Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2023 – 06:39 PM EDT

PDB ID	:	5UJT
Title	:	Crystal structure of human HLA-DQ8 in complex with insulin mimotope binding in register 3
Authors	:	Wang, Y.; Dai, S.
Deposited on	:	2017-01-18
Resolution	:	1.94 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:

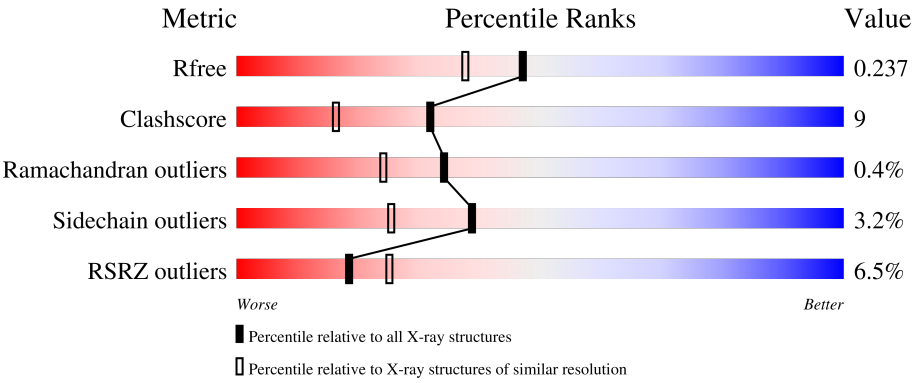
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.94 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	185	2% 82% 15%
1	D	185	9% 85% 12%
1	G	185	6% 86% 11%
2	B	189	5% 79% 17%
2	E	189	6% 72% 26%

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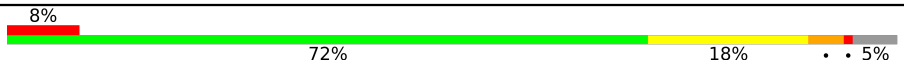
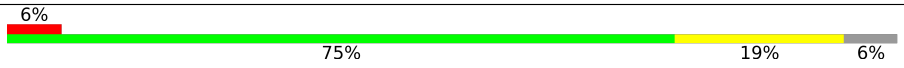
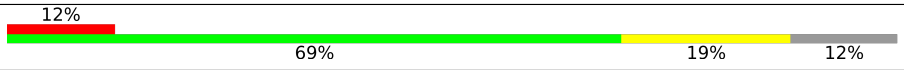
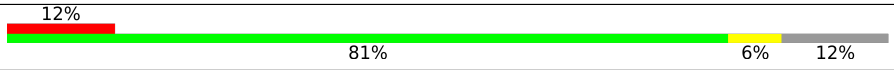
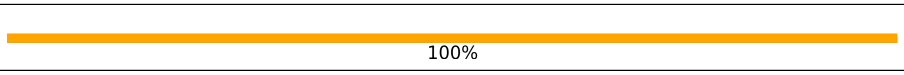
Mol	Chain	Length	Quality of chain
2	H	189	
3	C	16	
3	F	16	
3	I	16	
4	J	3	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10048 atoms, of which 13 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 MHC class II antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	0	1	0
			1485	954	243	285	3			
1	D	181	Total	C	N	O	S	0	0	0
			1463	941	240	279	3			
1	G	182	Total	C	N	O	S	0	0	0
			1467	943	241	280	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	CYS	ILE	conflict	UNP Q5Y7C3
D	72	CYS	ILE	conflict	UNP Q5Y7C3
G	72	CYS	ILE	conflict	UNP Q5Y7C3

- Molecule 2 is a protein called MHC class II HLA-DQ-beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	188	Total	C	N	O	S	0	0	0
			1552	979	275	291	7			
2	E	188	Total	C	N	O	S	0	0	0
			1549	978	274	290	7			
2	H	179	Total	C	N	O	S	0	0	0
			1483	940	260	276	7			

- Molecule 3 is a protein called insulin mimotope.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	15	Total	C	N	O	S	0	0	0
			105	65	15	24	1			
3	F	14	Total	C	N	O	S	0	0	0
			101	63	14	23	1			

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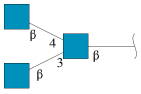
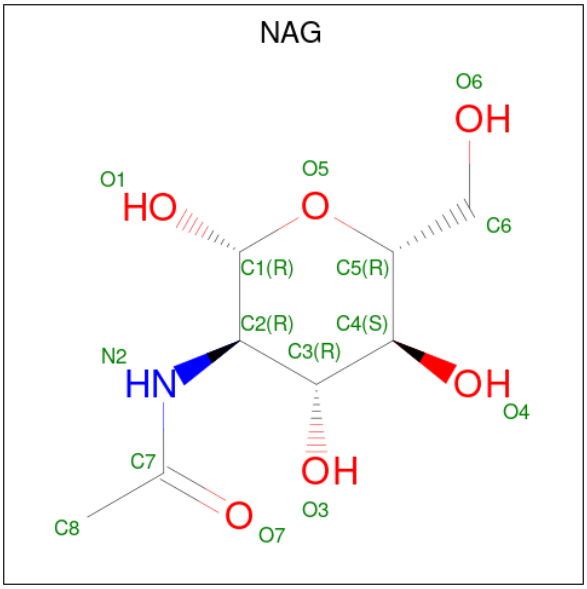
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	I	14	Total C N O S 101 63 14 23 1	0	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	J	3	Total C N O 42 24 3 15	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H N O 27 8 13 1 5	0	0
5	D	1	Total C N O 14 8 1 5	0	0
5	G	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is water.

