WORLDWIDE PDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 10, 2023 – 09:42 am GMT

PDB ID	:	2WBJ
Title	:	TCR complex
Authors	:	Harkiolaki, M.; Holmes, S.L.; Svendsen, P.; Gregersen, J.W.; Jensen, L.T.; McMahon, R.; Friese, M.A.; van Boxel, G.; Etzensperger, R.; Tzartos, J.S.; Kranc, K.; Sainsbury, S.; Harlos, K.; Mellins, E.D.; Palace, J.; Esiri, M.M.; van der Merwe, P.A.; Jones, E.Y.; Fugger, L.
Deposited on	:	2009-03-02
Resolution	:	3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

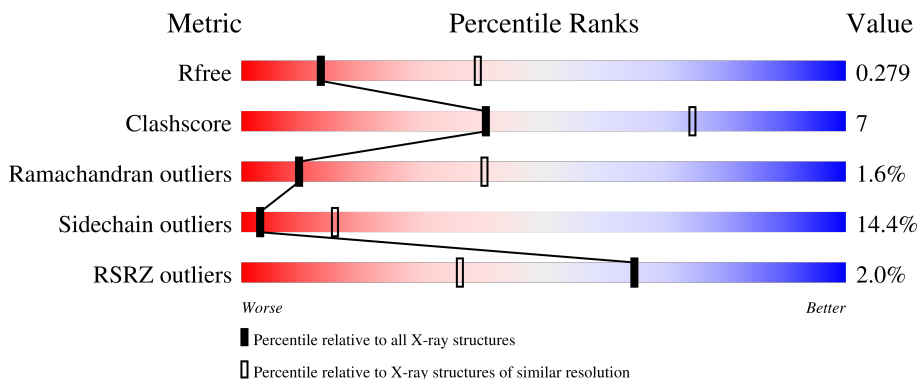|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.279
Clashscore		7
Ramachandran outliers		1.6%
Sidechain outliers		14.4%
RSRZ outliers		2.0%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	194	% 74% 15% · 8%
1	E	194	71% 18% · 9%
2	B	200	2% 76% 10% · 10%
2	F	200	2% 74% 19% · 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	219	4% 65% 18% · · 12%
3	G	219	% 59% 21% 6% 13%
4	D	279	2% 67% 25% · · ·
4	H	279	3% 66% 20% 6% · 7%
5	I	5	20% 40% 40%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	I	1	X	-	-	-
5	MAN	I	5	-	-	-	X
6	NAG	A	1181	X	-	-	-
6	NAG	E	1186	X	-	-	X
6	NAG	F	1191	X	-	-	X

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 13235 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	178	Total 1465	C 950	N 238	O 272	S 5	0	0	0
1	E	177	Total 1456	C 945	N 237	O 269	S 5	0	0	0

- Molecule 2 is a protein called HLA CLASS II HISTOCOMPATIBILITY ANTIGEN, DRB1-15 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	179	Total 1478	C 939	N 259	O 274	S 6	0	0	0
2	F	188	Total 1548	C 980	N 275	O 287	S 6	0	0	0

- Molecule 3 is a protein called OB TCR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	193	Total 1511	C 934	N 263	O 307	S 7	0	0	0
3	G	190	Total 1484	C 919	N 258	O 300	S 7	0	0	0

- Molecule 4 is a protein called OB TCR.

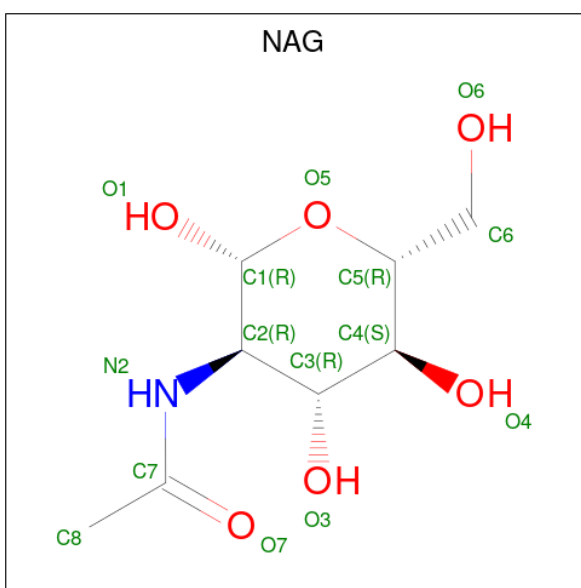| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	270	Total 2105	C 1323	N 366	O 408	S 8	0	0	0
4	H	260	Total 2056	C 1297	N 356	O 396	S 7	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.
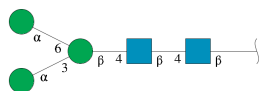
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	5	Total 61	C 34	N 2	O 25	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

