Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 09:30 AM EDT

PDB ID	:	4KDM
Title	:	Crystal structure of the hemagglutinin of ferret-transmissible H5N1 virus
Authors	:	Lu, X.; Shi, Y.; Zhang, W.; Zhang, Y.; Qi, J.; Gao, G.F.
Deposited on	:	2013-04-25
Resolution	:	2.50 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 (i) 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 (1)) were used in the production of this report:

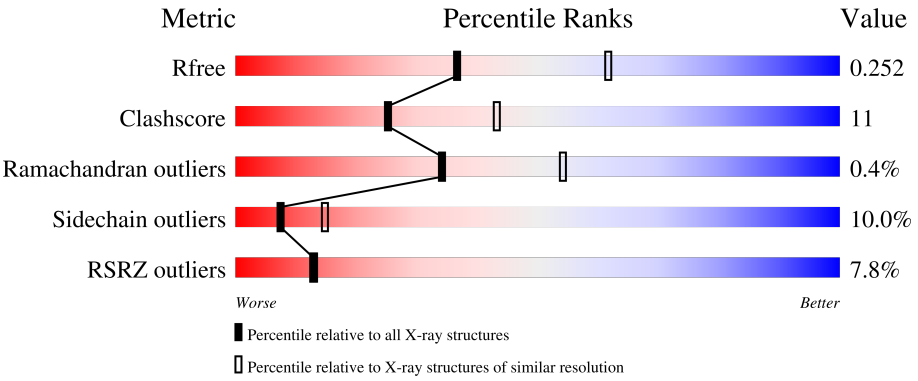
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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% 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	322	% 72% 23% 5%
1	C	322	4% 70% 25% 6%
1	E	322	4% 66% 29% 5%
2	B	175	3% 82% 14% ·
2	D	175	21% 75% 23% ·

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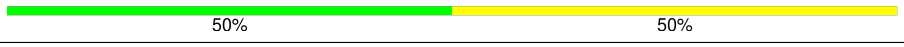
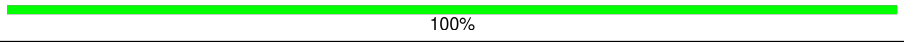
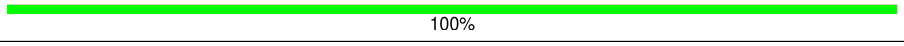
Mol	Chain	Length	Quality of chain
2	F	175	
3	G	2	
3	H	2	
3	I	2	

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	NAG	I	2	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12221 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2559	1621	440	483	15			
1	C	322	Total	C	N	O	S	0	0	0
			2559	1621	440	483	15			
1	E	322	Total	C	N	O	S	0	0	0
			2559	1621	440	483	15			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLN	-	expression tag	UNP Q6DQ33
A	158	ASP	ASN	engineered mutation	UNP Q6DQ33
A	224	LYS	ASN	engineered mutation	UNP Q6DQ33
A	226	LEU	GLN	engineered mutation	UNP Q6DQ33
A	319	ILE	THR	engineered mutation	UNP Q6DQ33
C	4	GLN	-	expression tag	UNP Q6DQ33
C	158	ASP	ASN	engineered mutation	UNP Q6DQ33
C	224	LYS	ASN	engineered mutation	UNP Q6DQ33
C	226	LEU	GLN	engineered mutation	UNP Q6DQ33
C	319	ILE	THR	engineered mutation	UNP Q6DQ33
E	4	GLN	-	expression tag	UNP Q6DQ33
E	158	ASP	ASN	engineered mutation	UNP Q6DQ33
E	224	LYS	ASN	engineered mutation	UNP Q6DQ33
E	226	LEU	GLN	engineered mutation	UNP Q6DQ33
E	319	ILE	THR	engineered mutation	UNP Q6DQ33

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			

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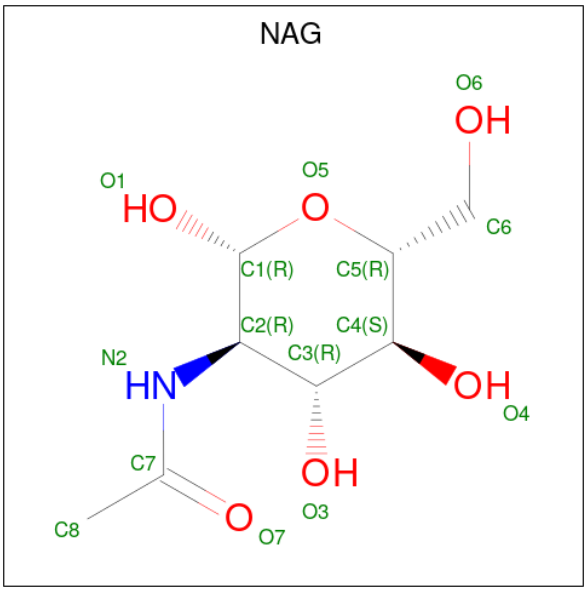
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	F	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C N O 14 8 1 5	0	0
4	E	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is water.

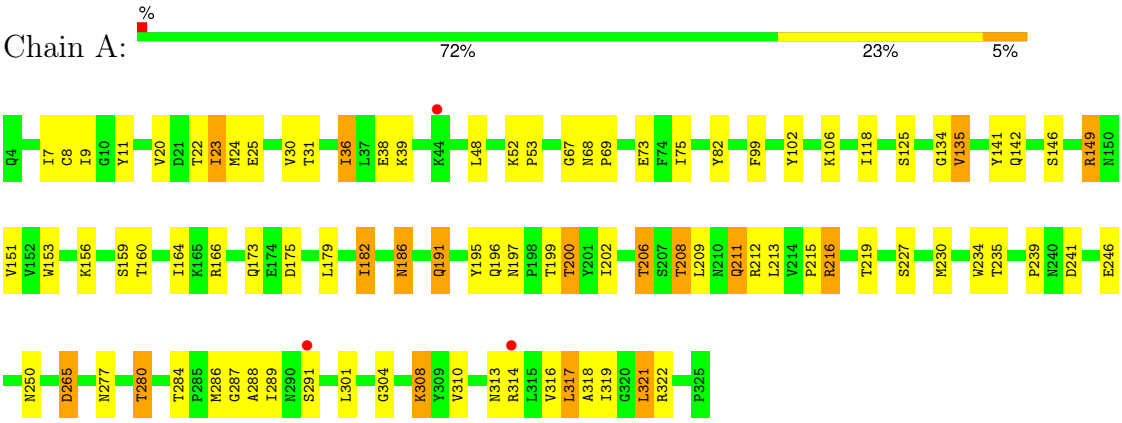
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	53	Total O 53 53	0	0
5	B	13	Total O 13 13	0	0
5	C	42	Total O 42 42	0	0
5	D	17	Total O 17 17	0	0
5	E	33	Total O 33 33	0	0
5	F	12	Total O 12 12	0	0

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.

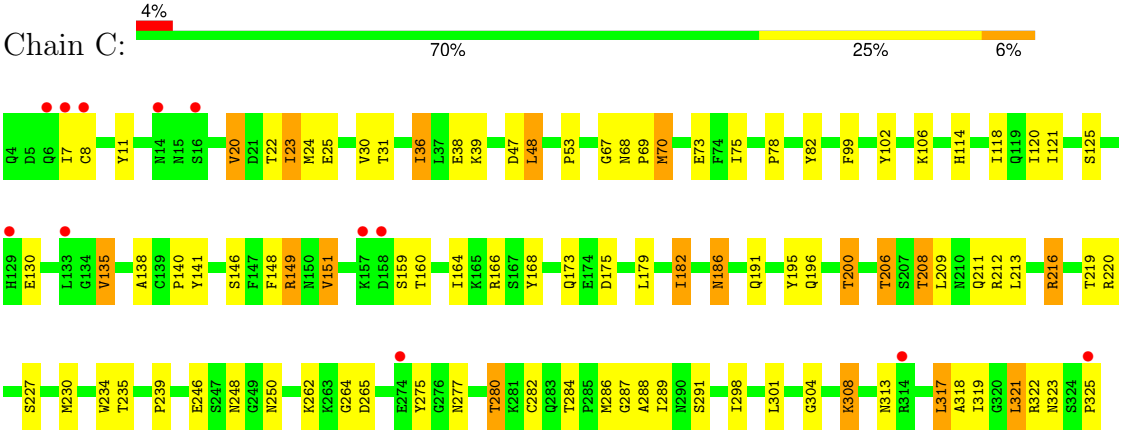
• Molecule 1: Hemagglutinin

Chain A:



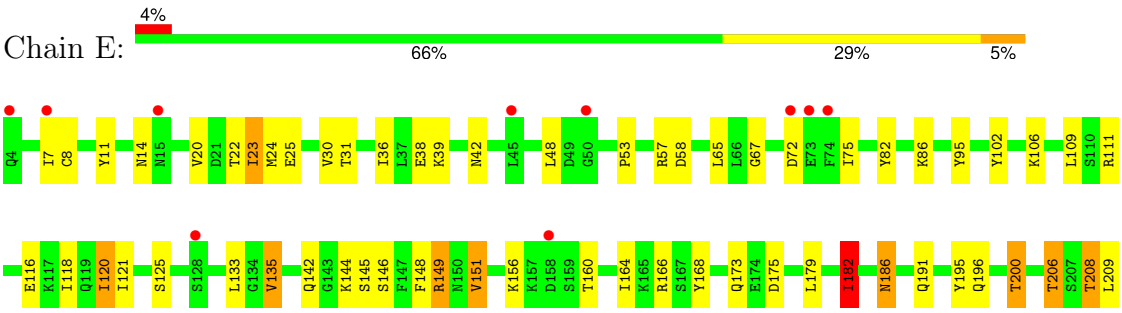
• Molecule 1: Hemagglutinin

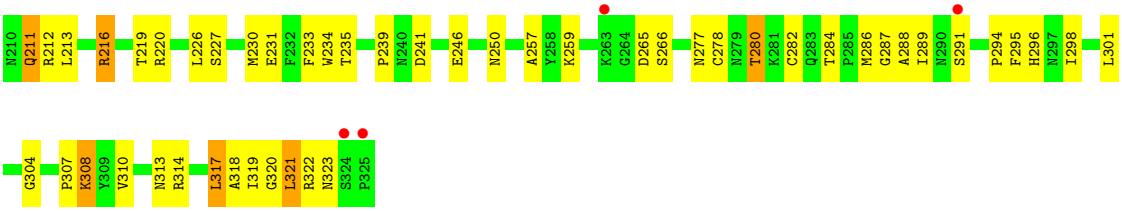
Chain C:



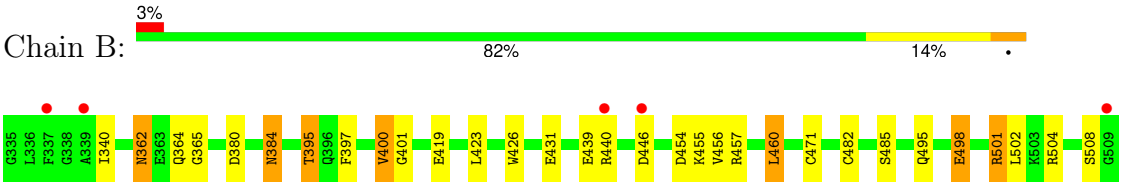
• Molecule 1: Hemagglutinin

Chain E:

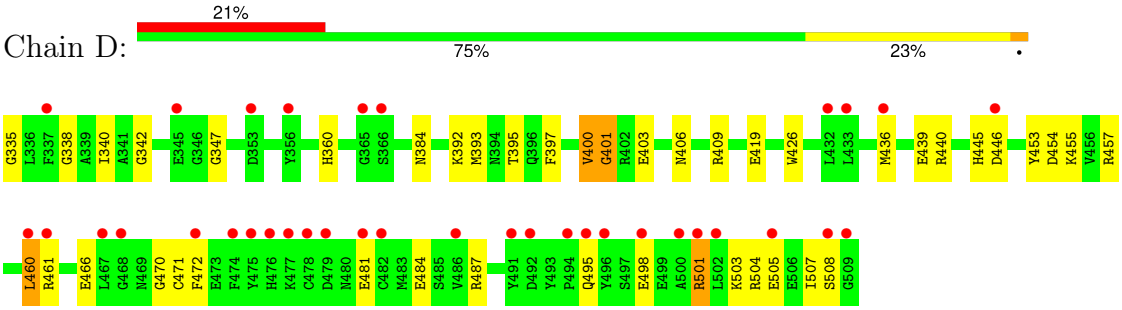




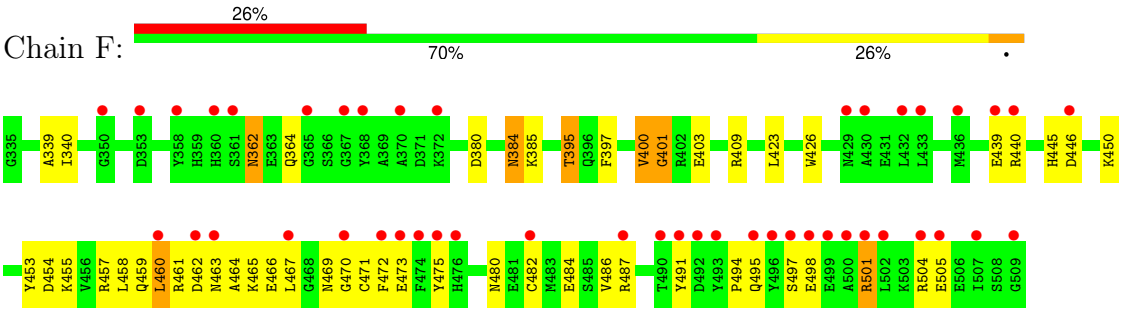
• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin

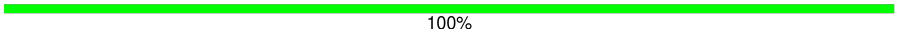


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.76Å 243.85Å 71.61Å 90.00° 110.01° 90.00°	Depositor
Resolution (Å)	35.07 – 2.50 35.61 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (35.07-2.50) 99.5 (35.61-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.215 , 0.251 0.217 , 0.252	Depositor DCC
R_{free} test set	3723 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	54.8	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12221	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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	0.30	0/2621	0.55	0/3558
1	C	0.29	0/2621	0.53	0/3558
1	E	0.29	0/2621	0.55	1/3558 (0.0%)
2	B	0.37	0/1443	0.51	1/1939 (0.1%)
2	D	0.37	0/1443	0.48	1/1939 (0.1%)
2	F	0.36	0/1443	0.50	0/1939
All	All	0.32	0/12192	0.53	3/16491 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	460	LEU	CB-CA-C	7.13	123.75	110.20
1	E	182	ILE	CB-CA-C	-5.44	100.72	111.60
2	D	460	LEU	CB-CA-C	5.20	120.09	110.20

