



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:53 AM UTC

PDB ID : 4P2O / pdb_00004p2o
Title : Crystal structure of the 2B4 TCR in complex with 2A/I-Ek
Authors : Birnbaum, M.E.; Ozkan, E.; Garcia, K.C.
Deposited on : 2014-03-04
Resolution : 2.60 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

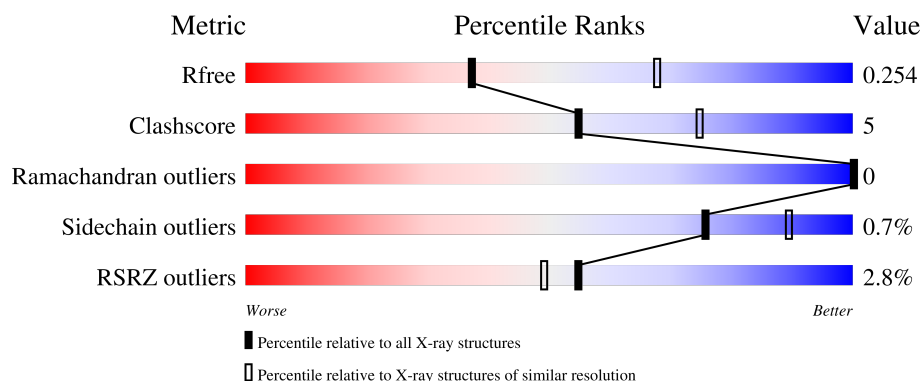
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	204	18% 75% 10% 14%
2	B	236	3% 64% 11% 25%
3	C	220	3% 82% 8% 9%
4	D	255	0% 82% 14% 0%
5	P	22	18% 86% 5% 9%

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Mol	Chain	Length	Quality of chain
6	E	4	 A horizontal bar chart showing the quality of chain 6. The bar is divided into two segments: a yellow segment on the left representing 25% and an orange segment on the right representing 75%. The labels '25%' and '75%' are positioned below their respective segments.

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6701 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 H-2 class II histocompatibility antigen, E-K alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	0	0
			1431	928	236	263	4			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ALA	-	expression tag	UNP P04224
A	-1	ASP	-	expression tag	UNP P04224
A	0	PRO	-	expression tag	UNP P04224
A	192	SER	-	expression tag	UNP P04224
A	193	ARG	-	expression tag	UNP P04224
A	194	GLY	-	expression tag	UNP P04224
A	195	GLY	-	expression tag	UNP P04224
A	196	LEU	-	expression tag	UNP P04224
A	197	GLU	-	expression tag	UNP P04224
A	198	VAL	-	expression tag	UNP P04224
A	199	LEU	-	expression tag	UNP P04224
A	200	PHE	-	expression tag	UNP P04224
A	201	GLN	-	expression tag	UNP P04224

- Molecule 2 is a protein called MHC class II E-beta-k.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	176	Total	C	N	O	S	0	0	0
			1450	926	247	271	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-27	ALA	-	expression tag	UNP Q31163
B	-26	ASP	-	expression tag	UNP Q31163
B	-25	PRO	-	expression tag	UNP Q31163

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-24	ALA	-	expression tag	UNP Q31163
B	-23	ASP	-	expression tag	UNP Q31163
B	-22	PRO	-	expression tag	UNP Q31163
B	-21	LEU	-	expression tag	UNP Q31163
B	-20	ALA	-	expression tag	UNP Q31163
B	-19	PHE	-	expression tag	UNP Q31163
B	-18	PHE	-	expression tag	UNP Q31163
B	-17	SER	-	expression tag	UNP Q31163
B	-16	SER	-	expression tag	UNP Q31163
B	-15	ALA	-	expression tag	UNP Q31163
B	-14	ILE	-	expression tag	UNP Q31163
B	-13	LYS	-	expression tag	UNP Q31163
B	-12	GLY	-	expression tag	UNP Q31163
B	-11	GLY	-	expression tag	UNP Q31163
B	-10	GLY	-	expression tag	UNP Q31163
B	-9	GLY	-	expression tag	UNP Q31163
B	-8	SER	-	expression tag	UNP Q31163
B	-7	LEU	-	expression tag	UNP Q31163
B	-6	VAL	-	expression tag	UNP Q31163
B	-5	PRO	-	expression tag	UNP Q31163
B	-4	ARG	-	expression tag	UNP Q31163
B	-3	GLY	-	expression tag	UNP Q31163
B	-2	SER	-	expression tag	UNP Q31163
B	-1	GLY	-	expression tag	UNP Q31163
B	0	GLY	-	expression tag	UNP Q31163
B	1	GLY	-	expression tag	UNP Q31163
B	2	GLY	-	expression tag	UNP Q31163
B	199	SER	-	expression tag	UNP Q31163
B	200	ARG	-	expression tag	UNP Q31163
B	201	GLY	-	expression tag	UNP Q31163
B	202	GLY	-	expression tag	UNP Q31163
B	203	LEU	-	expression tag	UNP Q31163
B	204	GLU	-	expression tag	UNP Q31163
B	205	VAL	-	expression tag	UNP Q31163
B	206	LEU	-	expression tag	UNP Q31163
B	207	PHE	-	expression tag	UNP Q31163
B	208	GLN	-	expression tag	UNP Q31163