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

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

O1

O3 O⁻ — S — O⁻ O4

S

O2

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	F	1	Total	O	S	0	0
			5	4	1		

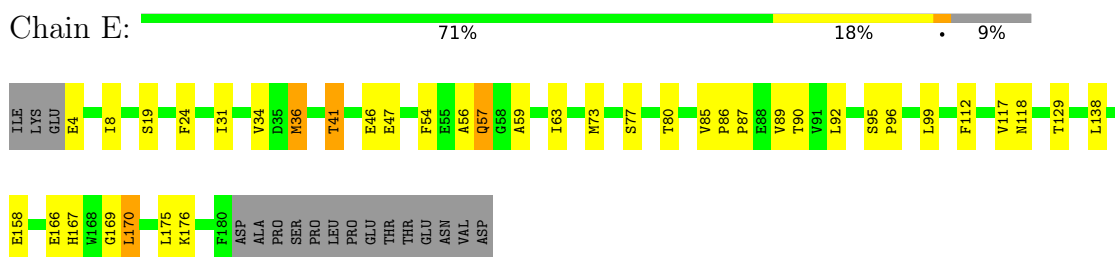# 3 Residue-property plots ⓘ

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.
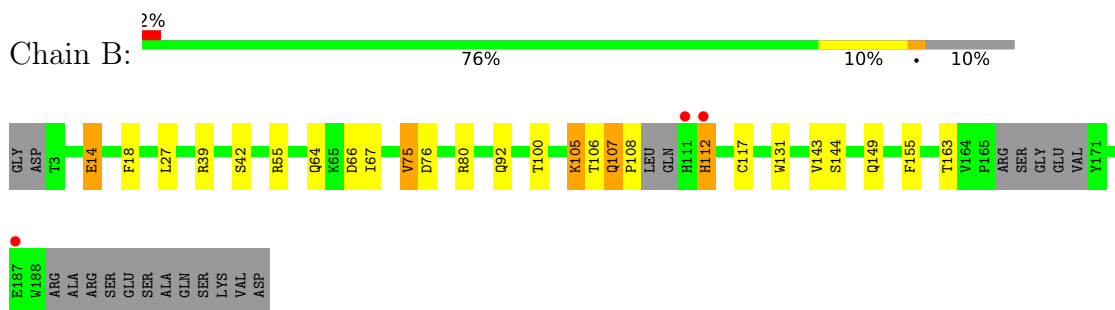
• Molecule 1: HLA CLASS II HISTOCOMPATIBILITY ANTIGEN, DR ALPHA CHAIN
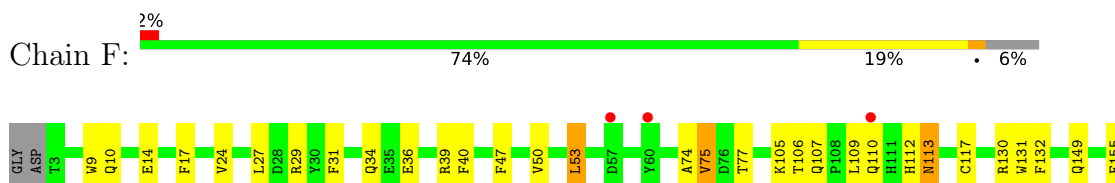

• Molecule 1: HLA CLASS II HISTOCOMPATIBILITY ANTIGEN, DR ALPHA CHAIN

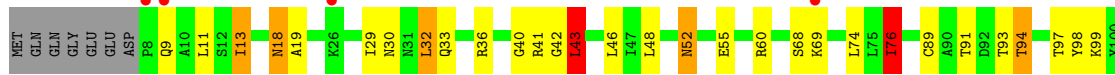• Molecule 2: HLA CLASS II HISTOCOMPATIBILITY ANTIGEN, DRB1-15 BETA CHAIN