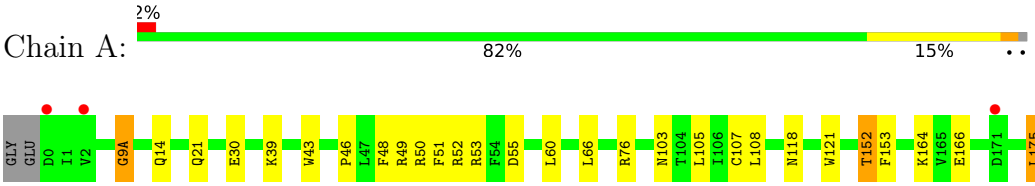
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	136	Total O 136 136	0	0
6	B	100	Total O 100 100	0	0
6	C	12	Total O 12 12	0	0
6	D	101	Total O 101 101	0	0
6	E	88	Total O 88 88	0	0
6	F	8	Total O 8 8	0	0
6	G	110	Total O 110 110	0	0
6	H	80	Total O 80 80	0	0
6	I	10	Total O 10 10	0	0

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.

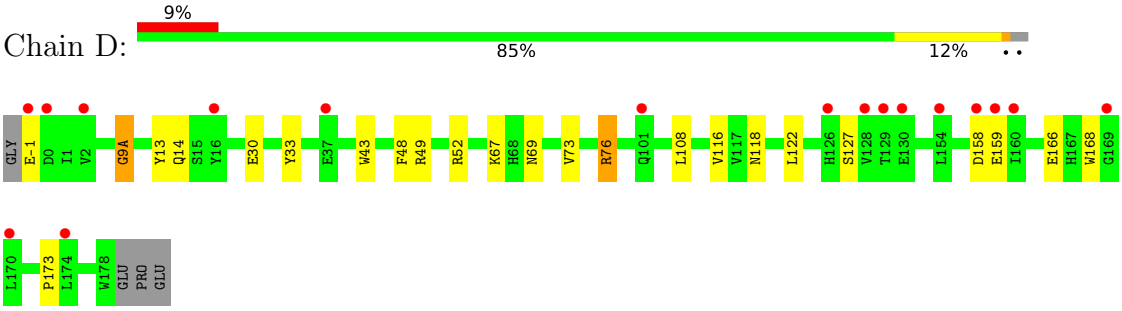
• Molecule 1: MHC class II antigen

Chain A:



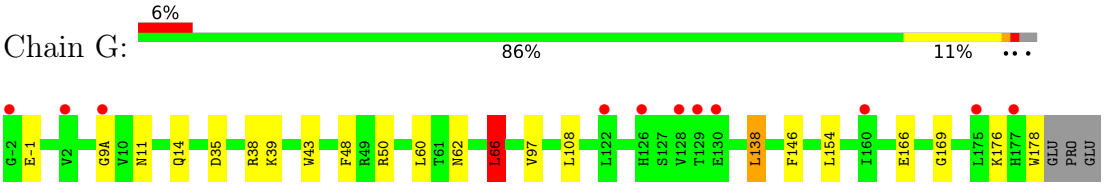
• Molecule 1: MHC class II antigen

Chain D:



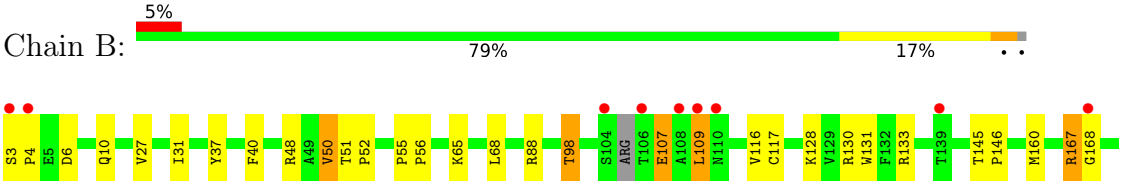
• Molecule 1: MHC class II antigen

Chain G:



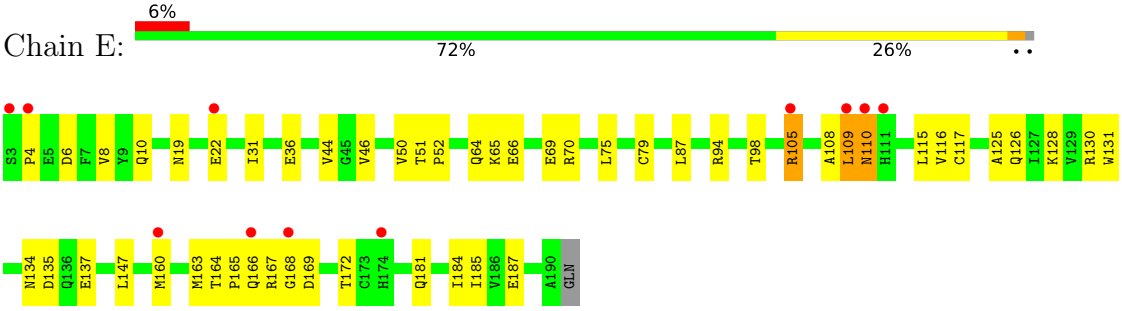
• Molecule 2: MHC class II HLA-DQ-beta-1

Chain B:



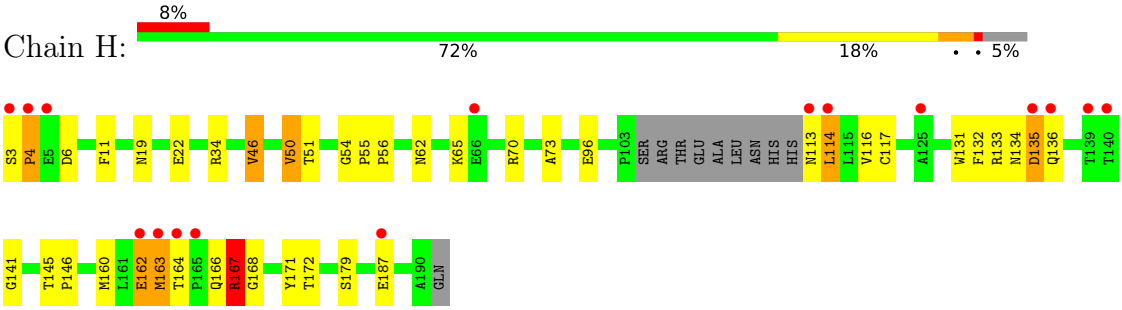
• Molecule 2: MHC class II HLA-DQ-beta-1