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	2559	0	2513	61	0
1	C	2559	0	2513	60	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2559	0	2513	69	1
2	B	1416	0	1319	23	0
2	D	1416	0	1319	33	0
2	F	1416	0	1319	42	0
3	G	28	0	25	1	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0
4	A	14	0	13	0	0
4	C	14	0	13	0	0
4	E	14	0	13	0	0
5	A	53	0	0	8	0
5	B	13	0	0	2	0
5	C	42	0	0	4	0
5	D	17	0	0	6	0
5	E	33	0	0	6	0
5	F	12	0	0	2	0
All	All	12221	0	11610	253	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (253) 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:E:206:THR:HG22	1:E:208:THR:H	1.37	0.89
5:A:753:HOH:O	3:G:1:NAG:O3	1.88	0.89
1:E:58:ASP:OD1	5:E:726:HOH:O	1.90	0.88
1:E:38:GLU:OE1	5:E:725:HOH:O	1.92	0.87
1:C:138:ALA:O	5:C:705:HOH:O	1.94	0.84
2:D:461:ARG:NH2	2:F:466:GLU:O	2.10	0.84
1:A:206:THR:HG22	1:A:208:THR:H	1.42	0.83
1:A:284:THR:HG22	1:A:286:MET:H	1.44	0.82
1:A:182:ILE:HD11	1:A:213:LEU:HD13	1.63	0.81
1:E:318:ALA:O	5:E:730:HOH:O	1.98	0.81
1:A:38:GLU:OE1	5:A:727:HOH:O	1.98	0.80
1:A:199:THR:OG1	5:A:752:HOH:O	1.99	0.80
1:E:57:ARG:NH1	1:E:72:ASP:OD1	2.15	0.79
1:C:206:THR:HG22	1:C:208:THR:H	1.48	0.78
1:E:67:GLY:HA3	1:E:149:ARG:HG2	1.66	0.77
1:C:135:VAL:HG22	1:C:146:SER:HA	1.67	0.77
1:E:284:THR:HG22	1:E:286:MET:H	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:GLU:OE1	5:C:734:HOH:O	2.03	0.76
2:B:419:GLU:O	5:B:608:HOH:O	2.04	0.75
1:C:186:ASN:OD1	1:C:186:ASN:N	2.20	0.74
1:C:284:THR:HG22	1:C:286:MET:H	1.50	0.74
1:E:280:THR:HG21	1:E:288:ALA:HB1	1.69	0.74
2:F:403:GLU:OE2	5:F:604:HOH:O	2.05	0.74
1:E:186:ASN:OD1	1:E:186:ASN:N	2.21	0.74
1:A:22:THR:HG22	1:A:24:MET:H	1.53	0.73
1:A:135:VAL:HG22	1:A:146:SER:HA	1.70	0.73
1:A:186:ASN:N	1:A:186:ASN:OD1	2.19	0.72
1:C:280:THR:HG21	1:C:288:ALA:HB1	1.72	0.72
2:D:347:GLY:O	5:D:607:HOH:O	2.08	0.71
1:E:25:GLU:OE2	1:E:322:ARG:NH2	2.22	0.70
2:D:453:TYR:HE1	2:D:470:GLY:HA2	1.56	0.70
1:E:22:THR:HG22	1:E:24:MET:H	1.58	0.69
1:C:130:GLU:O	5:C:703:HOH:O	2.11	0.69
1:E:156:LYS:HD2	1:E:196:GLN:HG2	1.75	0.69
1:A:125:SER:OG	1:A:166:ARG:NH2	2.26	0.68
2:F:484:GLU:HG2	2:F:487:ARG:HH12	1.58	0.67
1:A:265:ASP:OD2	2:D:409:ARG:NH2	2.27	0.67
1:C:25:GLU:OE2	1:C:322:ARG:NH2	2.28	0.67
2:F:494:PRO:HA	2:F:497:SER:HB3	1.75	0.67
1:C:182:ILE:HD11	1:C:213:LEU:HD13	1.77	0.66
1:A:301:LEU:HA	2:B:400:VAL:HG22	1.77	0.66
1:C:22:THR:HG22	1:C:24:MET:H	1.61	0.65
1:C:216:ARG:O	1:C:220:ARG:NH2	2.30	0.65
2:B:362:ASN:OD1	2:B:364:GLN:NE2	2.30	0.65
1:A:25:GLU:OE2	1:A:322:ARG:NH2	2.29	0.64
1:C:284:THR:HB	1:C:287:GLY:O	1.97	0.64
1:E:39:LYS:NZ	1:E:313:ASN:O	2.27	0.64
1:E:179:LEU:HD23	1:E:234:TRP:HB3	1.79	0.64
2:D:453:TYR:CE1	2:D:470:GLY:HA2	2.32	0.64
2:F:466:GLU:HG2	2:F:472:PHE:HE2	1.63	0.63
1:E:8:CYS:HA	2:F:471:CYS:HA	1.79	0.62
1:A:212:ARG:NH1	5:A:732:HOH:O	2.14	0.62
1:C:39:LYS:NZ	1:C:313:ASN:O	2.22	0.62
1:A:289:ILE:HG22	1:A:291:SER:HB3	1.81	0.62
1:A:39:LYS:NZ	1:A:313:ASN:O	2.21	0.61
2:B:508:SER:OG	2:F:501:ARG:NE	2.28	0.61
1:E:145:SER:OG	5:E:732:HOH:O	2.16	0.61
2:D:440:ARG:NH1	2:F:439:GLU:OE2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:GLY:HA3	1:C:149:ARG:HB2	1.81	0.60
2:B:431:GLU:OE1	5:B:605:HOH:O	2.17	0.60
2:D:393:MET:O	5:D:617:HOH:O	2.17	0.60
1:C:120:ILE:HG23	1:C:121:ILE:HG13	1.84	0.60
1:C:289:ILE:HG22	1:C:291:SER:HB3	1.83	0.59
2:D:360:HIS:HD2	2:D:487:ARG:HH21	1.50	0.59
1:A:20:VAL:HG11	1:A:318:ALA:HB2	1.82	0.59
1:A:280:THR:HG21	1:A:288:ALA:HB1	1.84	0.59
1:E:125:SER:OG	1:E:166:ARG:NH2	2.35	0.59
2:F:364:GLN:HE22	2:F:480:ASN:H	1.50	0.59
1:A:191:GLN:OE1	1:A:250:ASN:ND2	2.34	0.59
1:A:314:ARG:HG3	1:A:316:VAL:HG23	1.85	0.59
1:A:31:THR:HB	1:A:321:LEU:H	1.68	0.58
1:C:23:ILE:HG22	1:C:24:MET:HG3	1.86	0.58
1:A:179:LEU:HD23	1:A:234:TRP:HB3	1.86	0.57
1:A:206:THR:HG21	5:A:708:HOH:O	2.03	0.57
2:D:335:GLY:N	5:D:601:HOH:O	2.38	0.57
2:D:466:GLU:HG2	2:D:472:PHE:HE2	1.68	0.57
1:A:156:LYS:HD2	1:A:196:GLN:HG2	1.87	0.56
1:C:22:THR:HG23	2:D:439:GLU:HB2	1.86	0.56
1:E:23:ILE:HG22	1:E:24:MET:HG3	1.86	0.56
1:A:36:ILE:HG12	1:A:317:LEU:HD22	1.88	0.56
1:A:11:TYR:CZ	2:B:340:ILE:HG23	2.41	0.56
1:A:284:THR:HB	1:A:287:GLY:O	2.06	0.56
2:B:440:ARG:HH21	2:F:440:ARG:HH21	1.54	0.56
1:E:182:ILE:CD1	1:E:213:LEU:HD13	2.36	0.55
1:E:206:THR:HB	1:E:209:LEU:HB3	1.88	0.55
1:A:23:ILE:HG22	1:A:24:MET:HG3	1.89	0.55
2:F:362:ASN:H	2:F:362:ASN:HD22	1.55	0.55
1:E:284:THR:HB	1:E:287:GLY:O	2.06	0.55
2:F:501:ARG:HD3	2:F:505:GLU:HG3	1.88	0.55
1:A:164:ILE:O	1:A:246:GLU:HA	2.07	0.55
1:E:120:ILE:HD13	1:E:257:ALA:HB3	1.89	0.54
1:E:289:ILE:HD11	1:E:298:ILE:HG13	1.89	0.54
1:C:179:LEU:HD23	1:C:234:TRP:HB3	1.90	0.54
1:E:289:ILE:HG22	1:E:291:SER:HB3	1.89	0.54
1:C:301:LEU:HA	2:D:400:VAL:HG22	1.89	0.54
1:E:116:GLU:HB3	1:E:259:LYS:HB2	1.90	0.54
2:F:466:GLU:HG2	2:F:472:PHE:CE2	2.41	0.54
1:C:304:GLY:HA2	2:D:397:PHE:CD1	2.43	0.53
1:A:22:THR:HG23	2:B:439:GLU:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:THR:HG21	1:C:250:ASN:OD1	2.08	0.53
1:E:11:TYR:CZ	2:F:340:ILE:HG23	2.44	0.53
1:A:73:GLU:OE2	1:A:141:TYR:OH	2.24	0.53
1:A:200:THR:HG21	1:A:250:ASN:OD1	2.09	0.53
1:C:200:THR:HA	1:C:248:ASN:HD22	1.74	0.53
1:E:182:ILE:HD11	1:E:213:LEU:HD13	1.91	0.53
2:D:466:GLU:HG2	2:D:472:PHE:CE2	2.44	0.52
2:D:454:ASP:OD1	2:D:457:ARG:NH1	2.42	0.52
2:B:362:ASN:ND2	2:B:365:GLY:O	2.43	0.52
1:A:197:ASN:ND2	5:A:712:HOH:O	1.92	0.52
1:E:148:PHE:HB2	1:E:151:VAL:HG12	1.92	0.52
1:E:182:ILE:HD11	1:E:233:PHE:CE1	2.45	0.52
2:D:403:GLU:OE2	5:D:612:HOH:O	2.18	0.52
1:A:102:TYR:CE2	1:A:106:LYS:HD2	2.45	0.51
1:C:102:TYR:CZ	1:C:106:LYS:HD2	2.46	0.51
1:C:280:THR:HB	1:C:282:CYS:H	1.75	0.51
2:B:362:ASN:HD22	2:B:362:ASN:H	1.59	0.51
2:F:482:CYS:O	2:F:486:VAL:HG23	2.11	0.51
1:E:320:GLY:O	2:F:445:HIS:NE2	2.44	0.51
1:E:301:LEU:HA	2:F:400:VAL:HG22	1.93	0.51
1:E:135:VAL:HG22	1:E:146:SER:HA	1.92	0.50
1:E:200:THR:HG21	1:E:250:ASN:OD1	2.10	0.50
