Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2024 – 06:16 am GMT

PDB ID	:	5NAN
Title	:	Crystal Structure of human IL-17AF in complex with human IL-17RA
Authors	:	Rondeau, J.-M.; Goepfert, A.
Deposited on	:	2017-02-28
Resolution	:	3.30 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 (i)) were used in the production of this report:

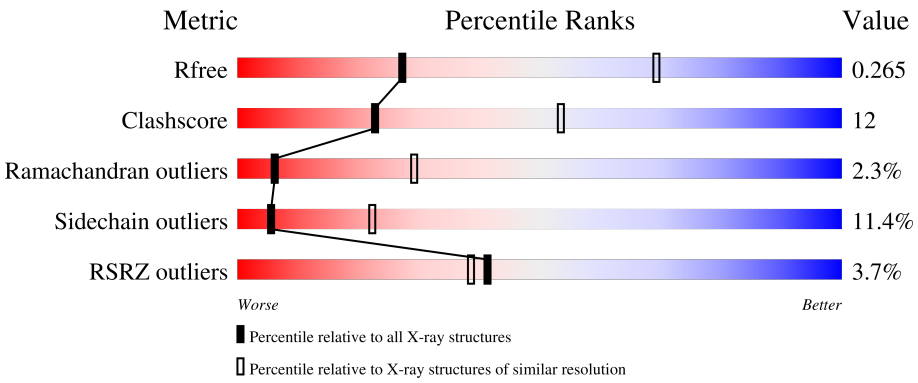
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	132	4% 54% 21% • 24%
1	D	132	7% 55% 22% • 21%
2	B	311	2% 53% 30% • • 13%
2	C	311	2% 54% 30% • 13%
3	E	139	6% 59% 17% 5% 19%

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Mol	Chain	Length	Quality of chain
3	F	139	% 60% 19% • 19%
4	G	3	100%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7923 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 Interleukin-17A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	100	811	508	150	146	7	0	0	0
1	D	104	849	528	162	152	7	0	0	0

- Molecule 2 is a protein called Interleukin-17 receptor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	271	2211	1391	405	399	16	0	0	0
2	C	271	2211	1391	405	399	16	0	0	0

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	321	GLU	-	expression tag	UNP Q96F46
B	322	PHE	-	expression tag	UNP Q96F46
B	323	ARG	-	expression tag	UNP Q96F46
B	324	HIS	-	expression tag	UNP Q96F46
B	325	ASP	-	expression tag	UNP Q96F46
B	326	SER	-	expression tag	UNP Q96F46
B	327	GLY	-	expression tag	UNP Q96F46
B	328	GLY	-	expression tag	UNP Q96F46
B	329	GLY	-	expression tag	UNP Q96F46
B	330	LEU	-	expression tag	UNP Q96F46
B	331	ASN	-	expression tag	UNP Q96F46
B	332	ASP	-	expression tag	UNP Q96F46
B	333	ILE	-	expression tag	UNP Q96F46
B	334	PHE	-	expression tag	UNP Q96F46
B	335	GLU	-	expression tag	UNP Q96F46
B	336	ALA	-	expression tag	UNP Q96F46

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Chain	Residue	Modelled	Actual	Comment	Reference
B	337	GLN	-	expression tag	UNP Q96F46
B	338	LYS	-	expression tag	UNP Q96F46
B	339	ILE	-	expression tag	UNP Q96F46
B	340	GLU	-	expression tag	UNP Q96F46
B	341	TRP	-	expression tag	UNP Q96F46
B	342	HIS	-	expression tag	UNP Q96F46
B	343	GLU	-	expression tag	UNP Q96F46
C	321	GLU	-	expression tag	UNP Q96F46
C	322	PHE	-	expression tag	UNP Q96F46
C	323	ARG	-	expression tag	UNP Q96F46
C	324	HIS	-	expression tag	UNP Q96F46
C	325	ASP	-	expression tag	UNP Q96F46
C	326	SER	-	expression tag	UNP Q96F46
C	327	GLY	-	expression tag	UNP Q96F46
C	328	GLY	-	expression tag	UNP Q96F46
C	329	GLY	-	expression tag	UNP Q96F46
C	330	LEU	-	expression tag	UNP Q96F46
C	331	ASN	-	expression tag	UNP Q96F46
C	332	ASP	-	expression tag	UNP Q96F46
C	333	ILE	-	expression tag	UNP Q96F46
C	334	PHE	-	expression tag	UNP Q96F46
C	335	GLU	-	expression tag	UNP Q96F46
C	336	ALA	-	expression tag	UNP Q96F46
C	337	GLN	-	expression tag	UNP Q96F46
C	338	LYS	-	expression tag	UNP Q96F46
C	339	ILE	-	expression tag	UNP Q96F46
C	340	GLU	-	expression tag	UNP Q96F46
C	341	TRP	-	expression tag	UNP Q96F46
C	342	HIS	-	expression tag	UNP Q96F46
C	343	GLU	-	expression tag	UNP Q96F46

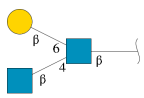
- Molecule 3 is a protein called Interleukin-17F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	113	866	533	157	167	9	0	0	0
			Total	C	N	O	S			
3	F	113	866	533	157	167	9	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