Chain E:



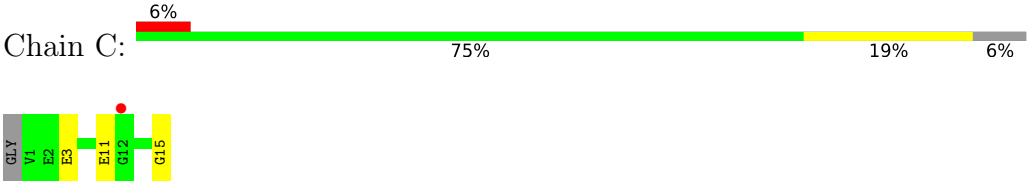
• Molecule 2: MHC class II HLA-DQ-beta-1

Chain H:



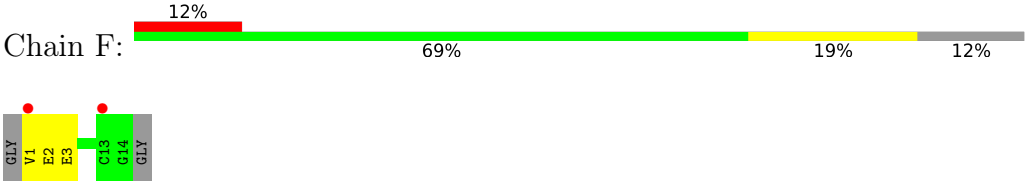
• Molecule 3: insulin mimotope

Chain C:



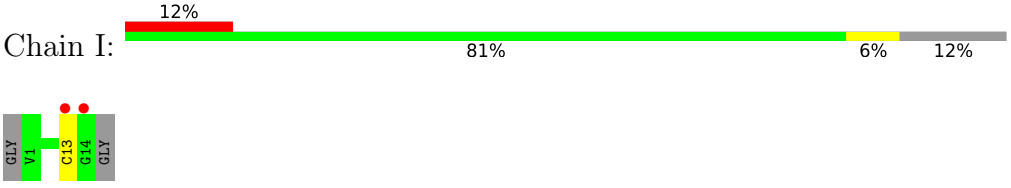
• Molecule 3: insulin mimotope

Chain F:



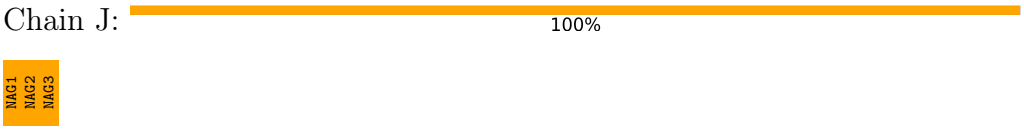
• Molecule 3: insulin mimotope

Chain I:



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

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.04Å 138.77Å 159.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.87 – 1.94 79.87 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.6 (79.87-1.94) 99.6 (79.87-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 1.94Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.209 , 0.238 0.211 , 0.237	Depositor DCC
R_{free} test set	5832 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	28.1	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.3	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	0.94	EDS
Total number of atoms	10048	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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	0.53	0/1532	0.66	0/2090
1	D	0.47	0/1506	0.63	1/2055 (0.0%)
1	G	0.51	0/1510	0.65	1/2060 (0.0%)
2	B	0.44	0/1591	0.63	0/2169
2	E	0.49	0/1589	0.67	3/2168 (0.1%)
2	H	0.46	0/1520	0.66	2/2072 (0.1%)
3	C	0.64	0/105	0.59	0/140
3	F	0.43	0/101	0.76	0/135
3	I	0.63	0/101	0.86	0/135
All	All	0.49	0/9555	0.65	7/13024 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	108	ALA	N-CA-C	-5.81	95.30	111.00
1	D	76	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	G	66	LEU	CA-CB-CG	5.21	127.27	115.30
2	E	87	LEU	CA-CB-CG	5.13	127.10	115.30
2	H	135	ASP	N-CA-C	5.11	124.80	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	34	ARG	NE-CZ-NH1	-5.01	117.79	120.30
2	E	109	LEU	CA-CB-CG	-5.01	103.78	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	9(A)	GLY	Peptide
1	D	9(A)	GLY	Peptide

5.2 Too-close contacts (i)

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	1485	0	1411	21	0
1	D	1463	0	1393	20	0
1	G	1467	0	1396	18	0
2	B	1552	0	1488	31	0
2	E	1549	0	1485	39	0
2	H	1483	0	1435	36	0
3	C	105	0	96	3	0
3	F	101	0	93	5	0
3	I	101	0	93	0	0
4	J	42	0	37	5	0
5	A	14	13	13	0	0
5	D	14	0	13	0	0
5	G	14	0	13	3	0
6	A	136	0	0	6	0
6	B	100	0	0	6	0
6	C	12	0	0	0	0
6	D	101	0	0	0	0
6	E	88	0	0	5	0
6	F	8	0	0	1	0
6	G	110	0	0	5	0
6	H	80	0	0	3	0
6	I	10	0	0	1	0
All	All	10035	13	8966	164	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 9.