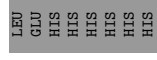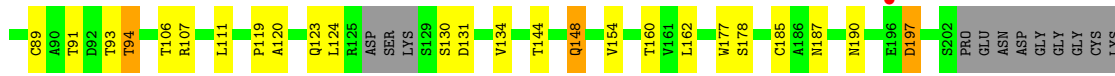• Molecule 2: HLA CLASS II HISTOCOMPATIBILITY ANTIGEN, DRB1-15 BETA CHAIN

E162 E169 T172 E176 H177 P178 V186 E187 W188 R189 A190 ARG SER GLU SER ALA GLN SER LYS VAL ASP

● Molecule 3: OB TCR

Chain C:

4%
65%　　　18%　　· ·　12%

MET GLN GLN GLY GLU GLU ASP P8 Q9 A10 L11 S12 I13 N18 A19 K26 I29 N30 N31 L32 Q33 R36 G40 R41 G42 L43 L46 I47 L48 N52 E55 R60 S68 K69 L74 L75 I76 C89 A90 T91 D92 T93 T94 T97 Y98 K99 Y100

I101 K109 V110 L111 P119 A120 L124 R125 K128 S129 S130 D131 S142 S147 K150 D151 S152 D153 T160 V161 L162 R165 S178 N179 K180 S181 D182 S192 I193 I194 D197 F200 PRO SER PRO GLU ASN ASP GLY GLY CYS LYS LEU GLU HIS HIS

HIS HIS HIS HIS

● Molecule 3: OB TCR

Chain G:

%
59%　　　21%　　6%　　13%

MET GLN GLN GLY GLU GLU ASP PRO GLN A10 L11 A19 T20 C23 S24 Y25 K26 I29 N30 N31 L32 Q33 W34 Y35 R36 Q37 N38 S39 G40 R41 G42 L43 V44 H45 L46 I47 L48 S51 R54 E55 K56 R60 K69 K70 S73 L74 L75 I76 D83 S86

C89 A90 T91 D92 T93 T94 T106 R107 L111 P119 A120 Q123 L124 R125 ASP SER LYS S129 S130 D131 V134 T144 Q148 V154 T160 V161 L162 W177 S178 C185 A186 N187 N190 E196 D197 S202 PRO GLU ASN ASP GLY GLY CYS LYS

LEU GLU HIS HIS HIS HIS HIS HIS

● Molecule 4: OB TCR

Chain D:

2%
67%　　　25%　　· · ·

M-1 D1 F2 A3 R4 I8 G15 G19 G23 A24 V25 W32 V33 I34 S35 K36 K42 D49 W57 P62 K63 Q64 M67 L68 E74 G75 S76 K77 A78 T79 Y80 G83 V84 E85 K86 D87 K88 F89 L90 I91 S95 L98 S99 T100 L101 T102

H107 P108 F113 L121 T122 S123 N126 N127 E128 R136 L137 T138 V139 T140 E141 D142 P148 P149 P156 Q165 L169 V170 H180 L183 W186 V187 E191 G195 V196 S197 Q206 L209 S212 S215 L216 R219 L220 R221 V222 S223 A224

T225 F226 N229 N232 C236 Q237 S244 P256 V257 T258 Q259 I260 V261 S262 A263 E264 R268 S269 ARG GLN ASP ARG GLY GLY GLY CYS ASP

● Molecule 4: OB TCR

Chain H:

3%
66%　　　20%　　6%　·　7%

MET D1 S9 S14 G15 G16 GLY SER GLY GLY GLY GLY ALA V25 V26 S27 I34 S35 V41 K42 W57 K63 Q64 M67 L68 E74 G75 S76 K77 A78 T79 Y80 E81 Q82 G83 V84 E85 K86 D87 K88 F89 L96 T97 L98 S99 T100 L101 T102 V103 T104

S105 A106 H107 P108 S112 F113 L121 T122 S123 N126 N127 E128 Q129 R136 L137 T138 V139 T140 E141 Q165 T168 L169 V170 C171 L172 A173 T174 P178 V192 G195 D199 P200 L203 Q206 L209 S212 S215 L216 R219 L220 R221 V222 S223 A224

T225 F226 N229 P230 R235 Y241 N246 T250 K255 P256 V257 T258 V261 R268 SER ARG GLN ASP ARG GLY GLY CYS ASP
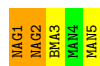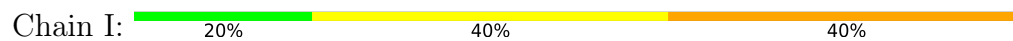
• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

