



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:50 PM UTC

PDB ID : 8EUQ / pdb_00008euq
Title : Crystal structure of HLA-DRA*01:01/HLA-DRB1*04:01 in complex with c44H10 Fab
Authors : Kassardjian, A.; Julien, J.-P.
Deposited on : 2022-10-19
Resolution : 3.09 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

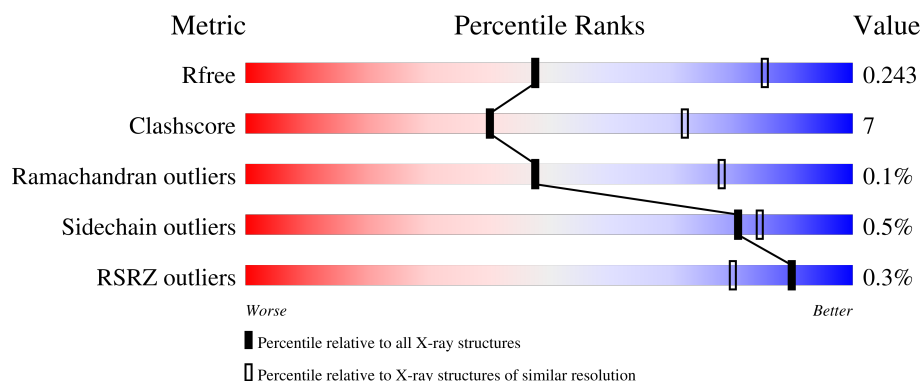
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	188	
1	F	188	
2	D	214	
2	H	214	
3	B	226	

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Mol	Chain	Length	Quality of chain
3	G	226	% 78%13%9%
4	C	223	82%18%
4	I	223	78%21%
5	E	2	100%
5	J	2	100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13053 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 HLA class II histocompatibility antigen, DR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	0	0
			1515	978	246	286	5			
1	F	185	Total	C	N	O	S	0	0	0
			1515	978	246	286	5			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	THR	-	expression tag	UNP P01903
A	183	SER	-	expression tag	UNP P01903
A	184	GLY	-	expression tag	UNP P01903
A	185	GLU	-	expression tag	UNP P01903
A	186	ASN	-	expression tag	UNP P01903
A	187	LEU	-	expression tag	UNP P01903
A	188	TYR	-	expression tag	UNP P01903
A	189	PHE	-	expression tag	UNP P01903
A	190	GLN	-	expression tag	UNP P01903
F	182	THR	-	expression tag	UNP P01903
F	183	SER	-	expression tag	UNP P01903
F	184	GLY	-	expression tag	UNP P01903
F	185	GLU	-	expression tag	UNP P01903
F	186	ASN	-	expression tag	UNP P01903
F	187	LEU	-	expression tag	UNP P01903
F	188	TYR	-	expression tag	UNP P01903
F	189	PHE	-	expression tag	UNP P01903
F	190	GLN	-	expression tag	UNP P01903

- Molecule 2 is a protein called c44H10 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	212	Total	C	N	O	S	0	0	0
			1624	1012	272	335	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	213	Total	C	N	O	S	0	0	0
			1644	1026	275	338	5			

- Molecule 3 is a protein called Hemagglutinin HA1 chain,HLA class II histocompatibility antigen DR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	201	Total	C	N	O	S	0	0	0
			1617	1023	285	304	5			
3	G	205	Total	C	N	O	S	0	0	0
			1663	1050	294	314	5			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	3	GLY	ALA	engineered mutation	UNP P04664
B	4	ALA	CYS	engineered mutation	UNP P04664
B	18	SER	-	linker	UNP P04664
B	19	GLY	-	linker	UNP P04664
B	20	GLY	-	linker	UNP P04664
B	21	SER	-	linker	UNP P04664
B	22	GLY	-	linker	UNP P04664
B	23	SER	-	linker	UNP P04664
B	24	ILE	-	linker	UNP P04664
B	25	GLU	-	linker	UNP P04664
B	26	GLY	-	linker	UNP P04664
B	27	ARG	-	linker	UNP P04664
B	28	GLY	-	linker	UNP P04664
B	29	SER	-	linker	UNP P04664
B	220	THR	-	expression tag	UNP A0A1V1IGJ9
B	221	GLY	-	expression tag	UNP A0A1V1IGJ9
B	222	GLY	-	expression tag	UNP A0A1V1IGJ9
B	223	GLU	-	expression tag	UNP A0A1V1IGJ9
B	224	ASN	-	expression tag	UNP A0A1V1IGJ9
B	225	LEU	-	expression tag	UNP A0A1V1IGJ9
B	226	TYR	-	expression tag	UNP A0A1V1IGJ9
B	227	PHE	-	expression tag	UNP A0A1V1IGJ9
B	228	GLN	-	expression tag	UNP A0A1V1IGJ9
G	3	GLY	ALA	engineered mutation	UNP P04664
G	4	ALA	CYS	engineered mutation	UNP P04664
G	18	SER	-	linker	UNP P04664
G	19	GLY	-	linker	UNP P04664

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Chain	Residue	Modelled	Actual	Comment	Reference
G	20	GLY	-	linker	UNP P04664
G	21	SER	-	linker	UNP P04664
G	22	GLY	-	linker	UNP P04664
G	23	SER	-	linker	UNP P04664
G	24	ILE	-	linker	UNP P04664
G	25	GLU	-	linker	UNP P04664
G	26	GLY	-	linker	UNP P04664
G	27	ARG	-	linker	UNP P04664
G	28	GLY	-	linker	UNP P04664
G	29	SER	-	linker	UNP P04664
G	220	THR	-	expression tag	UNP A0A1V1IGJ9
G	221	GLY	-	expression tag	UNP A0A1V1IGJ9
G	222	GLY	-	expression tag	UNP A0A1V1IGJ9
G	223	GLU	-	expression tag	UNP A0A1V1IGJ9
G	224	ASN	-	expression tag	UNP A0A1V1IGJ9
G	225	LEU	-	expression tag	UNP A0A1V1IGJ9
G	226	TYR	-	expression tag	UNP A0A1V1IGJ9
G	227	PHE	-	expression tag	UNP A0A1V1IGJ9
G	228	GLN	-	expression tag	UNP A0A1V1IGJ9

- Molecule 4 is a protein called c44H10 Fab heavy chain.