All (164) 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)
2:E:109:LEU:O	2:E:165:PRO:O	1.57	1.23
2:H:172:THR:HG22	2:H:187:GLU:HG2	1.38	1.05
2:H:166:GLN:O	2:H:167:ARG:HB3	1.53	1.04
1:G:35:ASP:OD2	1:G:38:ARG:NH1	2.02	0.92
2:E:164:THR:HG22	2:E:166:GLN:HE21	1.37	0.89
2:B:116:VAL:HG22	2:B:160:MET:HG2	1.56	0.87
2:H:166:GLN:O	2:H:167:ARG:CB	2.21	0.85
2:E:19:ASN:ND2	2:E:22:GLU:OE1	2.09	0.85
2:E:110:ASN:HA	2:E:166:GLN:HE22	1.43	0.84
1:G:-1:GLU:OE2	6:G:301:HOH:O	1.94	0.84
2:B:130:ARG:HD3	6:B:340:HOH:O	1.80	0.80
2:B:133:ARG:HD2	2:B:171:TYR:CE2	2.19	0.77
2:E:116:VAL:HG22	2:E:160:MET:HG2	1.65	0.77
2:H:172:THR:CG2	2:H:187:GLU:HG2	2.15	0.76
2:H:133:ARG:O	2:H:136:GLN:HB2	1.87	0.75
2:H:70:ARG:NH1	6:H:201:HOH:O	2.07	0.74
2:E:105:ARG:HD2	6:E:215:HOH:O	1.87	0.73
2:H:134:ASN:O	2:H:136:GLN:HG2	1.88	0.72
1:D:14:GLN:NE2	2:E:6:ASP:OD2	2.24	0.71
1:D:14:GLN:HG3	2:E:8:VAL:HG22	1.71	0.71
2:B:128:LYS:NZ	6:B:302:HOH:O	2.12	0.71
2:B:172:THR:HG22	2:B:187:GLU:HB3	1.74	0.69
2:B:187:GLU:OE2	2:B:189:ARG:NH2	2.27	0.68
2:B:128:LYS:HD3	2:B:130:ARG:HD2	1.76	0.68
1:A:181:GLU:OXT	2:E:105:ARG:NH2	2.27	0.67
1:D:9(A):GLY:HA3	6:F:107:HOH:O	1.94	0.67
3:F:1:VAL:HG12	3:F:2:GLU:N	2.08	0.67
2:B:133:ARG:HD2	2:B:171:TYR:CZ	2.31	0.66
2:H:166:GLN:OE1	6:H:202:HOH:O	2.14	0.66
2:H:19:ASN:ND2	2:H:22:GLU:OE1	2.29	0.65
1:D:158:ASP:C	1:D:159:GLU:HG3	2.17	0.65
4:J:1:NAG:O3	4:J:2:NAG:H83	1.97	0.65
2:E:130:ARG:HD2	2:E:137:GLU:OE2	1.98	0.64
2:E:164:THR:HG22	2:E:166:GLN:NE2	2.08	0.64
2:H:116:VAL:HG22	2:H:160:MET:HG3	1.80	0.63
2:B:172:THR:HG22	2:B:187:GLU:CB	2.30	0.61
4:J:1:NAG:H4	4:J:2:NAG:H83	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:166:GLU:HB3	5:G:201:NAG:H83	1.83	0.61
1:G:39:LYS:HG2	1:G:60:LEU:HD11	1.83	0.60
2:H:3:SER:HB3	2:H:4:PRO:CD	2.31	0.60
2:E:130:ARG:HH11	2:E:130:ARG:HG3	1.65	0.60
2:B:187:GLU:OE2	2:B:189:ARG:CZ	2.49	0.59
2:H:96:GLU:HG2	2:H:179:SER:OG	2.02	0.59
2:E:115:LEU:HD13	2:E:163:MET:SD	2.42	0.59
2:E:94:ARG:HH11	2:E:94:ARG:HG3	1.68	0.59
1:D:14:GLN:HG2	2:E:6:ASP:OD1	2.03	0.59
2:B:190:ALA:C	2:B:191:GLN:HG3	2.24	0.58
1:D:76:ARG:HD3	6:E:245:HOH:O	2.03	0.58
4:J:2:NAG:H82	4:J:3:NAG:C6	2.34	0.58
1:A:43:TRP:CE3	1:A:48:PHE:HB3	2.38	0.58
2:E:134:ASN:ND2	2:E:169:ASP:OD1	2.36	0.58
2:B:107:GLU:HA	6:B:325:HOH:O	2.03	0.57
2:E:36:GLU:O	2:E:50:VAL:HG22	2.04	0.57
2:B:48:ARG:NE	6:B:301:HOH:O	2.07	0.57
1:G:9(A):GLY:HA3	6:I:206:HOH:O	2.05	0.57
2:E:172:THR:HG22	2:E:187:GLU:HG2	1.86	0.56
1:G:138:LEU:HD23	1:G:146:PHE:CE2	2.40	0.56
1:A:180:PRO:O	6:A:301:HOH:O	2.18	0.56
3:F:1:VAL:HG12	3:F:2:GLU:H	1.71	0.56
1:A:9(A):GLY:HA3	6:A:340:HOH:O	2.05	0.55
1:D:14:GLN:HE22	1:D:116:VAL:HG23	1.71	0.55
2:H:163:MET:HG3	2:H:171:TYR:CZ	2.42	0.54
2:B:128:LYS:HD2	2:B:176:GLU:OE2	2.06	0.54
1:D:168:TRP:CE2	2:E:4:PRO:HD2	2.43	0.54
1:A:39:LYS:HG2	1:A:60:LEU:HD11	1.90	0.53
2:E:168:GLY:N	6:E:201:HOH:O	2.25	0.53
2:E:10:GLN:HB2	2:E:31:ILE:HB	1.91	0.53
2:B:3:SER:HB2	2:B:4:PRO:HD2	1.90	0.52
2:H:135:ASP:N	2:H:136:GLN:HB2	2.24	0.52
1:G:43:TRP:CE3	1:G:48:PHE:HB3	2.45	0.52
1:A:50:ARG:HG3	1:A:51:PHE:CD2	2.45	0.52
1:D:158:ASP:O	1:D:159:GLU:HG3	2.10	0.51
2:E:117:CYS:HB2	2:E:131:TRP:CZ2	2.46	0.51
2:E:51:THR:HB	2:E:52:PRO:CD	2.41	0.50
1:A:30:GLU:OE1	6:A:302:HOH:O	2.19	0.50
2:B:98:THR:HB	6:B:392:HOH:O	2.11	0.50
2:B:51:THR:HB	2:B:52:PRO:CD	2.41	0.50
2:E:130:ARG:HG3	2:E:130:ARG:NH1	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:141:GLY:CA	2:H:162:GLU:HG3	2.41	0.50
1:D:168:TRP:CZ2	2:E:4:PRO:HD2	2.47	0.49
1:D:43:TRP:CE3	1:D:48:PHE:HB3	2.48	0.49