1:A:52:LYS:HG2	1:A:53:PRO:HD2	1.93	0.50
1:E:53:PRO:HB3	1:E:82:TYR:CE2	2.47	0.50
1:E:133:LEU:N	5:E:714:HOH:O	2.44	0.50
2:F:463:ASN:ND2	2:F:491:TYR:OH	2.26	0.50
1:E:164:ILE:O	1:E:246:GLU:HA	2.12	0.50
1:E:156:LYS:NZ	1:E:196:GLN:OE1	2.42	0.49
1:A:206:THR:HB	1:A:209:LEU:HB3	1.93	0.49
1:A:212:ARG:HB2	1:C:216:ARG:HG2	1.93	0.49
1:E:216:ARG:O	1:E:220:ARG:NH2	2.45	0.49
2:B:508:SER:HG	2:F:501:ARG:HE	1.58	0.49
1:C:125:SER:CB	1:C:166:ARG:HH22	2.25	0.49
2:F:453:TYR:CE1	2:F:470:GLY:HA2	2.47	0.49
1:A:159:SER:O	1:A:196:GLN:HG3	2.12	0.49
1:C:206:THR:HB	1:C:209:LEU:HB3	1.94	0.49
1:C:164:ILE:O	1:C:246:GLU:HA	2.12	0.49
2:F:364:GLN:HE22	2:F:480:ASN:N	2.09	0.49
2:D:481:GLU:O	2:D:484:GLU:HB3	2.13	0.49
2:F:339:ALA:HB2	2:F:450:LYS:HB2	1.94	0.48
2:B:454:ASP:OD1	2:B:457:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:380:ASP:O	2:F:384:ASN:HB2	2.14	0.48
2:F:454:ASP:OD1	2:F:457:ARG:NH1	2.45	0.48
2:B:482:CYS:O	2:B:485:SER:OG	2.21	0.48
1:C:125:SER:HB2	1:C:166:ARG:HH22	1.79	0.48
1:E:211:GLN:OE1	1:E:213:LEU:HD11	2.14	0.48
1:C:308:LYS:HD2	2:D:426:TRP:CE2	2.49	0.48
2:F:465:LYS:HB2	2:F:475:TYR:CZ	2.48	0.48
1:E:14:ASN:O	1:E:323:ASN:ND2	2.42	0.48
2:D:505:GLU:HA	2:D:508:SER:HB3	1.95	0.47
1:C:323:ASN:O	1:C:325:PRO:HD3	2.15	0.47
2:D:501:ARG:HD3	2:D:505:GLU:HG3	1.97	0.47
1:A:200:THR:HG22	1:A:215:PRO:HG3	1.97	0.47
1:C:53:PRO:HB3	1:C:82:TYR:CE2	2.50	0.47
1:C:102:TYR:CE2	1:C:106:LYS:HD2	2.50	0.47
1:E:111:ARG:HH11	1:E:266:SER:HB3	1.79	0.47
1:E:120:ILE:HG13	1:E:168:TYR:CE1	2.50	0.47
1:E:321:LEU:HB3	2:F:445:HIS:CD2	2.50	0.47
1:C:70:MET:SD	1:C:140:PRO:HD2	2.55	0.47
2:D:503:LYS:O	2:D:507:ILE:HG12	2.15	0.47
2:F:462:ASP:O	2:F:504:ARG:NH1	2.48	0.47
1:A:99:PHE:HB3	1:A:102:TYR:HB2	1.97	0.46
1:C:73:GLU:OE2	1:C:141:TYR:OH	2.19	0.46
2:F:460:LEU:HD13	2:F:464:ALA:HB3	1.98	0.46
1:A:211:GLN:NE2	5:A:725:HOH:O	2.37	0.46
1:A:308:LYS:HD2	2:B:426:TRP:CE2	2.51	0.46
1:E:296:HIS:CD2	1:E:307:PRO:HG2	2.51	0.46
1:A:211:GLN:OE1	1:A:213:LEU:HD11	2.14	0.46
1:E:57:ARG:O	1:E:86:LYS:HG3	2.14	0.46
2:F:362:ASN:OD1	2:F:364:GLN:NE2	2.48	0.46
1:C:99:PHE:HB3	1:C:102:TYR:HB2	1.98	0.46
1:C:182:ILE:HD11	1:C:213:LEU:CD1	2.44	0.46
1:C:291:SER:HA	5:C:734:HOH:O	2.16	0.46
1:A:102:TYR:CZ	1:A:106:LYS:HD2	2.50	0.46
1:C:36:ILE:HG12	1:C:317:LEU:HD22	1.97	0.45
2:D:360:HIS:CD2	2:D:487:ARG:HH21	2.31	0.45
1:E:125:SER:C	1:E:166:ARG:HH22	2.20	0.45
1:C:120:ILE:HD11	1:C:168:TYR:CZ	2.50	0.45
1:A:23:ILE:HG23	2:F:385:LYS:HG3	1.98	0.45
1:E:120:ILE:HG23	1:E:121:ILE:HG13	1.99	0.45
1:E:280:THR:HB	1:E:282:CYS:H	1.82	0.45
2:F:454:ASP:O	2:F:458:LEU:HG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:PRO:HB3	1:A:82:TYR:CE2	2.52	0.45
2:B:498:GLU:O	2:B:502:LEU:HG	2.16	0.45
1:E:294:PRO:HG2	1:E:295:PHE:CD1	2.51	0.45
1:A:289:ILE:CG2	1:A:291:SER:HB3	2.46	0.45
1:C:175:ASP:OD1	1:C:239:PRO:HD3	2.16	0.45
1:E:31:THR:HB	1:E:321:LEU:H	1.82	0.45
2:F:457:ARG:HD2	2:F:466:GLU:OE2	2.17	0.45
1:C:24:MET:HE2	2:D:439:GLU:OE1	2.17	0.45
1:C:289:ILE:HD11	1:C:298:ILE:HG13	1.98	0.44
1:E:25:GLU:CD	1:E:322:ARG:HH22	2.17	0.44
1:A:11:TYR:HB2	1:A:321:LEU:HD11	2.00	0.44
1:A:182:ILE:HG23	1:A:202:ILE:HD12	1.99	0.44
1:A:216:ARG:HG2	1:E:212:ARG:HB2	1.99	0.44
1:A:304:GLY:HA2	2:B:397:PHE:CE1	2.53	0.44
1:E:65:LEU:HD11	1:E:109:LEU:HD11	1.98	0.44
1:E:102:TYR:CE2	1:E:106:LYS:HD2	2.52	0.44
1:E:308:LYS:HD2	2:F:426:TRP:CE2	2.53	0.44
1:A:8:CYS:HA	2:B:471:CYS:HA	2.00	0.44
1:C:67:GLY:HA3	1:C:149:ARG:H	1.82	0.44
1:C:67:GLY:CA	1:C:149:ARG:H	2.30	0.44
2:D:406:ASN:O	5:D:615:HOH:O	2.21	0.44
1:E:175:ASP:OD1	1:E:239:PRO:HD3	2.18	0.44
2:F:484:GLU:HG2	2:F:487:ARG:NH1	2.30	0.44
2:F:467:LEU:HD21	2:F:473:GLU:HB2	2.00	0.44
1:C:20:VAL:HG21	1:C:318:ALA:HB2	2.00	0.43
1:E:142:GLN:C	1:E:144:LYS:H	2.22	0.43
2:F:469:ASN:HB2	2:F:471:CYS:HB2	2.00	0.43
1:C:262:LYS:NZ	1:C:264:GLY:O	2.46	0.43
1:E:65:LEU:HD11	1:E:109:LEU:CD1	2.48	0.43
1:A:142:GLN:N	5:A:704:HOH:O	2.20	0.43
1:C:148:PHE:HB2	1:C:151:VAL:HG12	2.00	0.42
1:E:304:GLY:HA2	2:F:397:PHE:CD1	2.53	0.42
1:E:22:THR:HG23	2:F:439:GLU:HB2	1.99	0.42
1:A:67:GLY:HA3	1:A:149:ARG:HB2	2.02	0.42
1:C:78:PRO:O	1:C:114:HIS:HA	2.19	0.42
1:E:308:LYS:HD2	2:F:426:TRP:NE1	2.35	0.42
2:F:400:VAL:HA	2:F:401:GLY:HA3	1.68	0.42
1:C:11:TYR:CZ	2:D:340:ILE:HG23	2.54	0.42
1:C:48:LEU:HD23	1:C:48:LEU:HA	1.92	0.42
1:A:9:ILE:HD11	2:B:456:VAL:HG21	2.02	0.42
1:A:25:GLU:CD	1:A:322:ARG:HH22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:440:ARG:HH22	2:D:436:MET:HB3	1.84	0.42
1:C:68:ASN:HA	1:C:69:PRO:HD3	1.85	0.42
2:B:395:THR:O	2:B:395:THR:OG1	2.38	0.42
1:C:321:LEU:HB3	2:D:445:HIS:CD2	2.54	0.42
2:D:392:LYS:HD3	2:D:392:LYS:HA	1.91	0.42
1:E:206:THR:HG23	1:E:241:ASP:OD2	2.20	0.42
1:C:31:THR:HB	1:C:321:LEU:H	1.85	0.41
2:D:338:GLY:O	2:D:342:GLY:HA3	2.20	0.41
2:D:400:VAL:HA	2:D:401:GLY:HA3	1.70	0.41
2:F:395:THR:O	2:F:395:THR:OG1	2.38	0.41
1:A:134:GLY:HA3	1:A:153:TRP:HB3	2.01	0.41
1:A:206:THR:HG23	1:A:241:ASP:OD2	2.21	0.41
1:C:47:ASP:OD1	1:C:275:TYR:OH	2.34	0.41
1:C:212:ARG:HB2	1:E:216:ARG:HG2	2.01	0.41
1:E:314:ARG:HE	1:E:314:ARG:HB3	1.57	0.41
1:A:304:GLY:HA2	2:B:397:PHE:CD1	2.55	0.41
1:E:42:ASN:ND2	1:E:278:CYS:SG	2.94	0.41
2:D:419:GLU:OE2	5:D:613:HOH:O	2.22	0.41
1:E:212:ARG:NE	5:E:703:HOH:O	1.92	0.41
2:B:501:ARG:HG2	2:B:504:ARG:NH2	2.36	0.41
2:D:501:ARG:HG2	2:D:504:ARG:NH2	2.36	0.41
1:E:95:TYR:CE1	1:E:226:LEU:HD13	2.56	0.41
1:A:159:SER:C	1:A:196:GLN:HG3	2.42	0.41
1:E:182:ILE:HG12	1:E:231:GLU:HB3	2.03	0.40
1:C:8:CYS:HA	2:D:471:CYS:HA	2.03	0.40
1:C:159:SER:O	1:C:196:GLN:HG3	2.21	0.40
1:A:175:ASP:OD1	1:A:239:PRO:HD3	2.22	0.40
1:E:317:LEU:HD12	1:E:317:LEU:HA	1.83	0.40
1:A:68:ASN:HA	1:A:69:PRO:HD3	1.91	0.40
2:B:380:ASP:O	2:B:384:ASN:HB2	2.22	0.40
2:F:409:ARG:NH1	5:F:611:HOH:O	2.55	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:TYR:O	1:E:144:LYS:NZ[1_655]	2.14	0.06