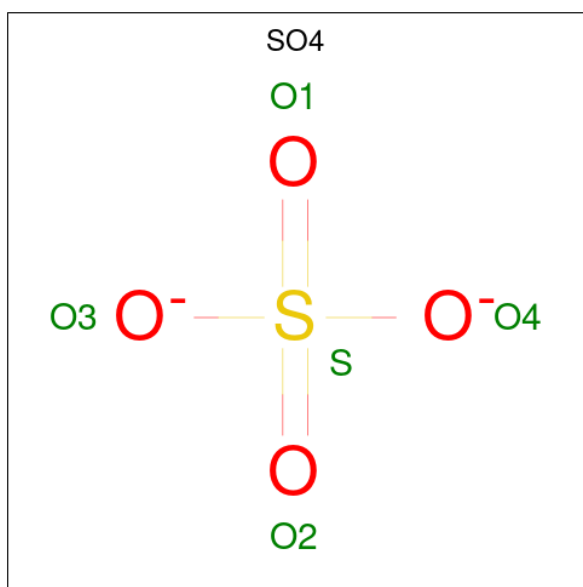
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	222	Total	C	N	O	S	0	0	0
			1655	1050	273	324	8			
4	I	222	Total	C	N	O	S	0	0	0
			1656	1050	273	325	8			

- Molecule 5 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
5	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



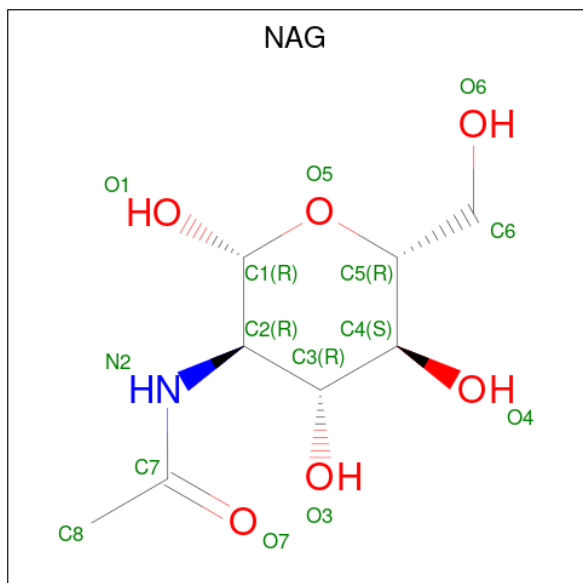
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	O	S	0	0
			5	4	1		
6	I	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

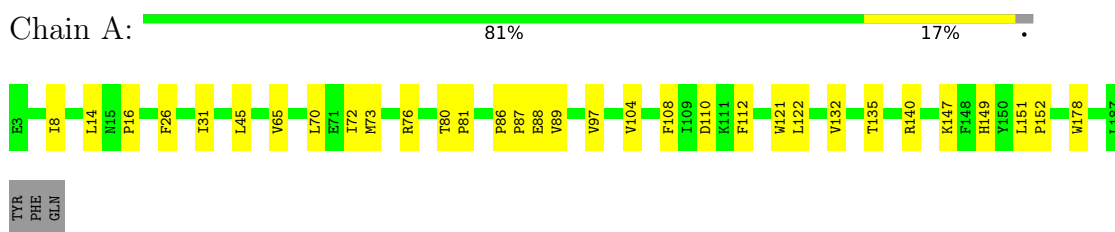


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		

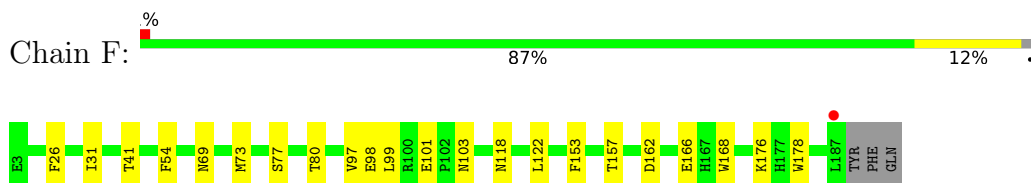
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

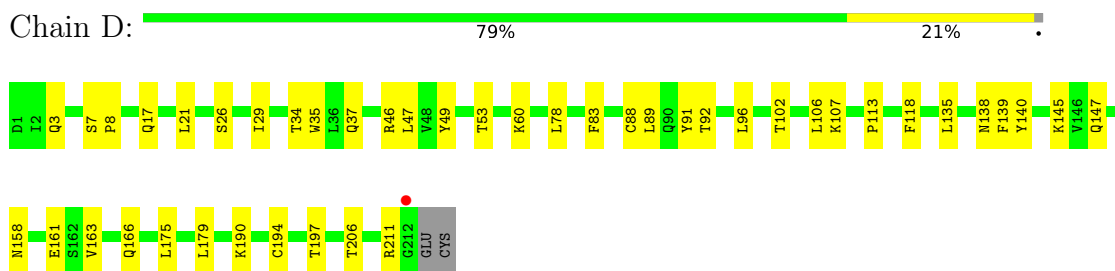
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain



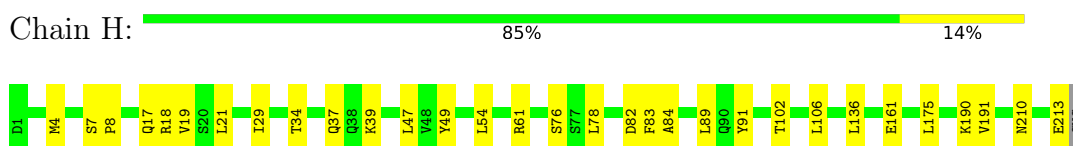
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain



- Molecule 2: c44H10 Fab light chain

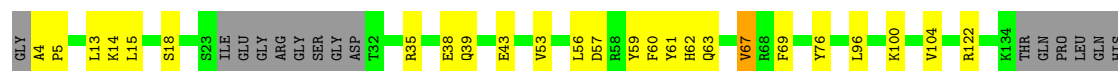


- Molecule 2: c44H10 Fab light chain

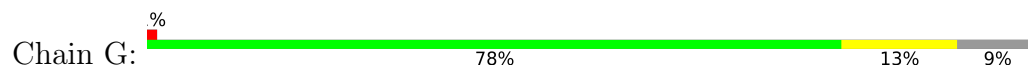


- Molecule 3: Hemagglutinin HA1 chain, HLA class II histocompatibility antigen DR beta chain

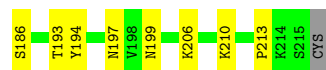
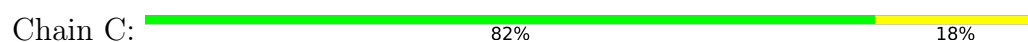