2:E:134:ASN:HD21	2:E:169:ASP:HA	1.78	0.49
2:H:50:VAL:HG22	2:H:51:THR:HG23	1.94	0.49
1:D:52:ARG:NE	3:F:3:GLU:OE1	2.28	0.49
4:J:2:NAG:H82	4:J:3:NAG:O6	2.13	0.49
1:D:43:TRP:HB2	1:D:49:ARG:HG2	1.94	0.48
2:H:113:ASN:O	2:H:114:LEU:HD12	2.13	0.48
1:G:14:GLN:NE2	2:H:6:ASP:OD2	2.46	0.48
2:H:133:ARG:C	2:H:135:ASP:H	2.17	0.48
2:H:163:MET:HG2	2:H:164:THR:N	2.28	0.47
2:B:10:GLN:HB2	2:B:31:ILE:HB	1.97	0.47
2:H:54:GLY:N	2:H:55:PRO:CD	2.78	0.47
3:F:1:VAL:CG1	3:F:2:GLU:N	2.73	0.47
2:H:135:ASP:O	2:H:135:ASP:OD1	2.33	0.46
2:E:44:VAL:HG12	2:E:46:VAL:H	1.79	0.46
2:B:37:TYR:C	2:B:50:VAL:HG13	2.35	0.46
2:B:133:ARG:HG2	2:B:133:ARG:NH1	2.30	0.46
2:E:105:ARG:CD	6:E:215:HOH:O	2.55	0.46
2:H:46:VAL:HG22	2:H:62:ASN:OD1	2.16	0.46
2:H:132:PHE:HB2	2:H:172:THR:OG1	2.16	0.46
1:G:97:VAL:HG21	1:G:178:TRP:CZ2	2.51	0.46
1:A:55:ASP:HB2	1:G:-1:GLU:HB3	1.98	0.46
1:A:76:ARG:NH2	3:C:11:GLU:OE1	2.34	0.46
2:E:94:ARG:HG3	2:E:94:ARG:NH1	2.30	0.46
2:E:128:LYS:HE3	2:E:130:ARG:NE	2.31	0.45
1:A:43:TRP:HB2	1:A:49:ARG:HG2	1.98	0.45
2:H:141:GLY:O	2:H:162:GLU:HG2	2.17	0.45
2:E:70:ARG:NH2	6:E:208:HOH:O	2.49	0.45
1:A:21:GLN:HG2	6:A:329:HOH:O	2.17	0.45
2:B:133:ARG:HG2	2:B:133:ARG:HH11	1.81	0.45
1:A:152:THR:HG22	6:A:312:HOH:O	2.16	0.45
2:H:117:CYS:HB2	2:H:131:TRP:CZ2	2.52	0.44
1:A:52:ARG:HH21	3:C:3:GLU:CD	2.20	0.44
1:A:105:LEU:HD21	1:A:178:TRP:CD2	2.52	0.44
1:D:118:ASN:HB2	1:D:166:GLU:HB2	2.00	0.44
2:B:27:VAL:HA	2:B:40:PHE:O	2.17	0.44
2:B:145:THR:HB	2:B:146:PRO:HD2	1.98	0.44
2:H:167:ARG:HA	2:H:168:GLY:HA2	1.63	0.44
1:D:13:TYR:CZ	1:D:67:LYS:HG2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:ARG:HA	2:B:168:GLY:HA2	1.82	0.44
1:G:166:GLU:HB3	5:G:201:NAG:C8	2.48	0.44
1:A:46:PRO:O	1:A:50:ARG:HG2	2.18	0.43
1:A:103:ASN:HB3	1:A:153:PHE:CE1	2.53	0.43
2:B:55:PRO:N	2:B:56:PRO:HD2	2.33	0.43
2:E:134:ASN:O	2:E:135:ASP:HB2	2.18	0.43
2:H:3:SER:HB3	2:H:4:PRO:HD3	1.99	0.43
3:C:15:GLY:HA3	1:G:169:GLY:O	2.18	0.43
2:B:109:LEU:HA	2:B:109:LEU:HD23	1.63	0.43
1:G:50:ARG:NE	6:G:307:HOH:O	2.52	0.43
2:B:117:CYS:HB2	2:B:131:TRP:CZ2	2.53	0.43
2:E:184:ILE:C	2:E:185:ILE:HD12	2.39	0.43
2:E:51:THR:HB	2:E:52:PRO:HD2	2.01	0.42
2:H:134:ASN:O	2:H:135:ASP:OD1	2.37	0.42
1:A:14:GLN:NE2	2:B:6:ASP:OD2	2.52	0.42
1:A:118:ASN:HB2	1:A:166:GLU:HB2	2.01	0.42
1:G:154:LEU:HD12	1:G:154:LEU:HA	1.91	0.42
2:B:50:VAL:HG22	2:B:51:THR:HG23	2.01	0.42
5:G:201:NAG:H81	6:G:396:HOH:O	2.20	0.42
2:E:36:GLU:O	2:E:50:VAL:CG2	2.68	0.42
2:E:125:ALA:HB1	2:E:147:LEU:HD21	2.01	0.42
2:B:65:LYS:N	2:B:65:LYS:HD2	2.34	0.42
1:D:52:ARG:HH21	3:F:3:GLU:CD	2.23	0.42
1:D:30:GLU:OE2	1:D:33:TYR:HB3	2.20	0.41
2:E:65:LYS:O	2:E:69:GLU:HG3	2.20	0.41
1:G:11:ASN:HB2	2:H:11:PHE:HB3	2.02	0.41
1:G:50:ARG:NH1	6:G:308:HOH:O	2.52	0.41
4:J:1:NAG:O3	4:J:2:NAG:C8	2.67	0.41
1:A:50:ARG:NH2	6:A:303:HOH:O	2.21	0.41
1:D:122:LEU:HD23	1:D:127:SER:HA	2.02	0.41
1:D:166:GLU:HG2	1:D:173:PRO:HG3	2.03	0.41
1:G:38:ARG:NH1	6:G:306:HOH:O	2.52	0.41
2:H:141:GLY:HA2	2:H:162:GLU:HG3	2.02	0.41
1:G:11:ASN:HB3	1:G:66:LEU:HD11	2.02	0.41
2:H:73:ALA:HB3	6:H:221:HOH:O	2.20	0.41
2:H:3:SER:CB	2:H:4:PRO:CD	2.98	0.41
1:A:164:LYS:HG3	1:A:175:LEU:CD2	2.51	0.41
2:E:75:LEU:O	2:E:79:CYS:HB2	2.21	0.41
2:E:165:PRO:O	2:E:166:GLN:NE2	2.53	0.41
1:A:107:CYS:HB2	1:A:121:TRP:CH2	2.56	0.40
2:B:88:ARG:NH1	6:B:310:HOH:O	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:ASN:O	1:D:73:VAL:HG22	2.20	0.40
2:H:55:PRO:HB2	2:H:56:PRO:HD3	2.04	0.40
2:H:145:THR:HB	2:H:146:PRO:HD2	2.03	0.40
2:H:55:PRO:N	2:H:56:PRO:HD2	2.37	0.40