- Molecule 3 is a protein called 2B4 T-cell receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	200	Total	C	N	O	S	0	0	0
			1526	946	261	311	8			

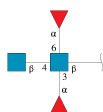
- Molecule 4 is a protein called 2B4 T-cell receptor beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	244	Total	C	N	O	S	0	0	0
			1953	1234	339	371	9			

- Molecule 5 is a protein called 2A peptide.

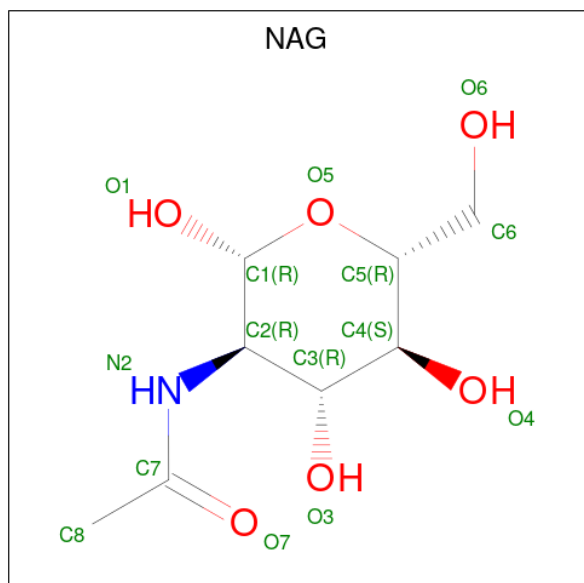
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	P	20	Total	C	N	O	0	0	0
			133	87	21	25			

- Molecule 6 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	E	4	Total	C	N	O	0	0	0
			48	28	2	18			

- 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	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		

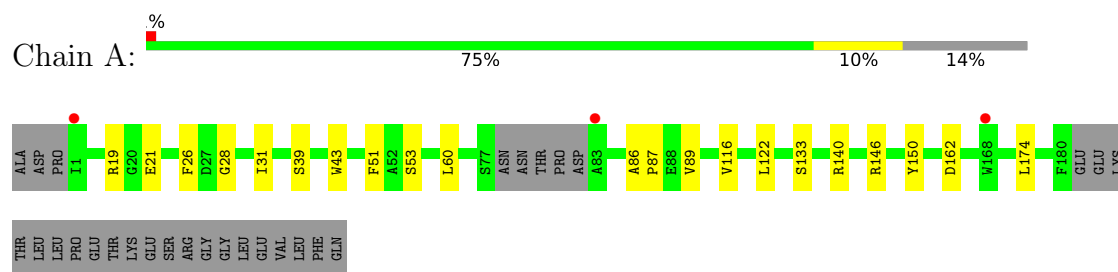
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	31	Total	O	0	0
			31	31		
8	B	28	Total	O	0	0
			28	28		
8	C	28	Total	O	0	0
			28	28		
8	D	30	Total	O	0	0
			30	30		
8	P	1	Total	O	0	0
			1	1		