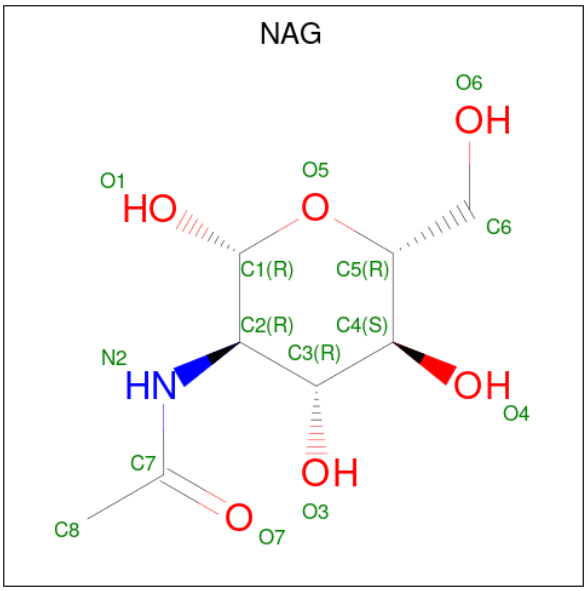
Chain	Residue	Modelled	Actual	Comment	Reference
E	25	GLU	-	expression tag	UNP Q96PD4
E	26	PHE	-	expression tag	UNP Q96PD4
E	27	ARG	-	expression tag	UNP Q96PD4
E	28	HIS	-	expression tag	UNP Q96PD4
E	29	ASP	-	expression tag	UNP Q96PD4
E	30	SER	-	expression tag	UNP Q96PD4
F	25	GLU	-	expression tag	UNP Q96PD4
F	26	PHE	-	expression tag	UNP Q96PD4
F	27	ARG	-	expression tag	UNP Q96PD4
F	28	HIS	-	expression tag	UNP Q96PD4
F	29	ASP	-	expression tag	UNP Q96PD4
F	30	SER	-	expression tag	UNP Q96PD4

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-D-galactopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	G	3	39	22	2	15	0	0	0

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



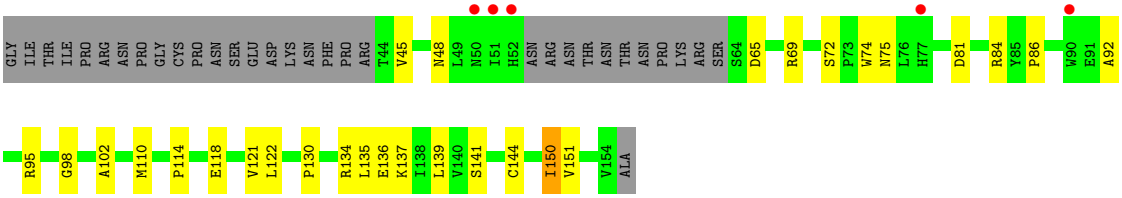
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	B	1	14	8	1	5	0	0
5	C	1	14	8	1	5	0	0
5	C	1	14	8	1	5	0	0
5	C	1	14	8	1	5	0	0
5	E	1	14	8	1	5	0	0

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.

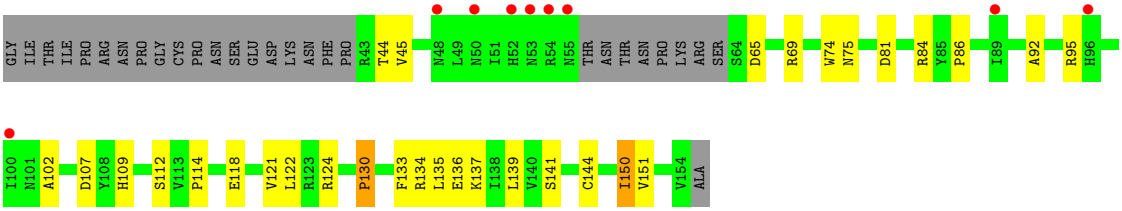
• Molecule 1: Interleukin-17A

Chain A:



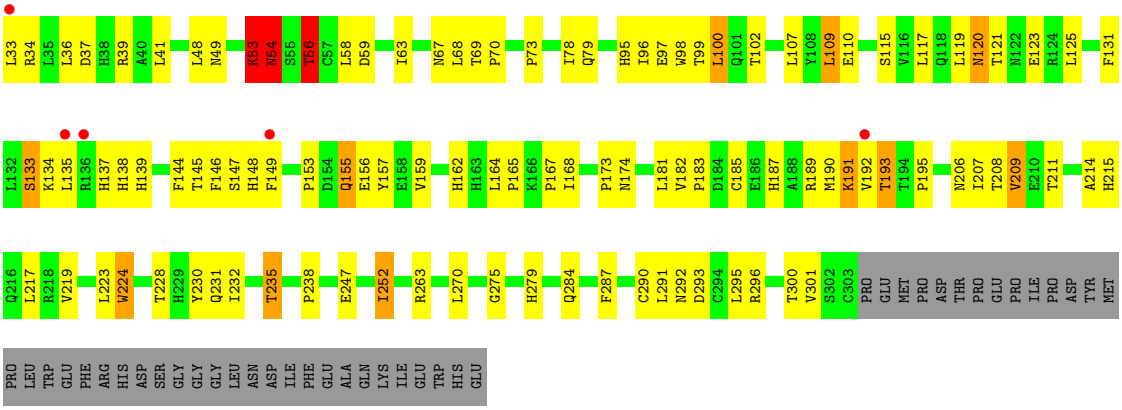
• Molecule 1: Interleukin-17A

Chain D:



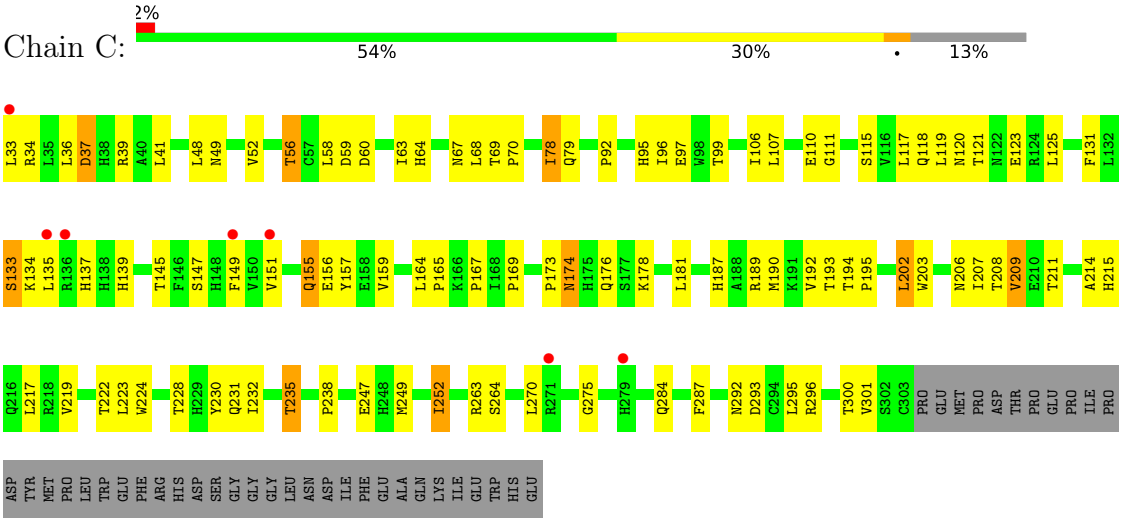
• Molecule 2: Interleukin-17 receptor A

Chain B:



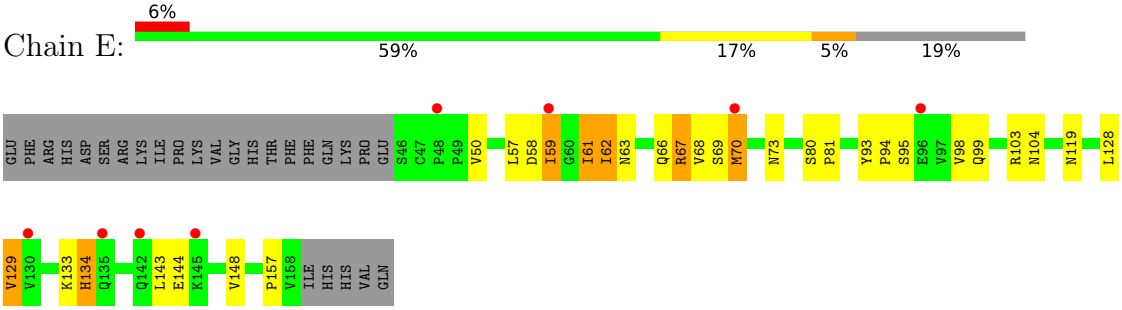
• Molecule 2: Interleukin-17 receptor A

Chain C:



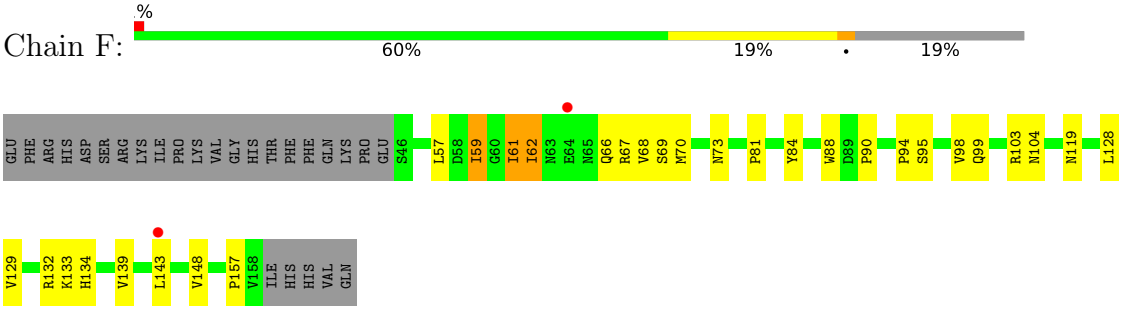
• Molecule 3: Interleukin-17F

Chain E:



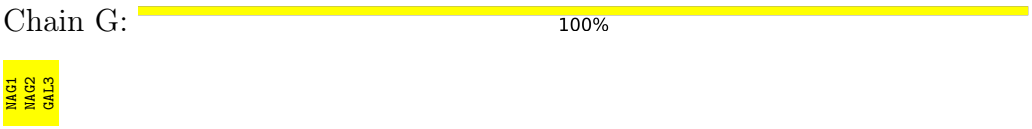
• Molecule 3: Interleukin-17F

Chain F:



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-D-galactopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	100.00Å 66.10Å 104.12Å 90.00° 90.13° 90.00°	Depositor
Resolution (Å)	66.10 – 3.30 66.10 – 3.30	Depositor EDS
% Data completeness (in resolution range)	96.8 (66.10-3.30) 96.8 (66.10-3.30)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 3.33Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.186 , 0.243 0.219 , 0.265	Depositor DCC
R_{free} test set	1009 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	127.6	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 127.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.028 for l,k,-h 0.046 for h,-k,-l 0.046 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7923	wwPDB-VP
Average B, all atoms (Å^2)	169.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.86% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, 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	0.46	0/833	0.75	0/1137
1	D	0.47	0/871	0.75	0/1187
2	B	0.56	0/2278	0.83	2/3104 (0.1%)
2	C	0.54	0/2278	0.82	1/3104 (0.0%)
3	E	0.51	0/881	0.83	0/1198
3	F	0.51	0/881	0.80	0/1198
All	All	0.52	0/8022	0.81	3/10928 (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	53	LYS	C-N-CA	6.13	137.03	121.70
2	B	56	THR	N-CA-C	-5.67	95.69	111.00
2	C	56	THR	N-CA-C	-5.66	95.71	111.00

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	811	0	780	17	0
1	D	849	0	818	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2211	0	2112	63	0
2	C	2211	0	2110	63	0
3	E	866	0	857	23	0
3	F	866	0	857	16	0
4	G	39	0	34	1	0
5	B	14	0	13	0	0
5	C	42	0	39	1	0
5	E	14	0	13	0	0
All	All	7923	0	7633	179	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 12.