20%   40%   40%

NAG1 NAG2 BMA3 MAN4 MAN5

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	109.71Å 130.27Å 180.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	105.41 – 3.00 29.62 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (105.41-3.00) 99.6 (29.62-3.00)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.247 , 0.288 0.240 , 0.279	Depositor DCC
R_{free} test set	2659 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	67.3	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 42.8	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	13235	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: MAN, BMA, SO4, 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	0.38	0/1510	0.50	0/2059
1	E	0.37	0/1501	0.53	0/2047
2	B	0.37	0/1519	0.49	0/2064
2	F	0.36	0/1591	0.48	0/2163
3	C	0.36	0/1537	0.53	0/2077
3	G	0.37	0/1509	0.58	1/2041 (0.0%)
4	D	0.37	0/2161	0.54	2/2936 (0.1%)
4	H	0.37	0/2111	0.54	1/2870 (0.0%)
All	All	0.37	0/13439	0.53	4/18257 (0.0%)

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
2	B	0	1
3	C	0	1
3	G	0	1
4	D	0	5
4	H	0	5
All	All	0	13

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	32	LEU	CA-CB-CG	5.83	128.71	115.30
4	H	121	LEU	CA-CB-CG	5.45	127.82	115.30
4	D	223	SER	N-CA-C	5.17	124.97	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	98	LEU	CA-CB-CG	5.11	127.05	115.30

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	112	HIS	Peptide
3	C	76	ILE	Peptide
4	D	15	GLY	Peptide
4	D	83	GLY	Peptide
4	D	84	VAL	Peptide

5.2   Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1465	0	1401	18	0
1	E	1456	0	1394	22	0
2	B	1478	0	1398	14	0
2	F	1548	0	1473	20	0
3	C	1511	0	1465	25	0
3	G	1484	0	1438	28	0
4	D	2105	0	2005	36	0
4	H	2056	0	1962	35	0
5	I	61	0	52	2	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
6	E	14	0	13	0	0
6	F	14	0	13	0	0
7	B	5	0	0	0	0
7	C	5	0	0	0	0
7	F	5	0	0	0	0
All	All	13235	0	12640	185	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.

The worst 5 of 185 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:H:223:SER:CB	4:H:226:PHE:HB3	1.57	1.32
4:H:223:SER:HB2	4:H:226:PHE:HB3	1.21	1.15
4:D:83:GLY:HA2	4:D:84:VAL:HB	1.27	1.15
4:H:223:SER:HB3	4:H:226:PHE:HB3	1.33	1.10
4:H:223:SER:HB2	4:H:226:PHE:CB	1.94	0.96

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	176/194 (91%)	170 (97%)	6 (3%)	0	100	100
1	E	175/194 (90%)	170 (97%)	5 (3%)	0	100	100
2	B	173/200 (86%)	165 (95%)	7 (4%)	1 (1%)	25	64
2	F	186/200 (93%)	175 (94%)	10 (5%)	1 (0%)	29	68
3	C	191/219 (87%)	166 (87%)	22 (12%)	3 (2%)	9	40
3	G	186/219 (85%)	160 (86%)	21 (11%)	5 (3%)	5	26
4	D	268/279 (96%)	237 (88%)	22 (8%)	9 (3%)	3	20
4	H	256/279 (92%)	234 (91%)	16 (6%)	6 (2%)	6	30
All	All	1611/1784 (90%)	1477 (92%)	109 (7%)	25 (2%)	9	40

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	84	VAL
4	D	223	SER
3	G	38	ASN
3	G	47	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	H	76	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	163/178 (92%)	146 (90%)	17 (10%)	7	27
1	E	162/178 (91%)	146 (90%)	16 (10%)	8	30
2	B	163/180 (91%)	153 (94%)	10 (6%)	18	53
2	F	170/180 (94%)	156 (92%)	14 (8%)	11	39
3	C	173/195 (89%)	142 (82%)	31 (18%)	2	9
3	G	170/195 (87%)	133 (78%)	37 (22%)	1	5
4	D	231/237 (98%)	188 (81%)	43 (19%)	1	8
4	H	228/237 (96%)	186 (82%)	42 (18%)	1	9
All	All	1460/1580 (92%)	1250 (86%)	210 (14%)	3	15