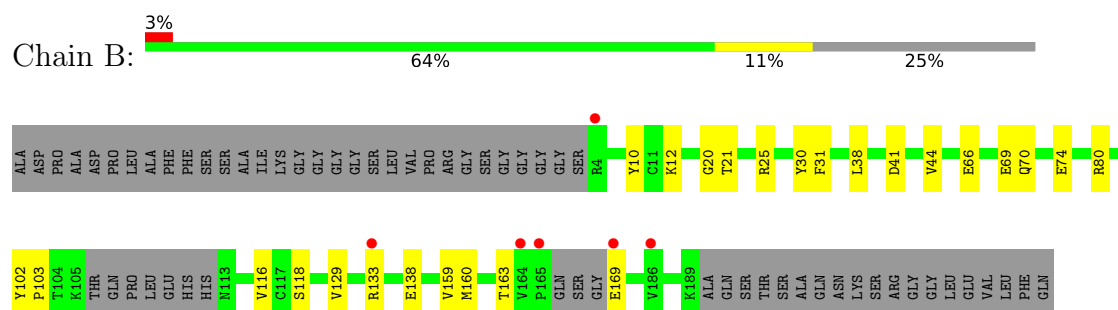
3 Residue-property plots [i](#)

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.

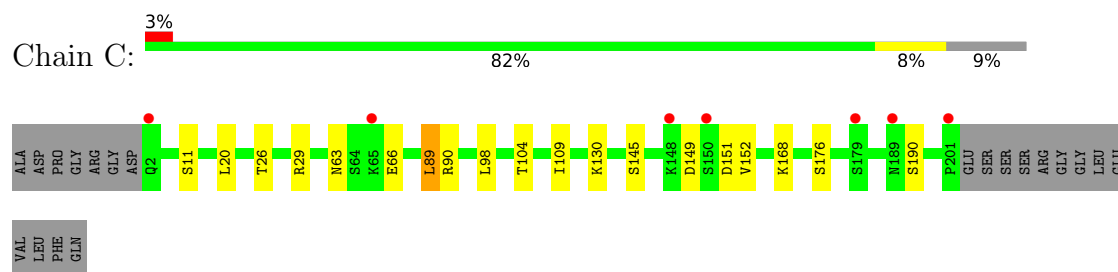
- Molecule 1: H-2 class II histocompatibility antigen, E-K alpha chain



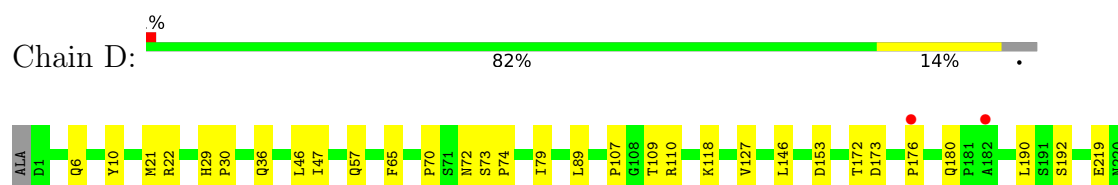
- Molecule 2: MHC class II E-beta-k



- Molecule 3: 2B4 T-cell receptor alpha chain

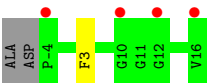
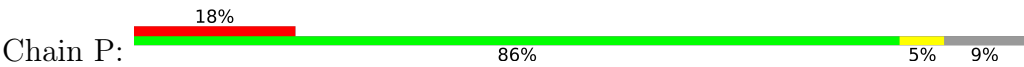


- Molecule 4: 2B4 T-cell receptor beta chain





• Molecule 5: 2A peptide



• Molecule 6: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	239.94Å 60.18Å 78.36Å 90.00° 104.33° 90.00°	Depositor
Resolution (Å)	47.67 – 2.60 47.67 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.8 (47.67-2.60) 96.9 (47.67-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.189 , 0.245 0.202 , 0.254	Depositor DCC
R_{free} test set	1649 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.677	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6701	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% 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, FUC

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	0.24	0/1472	0.69	0/1999
2	B	0.28	0/1489	0.73	0/2029
3	C	0.25	0/1556	0.68	0/2112
4	D	0.26	0/2006	0.71	2/2730 (0.1%)
5	P	0.26	0/136	0.59	0/182
All	All	0.26	0/6659	0.70	2/9052 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	180	GLN	CA-C-N	5.73	126.12	119.47
4	D	180	GLN	C-N-CA	5.73	126.12	119.47

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	1431	0	1367	12	0
2	B	1450	0	1359	18	0
3	C	1526	0	1424	12	0
4	D	1953	0	1861	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	133	0	135	1	0
6	E	48	0	43	5	0
7	A	14	0	13	0	0
7	C	28	0	26	1	0
8	A	31	0	0	2	0
8	B	28	0	0	5	0
8	C	28	0	0	2	0
8	D	30	0	0	0	0
8	P	1	0	0	0	0
All	All	6701	0	6228	62	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 5.