There are no symmetry-related clashes.

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	182/185 (98%)	178 (98%)	4 (2%)	0	100 100
1	D	179/185 (97%)	175 (98%)	4 (2%)	0	100 100
1	G	180/185 (97%)	175 (97%)	5 (3%)	0	100 100
2	B	184/189 (97%)	178 (97%)	4 (2%)	2 (1%)	14 5
2	E	186/189 (98%)	180 (97%)	5 (3%)	1 (0%)	29 17
2	H	175/189 (93%)	165 (94%)	8 (5%)	2 (1%)	14 5
3	C	13/16 (81%)	12 (92%)	1 (8%)	0	100 100
3	F	12/16 (75%)	12 (100%)	0	0	100 100
3	I	12/16 (75%)	12 (100%)	0	0	100 100
All	All	1123/1170 (96%)	1087 (97%)	31 (3%)	5 (0%)	34 24

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	4	PRO
2	B	109	LEU
2	E	167	ARG
2	B	107	GLU
2	H	167	ARG

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	169/170 (99%)	163 (96%)	6 (4%)	35 20
1	D	166/170 (98%)	164 (99%)	2 (1%)	71 64
1	G	166/170 (98%)	161 (97%)	5 (3%)	41 27
2	B	172/174 (99%)	167 (97%)	5 (3%)	42 28
2	E	171/174 (98%)	164 (96%)	7 (4%)	30 15
2	H	165/174 (95%)	158 (96%)	7 (4%)	30 14
3	C	10/10 (100%)	10 (100%)	0	100 100
3	F	10/10 (100%)	10 (100%)	0	100 100
3	I	10/10 (100%)	9 (90%)	1 (10%)	7 1
All	All	1039/1062 (98%)	1006 (97%)	33 (3%)	39 25

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ARG
1	A	66	LEU
1	A	108	LEU
1	A	152	THR
1	A	175	LEU
1	A	181	GLU
2	B	50	VAL
2	B	68	LEU
2	B	98	THR
2	B	167	ARG
2	B	191	GLN
1	D	-1	GLU
1	D	108	LEU
2	E	64	GLN
2	E	66	GLU
2	E	98	THR
2	E	105	ARG
2	E	110	ASN

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Mol	Chain	Res	Type
2	E	126	GLN
2	E	181	GLN
1	G	62	ASN
1	G	66	LEU
1	G	108	LEU
1	G	138	LEU
1	G	176	LYS
2	H	46	VAL
2	H	50	VAL
2	H	65	LYS
2	H	114	LEU
2	H	162	GLU
2	H	163	MET
2	H	167	ARG
3	I	13	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	191	GLN
2	E	19	ASN
2	E	111	HIS
2	E	166	GLN

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)

3 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	$\#\|Z\| > 2$
4	NAG	J	1	1,4	14,14,15	0.36	0	17,19,21	1.23	2 (11%)
4	NAG	J	2	4	14,14,15	1.25	2 (14%)	17,19,21	1.24	1 (5%)
4	NAG	J	3	4	14,14,15	0.76	1 (7%)	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	J	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	3/6/23/26	0/1/1/1
4	NAG	J	3	4	-	4/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	2	NAG	O5-C1	-3.93	1.37	1.43
4	J	3	NAG	C1-C2	2.65	1.56	1.52
4	J	2	NAG	C1-C2	-2.38	1.48	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	2	NAG	C1-O5-C5	4.16	117.83	112.19
4	J	1	NAG	O3-C3-C2	-3.86	101.47	109.47
4	J	1	NAG	C1-O5-C5	2.06	114.99	112.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
4	J	3	NAG	C8-C7-N2-C2
4	J	3	NAG	O7-C7-N2-C2