5 of 210 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	170	LEU
3	G	48	LEU
4	H	203	LEU
2	F	50	VAL
2	F	189	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
3	G	38	ASN
3	G	148	GLN
4	H	188	ASN
4	D	73	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	60	GLN

5.3.3   RNA   ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates   ⓘ

5 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	I	1	1,5	14,14,15	0.47	0	17,19,21	1.09	1 (5%)
5	NAG	I	2	5	14,14,15	0.53	0	17,19,21	1.05	2 (11%)
5	BMA	I	3	5	11,11,12	0.43	0	15,15,17	1.00	1 (6%)
5	MAN	I	4	5	11,11,12	0.57	0	15,15,17	0.66	0
5	MAN	I	5	5	11,11,12	0.71	0	15,15,17	1.14	2 (13%)

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	I	1	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	3/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1
5	MAN	I	4	5	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	I	5	5	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	1	NAG	C1-O5-C5	3.28	116.64	112.19
5	I	5	MAN	C3-C4-C5	2.76	115.16	110.24
5	I	3	BMA	C1-C2-C3	2.65	112.93	109.67
5	I	2	NAG	C4-C3-C2	2.36	114.47	111.02
5	I	5	MAN	C2-C3-C4	2.22	114.75	110.89

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	I	1	NAG	C1

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	5	MAN	O5-C5-C6-O6
5	I	5	MAN	C4-C5-C6-O6
5	I	2	NAG	C8-C7-N2-C2
5	I	2	NAG	O5-C5-C6-O6
5	I	2	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

Bond lengths

Bond angles

Torsions

Rings
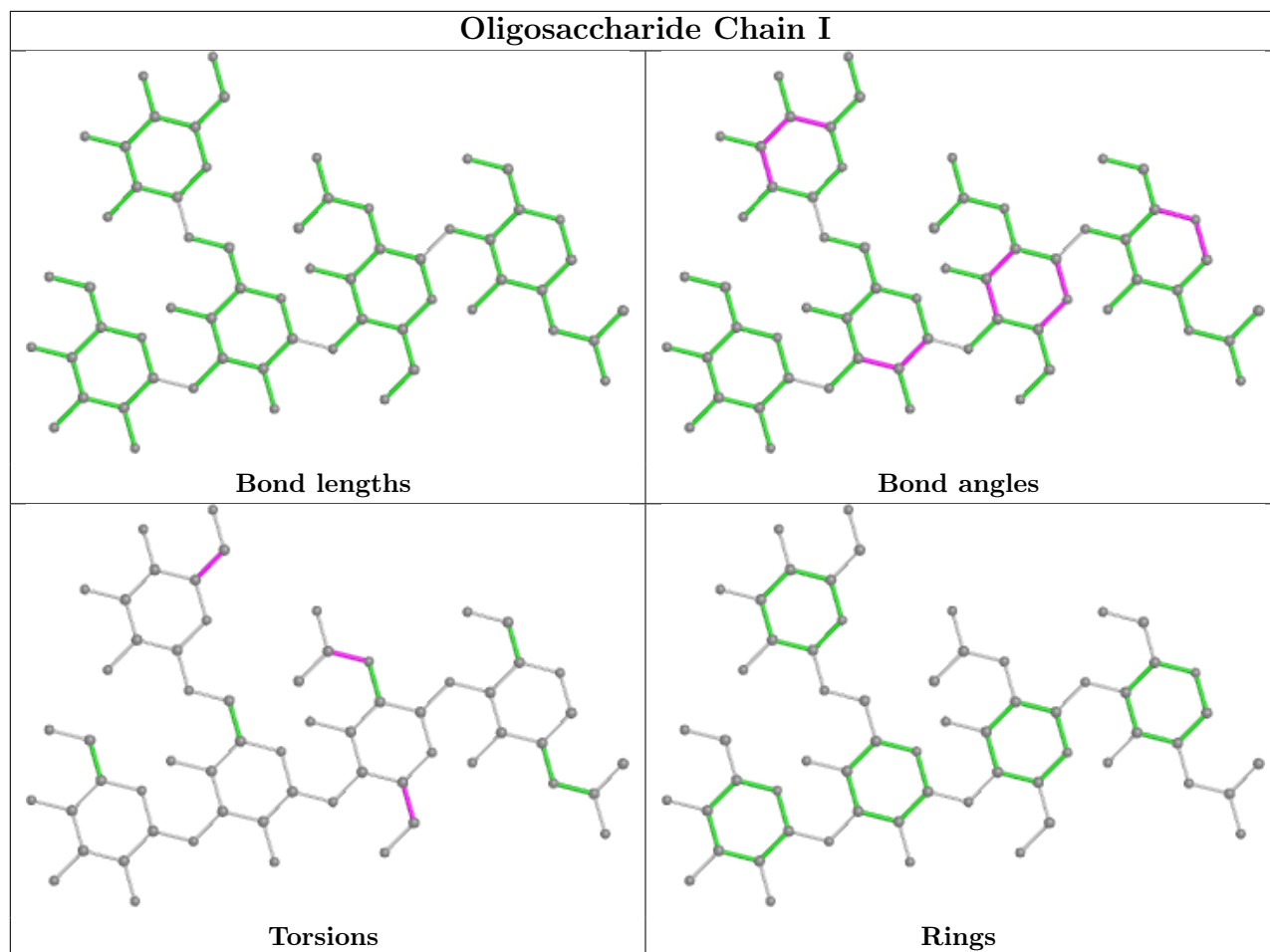
5.6 Ligand geometry (i)