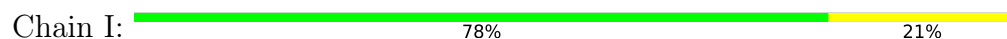
- Molecule 3: Hemagglutinin HA1 chain, HLA class II histocompatibility antigen DR beta chain



- Molecule 4: c44H10 Fab heavy chain



- Molecule 4: c44H10 Fab heavy chain



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.15Å 178.72Å 182.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.51 – 3.09 39.51 – 3.09	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.51-3.09) 99.8 (39.51-3.09)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.200 , 0.244 0.201 , 0.243	Depositor DCC
R_{free} test set	1998 reflections (3.93%)	wwPDB-VP
Wilson B-factor (Å ²)	87.6	Xtriage
Anisotropy	0.723	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 72.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13053	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SO4

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	0.19	0/1560	0.39	0/2127
1	F	0.17	0/1560	0.38	0/2127
2	D	0.16	0/1656	0.41	0/2248
2	H	0.19	0/1676	0.42	0/2272
3	B	0.17	0/1656	0.35	1/2245 (0.0%)
3	G	0.17	0/1704	0.34	0/2309
4	C	0.17	0/1698	0.40	0/2315
4	I	0.15	0/1699	0.38	0/2316
All	All	0.17	0/13209	0.38	1/17959 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	62	HIS	CB-CA-C	-5.36	109.94	117.23

There are no chirality outliers.

There are no planarity outliers.

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	1515	0	1444	23	0
1	F	1515	0	1444	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1624	0	1565	29	0
2	H	1644	0	1602	20	0
3	B	1617	0	1527	29	0
3	G	1663	0	1570	17	0
4	C	1655	0	1623	28	0
4	I	1656	0	1626	29	0
5	E	28	0	25	0	0
5	J	28	0	25	2	0
6	A	10	0	0	0	0
6	B	30	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	0	0
6	F	5	0	0	0	0
6	G	20	0	0	0	0
6	I	5	0	0	0	0
7	B	14	0	13	0	0
7	G	14	0	13	0	0
All	All	13053	0	12477	168	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 7.