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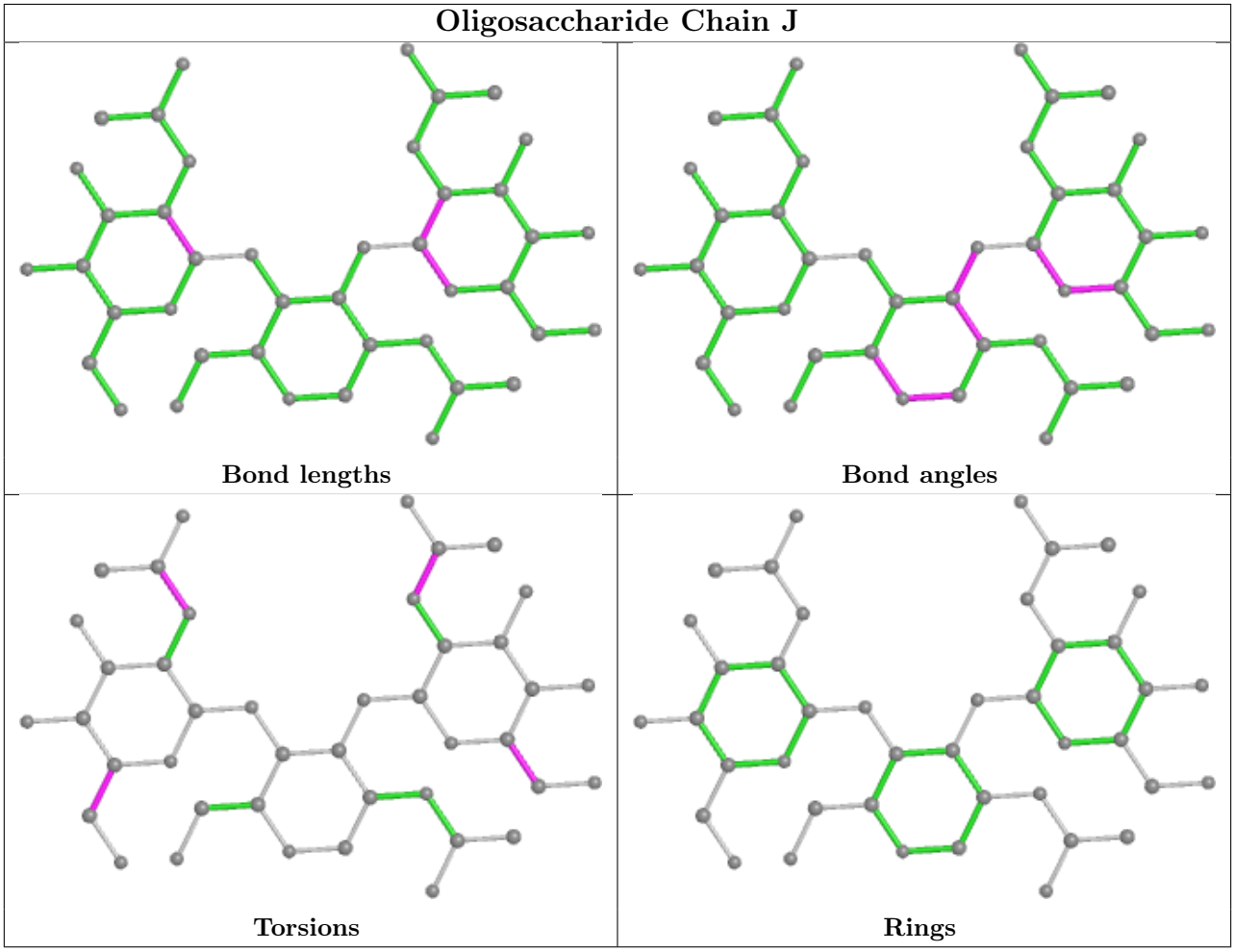
Mol	Chain	Res	Type	Atoms
4	J	3	NAG	O5-C5-C6-O6
4	J	3	NAG	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	1	NAG	3	0
4	J	3	NAG	2	0
4	J	2	NAG	5	0

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



5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	A	204	1	14,14,15	0.56	0	17,19,21	0.80	1 (5%)
5	NAG	G	201	1	14,14,15	0.65	1 (7%)	17,19,21	0.62	0
5	NAG	D	201	1	14,14,15	0.59	1 (7%)	17,19,21	0.78	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
5	NAG	A	204	1	-	2/6/23/26	0/1/1/1
5	NAG	G	201	1	-	2/6/23/26	0/1/1/1
5	NAG	D	201	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	201	NAG	O5-C1	-2.31	1.40	1.43
5	D	201	NAG	O5-C1	-2.05	1.40	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	204	NAG	C2-N2-C7	2.19	126.02	122.90

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	204	NAG	C8-C7-N2-C2
5	A	204	NAG	O7-C7-N2-C2
5	D	201	NAG	C8-C7-N2-C2
5	D	201	NAG	O7-C7-N2-C2
5	G	201	NAG	C8-C7-N2-C2
5	G	201	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	201	NAG	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	183/185 (98%)	0.60	4 (2%) 62 69	16, 24, 38, 62	0
1	D	181/185 (97%)	0.74	17 (9%) 8 12	19, 29, 50, 71	0
1	G	182/185 (98%)	0.70	11 (6%) 21 28	21, 30, 53, 67	0
2	B	188/189 (99%)	0.63	10 (5%) 26 33	16, 26, 48, 62	0
2	E	188/189 (99%)	0.71	11 (5%) 22 28	18, 26, 46, 70	0
2	H	179/189 (94%)	0.88	16 (8%) 9 14	21, 31, 54, 73	0
3	C	15/16 (93%)	0.82	1 (6%) 17 24	18, 26, 39, 47	0
3	F	14/16 (87%)	0.95	2 (14%) 2 3	21, 27, 54, 59	0
3	I	14/16 (87%)	1.16	2 (14%) 2 3	25, 30, 45, 45	0
All	All	1144/1170 (97%)	0.72	74 (6%) 18 25	16, 28, 51, 73	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	3	SER	8.5
2	H	4	PRO	7.0
2	E	4	PRO	6.1
3	F	1	VAL	6.0
3	I	14	GLY	5.9
2	E	109	LEU	5.8
1	D	158	ASP	5.5
1	G	129	THR	5.3
2	B	109	LEU	5.2
2	H	162	GLU	5.2
2	H	3	SER	5.1
2	H	114	LEU	4.9
2	H	165	PRO	4.6
2	B	3	SER	4.5
2	H	113	ASN	4.5