7 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	$\#|Z| > 2$
7	SO4	C	1201	-	4,4,4	0.13	0	6,6,6	0.09	0
6	NAG	B	1189	2	14,14,15	0.54	0	17,19,21	1.08	1 (5%)
6	NAG	E	1186	1	14,14,15	0.56	0	17,19,21	0.91	0
6	NAG	F	1191	2	14,14,15	0.51	0	17,19,21	0.67	0
7	SO4	B	1190	-	4,4,4	0.18	0	6,6,6	0.13	0
6	NAG	A	1181	1	14,14,15	0.48	0	17,19,21	0.92	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z \rvert > 2$	Counts	RMSZ	$\#\lvert Z \rvert > 2$
7	SO4	F	1192	-	4,4,4	0.16	0	6,6,6	0.12	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
6	NAG	E	1186	1	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	F	1191	2	1/1/5/7	4/6/23/26	0/1/1/1
6	NAG	A	1181	1	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	B	1189	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1181	NAG	C1-O5-C5	2.39	115.43	112.19
6	B	1189	NAG	O5-C5-C6	2.38	110.94	107.20
6	A	1181	NAG	O5-C5-C6	2.03	110.39	107.20

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	1181	NAG	C1
6	E	1186	NAG	C1
6	F	1191	NAG	C1

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	1191	NAG	C8-C7-N2-C2
6	F	1191	NAG	O7-C7-N2-C2
6	E	1186	NAG	C8-C7-N2-C2
6	E	1186	NAG	O7-C7-N2-C2
6	A	1181	NAG	C8-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7　Other polymers ⓘ

There are no such residues in this entry.

5.8　Polymer linkage issues ⓘ

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	178/194 (91%)	-0.18	2 (1%)	80	56	55, 61, 69, 78	0
1	E	177/194 (91%)	-0.29	0	100	100	55, 61, 69, 71	0
2	B	179/200 (89%)	-0.04	3 (1%)	70	41	49, 62, 71, 96	0
2	F	188/200 (94%)	-0.08	3 (1%)	72	44	49, 63, 71, 86	0
3	C	193/219 (88%)	0.10	9 (4%)	31	11	53, 66, 78, 88	0
3	G	190/219 (86%)	0.01	2 (1%)	80	56	53, 66, 74, 89	0
4	D	270/279 (96%)	0.01	6 (2%)	62	33	50, 64, 76, 95	0
4	H	260/279 (93%)	0.07	8 (3%)	49	21	51, 63, 73, 83	0
All	All	1635/1784 (91%)	-0.04	33 (2%)	65	36	49, 63, 73, 96	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	112	HIS	4.7
4	H	1	ASP	4.1
2	B	111	HIS	3.8
3	C	26	LYS	3.5
3	C	69	LYS	3.4