All (179) 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:B:58:LEU:HD21	2:B:63:ILE:HD11	1.50	0.90
1:D:134:ARG:HH12	3:E:62:ILE:H	1.21	0.88
2:C:187:HIS:HB3	2:C:190:MET:HB2	1.57	0.84
1:A:134:ARG:HH12	3:F:62:ILE:H	1.29	0.80
2:C:155:GLN:HE21	2:C:155:GLN:HA	1.47	0.80
1:D:135:LEU:HB3	3:E:61:ILE:HG12	1.63	0.80
2:C:190:MET:O	2:C:193:THR:HG22	1.82	0.79
1:A:121:VAL:HG23	1:A:136:GLU:HB3	1.66	0.77
1:D:121:VAL:HG23	1:D:136:GLU:HB3	1.66	0.77
2:B:53:LYS:HG3	2:B:54:ASN:H	1.49	0.76
2:C:97:GLU:HG2	2:C:145:THR:HG22	1.67	0.75
2:B:97:GLU:HG2	2:B:145:THR:HG22	1.68	0.75
2:B:119:LEU:HD12	2:B:156:GLU:HB3	1.68	0.74
2:C:69:THR:HG21	2:C:167:PRO:HA	1.68	0.74
2:B:69:THR:HG21	2:B:167:PRO:HA	1.67	0.74
1:D:134:ARG:NH1	3:E:62:ILE:H	1.86	0.72
2:B:70:PRO:HB2	2:B:109:LEU:HD12	1.71	0.72
2:B:58:LEU:HD21	2:B:63:ILE:CD1	2.19	0.72
2:C:187:HIS:HB3	2:C:190:MET:CB	2.21	0.71
3:F:94:PRO:HD2	3:F:129:VAL:HG12	1.73	0.71
2:B:120:ASN:ND2	2:B:120:ASN:H	1.91	0.69
2:C:119:LEU:HD12	2:C:156:GLU:HB3	1.75	0.68
4:G:1:NAG:H62	4:G:3:GAL:O2	1.94	0.68
1:A:74:TRP:CD1	1:A:92:ALA:HB1	2.28	0.68
1:D:74:TRP:CD1	1:D:92:ALA:HB1	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:PRO:HD2	1:A:121:VAL:HG12	1.76	0.67
2:C:296:ARG:HB2	1:D:151:VAL:HG22	1.75	0.67
2:B:56:THR:HG23	3:F:61:ILE:HD12	1.76	0.66
2:C:58:LEU:HD22	3:E:59:ILE:HG21	1.78	0.66
2:C:167:PRO:HD3	2:C:174:ASN:OD1	1.95	0.66
2:B:49:ASN:HB2	2:B:133:SER:HB3	1.79	0.63
2:B:232:ILE:HG12	2:B:252:ILE:HD11	1.79	0.63
2:C:232:ILE:HG12	2:C:252:ILE:HD11	1.82	0.62
2:C:63:ILE:HG22	2:C:64:HIS:CD2	2.34	0.62
1:A:45:VAL:HG22	3:F:59:ILE:HD11	1.79	0.62
2:B:36:LEU:HB3	2:B:148:HIS:CD2	2.34	0.61
1:D:86:PRO:HD2	1:D:121:VAL:HG12	1.81	0.61
2:C:187:HIS:CD2	2:C:190:MET:HB2	2.36	0.61
2:C:209:VAL:HG13	2:C:219:VAL:HG22	1.83	0.61
2:C:49:ASN:HB2	2:C:133:SER:HB3	1.83	0.60
1:A:75:ASN:HD21	1:A:95:ARG:HE	1.50	0.60
2:B:120:ASN:H	2:B:120:ASN:HD22	1.49	0.59
2:B:209:VAL:HG13	2:B:219:VAL:HG22	1.84	0.59
2:C:137:HIS:HB2	2:C:139:HIS:CE1	2.37	0.59
3:E:129:VAL:HG23	3:E:144:GLU:HB2	1.84	0.58
2:B:37:ASP:C	2:B:39:ARG:H	2.07	0.57
1:D:75:ASN:HD21	1:D:95:ARG:HE	1.51	0.57
2:C:209:VAL:HG12	2:C:217:LEU:HD22	1.86	0.57
2:B:117:LEU:O	2:B:157:TYR:HA	2.05	0.56
2:B:137:HIS:HB2	2:B:139:HIS:CE1	2.39	0.56
2:B:206:ASN:HB3	2:B:263:ARG:HH12	1.71	0.56
2:C:121:THR:OG1	2:C:123:GLU:HB2	2.05	0.56
2:C:206:ASN:HB3	2:C:263:ARG:HH12	1.71	0.56
2:C:264:SER:HA	5:C:403:NAG:H82	1.88	0.56
2:C:41:LEU:HB2	2:C:52:VAL:HG11	1.89	0.55
2:B:121:THR:OG1	2:B:123:GLU:HB2	2.07	0.54
2:C:202:LEU:H	2:C:202:LEU:HD12	1.71	0.54
2:B:209:VAL:HG12	2:B:217:LEU:HD22	1.90	0.54
2:C:117:LEU:O	2:C:157:TYR:HA	2.07	0.54
3:E:66:GLN:O	3:E:68:VAL:HG23	2.07	0.54
2:B:187:HIS:HB3	2:B:190:MET:HB2	1.90	0.53
2:B:193:THR:HG23	2:B:195:PRO:HG2	1.90	0.53
1:D:118:GLU:HG2	1:D:137:LYS:HE2	1.91	0.53
1:A:135:LEU:HB3	3:F:61:ILE:HG12	1.90	0.52
2:C:56:THR:HG23	3:E:61:ILE:HD12	1.90	0.52
1:D:45:VAL:HG22	3:E:59:ILE:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:HIS:HD2	2:B:139:HIS:H	1.57	0.52
1:D:107:ASP:OD1	1:D:109:HIS:HB2	2.10	0.52
3:E:99:GLN:HE22	3:E:148:VAL:HA	1.74	0.52
1:D:69:ARG:HH21	3:E:157:PRO:HA	1.74	0.52
1:A:118:GLU:HG2	1:A:137:LYS:HE2	1.91	0.52
2:B:137:HIS:HD2	2:B:139:HIS:N	2.09	0.51
2:C:187:HIS:CB	2:C:190:MET:HB2	2.35	0.51
3:F:99:GLN:HE22	3:F:148:VAL:HA	1.76	0.50
1:A:134:ARG:HH12	3:F:62:ILE:N	2.04	0.50
2:B:48:LEU:HD11	2:B:131:PHE:CD1	2.47	0.50
2:B:110:GLU:HG2	2:B:134:LYS:HE3	1.92	0.49
2:C:110:GLU:HG2	2:C:134:LYS:HE3	1.94	0.49
2:B:36:LEU:HB3	2:B:148:HIS:HD2	1.77	0.49
2:B:238:PRO:HA	2:B:275:GLY:O	2.13	0.49
2:C:137:HIS:HD2	2:C:139:HIS:N	2.10	0.49
2:C:238:PRO:HA	2:C:275:GLY:O	2.12	0.49
3:F:66:GLN:O	3:F:68:VAL:HG23	2.13	0.49
2:C:58:LEU:HD12	3:E:93:TYR:CG	2.48	0.49
2:C:56:THR:HG22	2:C:58:LEU:H	1.77	0.48
3:E:128:LEU:HD22	3:E:143:LEU:HD22	1.94	0.48
3:F:81:PRO:HB2	3:F:103:ARG:HD2	1.94	0.48
2:B:48:LEU:HD13	2:B:135:LEU:HD21	1.95	0.48
2:B:70:PRO:HG3	2:B:109:LEU:HA	1.94	0.48
2:B:185:CYS:O	2:B:191:LYS:HB3	2.14	0.48
2:C:58:LEU:HD21	2:C:63:ILE:CD1	2.43	0.48
2:B:56:THR:HG22	2:B:58:LEU:H	1.77	0.48
3:F:88:TRP:CD1	3:F:90:PRO:HD3	2.48	0.48
2:B:100:LEU:HD21	2:B:144:PHE:CE1	2.49	0.47