All (168) 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)
4:C:30:THR:HG22	4:C:73:ASN:HD22	1.50	0.76
4:I:159:LEU:HD21	4:I:182:VAL:HG11	1.69	0.74
4:C:126:PRO:HG3	4:C:138:LEU:HB3	1.71	0.72
2:H:190:LYS:HG3	2:H:191:VAL:HG23	1.71	0.70
2:H:7:SER:HB2	2:H:8:PRO:HD3	1.74	0.69
2:H:136:LEU:HD22	2:H:175:LEU:HD23	1.75	0.69
3:B:143:LEU:HD22	3:B:191:GLU:HA	1.75	0.67
2:H:34:THR:HG22	2:H:49:TYR:HA	1.77	0.67
4:I:18:LEU:O	4:I:81:LYS:HA	1.95	0.67
2:H:18:ARG:HG2	2:H:76:SER:HA	1.78	0.64
4:C:132:SER:HB2	4:I:133:GLY:HA3	1.79	0.63
3:B:13:LEU:HD13	3:B:96:LEU:HD11	1.81	0.63
4:I:119:PRO:HB3	4:I:145:TYR:HB3	1.79	0.63
2:D:7:SER:HB2	2:D:8:PRO:HD3	1.79	0.62
4:I:153:SER:HB2	4:I:197:ASN:HB2	1.80	0.62
1:A:135:THR:O	1:A:147:LYS:NZ	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:118:ASN:HB2	1:F:166:GLU:HB3	1.82	0.62
3:B:53:VAL:HB	3:B:104:VAL:HG13	1.82	0.61
3:G:150:GLY:HA2	3:G:183:THR:HB	1.82	0.61
3:G:143:LEU:HD13	3:G:191:GLU:HA	1.82	0.60
2:D:161:GLU:HB2	2:D:175:LEU:HD11	1.82	0.60
3:B:13:LEU:HD11	3:B:100:LYS:HE3	1.83	0.59
4:C:126:PRO:HD2	4:C:213:PRO:HA	1.85	0.59
4:C:18:LEU:HB3	4:C:82:MET:HB2	1.86	0.58
1:A:45:LEU:HD11	3:B:182:TRP:HB2	1.85	0.58
2:H:37:GLN:HB2	2:H:47:LEU:HD11	1.87	0.56
4:I:87:THR:HG23	4:I:110:THR:HA	1.88	0.56
2:D:106:LEU:O	2:D:166:GLN:NE2	2.35	0.56
2:D:145:LYS:HB3	2:D:197:THR:HB	1.87	0.55
4:I:29:LEU:HB3	4:I:71:LYS:HD2	1.88	0.55
1:F:98:GLU:HG3	1:F:101:GLU:HB2	1.89	0.55
3:G:161:PHE:HB2	3:G:201:THR:HB	1.88	0.55
2:D:34:THR:HG22	2:D:49:TYR:HA	1.89	0.55
2:H:161:GLU:HB2	2:H:175:LEU:HD11	1.88	0.55
4:C:63:LEU:HB3	4:C:67:LEU:HD23	1.88	0.54
1:F:77:SER:OG	1:F:80:THR:HB	2.07	0.54
1:F:26:PHE:HB2	1:F:31:ILE:HD11	1.90	0.54
1:A:88:GLU:HG3	4:C:96:TYR:CZ	2.44	0.53
3:B:145:VAL:HG22	3:B:189:MET:HE2	1.91	0.53
3:B:150:GLY:HA2	3:B:183:THR:HB	1.91	0.53
4:I:116:THR:HG22	4:I:147:PRO:HD3	1.90	0.53
4:I:69:ILE:HG12	4:I:80:LEU:HD23	1.90	0.52
2:D:190:LYS:HD2	2:D:211:ARG:HE	1.74	0.52
1:F:73:MET:HE3	3:G:15:LEU:HD11	1.90	0.52
4:C:47:TRP:HZ2	4:C:50:VAL:HG12	1.74	0.52
3:B:122:ARG:NH1	3:B:182:TRP:O	2.41	0.52
2:D:37:GLN:HB2	2:D:47:LEU:HD11	1.92	0.52
1:F:97:VAL:HG21	1:F:178:TRP:HZ2	1.75	0.52
4:C:135:THR:HG23	4:I:135:THR:HG23	1.93	0.51
1:F:99:LEU:HD21	1:F:157:THR:HG23	1.92	0.51
3:B:154:GLY:HA3	3:B:176:LEU:HD21	1.93	0.51
2:D:17:GLN:O	2:D:78:LEU:HB2	2.11	0.51
4:I:59:TYR:HE1	4:I:69:ILE:HG13	1.76	0.51
3:G:69:PHE:HB2	3:G:76:TYR:CE1	2.46	0.51
2:D:135:LEU:HD22	4:C:181:VAL:HG11	1.93	0.51
2:H:21:LEU:HD22	2:H:102:THR:HG21	1.93	0.50
4:I:39:GLN:HB2	4:I:45:LEU:HD23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:35:TRP:CZ3	2:D:88:CYS:HB3	2.47	0.50
4:C:159:LEU:HD21	4:C:182:VAL:HG11	1.94	0.49
3:B:57:ASP:HB3	3:B:69:PHE:HB3	1.93	0.49
4:C:18:LEU:HB2	4:C:82(C):LEU:HD11	1.93	0.49
1:A:86:PRO:HB2	4:C:100(B):TYR:CE1	2.47	0.49
4:C:163:VAL:HG22	4:C:182:VAL:HG22	1.95	0.49
3:B:69:PHE:HB2	3:B:76:TYR:CE1	2.48	0.49
2:H:34:THR:HG23	2:H:91:TYR:CE1	2.48	0.48
2:H:210:ASN:HB2	2:H:213:GLU:HG2	1.94	0.48
2:H:39:LYS:HD2	2:H:84:ALA:HB2	1.95	0.48
1:A:26:PHE:HB2	1:A:31:ILE:HD11	1.95	0.48
1:A:65:VAL:HG13	3:B:14:LYS:HG2	1.94	0.48
3:G:47:PHE:HB2	3:G:52:ARG:HB2	1.94	0.48
4:C:135:THR:CG2	4:I:135:THR:HG23	2.43	0.48
1:F:103:ASN:HB3	1:F:153:PHE:CE1	2.49	0.48
2:D:138:ASN:HB3	4:I:187:SER:HB3	1.95	0.47
2:D:145:LYS:HE3	2:D:147:GLN:NE2	2.29	0.47
3:B:209:LEU:HD13	3:B:213:LEU:HG	1.95	0.47
3:G:58:ARG:HD2	3:G:65:GLU:OE2	2.14	0.47
2:D:3:GLN:HB3	2:D:26:SER:HB3	1.97	0.47
3:G:91:ASN:HA	3:G:97:LEU:HD11	1.96	0.47
1:A:132:VAL:HG22	1:A:151:LEU:HD13	1.96	0.47
1:A:147:LYS:HE3	1:A:149:HIS:NE2	2.30	0.47
4:I:117:LYS:HD3	4:I:175:LEU:HD21	1.96	0.47
2:H:19:VAL:HG13	2:H:78:LEU:HD11	1.97	0.47
4:I:163:VAL:HG22	4:I:182:VAL:HG22	1.97	0.47
1:A:87:PRO:HA	1:A:112:PHE:HB3	1.96	0.46
4:C:65:SER:C	4:C:67:LEU:H	2.22	0.46
2:D:118:PHE:CD2	4:C:124:LEU:HB3	2.51	0.46
1:A:14:LEU:HD11	3:B:35:ARG:HB3	1.97	0.46
4:I:89:MET:HE2	4:I:108:SER:OG	2.15	0.46
1:A:104:VAL:HA	1:A:152:PRO:HA	1.96	0.46
4:C:53:ALA:O	4:C:71:LYS:NZ	2.49	0.46
3:B:63:GLN:OE1	3:B:63:GLN:N	2.49	0.46
2:D:34:THR:HG23	2:D:91:TYR:CE1	2.51	0.45
2:H:4:MET:HE1	2:H:29:ILE:HD13	1.97	0.45
4:C:135:THR:O	4:C:186:SER:HB3	2.16	0.45