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

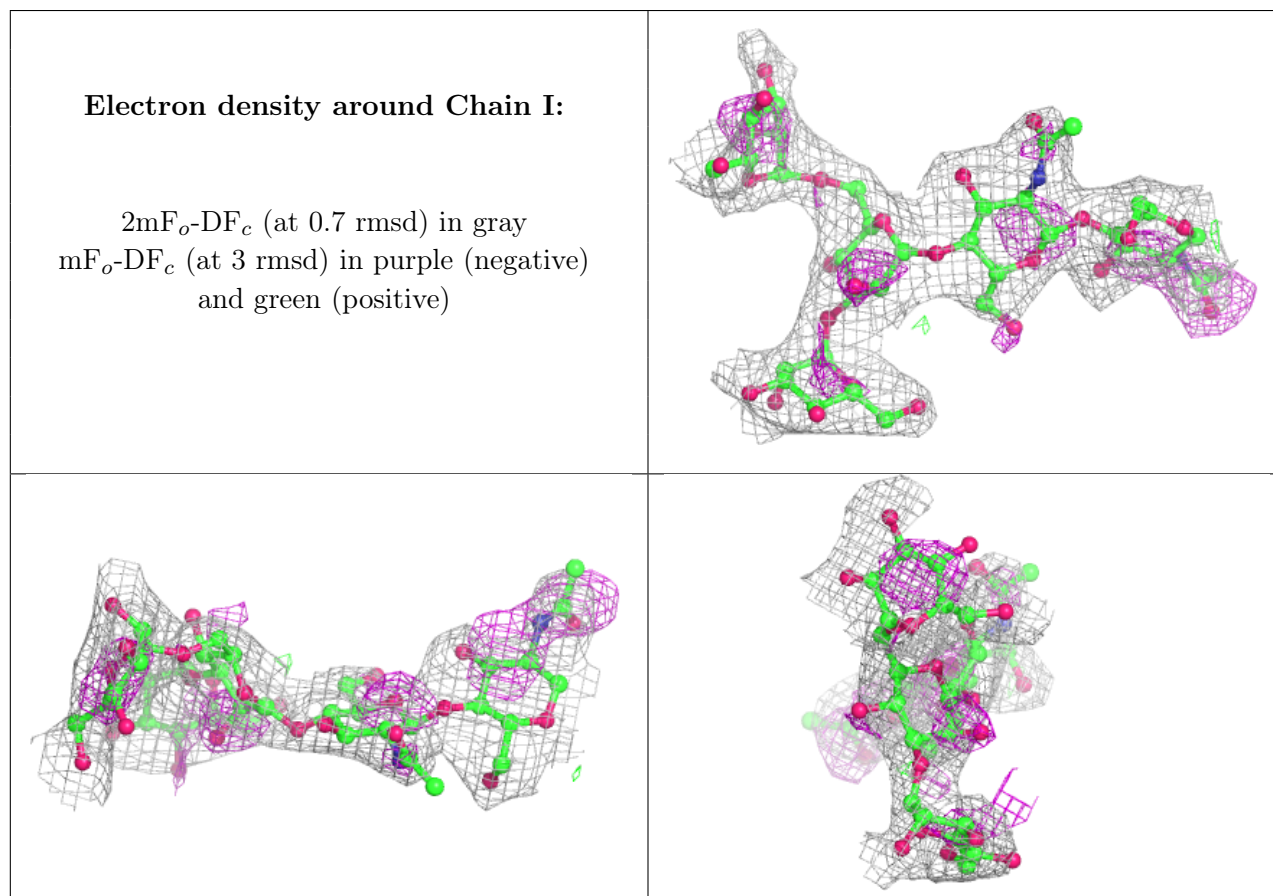There are no non-standard protein/DNA/RNA residues in this entry.

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	MAN	I	5	11/12	0.55	0.49	105,109,111,112	0
5	MAN	I	4	11/12	0.86	0.42	87,91,92,93	0
5	BMA	I	3	11/12	0.90	0.39	83,86,89,98	0
5	NAG	I	1	14/15	0.91	0.27	51,60,65,66	0
5	NAG	I	2	14/15	0.92	0.44	72,76,77,79	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 I:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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, 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(Å²)	Q<0.9
6	NAG	E	1186	14/15	0.76	0.43	94,99,103,104	0
6	NAG	F	1191	14/15	0.77	0.42	95,101,104,106	0
6	NAG	A	1181	14/15	0.83	0.34	86,92,95,96	0
6	NAG	B	1189	14/15	0.86	0.36	74,82,87,89	0
7	SO4	C	1201	5/5	0.92	0.19	91,91,92,93	0
7	SO4	F	1192	5/5	0.93	0.23	56,58,59,61	0
7	SO4	B	1190	5/5	0.97	0.26	51,52,54,54	0

6.5   Other polymers ⓘ

There are no such residues in this entry.