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	320/322 (99%)	297 (93%)	22 (7%)	1 (0%)	41	61
1	C	320/322 (99%)	301 (94%)	18 (6%)	1 (0%)	41	61
1	E	320/322 (99%)	299 (93%)	20 (6%)	1 (0%)	41	61
2	B	173/175 (99%)	164 (95%)	8 (5%)	1 (1%)	25	43
2	D	173/175 (99%)	165 (95%)	7 (4%)	1 (1%)	25	43
2	F	173/175 (99%)	166 (96%)	6 (4%)	1 (1%)	25	43
All	All	1479/1491 (99%)	1392 (94%)	81 (6%)	6 (0%)	34	54

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	277	ASN
1	C	277	ASN
1	E	277	ASN
2	B	401	GLY
2	D	401	GLY
2	F	401	GLY

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	290/290 (100%)	258 (89%)	32 (11%)	6	12
1	C	290/290 (100%)	257 (89%)	33 (11%)	5	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	290/290 (100%)	256 (88%)	34 (12%)	5 10
2	B	149/149 (100%)	138 (93%)	11 (7%)	13 27
2	D	149/149 (100%)	140 (94%)	9 (6%)	19 37
2	F	149/149 (100%)	136 (91%)	13 (9%)	10 20
All	All	1317/1317 (100%)	1185 (90%)	132 (10%)	7 15

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	23	ILE
1	A	30	VAL
1	A	36	ILE
1	A	48	LEU
1	A	75	ILE
1	A	118	ILE
1	A	135	VAL
1	A	149	ARG
1	A	151	VAL
1	A	160	THR
1	A	173	GLN
1	A	182	ILE
1	A	186	ASN
1	A	191	GLN
1	A	195	TYR
1	A	200	THR
1	A	206	THR
1	A	208	THR
1	A	211	GLN
1	A	216	ARG
1	A	219	THR
1	A	227	SER
1	A	230	MET
1	A	235	THR
1	A	265	ASP
1	A	280	THR
1	A	308	LYS
1	A	310	VAL
1	A	317	LEU
1	A	319	ILE
1	A	321	LEU

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Mol	Chain	Res	Type
2	B	362	ASN
2	B	384	ASN
2	B	395	THR
2	B	400	VAL
2	B	423	LEU
2	B	446	ASP
2	B	455	LYS
2	B	460	LEU
2	B	495	GLN
2	B	498	GLU
2	B	501	ARG
1	C	7	ILE
1	C	20	VAL
1	C	23	ILE
1	C	30	VAL
1	C	36	ILE
1	C	48	LEU
1	C	70	MET
1	C	75	ILE
1	C	118	ILE
1	C	135	VAL
1	C	149	ARG
1	C	151	VAL
1	C	160	THR
1	C	173	GLN
1	C	182	ILE
1	C	186	ASN
1	C	191	GLN
1	C	195	TYR
1	C	200	THR
1	C	206	THR
1	C	208	THR
1	C	211	GLN
1	C	216	ARG
1	C	219	THR
1	C	227	SER
1	C	230	MET
1	C	235	THR
1	C	265	ASP
1	C	280	THR
1	C	308	LYS
1	C	317	LEU

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Mol	Chain	Res	Type
1	C	319	ILE
1	C	321	LEU
2	D	384	ASN
2	D	395	THR
2	D	400	VAL
2	D	446	ASP
2	D	455	LYS
2	D	460	LEU
2	D	495	GLN
2	D	498	GLU
2	D	501	ARG
1	E	7	ILE
1	E	20	VAL
1	E	23	ILE
1	E	30	VAL
1	E	36	ILE
1	E	48	LEU
1	E	75	ILE
1	E	118	ILE
1	E	120	ILE
1	E	135	VAL
1	E	149	ARG
1	E	151	VAL
1	E	160	THR
1	E	173	GLN
1	E	182	ILE
1	E	186	ASN
1	E	191	GLN
1	E	195	TYR
1	E	200	THR
1	E	206	THR
1	E	208	THR
1	E	211	GLN
1	E	216	ARG
1	E	219	THR
1	E	227	SER
1	E	230	MET
1	E	235	THR
1	E	265	ASP
1	E	280	THR
1	E	308	LYS
1	E	310	VAL

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Mol	Chain	Res	Type
1	E	317	LEU
1	E	319	ILE
1	E	321	LEU
2	F	362	ASN
2	F	384	ASN
2	F	395	THR
2	F	400	VAL
2	F	423	LEU
2	F	446	ASP
2	F	455	LYS
2	F	459	GLN
2	F	460	LEU
2	F	461	ARG
2	F	495	GLN
2	F	498	GLU
2	F	501	ARG

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

Mol	Chain	Res	Type
2	B	364	GLN
1	C	248	ASN
2	D	360	HIS
2	F	364	GLN
2	F	429	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

6 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	G	1	3,1	14,14,15	0.52	0	17,19,21	0.66	0
3	NAG	G	2	3	14,14,15	0.44	0	17,19,21	0.88	0
3	NAG	H	1	3,1	14,14,15	0.54	0	17,19,21	0.66	0
3	NAG	H	2	3	14,14,15	0.55	0	17,19,21	0.68	0
3	NAG	I	1	3,1	14,14,15	0.52	0	17,19,21	0.80	0
3	NAG	I	2	3	14,14,15	0.42	0	17,19,21	0.88	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	1/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	1	NAG	C8-C7-N2-C2
3	I	1	NAG	O7-C7-N2-C2
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
3	H	2	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6

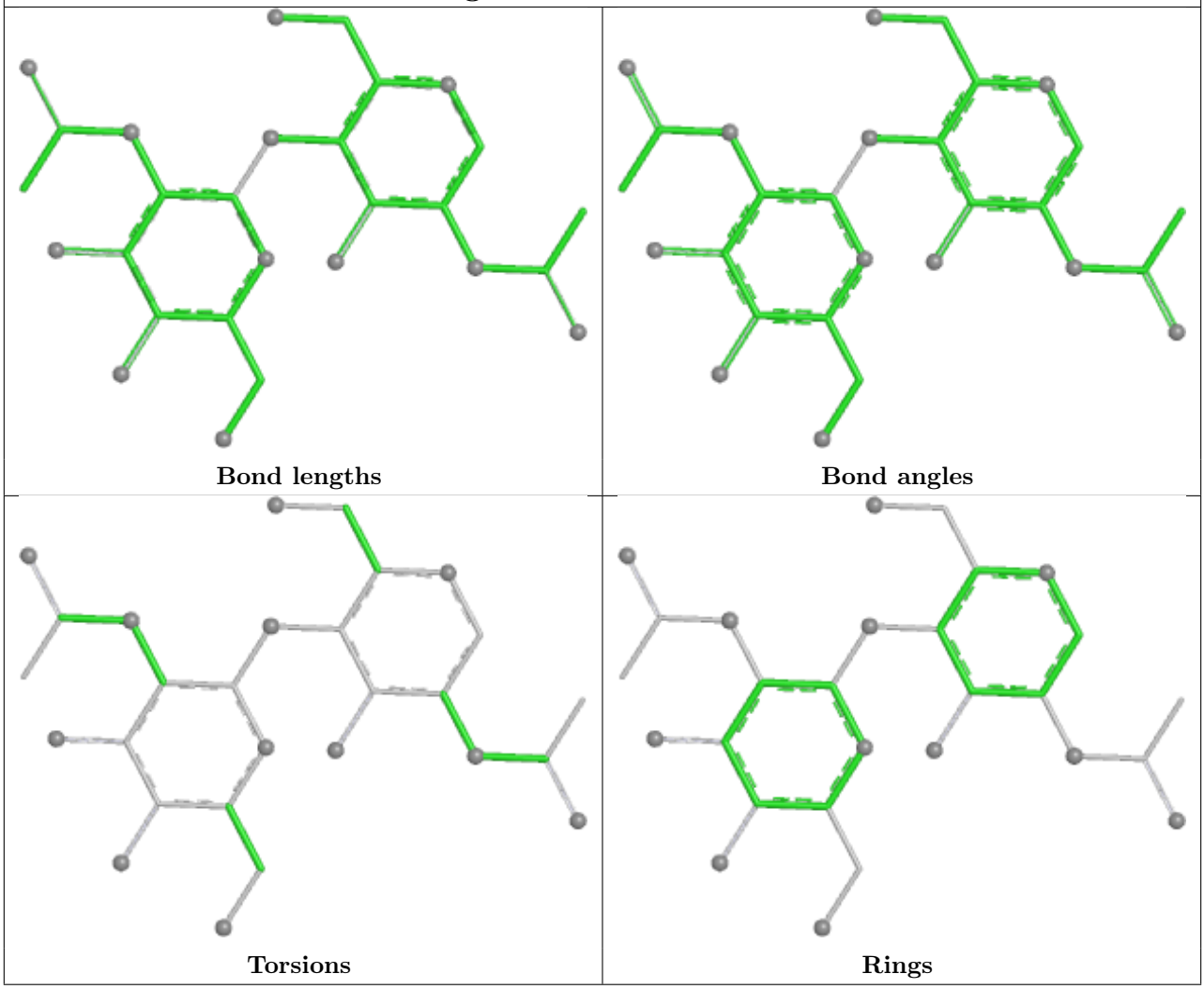
There are no ring outliers.