3:G:36:PHE:HA	3:G:62:HIS:HE1	1.82	0.45
4:I:18:LEU:HB2	4:I:82(C):LEU:HD11	1.98	0.45
2:D:29:ILE:HA	2:D:92:THR:HG21	1.98	0.45
1:F:122:LEU:HB2	1:F:162:ASP:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:17:GLN:O	2:H:78:LEU:HG	2.16	0.45
1:A:73:MET:HE3	3:B:15:LEU:HD11	1.98	0.45
3:B:146:CYS:HB2	3:B:160:TRP:CZ2	2.51	0.45
4:C:29:LEU:HB3	4:C:71:LYS:HD2	1.99	0.45
4:C:184:VAL:HG11	4:C:194:TYR:CE1	2.52	0.45
1:A:73:MET:HB3	3:B:61:TYR:CD1	2.52	0.45
1:A:97:VAL:HG11	1:A:178:TRP:HZ2	1.82	0.45
2:D:163:VAL:HG22	2:D:175:LEU:HD13	1.99	0.45
2:H:34:THR:OG1	2:H:89:LEU:HB3	2.17	0.45
1:F:41:THR:HG21	1:F:54:PHE:HB3	1.99	0.45
4:C:59:TYR:HE1	4:C:69:ILE:HG13	1.82	0.45
2:D:34:THR:OG1	2:D:89:LEU:HB3	2.17	0.44
3:B:59:TYR:HB2	3:B:67:VAL:HG13	1.99	0.44
4:C:68:SER:HB3	4:C:81:LYS:HB3	1.98	0.44
3:G:104:VAL:HG12	3:G:109:ARG:NH1	2.33	0.44
3:B:199:VAL:HG22	3:B:218:ARG:HD3	2.00	0.44
5:J:1:NAG:H61	5:J:2:NAG:C7	2.48	0.44
2:H:61:ARG:NE	2:H:82:ASP:OD2	2.45	0.44
4:C:193:THR:HG23	4:C:210:LYS:HE3	1.99	0.44
2:H:54:LEU:HD12	2:H:54:LEU:HA	1.89	0.43
1:A:97:VAL:HG11	1:A:178:TRP:CZ2	2.53	0.43
2:H:83:PHE:CZ	2:H:106:LEU:HD13	2.53	0.43
2:D:21:LEU:CD2	2:D:102:THR:HG21	2.48	0.43
2:H:21:LEU:CD2	2:H:102:THR:HG21	2.48	0.43
3:B:171:VAL:HG13	3:B:188:VAL:HG13	2.00	0.43
3:G:143:LEU:HD12	3:G:189:MET:HE2	2.00	0.43
1:F:176:LYS:HD3	1:F:176:LYS:HA	1.92	0.43
4:I:146:PHE:HA	4:I:147:PRO:HA	1.86	0.43
3:G:206:HIS:CG	3:G:207:PRO:HD2	2.54	0.43
1:A:16:PRO:HD2	3:B:35:ARG:HD3	2.00	0.43
1:A:70:LEU:HD13	3:B:38:GLU:HB2	2.01	0.42
2:D:96:LEU:HB2	4:C:47:TRP:CG	2.54	0.42
2:D:107:LYS:HA	2:D:140:TYR:OH	2.19	0.42
4:C:199:ASN:HD21	4:C:206:LYS:HE2	1.84	0.42
4:I:11:LEU:HB2	4:I:147:PRO:HG3	2.02	0.42
4:I:67:LEU:HD23	4:I:67:LEU:HA	1.81	0.42
1:A:121:TRP:O	1:A:122:LEU:HD23	2.19	0.42
4:C:153:SER:OG	4:C:197:ASN:HB2	2.19	0.42
1:A:72:ILE:HG22	1:A:76:ARG:HD3	2.02	0.42
3:B:206:HIS:CG	3:B:207:PRO:HD2	2.54	0.42
3:B:39:GLN:HB2	3:B:60:PHE:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ILE:HA	3:B:43:GLU:HA	2.02	0.41
2:D:190:LYS:HD2	2:D:190:LYS:HA	1.88	0.41
4:I:13:ALA:HB3	4:I:16:GLN:HG3	2.02	0.41
4:I:52:TRP:O	4:I:71:LYS:NZ	2.41	0.41
2:D:158:ASN:O	2:D:179:LEU:HA	2.19	0.41
4:I:66:ARG:O	4:I:82:MET:HA	2.20	0.41
3:B:56:LEU:HD12	3:B:56:LEU:HA	1.89	0.41
4:I:35:HIS:ND1	4:I:50:VAL:HB	2.35	0.41
4:I:39:GLN:HG3	4:I:44:GLY:O	2.21	0.41
1:A:80:THR:HA	1:A:81:PRO:HD3	1.86	0.41
1:F:168:TRP:CE2	5:J:1:NAG:H83	2.55	0.41
1:A:89:VAL:HA	1:A:108:PHE:O	2.21	0.41
2:D:21:LEU:HD22	2:D:102:THR:HG21	2.03	0.41
2:D:113:PRO:HB3	2:D:139:PHE:HB3	2.01	0.41
3:G:13:LEU:HD13	3:G:96:LEU:HD11	2.03	0.41
3:G:36:PHE:HA	3:G:62:HIS:CE1	2.56	0.41
3:G:154:GLY:HA3	3:G:176:LEU:HD21	2.02	0.41
4:I:11:LEU:HD21	4:I:114:ALA:O	2.21	0.41
2:D:53:THR:OG1	3:B:63:GLN:HG3	2.21	0.41
2:H:4:MET:CE	2:H:29:ILE:HD13	2.51	0.41
4:I:184:VAL:HG11	4:I:194:TYR:CE1	2.55	0.41
4:I:212:GLU:HA	4:I:213:PRO:HD3	1.98	0.41
2:D:46:ARG:HD3	4:C:100(D):MET:O	2.21	0.40
3:B:4:ALA:HB3	3:B:5:PRO:HD3	2.03	0.40
1:A:110:ASP:OD1	1:A:140:ARG:HD2	2.22	0.40
2:D:194:CYS:O	2:D:206:THR:HA	2.20	0.40
2:D:83:PHE:CZ	2:D:106:LEU:HD13	2.56	0.40
1:F:69:ASN:CG	3:G:15:LEU:HG	2.46	0.40
3:G:156:ILE:HD11	3:G:204:VAL:HG13	2.03	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	183/188 (97%)	175 (96%)	8 (4%)	0	100	100
1	F	183/188 (97%)	176 (96%)	7 (4%)	0	100	100
2	D	210/214 (98%)	197 (94%)	13 (6%)	0	100	100
2	H	211/214 (99%)	196 (93%)	15 (7%)	0	100	100
3	B	195/226 (86%)	182 (93%)	12 (6%)	1 (0%)	24	57
3	G	199/226 (88%)	188 (94%)	11 (6%)	0	100	100
4	C	220/223 (99%)	206 (94%)	13 (6%)	1 (0%)	24	57
4	I	220/223 (99%)	209 (95%)	11 (5%)	0	100	100
All	All	1621/1702 (95%)	1529 (94%)	90 (6%)	2 (0%)	48	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	131	THR
3	B	18	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	169/172 (98%)	169 (100%)	0	100	100
1	F	169/172 (98%)	169 (100%)	0	100	100
2	D	184/189 (97%)	183 (100%)	1 (0%)	81	85
2	H	188/189 (100%)	188 (100%)	0	100	100
3	B	172/197 (87%)	170 (99%)	2 (1%)	63	78
3	G	178/197 (90%)	177 (99%)	1 (1%)	78	83
4	C	187/189 (99%)	187 (100%)	0	100	100
4	I	188/189 (100%)	185 (98%)	3 (2%)	55	75
All	All	1435/1494 (96%)	1428 (100%)	7 (0%)	81	85