2:C:169:PRO:HB3	3:E:134:HIS:ND1	2.28	0.47
2:B:96:ILE:O	2:B:145:THR:HA	2.14	0.47
2:B:110:GLU:HG3	2:B:165:PRO:HD3	1.95	0.47
2:B:102:THR:HA	2:B:138:HIS:CE1	2.49	0.47
3:F:128:LEU:HD22	3:F:143:LEU:HD22	1.96	0.47
2:B:217:LEU:HD12	2:B:270:LEU:HD21	1.95	0.47
2:C:217:LEU:HD12	2:C:270:LEU:HD21	1.96	0.47
1:D:124:ARG:HG3	1:D:133:PHE:CE1	2.49	0.47
1:A:114:PRO:HA	1:A:144:CYS:HA	1.96	0.47
1:A:151:VAL:HG22	2:B:296:ARG:HB2	1.96	0.47
2:C:169:PRO:HB3	3:E:134:HIS:CE1	2.50	0.47
1:D:44:THR:HG22	3:E:58:ASP:HA	1.96	0.47
2:B:58:LEU:CD2	2:B:63:ILE:HD11	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:123:GLU:HG3	1:D:118:GLU:CD	2.36	0.46
2:C:96:ILE:O	2:C:145:THR:HA	2.16	0.46
2:B:70:PRO:HD3	2:B:165:PRO:HD2	1.97	0.46
2:B:79:GLN:O	2:B:95:HIS:HB3	2.16	0.46
2:C:92:PRO:HB2	2:C:151:VAL:HG23	1.98	0.46
2:C:123:GLU:HG3	1:D:118:GLU:OE1	2.16	0.46
2:C:223:LEU:HD22	2:C:230:TYR:CE1	2.51	0.46
2:B:284:GLN:HB2	2:B:296:ARG:HG2	1.98	0.45
2:C:284:GLN:HB2	2:C:296:ARG:HG2	1.97	0.45
2:C:193:THR:HG23	2:C:195:PRO:HG2	1.98	0.45
2:C:209:VAL:HB	2:C:301:VAL:HG21	1.99	0.45
2:B:96:ILE:HG12	2:B:159:VAL:HG11	1.99	0.45
2:C:70:PRO:HD3	2:C:165:PRO:HD2	1.99	0.45
1:A:150:ILE:H	1:A:150:ILE:HG13	1.66	0.45
2:B:223:LEU:HD22	2:B:230:TYR:CE1	2.52	0.45
2:B:73:PRO:HB3	2:B:98:TRP:CD1	2.52	0.45
3:E:81:PRO:HB2	3:E:103:ARG:HD2	1.97	0.45
2:B:228:THR:HG21	2:B:287:PHE:HA	1.99	0.45
2:C:120:ASN:ND2	2:C:121:THR:HG23	2.32	0.45
2:C:228:THR:HG21	2:C:287:PHE:HA	1.98	0.44
2:B:217:LEU:HG	2:B:270:LEU:HD11	1.99	0.44
1:D:137:LYS:HD3	3:E:63:ASN:HB3	1.99	0.44
1:A:74:TRP:CD1	1:A:92:ALA:CB	2.99	0.44
2:C:79:GLN:O	2:C:95:HIS:HB3	2.17	0.44
1:D:150:ILE:H	1:D:150:ILE:HG13	1.69	0.44
2:C:164:LEU:HA	2:C:165:PRO:C	2.37	0.44
2:B:206:ASN:HB3	2:B:263:ARG:NH1	2.33	0.44
2:B:146:PHE:CZ	2:B:148:HIS:HB2	2.53	0.44
2:B:182:VAL:HG12	2:B:183:PRO:HD2	2.00	0.44
2:C:187:HIS:HD2	2:C:190:MET:HB2	1.82	0.43
1:D:74:TRP:CD1	1:D:92:ALA:CB	3.01	0.43
2:B:153:PRO:HG3	2:B:190:MET:HE3	2.00	0.43
2:B:211:THR:HA	2:B:217:LEU:HD23	2.01	0.43
2:B:146:PHE:CE2	2:B:148:HIS:HB2	2.53	0.43
2:C:58:LEU:HD21	2:C:63:ILE:HD12	2.00	0.43
3:F:132:ARG:HG3	3:F:139:VAL:HG23	2.01	0.43
2:B:155:GLN:HB3	2:B:157:TYR:CE1	2.53	0.43
2:C:211:THR:HA	2:C:217:LEU:HD23	2.01	0.43
1:A:135:LEU:O	3:F:61:ILE:HA	2.18	0.43
2:B:235:THR:HG23	2:B:247:GLU:HG3	2.00	0.43
2:C:235:THR:HG23	2:C:247:GLU:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:118:GLN:HE21	2:C:157:TYR:HE1	1.67	0.42
2:C:78:ILE:HD11	2:C:178:LYS:HB2	2.01	0.42
3:E:73:ASN:CG	3:E:73:ASN:O	2.57	0.42
2:B:217:LEU:HD11	2:B:279:HIS:CD2	2.54	0.42
2:C:194:THR:N	2:C:195:PRO:HD2	2.34	0.42
2:B:137:HIS:CD2	2:B:139:HIS:H	2.37	0.42
2:C:96:ILE:HG12	2:C:159:VAL:HG11	2.00	0.42
2:C:203:TRP:HB2	2:C:224:TRP:CE3	2.54	0.42
1:A:69:ARG:HH21	3:F:157:PRO:HA	1.83	0.42
1:D:130:PRO:HG2	3:E:50:VAL:HG11	2.00	0.42
1:A:81:ASP:HB3	1:A:84:ARG:HB3	2.02	0.42
2:C:37:ASP:HB3	2:C:39:ARG:HG3	2.01	0.42
2:C:206:ASN:HB3	2:C:263:ARG:NH1	2.33	0.42
2:B:224:TRP:HA	2:B:224:TRP:CE3	2.55	0.41
2:B:209:VAL:HB	2:B:301:VAL:HG21	2.01	0.41
3:E:94:PRO:HD2	3:E:129:VAL:HG12	2.02	0.41
1:D:81:ASP:HB3	1:D:84:ARG:HB3	2.02	0.41
2:B:120:ASN:HA	3:F:84:TYR:CZ	2.55	0.41
1:D:135:LEU:O	3:E:61:ILE:HA	2.20	0.41
2:B:125:LEU:HG	2:B:149:PHE:HE1	1.86	0.41
2:C:111:GLY:HA2	2:C:131:PHE:CD2	2.56	0.41
1:D:137:LYS:HB3	3:E:63:ASN:HA	2.03	0.41
1:A:98:GLY:HA2	1:A:110:MET:O	2.21	0.41
1:D:114:PRO:HA	1:D:144:CYS:HA	2.03	0.41
2:B:156:GLU:HB2	3:F:73:ASN:HD21	1.86	0.41
2:C:120:ASN:HD22	2:C:121:THR:HG23	1.85	0.40
2:B:39:ARG:CG	2:B:41:LEU:HD23	2.51	0.40
2:C:155:GLN:HB3	2:C:157:TYR:CE2	2.57	0.40
2:C:125:LEU:HG	2:C:149:PHE:HE1	1.86	0.40
3:E:67:ARG:HH21	3:E:70:MET:HA	1.86	0.40
2:C:48:LEU:HD13	2:C:135:LEU:HD21	2.03	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	96/132 (73%)	90 (94%)	3 (3%)	3 (3%)	4	23
1	D	100/132 (76%)	94 (94%)	3 (3%)	3 (3%)	4	24
2	B	269/311 (86%)	236 (88%)	26 (10%)	7 (3%)	5	27
2	C	269/311 (86%)	241 (90%)	23 (9%)	5 (2%)	8	34
3	E	111/139 (80%)	98 (88%)	11 (10%)	2 (2%)	8	35
3	F	111/139 (80%)	102 (92%)	7 (6%)	2 (2%)	8	35
All	All	956/1164 (82%)	861 (90%)	73 (8%)	22 (2%)	6	29