1 monomer is involved in 1 short contact:

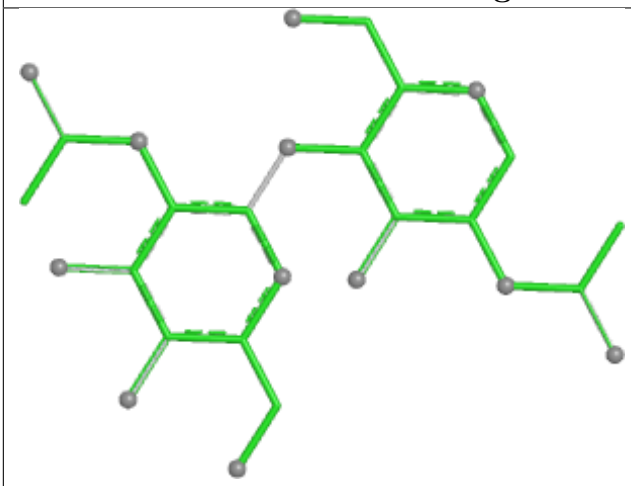
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

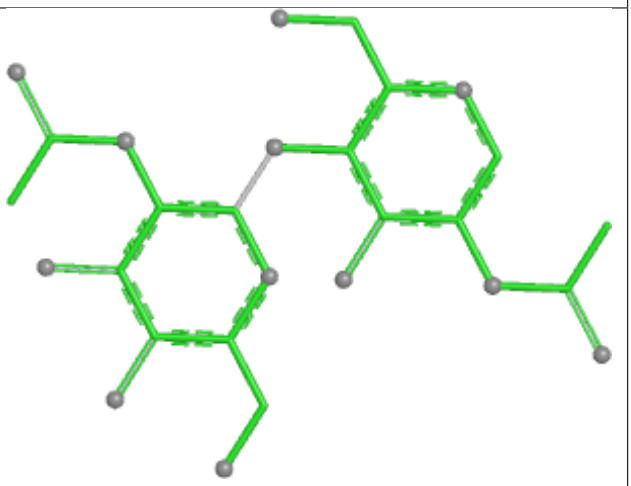
Oligosaccharide Chain G



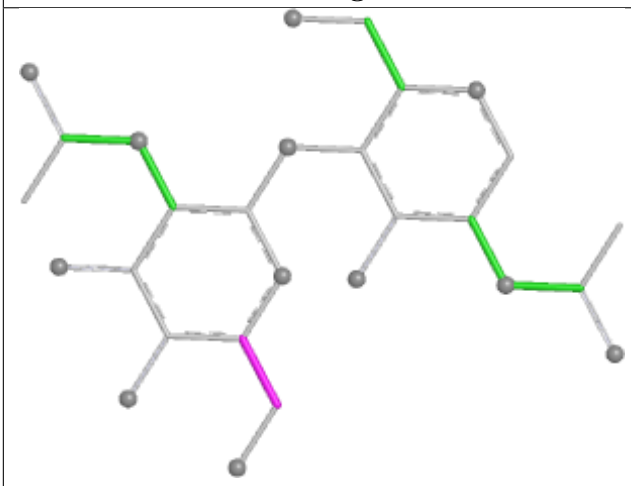
Oligosaccharide Chain H



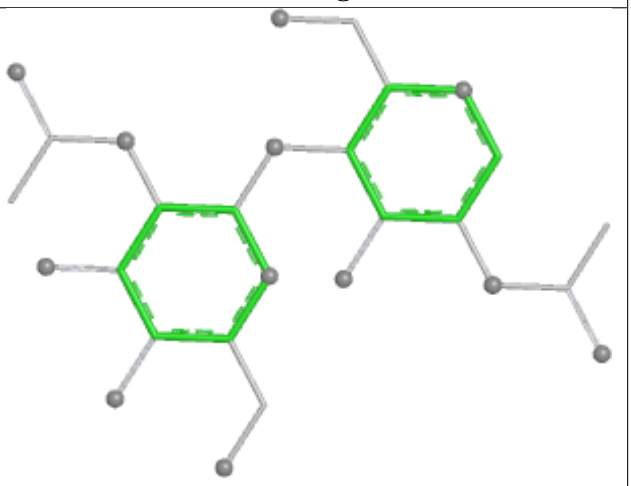
Bond lengths



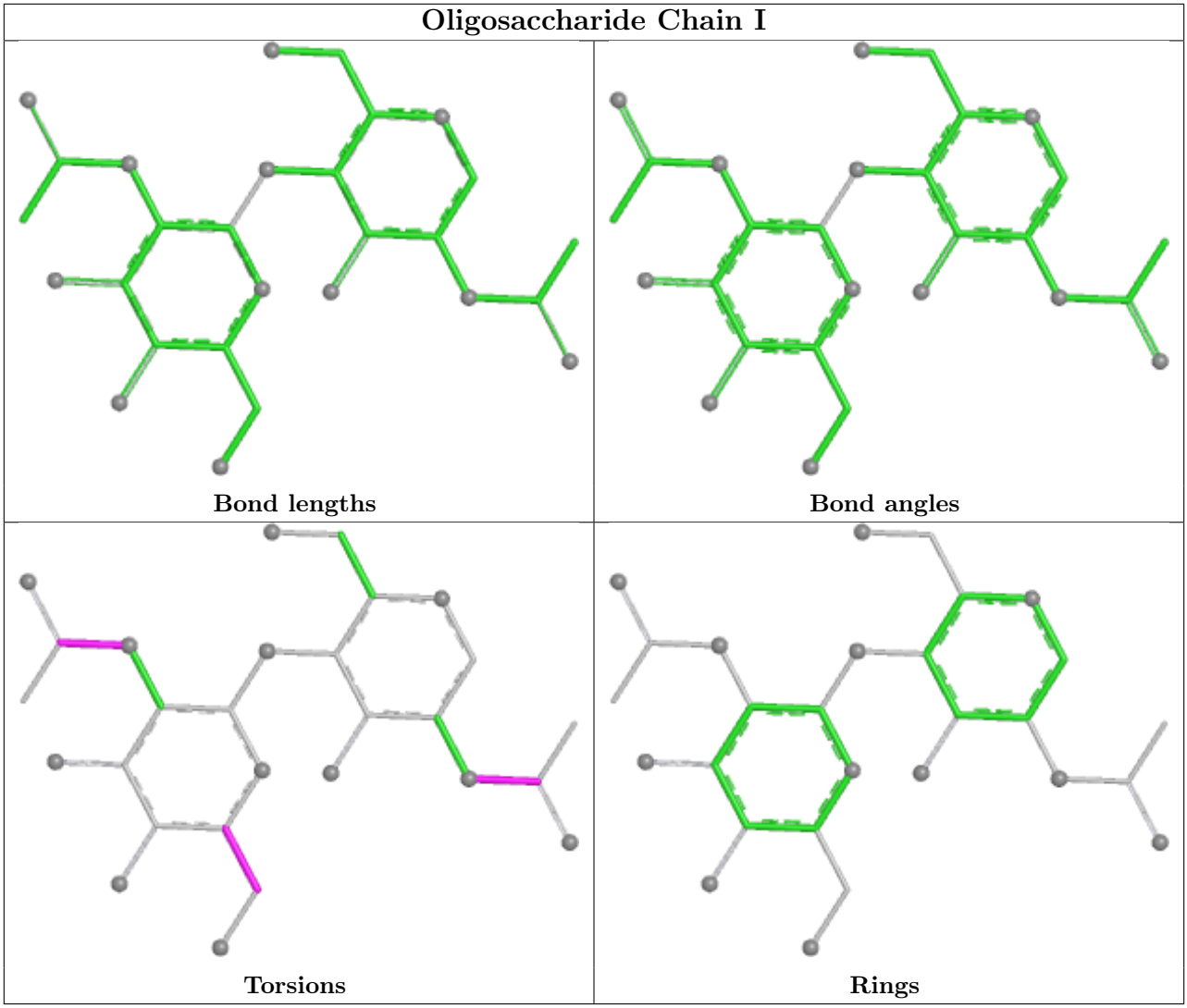
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	E	601	1	14,14,15	0.42	0	17,19,21	1.39	2 (11%)
4	NAG	C	601	1	14,14,15	0.49	0	17,19,21	0.79	0
4	NAG	A	601	1	14,14,15	0.47	0	17,19,21	0.75	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	601	1	-	2/6/23/26	0/1/1/1
4	NAG	C	601	1	-	2/6/23/26	0/1/1/1
4	NAG	A	601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	601	NAG	C1-O5-C5	4.25	117.88	112.19
4	E	601	NAG	C4-C3-C2	-2.29	107.66	111.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	601	NAG	C8-C7-N2-C2
4	E	601	NAG	O7-C7-N2-C2
4	C	601	NAG	C8-C7-N2-C2
4	C	601	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (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, 95^{th} 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	322/322 (100%)	0.11	3 (0%) 84 86	20, 44, 72, 119	0
1	C	322/322 (100%)	0.22	12 (3%) 41 45	23, 51, 89, 121	0
1	E	322/322 (100%)	0.32	14 (4%) 35 38	30, 56, 97, 143	0
2	B	175/175 (100%)	0.47	5 (2%) 51 55	30, 57, 88, 140	0
2	D	175/175 (100%)	1.07	36 (20%) 1 0	25, 75, 123, 191	0
2	F	175/175 (100%)	1.30	46 (26%) 0 0	29, 84, 147, 196	0
All	All	1491/1491 (100%)	0.47	116 (7%) 13 13	20, 54, 115, 196	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	509	GLY	8.2
1	C	325	PRO	7.6
2	B	509	GLY	7.1
2	D	353	ASP	6.3
2	F	475	TYR	6.1
2	F	507	ILE	5.8
2	D	477	LYS	5.7
2	F	474	PHE	5.7
2	D	505	GLU	5.5
2	F	509	GLY	5.5
2	F	501	ARG	5.4
2	D	498	GLU	5.4
2	F	504	ARG	5.3
1	C	16	SER	5.2
2	F	487	ARG	5.0
2	F	350	GLY	4.8
2	F	460	LEU	4.7
2	F	492	ASP	4.4
1	E	15	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	7	ILE	4.0
1	E	73	GLU	4.0
2	F	472	PHE	3.9
2	D	481	GLU	3.9
2	D	474	PHE	3.9