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

Mol	Chain	Res	Type
2	D	60	LYS
3	B	67	VAL
3	B	215	VAL
3	G	66	TYR
4	I	24	VAL
4	I	85	ASP
4	I	113	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	137	ASN
2	D	138	ASN
2	D	155	GLN
1	F	84	ASN
3	B	165	GLN
4	C	164	HIS
4	C	197	ASN
3	G	178	GLN
4	I	171	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](#)

4 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
5	NAG	E	1	1,5	14,14,15	0.49	0	17,19,21	0.56	0
5	NAG	E	2	5	14,14,15	0.32	0	17,19,21	0.47	0
5	NAG	J	1	1,5	14,14,15	0.51	0	17,19,21	0.50	0
5	NAG	J	2	5	14,14,15	0.57	0	17,19,21	0.45	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	E	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	NAG	J	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

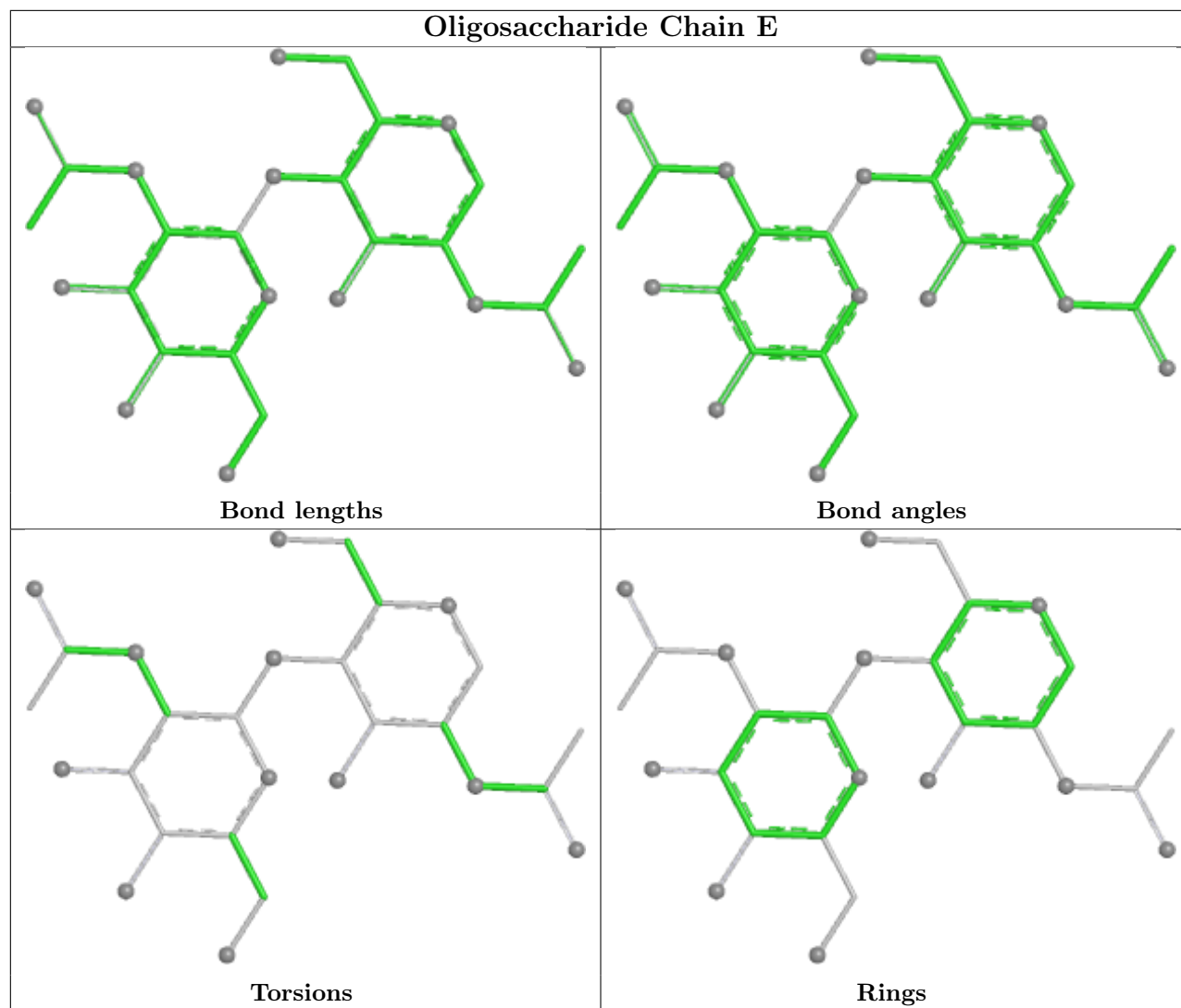
There are no torsion outliers.

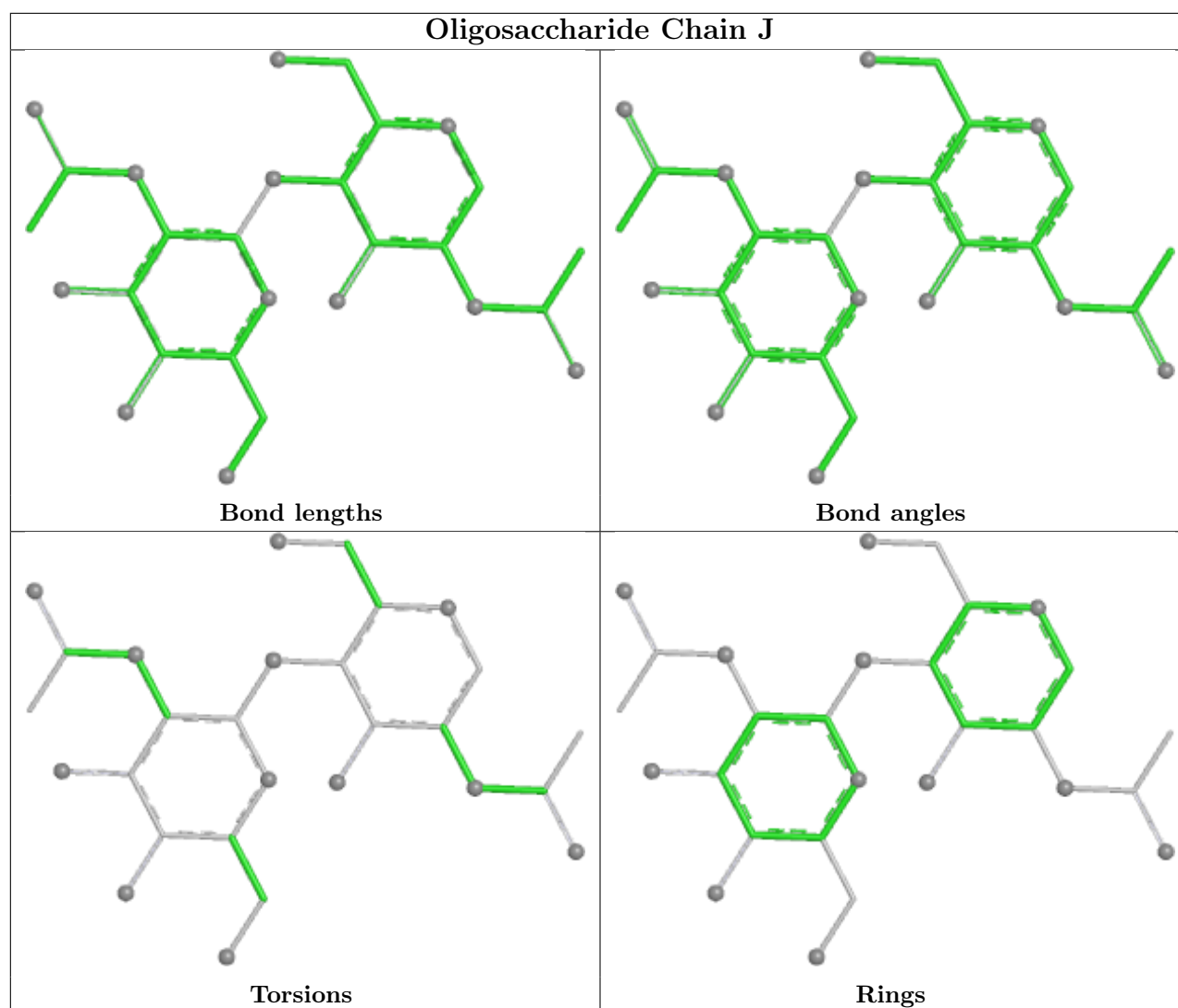
There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