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	ASP
2	B	173	PRO
2	C	36	LEU
2	C	173	PRO
1	D	65	ASP
3	E	61	ILE
3	E	67	ARG
3	F	61	ILE
3	F	67	ARG
1	A	102	ALA
2	B	54	ASN
2	B	293	ASP
2	C	293	ASP
1	A	130	PRO
2	B	53	LYS
1	D	102	ALA
2	B	214	ALA
2	B	291	LEU
2	C	214	ALA
1	D	130	PRO
2	B	207	ILE
2	C	207	ILE

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	95/124 (77%)	89 (94%)	6 (6%)	18	47
1	D	99/124 (80%)	94 (95%)	5 (5%)	24	54
2	B	256/292 (88%)	219 (86%)	37 (14%)	3	14
2	C	256/292 (88%)	224 (88%)	32 (12%)	4	19
3	E	103/129 (80%)	90 (87%)	13 (13%)	4	19
3	F	103/129 (80%)	92 (89%)	11 (11%)	6	25
All	All	912/1090 (84%)	808 (89%)	104 (11%)	5	22

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	72	SER
1	A	122	LEU
1	A	139	LEU
1	A	141	SER
1	A	150	ILE
2	B	33	LEU
2	B	34	ARG
2	B	54	ASN
2	B	56	THR
2	B	59	ASP
2	B	67	ASN
2	B	68	LEU
2	B	78	ILE
2	B	99	THR
2	B	100	LEU
2	B	107	LEU
2	B	109	LEU
2	B	115	SER
2	B	120	ASN
2	B	133	SER
2	B	147	SER
2	B	155	GLN
2	B	162	HIS
2	B	164	LEU
2	B	168	ILE

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Mol	Chain	Res	Type
2	B	174	ASN
2	B	181	LEU
2	B	189	ARG
2	B	191	LYS
2	B	192	VAL
2	B	193	THR
2	B	208	THR
2	B	209	VAL
2	B	215	HIS
2	B	224	TRP
2	B	231	GLN
2	B	235	THR
2	B	252	ILE
2	B	290	CYS
2	B	292	ASN
2	B	295	LEU
2	B	300	THR
2	C	33	LEU
2	C	34	ARG
2	C	37	ASP
2	C	59	ASP
2	C	60	ASP
2	C	67	ASN
2	C	68	LEU
2	C	78	ILE
2	C	99	THR
2	C	106	ILE
2	C	107	LEU
2	C	115	SER
2	C	133	SER
2	C	147	SER
2	C	155	GLN
2	C	174	ASN
2	C	176	GLN
2	C	181	LEU
2	C	189	ARG
2	C	192	VAL
2	C	202	LEU
2	C	208	THR
2	C	209	VAL
2	C	215	HIS
2	C	222	THR