1	C	158	ASP	3.9
2	D	491	TYR	3.9
2	F	365	GLY	3.8
2	F	490	THR	3.8
1	E	7	ILE	3.8
2	F	496	TYR	3.7
2	D	482	CYS	3.7
2	F	482	CYS	3.7
2	F	436	MET	3.6
2	D	475	TYR	3.6
2	D	492	ASP	3.5
1	E	291	SER	3.3
2	F	463	ASN	3.2
2	F	473	GLU	3.2
2	D	460	LEU	3.2
2	D	496	TYR	3.1
1	E	325	PRO	3.1
2	D	502	LEU	3.1
2	D	356	TYR	3.1
2	F	372	LYS	3.1
2	F	493	TYR	3.0
2	D	365	GLY	3.0
2	F	470	GLY	3.0
1	E	4	GLN	2.9
2	F	432	LEU	2.8
2	F	505	GLU	2.7
2	D	494	PRO	2.7
2	F	499	GLU	2.7
2	D	467	LEU	2.7
2	D	345	GLU	2.7
2	F	498	GLU	2.7
2	F	495	GLN	2.7
1	E	263	LYS	2.7
2	D	337	PHE	2.6
2	D	468	GLY	2.6
2	D	478	CYS	2.6
2	D	500	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	F	440	ARG	2.6
2	D	476	HIS	2.6
1	C	274	GLU	2.6
1	C	14	ASN	2.6
2	F	367	GLY	2.6
2	B	440	ARG	2.6
1	C	133	LEU	2.6
1	E	128	SER	2.6
1	E	72	ASP	2.5
2	B	446	ASP	2.5
1	A	314	ARG	2.5
1	A	291	SER	2.4
2	F	502	LEU	2.4
2	F	368	TYR	2.4
2	F	491	TYR	2.4
1	C	129	HIS	2.4
2	F	430	ALA	2.4
2	F	429	ASN	2.4
2	F	361	SER	2.4
2	D	501	ARG	2.4
1	A	44	LYS	2.4
1	E	74	PHE	2.4
2	D	446	ASP	2.4
1	C	157	LYS	2.3
2	D	366	SER	2.3
1	C	6	GLN	2.3
2	F	476	HIS	2.3
1	E	50	GLY	2.3
2	D	479	ASP	2.3
2	D	436	MET	2.3
2	F	497	SER	2.3
2	D	433	LEU	2.3
1	E	45	LEU	2.2
2	D	472	PHE	2.2
1	C	8	CYS	2.2
2	B	339	ALA	2.2
2	F	433	LEU	2.2
1	C	314	ARG	2.2
2	D	432	LEU	2.2
2	F	370	ALA	2.1
2	F	446	ASP	2.1
2	F	462	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	508	SER	2.1
1	E	158	ASP	2.1
2	D	461	ARG	2.1
2	F	500	ALA	2.1
2	F	467	LEU	2.1
2	F	358	TYR	2.1
2	F	353	ASP	2.1
1	E	324	SER	2.1
2	B	337	PHE	2.0
2	F	439	GLU	2.0
2	D	495	GLN	2.0
2	F	360	HIS	2.0
2	D	486	VAL	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)

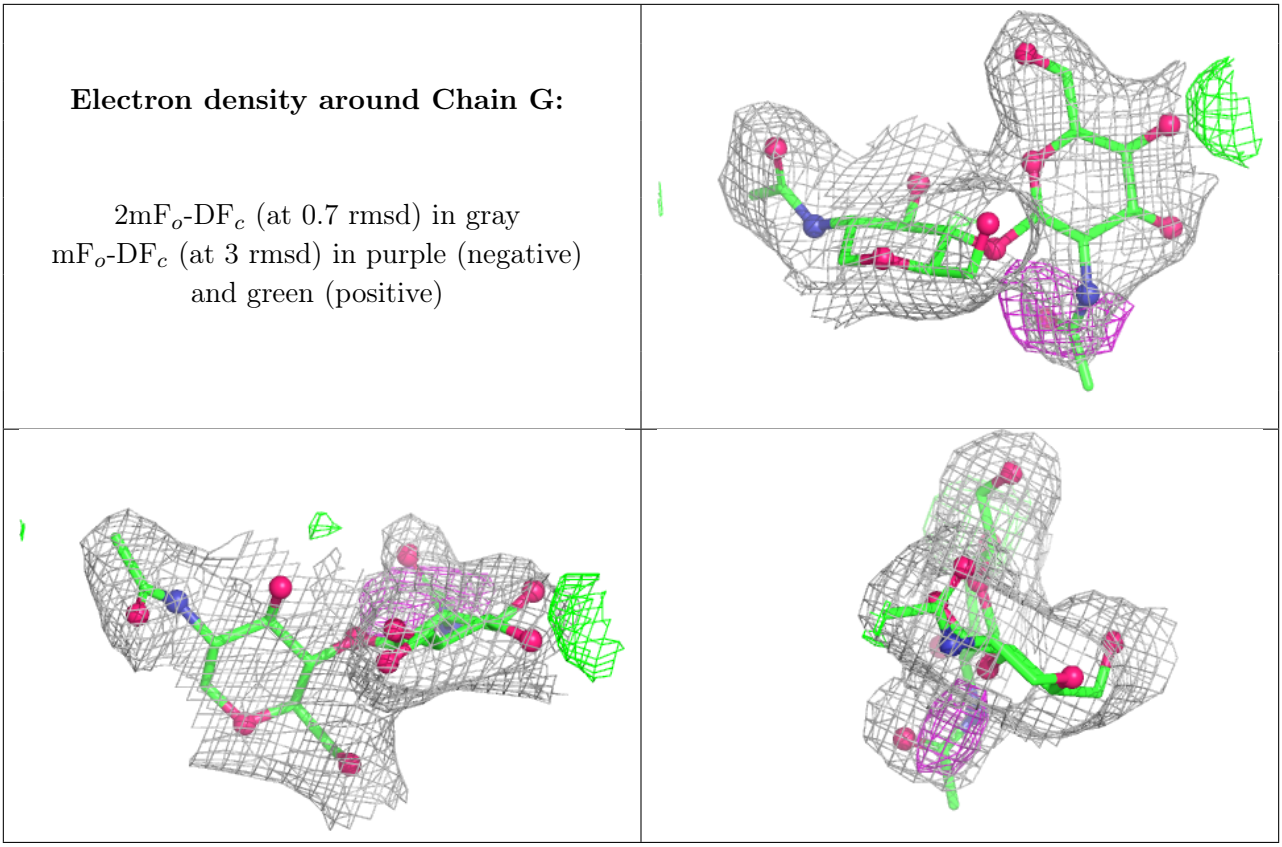
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	I	2	14/15	0.73	0.51	73,89,97,99	0
3	NAG	G	2	14/15	0.81	0.21	52,56,66,72	0
3	NAG	H	2	14/15	0.88	0.37	80,89,92,96	0
3	NAG	H	1	14/15	0.91	0.15	47,71,85,85	0
3	NAG	I	1	14/15	0.93	0.26	46,62,71,78	0
3	NAG	G	1	14/15	0.95	0.10	28,43,53,55	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.