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





5.6 Ligand geometry [i](#)

18 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	$\# Z > 2$
6	SO4	D	301	-	4,4,4	0.26	0	6,6,6	0.38	0
7	NAG	G	305	3	14,14,15	0.43	0	17,19,21	0.42	0
7	NAG	B	307	3	14,14,15	0.36	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	F	201	-	4,4,4	0.29	0	6,6,6	0.42	0
6	SO4	B	305	-	4,4,4	0.25	0	6,6,6	0.37	0
6	SO4	G	303	-	4,4,4	0.27	0	6,6,6	0.38	0
6	SO4	B	306	-	4,4,4	0.27	0	6,6,6	0.78	0
6	SO4	I	301	-	4,4,4	0.28	0	6,6,6	0.53	0
6	SO4	B	303	-	4,4,4	0.30	0	6,6,6	0.39	0
6	SO4	A	202	-	4,4,4	0.28	0	6,6,6	0.41	0
6	SO4	G	302	-	4,4,4	0.25	0	6,6,6	0.80	0
6	SO4	C	301	-	4,4,4	0.27	0	6,6,6	0.56	0
6	SO4	B	301	-	4,4,4	0.21	0	6,6,6	0.70	0
6	SO4	B	302	-	4,4,4	0.25	0	6,6,6	0.49	0
6	SO4	B	304	-	4,4,4	0.27	0	6,6,6	0.57	0
6	SO4	G	301	-	4,4,4	0.28	0	6,6,6	0.46	0
6	SO4	G	304	-	4,4,4	0.28	0	6,6,6	0.72	0
6	SO4	A	201	-	4,4,4	0.26	0	6,6,6	0.66	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
7	NAG	G	305	3	-	0/6/23/26	0/1/1/1
7	NAG	B	307	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	185/188 (98%)	-0.36	0 100 100	64, 88, 123, 169	0
1	F	185/188 (98%)	-0.32	1 (0%) 87 73	65, 86, 123, 148	0
2	D	212/214 (99%)	-0.13	1 (0%) 87 73	77, 120, 165, 187	0
2	H	213/214 (99%)	-0.17	0 100 100	71, 93, 128, 148	0
3	B	201/226 (88%)	-0.11	1 (0%) 87 73	73, 100, 151, 194	0
3	G	205/226 (90%)	-0.15	2 (0%) 79 61	63, 88, 157, 191	0
4	C	222/223 (99%)	-0.15	0 100 100	80, 122, 163, 196	0
4	I	222/223 (99%)	-0.10	0 100 100	76, 109, 145, 185	0
All	All	1645/1702 (96%)	-0.18	5 (0%) 90 80	63, 101, 154, 196	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	187	LEU	3.3
2	D	212	GLY	3.0
3	B	155	SER	2.4
3	G	142	ASN	2.3
3	G	219	ALA	2.2

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

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

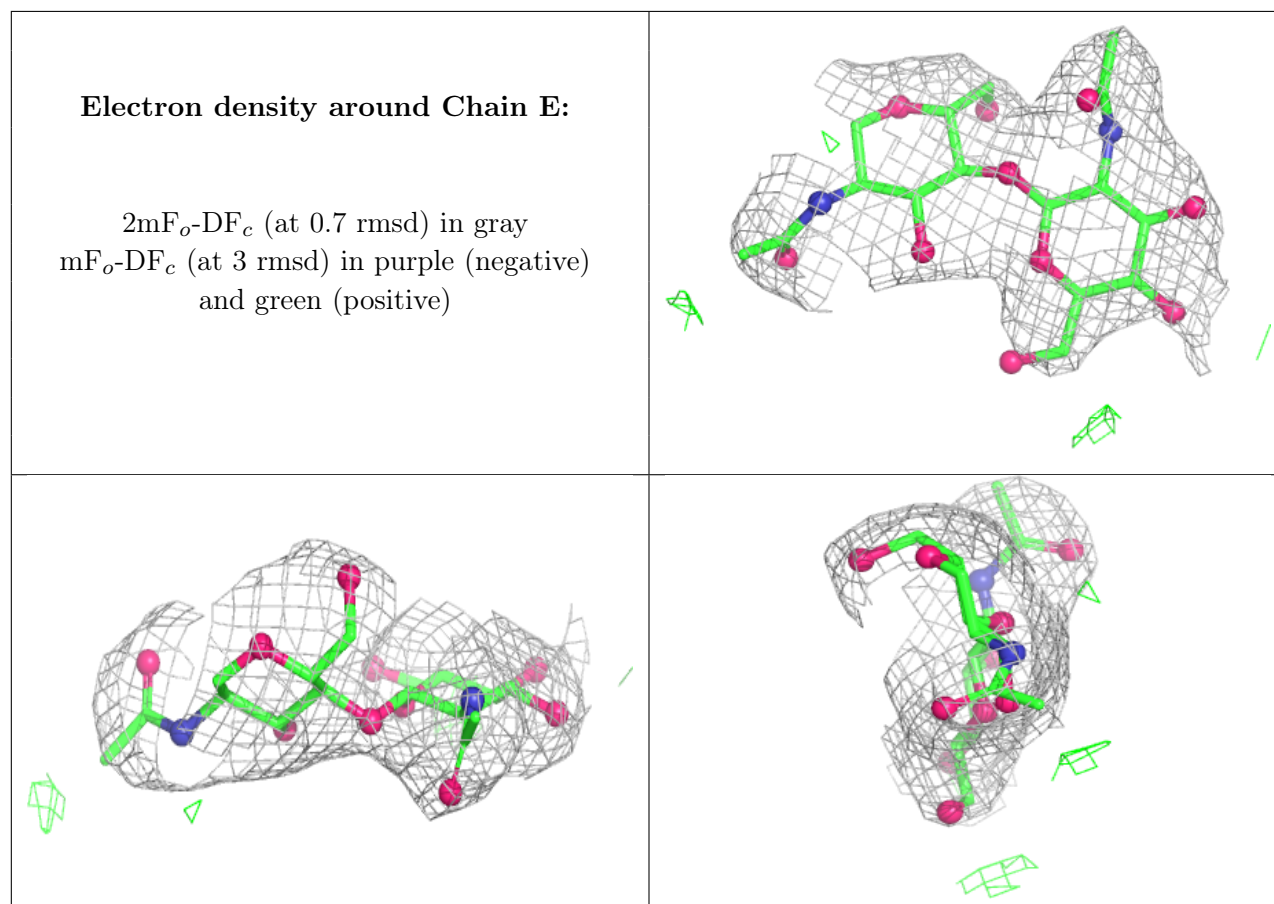
6.3 Carbohydrates [i](#)