All (62) 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:21:THR:O	2:B:80:ARG:NH1	2.07	0.88
7:C:901:NAG:O4	8:C:1007:HOH:O	1.91	0.87
8:B:1005:HOH:O	6:E:3:NAG:O4	1.95	0.85
2:B:10:TYR:HB3	2:B:31:PHE:HB2	1.67	0.77
2:B:20:GLY:HA3	6:E:4:FUC:H4	1.69	0.74
2:B:118:SER:OG	8:B:1023:HOH:O	2.06	0.73
3:C:29:ARG:NH2	5:P:3:PHE:O	2.23	0.70
2:B:25:ARG:NH1	2:B:41:ASP:OD2	2.25	0.69
3:C:149:ASP:HB3	3:C:152:VAL:HG22	1.77	0.66
4:D:36:GLN:HG3	4:D:46:LEU:HD11	1.79	0.63
1:A:21:GLU:OE1	8:A:1013:HOH:O	2.15	0.62
2:B:116:VAL:HG22	2:B:160:MET:HG2	1.81	0.61
4:D:22:ARG:HH21	4:D:74:PRO:HG2	1.66	0.60
2:B:69:GLU:O	8:B:1022:HOH:O	2.17	0.59
1:A:51:PHE:O	8:A:1030:HOH:O	2.17	0.59
3:C:145:SER:H	3:C:190:SER:HB3	1.67	0.59
6:E:2:FUC:H5	6:E:3:NAG:HN2	1.68	0.59
3:C:11:SER:HB3	3:C:109:ILE:HD11	1.86	0.58
2:B:21:THR:OG1	6:E:4:FUC:O3	2.22	0.58
3:C:63:ASN:ND2	3:C:66:GLU:OE1	2.37	0.57
1:A:140:ARG:O	2:B:12:LYS:NZ	2.40	0.55
1:A:133:SER:HB3	1:A:150:TYR:HB2	1.90	0.53
4:D:153:ASP:HB2	4:D:176:PRO:HG2	1.91	0.52
6:E:2:FUC:H3	6:E:3:NAG:H82	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:GLU:OE1	8:B:1010:HOH:O	2.19	0.51
4:D:89:LEU:HD13	4:D:110:ARG:HG3	1.93	0.51
3:C:20:LEU:HD22	3:C:104:THR:HG21	1.92	0.51
2:B:30:TYR:HB2	2:B:38:LEU:HB3	1.92	0.50
2:B:169:GLU:N	8:B:1016:HOH:O	2.44	0.50
4:D:21:MET:HG2	4:D:109:THR:HG21	1.94	0.50
4:D:226:ASP:OD1	4:D:226:ASP:N	2.44	0.50
4:D:172:THR:HG23	4:D:192:SER:HB2	1.95	0.48
4:D:70:PRO:HG2	4:D:73:SER:HB3	1.96	0.48
1:A:19:ARG:NH1	1:A:21:GLU:OE2	2.45	0.47
1:A:39:SER:HB2	1:A:60:LEU:HD11	1.95	0.47
1:A:26:PHE:HB2	1:A:31:ILE:HD11	1.96	0.47
2:B:133:ARG:HH21	2:B:138:GLU:HG2	1.80	0.46
4:D:127:VAL:HG23	4:D:237:ALA:HB3	1.96	0.46
4:D:47:ILE:HG13	4:D:57:GLN:HB3	1.98	0.45
1:A:86:ALA:HA	1:A:87:PRO:HD3	1.78	0.44
4:D:10:TYR:CE2	4:D:110:ARG:HD3	2.52	0.44
3:C:130:LYS:NZ	8:C:1002:HOH:O	2.50	0.44
3:C:152:VAL:HG12	3:C:176:SER:HB2	2.00	0.44
4:D:65:PHE:CE2	4:D:79:ILE:HG12	2.53	0.44
1:A:89:VAL:HG21	1:A:174:LEU:HD11	2.00	0.43
3:C:168:LYS:NZ	3:C:168:LYS:HB2	2.33	0.43
1:A:28:GLY:O	1:A:146:ARG:NH2	2.51	0.43
1:A:122:LEU:HB2	1:A:162:ASP:HB2	2.00	0.43
4:D:6:GLN:HB2	4:D:107:PRO:HD2	2.00	0.43
4:D:118:LYS:HD2	4:D:225:GLN:NE2	2.34	0.42
4:D:146:LEU:HD23	4:D:146:LEU:HA	1.90	0.42
4:D:173:ASP:HB2	4:D:190:LEU:HD12	2.02	0.42
2:B:129:VAL:HB	2:B:159:VAL:HG21	2.02	0.42
2:B:102:TYR:HA	2:B:103:PRO:HD3	1.77	0.42
2:B:133:ARG:CZ	2:B:163:THR:HG21	2.51	0.41
2:B:70:GLN:O	2:B:74:GLU:HG3	2.20	0.41
3:C:149:ASP:C	3:C:151:ASP:H	2.29	0.41
2:B:41:ASP:HB3	2:B:44:VAL:HG23	2.02	0.41
4:D:29:HIS:HA	4:D:30:PRO:HD3	1.85	0.40
1:A:43:TRP:HZ2	1:A:53:SER:HA	1.87	0.40
3:C:89:LEU:HD13	3:C:98:LEU:HD13	2.03	0.40
3:C:26:THR:HG21	3:C:90:ARG:HD2	2.04	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	171/204 (84%)	166 (97%)	5 (3%)	0	100	100
2	B	170/236 (72%)	163 (96%)	7 (4%)	0	100	100
3	C	198/220 (90%)	192 (97%)	6 (3%)	0	100	100
4	D	242/255 (95%)	232 (96%)	10 (4%)	0	100	100
5	P	18/22 (82%)	18 (100%)	0	0	100	100
All	All	799/937 (85%)	771 (96%)	28 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	155/184 (84%)	154 (99%)	1 (1%)	78	91
2	B	160/207 (77%)	160 (100%)	0	100	100
3	C	170/191 (89%)	169 (99%)	1 (1%)	78	91
4	D	215/225 (96%)	212 (99%)	3 (1%)	59	81
5	P	13/14 (93%)	13 (100%)	0	100	100
All	All	713/821 (87%)	708 (99%)	5 (1%)	76	89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	VAL
3	C	89	LEU
4	D	72	ASN
4	D	219	GLU
4	D	244	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	134	ASN
3	C	188	ASN
4	D	80	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 ⓘ