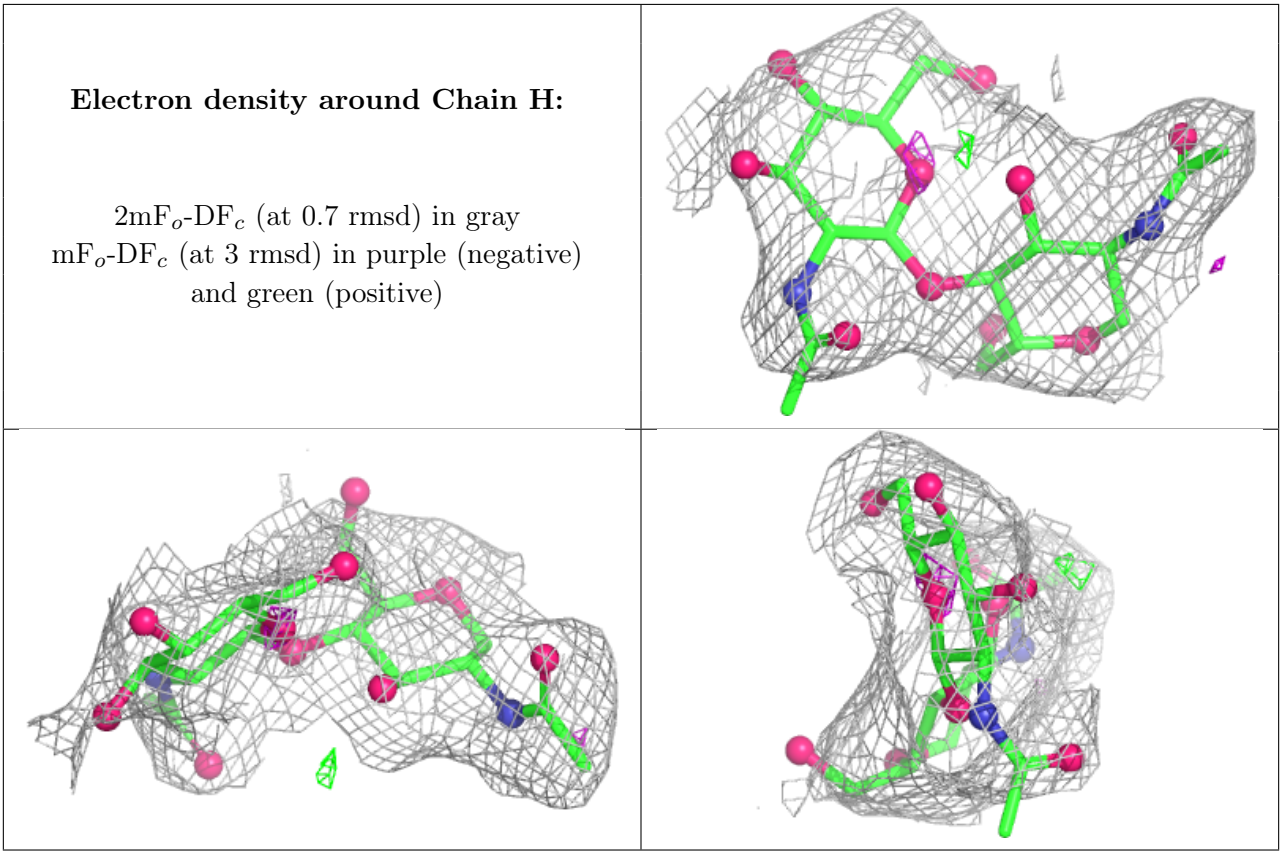
Electron density around Chain G:

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



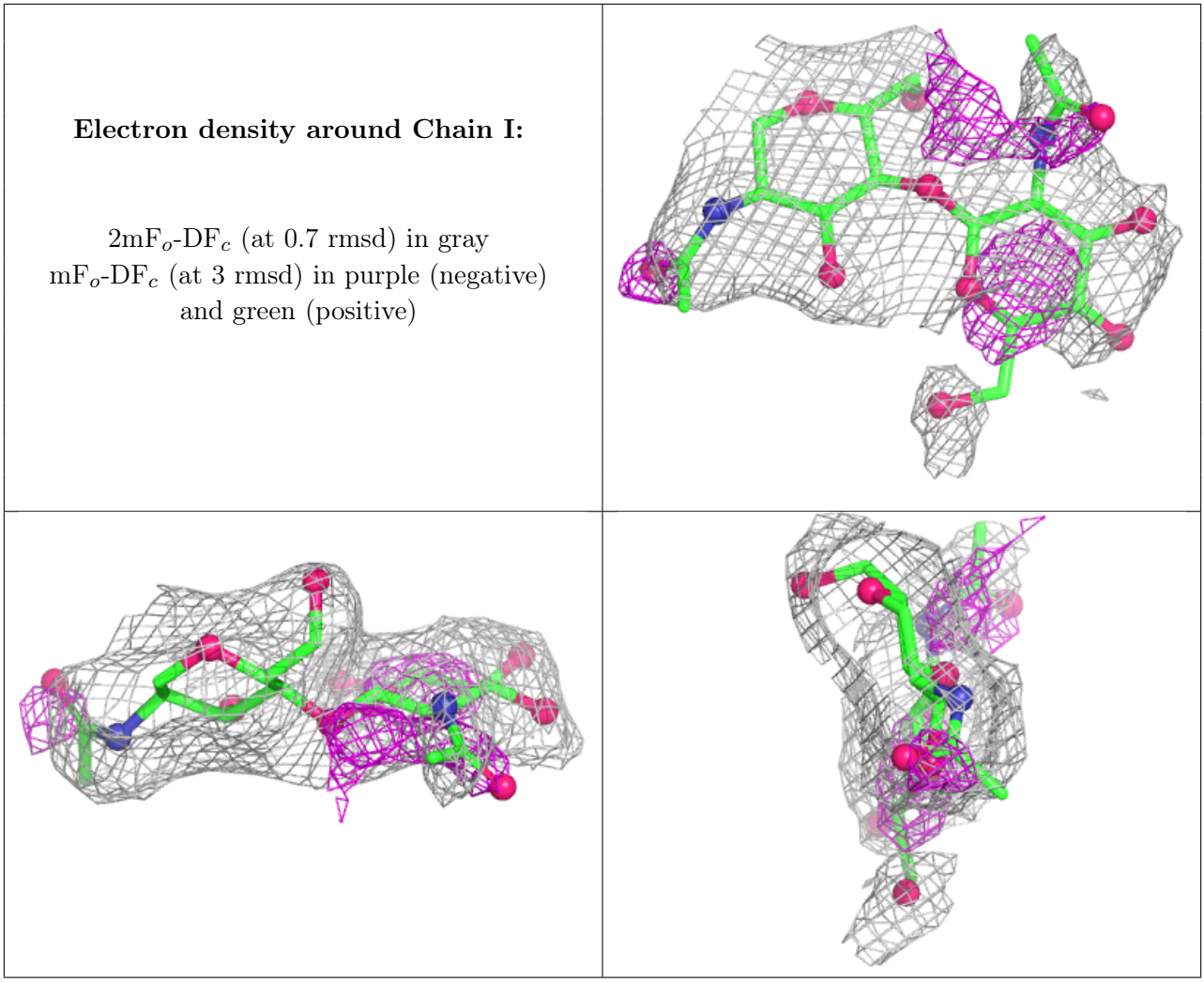
Electron density around Chain H:

$2mF_o$-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 I:

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



6.4 Ligands

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, 95^{th} 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
4	NAG	E	601	14/15	0.80	0.33	85,92,96,99	0
4	NAG	C	601	14/15	0.83	0.20	79,85,90,90	0
4	NAG	A	601	14/15	0.83	0.24	78,82,87,87	0

6.5 Other polymers

There are no such residues in this entry.