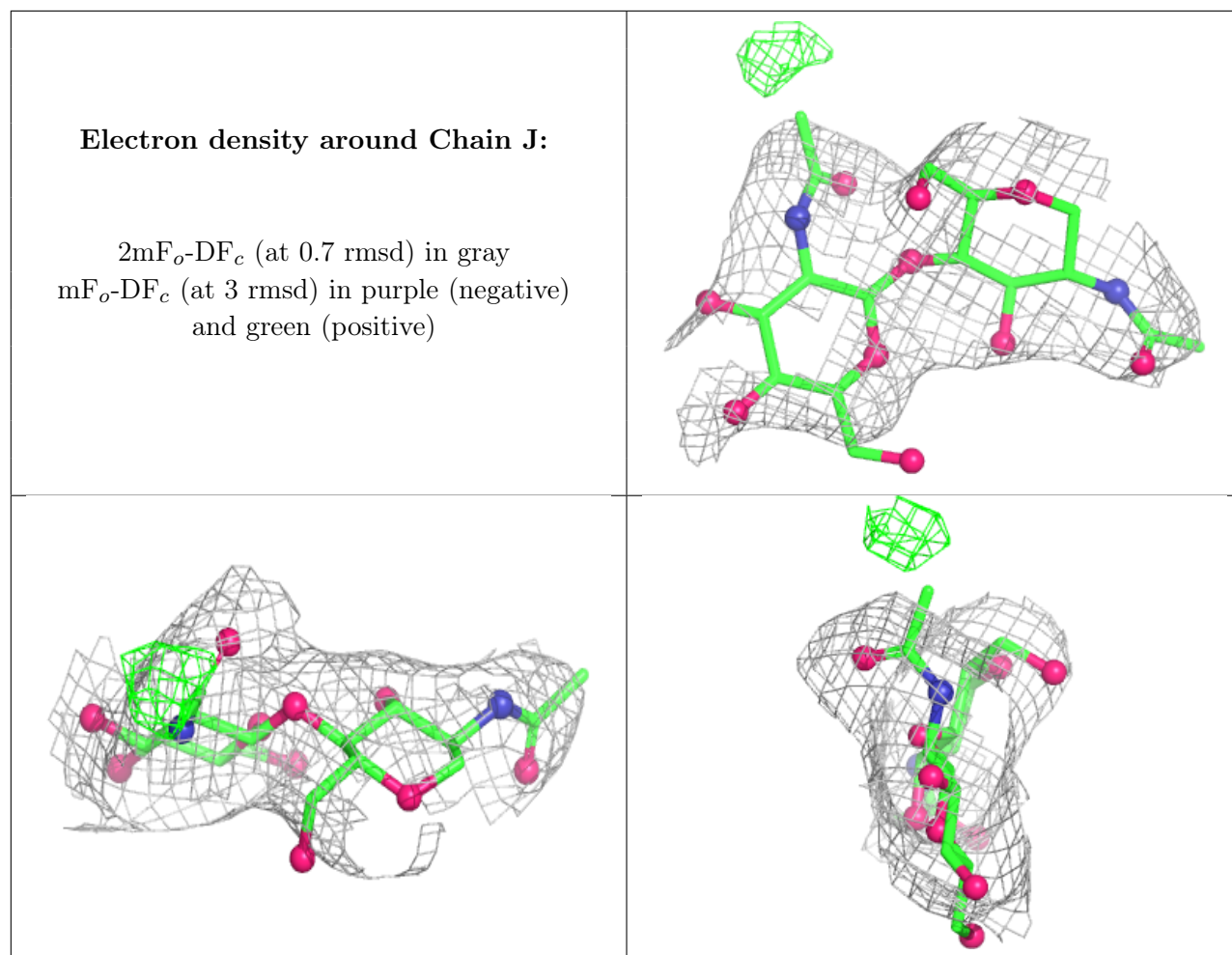
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	E	1	14/15	-	-	82,105,115,123	0
5	NAG	E	2	14/15	-	-	80,115,130,131	0
5	NAG	J	2	14/15	0.47	0.12	120,135,142,142	0
5	NAG	J	1	14/15	0.93	0.07	92,110,130,135	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.





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	SO4	G	301	5/5	0.44	0.09	163,166,186,240	0
6	SO4	D	301	5/5	0.52	0.09	134,163,187,236	0
7	NAG	B	307	14/15	0.53	0.10	130,150,160,167	0
7	NAG	G	305	14/15	0.55	0.14	122,139,148,155	0
6	SO4	B	304	5/5	0.57	0.07	144,152,165,172	0
6	SO4	B	303	5/5	0.59	0.10	130,148,166,192	0
6	SO4	B	306	5/5	0.70	0.08	132,155,176,225	0
6	SO4	C	301	5/5	0.71	0.09	109,148,170,204	0
6	SO4	I	301	5/5	0.71	0.09	132,136,179,204	0
6	SO4	G	303	5/5	0.74	0.14	119,124,128,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	A	202	5/5	0.75	0.07	125,134,185,200	0
6	SO4	F	201	5/5	0.78	0.14	122,125,153,166	0
6	SO4	G	304	5/5	0.81	0.15	107,119,130,141	0
6	SO4	B	302	5/5	0.82	0.11	103,114,124,145	0
6	SO4	B	305	5/5	0.82	0.09	143,150,189,198	0
6	SO4	B	301	5/5	0.83	0.11	145,146,158,175	0
6	SO4	G	302	5/5	0.85	0.28	109,129,142,174	0
6	SO4	A	201	5/5	0.91	0.27	113,124,154,173	0

6.5 Other polymers [i](#)

There are no such residues in this entry.