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Mol	Chain	Res	Type
2	C	231	GLN
2	C	235	THR
2	C	249	MET
2	C	252	ILE
2	C	292	ASN
2	C	295	LEU
2	C	300	THR
1	D	112	SER
1	D	122	LEU
1	D	139	LEU
1	D	141	SER
1	D	150	ILE
3	E	57	LEU
3	E	59	ILE
3	E	62	ILE
3	E	69	SER
3	E	70	MET
3	E	80	SER
3	E	95	SER
3	E	98	VAL
3	E	104	ASN
3	E	119	ASN
3	E	129	VAL
3	E	133	LYS
3	E	134	HIS
3	F	57	LEU
3	F	59	ILE
3	F	62	ILE
3	F	69	SER
3	F	70	MET
3	F	95	SER
3	F	98	VAL
3	F	104	ASN
3	F	119	ASN
3	F	133	LYS
3	F	134	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	77	HIS

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Mol	Chain	Res	Type
1	A	79	ASN
2	B	38	HIS
2	B	120	ASN
2	B	137	HIS
2	B	148	HIS
2	B	155	GLN
2	B	176	GLN
2	C	64	HIS
2	C	120	ASN
2	C	137	HIS
2	C	155	GLN
2	C	176	GLN
2	C	187	HIS
1	D	75	ASN
1	D	77	HIS
1	D	79	ASN
3	E	142	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	G	1	4,3	14,14,15	0.37	0	17,19,21	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	G	2	4	14,14,15	0.34	0	17,19,21	0.90	2 (11%)
4	GAL	G	3	4	11,11,12	0.42	0	15,15,17	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
4	NAG	G	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	GAL	G	3	4	-	2/2/19/22	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	G	2	NAG	O5-C1-C2	-2.51	107.33	111.29
4	G	2	NAG	C1-O5-C5	2.12	115.06	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	3	GAL	O5-C5-C6-O6
4	G	3	GAL	C4-C5-C6-O6

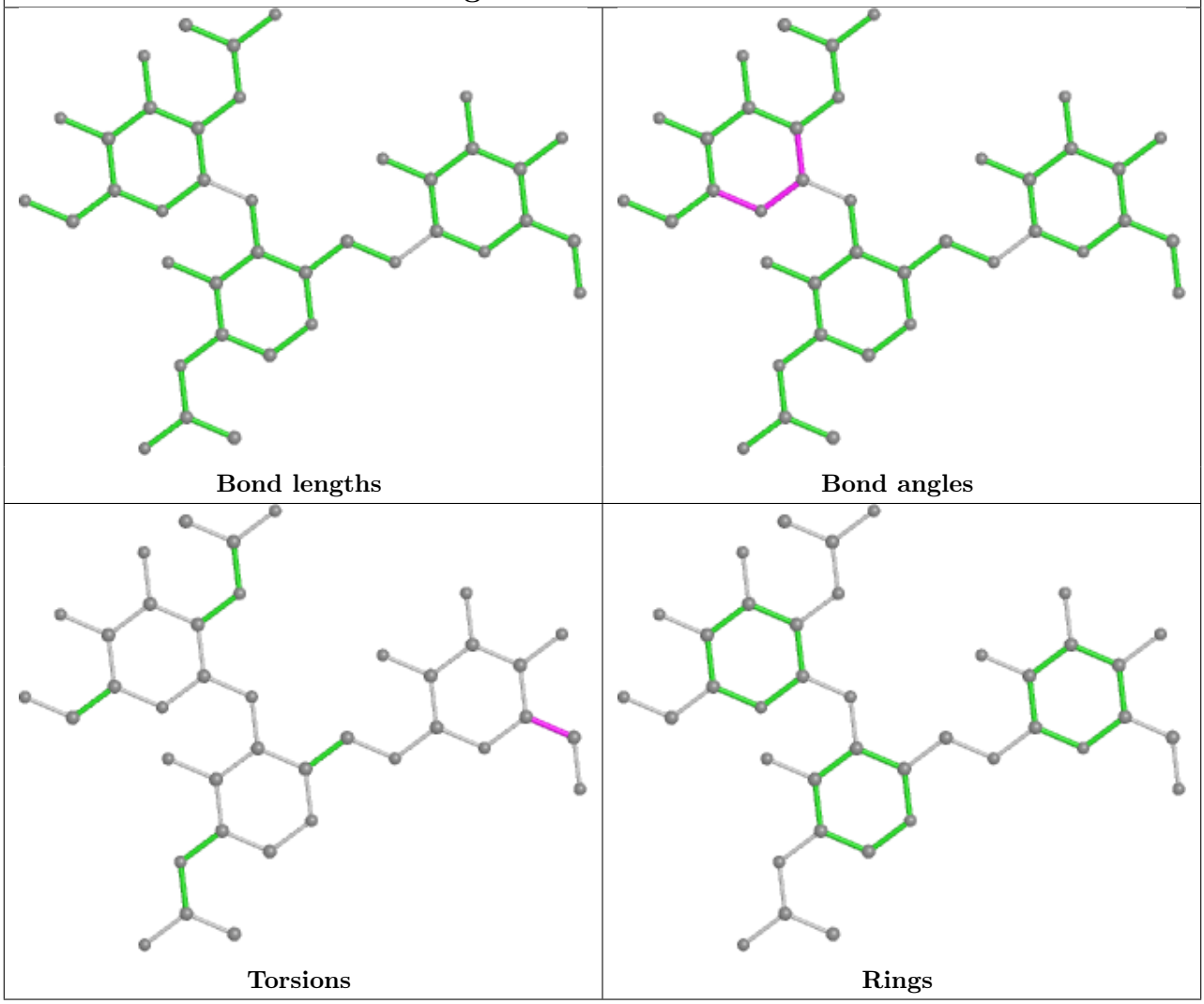
There are no ring outliers.

