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





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.