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Mol	Chain	Res	Type	RSRZ
2	E	111	HIS	4.3
1	A	0	ASP	4.2
1	G	128	VAL	4.0
1	A	2	VAL	4.0
1	G	-2	GLY	4.0
1	D	160	ILE	4.0
2	E	110	ASN	3.8
2	H	5	GLU	3.8
2	B	4	PRO	3.7
2	H	135	ASP	3.7
1	D	-1	GLU	3.6
1	G	126	HIS	3.5
1	D	101	GLN	3.5
1	D	129	THR	3.4
1	D	170	LEU	3.4
1	D	0	ASP	3.4
1	G	130	GLU	3.4
1	D	128	VAL	3.4
1	G	177	HIS	3.2
1	D	154	LEU	3.0
1	D	174	LEU	2.9
2	E	105	ARG	2.9
2	H	163	MET	2.9
2	B	139	THR	2.9
1	G	160	ILE	2.8
2	E	168	GLY	2.8
2	E	166	GLN	2.8
2	B	104	SER	2.8
2	H	164	THR	2.7
1	D	159	GLU	2.7
1	D	37	GLU	2.7
1	G	122	LEU	2.7
1	D	169	GLY	2.7
1	A	181	GLU	2.6
2	H	187	GLU	2.6
2	H	140	THR	2.6
1	D	16	TYR	2.5
2	E	174	HIS	2.5
2	B	168	GLY	2.4
1	D	126	HIS	2.4
3	F	13	CYS	2.4
1	D	130	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	175	LEU	2.3
2	B	108	ALA	2.3
1	D	2	VAL	2.2
2	B	106	THR	2.2
1	A	171	ASP	2.2
1	G	9(A)	GLY	2.2
2	E	160	MET	2.2
2	B	110	ASN	2.2
2	E	22	GLU	2.2
2	H	139	THR	2.2
2	B	191	GLN	2.1
2	H	66	GLU	2.1
2	H	125	ALA	2.1
3	I	13	CYS	2.1
2	H	136	GLN	2.0
3	C	12	GLY	2.0
1	G	2	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)

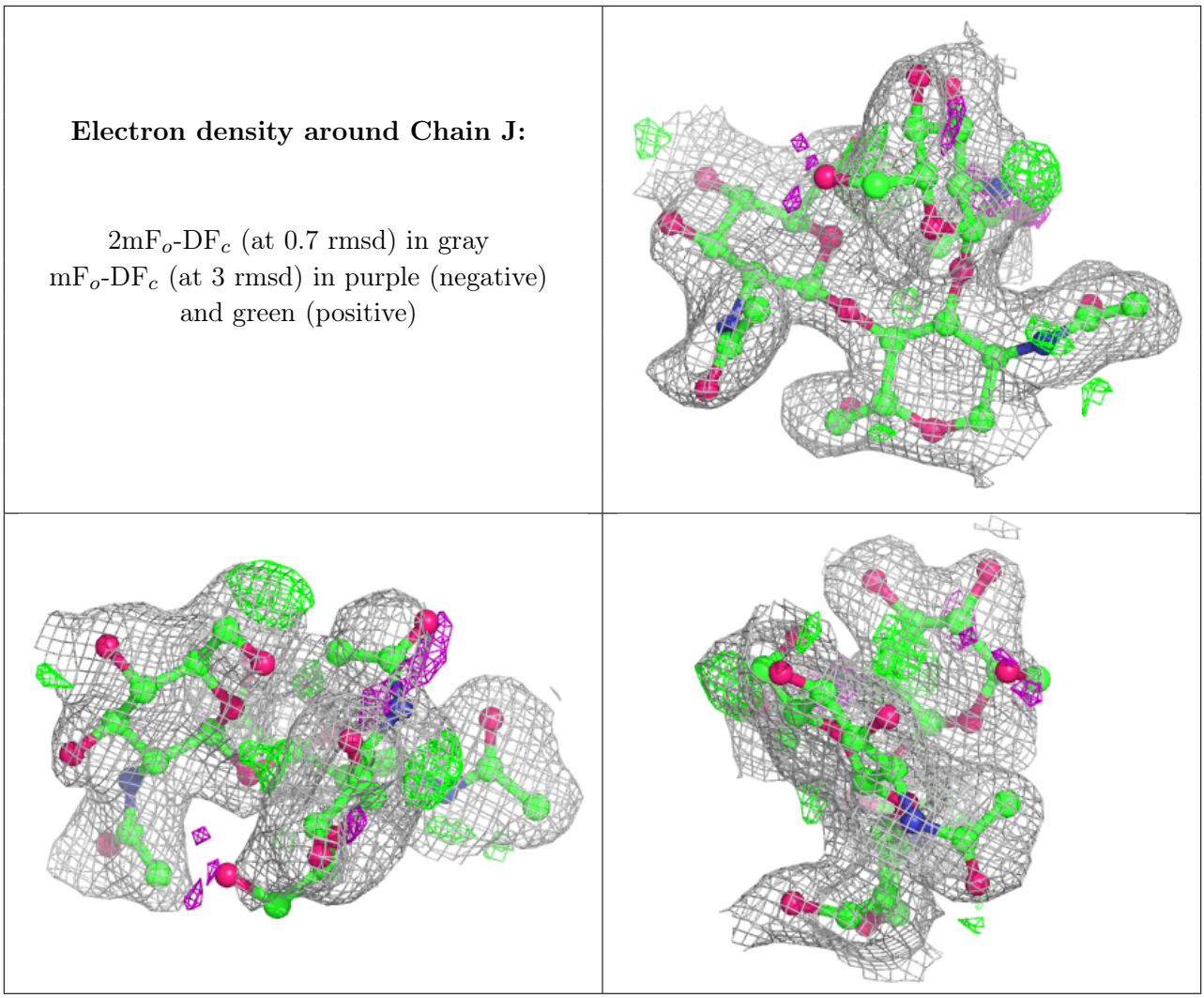
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	NAG	J	2	14/15	0.77	0.26	34,46,54,56	0
4	NAG	J	1	14/15	0.84	0.14	33,38,45,46	0
4	NAG	J	3	14/15	0.87	0.14	41,45,53,53	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 J:

$2mF_o$-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
5	NAG	D	201	14/15	0.72	0.22	38,45,53,55	0
5	NAG	A	204	14/15	0.82	0.15	34,46,60,63	0
5	NAG	G	201	14/15	0.84	0.20	39,48,54,54	0

6.5 Other polymers

There are no such residues in this entry.