2 monomers are involved in 1 short contact:

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

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

Oligosaccharide Chain G



5.6 Ligand geometry (i)

5 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	C	401	2	14,14,15	0.36	0	17,19,21	0.32	0
5	NAG	E	201	3	14,14,15	0.39	0	17,19,21	0.57	0
5	NAG	C	402	2	14,14,15	0.29	0	17,19,21	1.11	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	B	401	2	14,14,15	0.33	0	17,19,21	1.16	3 (17%)
5	NAG	C	403	2	14,14,15	0.33	0	17,19,21	0.81	1 (5%)

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	C	401	2	-	0/6/23/26	0/1/1/1
5	NAG	E	201	3	-	0/6/23/26	0/1/1/1
5	NAG	C	402	2	-	2/6/23/26	0/1/1/1
5	NAG	B	401	2	-	2/6/23/26	0/1/1/1
5	NAG	C	403	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	402	NAG	O5-C1-C2	-3.28	106.10	111.29
5	B	401	NAG	O5-C1-C2	-2.95	106.63	111.29
5	C	403	NAG	C1-C2-N2	2.83	115.32	110.49
5	B	401	NAG	C1-C2-N2	2.60	114.92	110.49
5	B	401	NAG	C1-O5-C5	2.21	115.18	112.19
5	C	402	NAG	C1-C2-N2	2.02	113.95	110.49
5	C	402	NAG	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	402	NAG	C4-C5-C6-O6
5	C	402	NAG	O5-C5-C6-O6
5	B	401	NAG	C4-C5-C6-O6
5	B	401	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
5	C	403	NAG	1	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 (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	100/132 (75%)	0.30	5 (5%)	28	27	126, 172, 222, 268	0
1	D	104/132 (78%)	0.53	9 (8%)	10	10	126, 177, 232, 242	0
2	B	271/311 (87%)	0.11	5 (1%)	68	67	111, 157, 223, 248	0
2	C	271/311 (87%)	0.04	7 (2%)	56	53	102, 154, 231, 245	0
3	E	113/139 (81%)	0.17	8 (7%)	16	16	122, 171, 243, 261	0
3	F	113/139 (81%)	-0.02	2 (1%)	68	67	116, 163, 233, 243	0
All	All	972/1164 (83%)	0.15	36 (3%)	41	38	102, 163, 231, 268	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	53	ASN	7.7
2	B	33	LEU	7.4
1	A	52	HIS	7.2
1	D	55	ASN	6.2
2	C	33	LEU	6.2
1	D	52	HIS	5.9
1	D	50	ASN	5.8
1	D	48	ASN	5.1
3	E	142	GLN	4.1
2	B	136	ARG	3.7
1	D	54	ARG	3.6
3	E	70	MET	3.6
2	B	135	LEU	3.5
2	C	271	ARG	3.3
3	F	143	LEU	3.1
2	C	136	ARG	3.1
1	D	96	HIS	3.0
3	E	145	LYS	2.8
2	C	135	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	50	ASN	2.8
3	E	59	ILE	2.6
2	B	149	PHE	2.6
3	E	130	VAL	2.6
1	A	51	ILE	2.5
1	A	90	TRP	2.4
3	E	135	GLN	2.4
2	C	149	PHE	2.4
2	C	151	VAL	2.4
2	B	192	VAL	2.4
1	D	100	ILE	2.3
3	F	64	GLU	2.3
1	A	77	HIS	2.2
3	E	96	GLU	2.2
2	C	279	HIS	2.1
3	E	48	PRO	2.1
1	D	89	ILE	2.0

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

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

6.3 Carbohydrates (i)

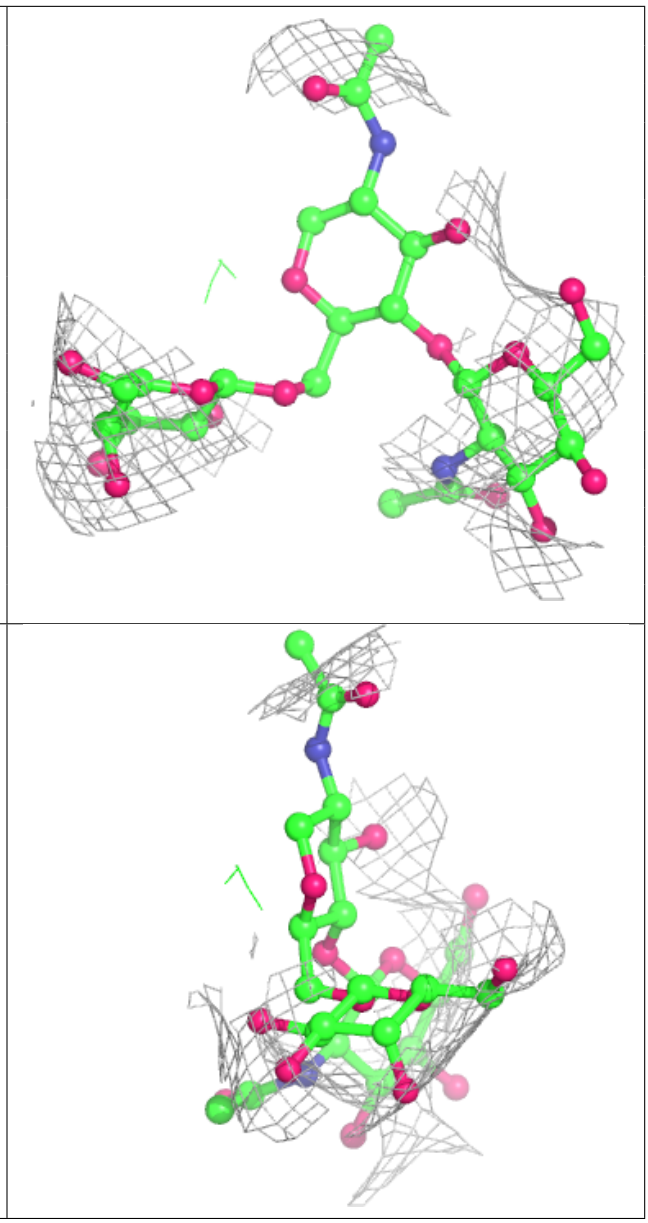
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	G	2	14/15	0.76	0.32	250,255,258,258	0
4	GAL	G	3	11/12	0.89	0.17	218,223,226,228	0
4	NAG	G	1	14/15	0.90	0.14	221,228,234,243	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)



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
5	NAG	C	401	14/15	0.77	0.21	185,211,216,220	0
5	NAG	C	403	14/15	0.83	0.23	250,253,258,259	0
5	NAG	B	401	14/15	0.86	0.22	225,229,233,237	0
5	NAG	E	201	14/15	0.88	0.14	186,201,213,217	0
5	NAG	C	402	14/15	0.92	0.18	198,201,204,206	0

6.5 Other polymers (i)

There are no such residues in this entry.