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	$\# Z > 2$
6	NAG	E	1	2,6	14,14,15	0.71	1 (7%)	17,19,21	1.40	3 (17%)
6	FUC	E	2	6	10,10,11	0.75	0	14,14,16	1.06	2 (14%)
6	NAG	E	3	6	14,14,15	0.38	0	17,19,21	0.76	1 (5%)
6	FUC	E	4	6	10,10,11	0.81	0	14,14,16	0.90	1 (7%)

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	1	2,6	-	1/6/23/26	0/1/1/1
6	FUC	E	2	6	-	-	0/1/1/1
6	NAG	E	3	6	-	3/6/23/26	0/1/1/1
6	FUC	E	4	6	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	1	NAG	C1-C2	2.18	1.55	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	1	NAG	O4-C4-C3	3.81	119.35	110.38
6	E	3	NAG	C1-O5-C5	2.64	115.72	112.19
6	E	1	NAG	C1-O5-C5	2.46	115.49	112.19
6	E	2	FUC	C1-O5-C5	2.31	118.42	112.97
6	E	2	FUC	O5-C5-C4	2.30	113.69	109.55
6	E	4	FUC	O5-C5-C4	2.14	113.40	109.55
6	E	1	NAG	C4-C3-C2	-2.11	107.93	111.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

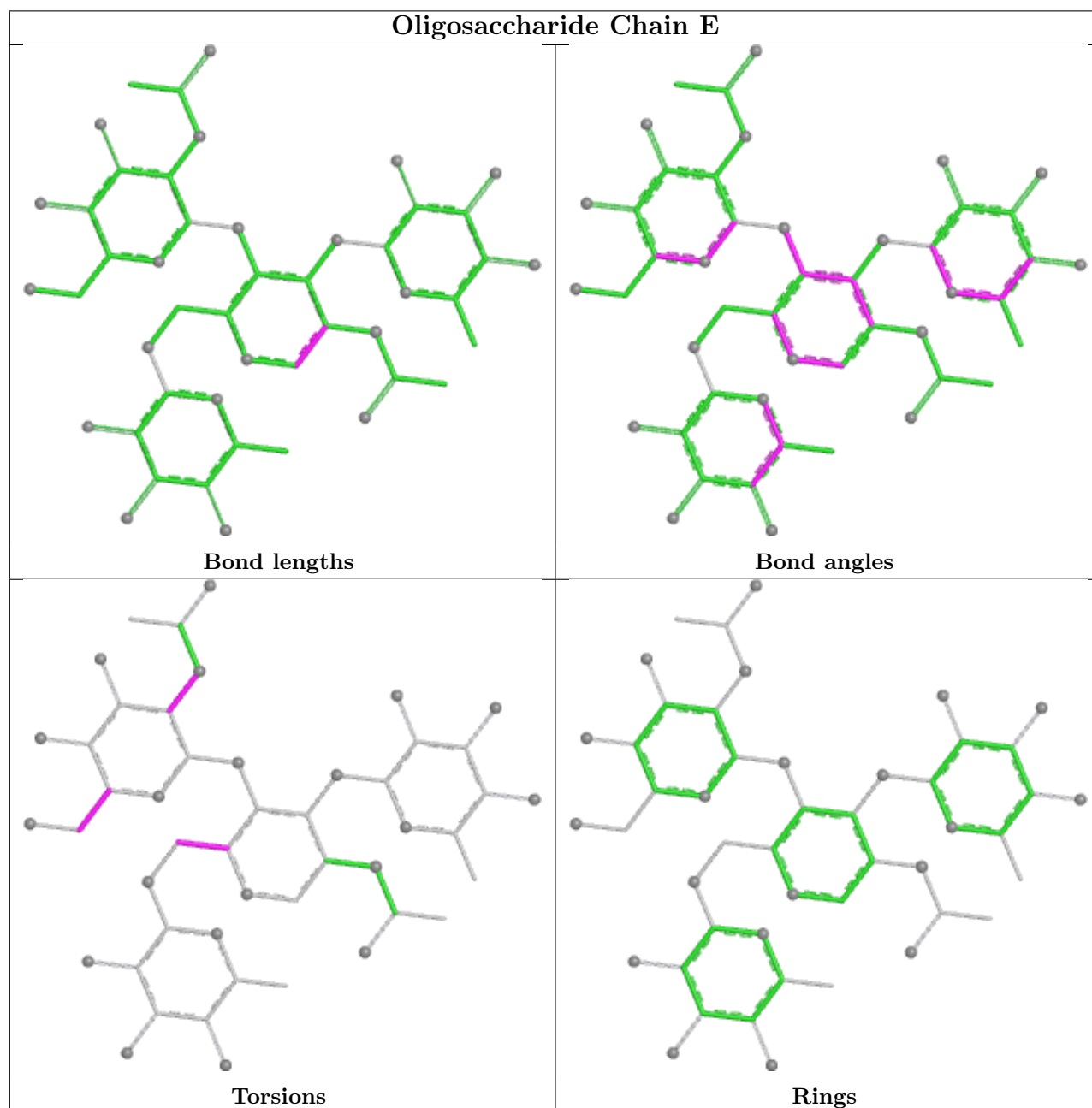
Mol	Chain	Res	Type	Atoms
6	E	3	NAG	O5-C5-C6-O6
6	E	3	NAG	C4-C5-C6-O6
6	E	1	NAG	O5-C5-C6-O6
6	E	3	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	4	FUC	2	0
6	E	2	FUC	2	0
6	E	3	NAG	3	0

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



5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	C	902	3	14,14,15	0.39	0	17,19,21	0.57	0
7	NAG	A	901	1	14,14,15	0.20	0	17,19,21	0.41	0
7	NAG	C	901	3	14,14,15	0.19	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
7	NAG	C	902	3	-	0/6/23/26	0/1/1/1
7	NAG	A	901	1	-	2/6/23/26	0/1/1/1
7	NAG	C	901	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.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	901	NAG	O5-C5-C6-O6
7	A	901	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	901	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	175/204 (85%)	0.08	3 (1%) 69 64	37, 53, 80, 89	0
2	B	176/236 (74%)	0.16	6 (3%) 48 42	37, 54, 99, 117	0
3	C	200/220 (90%)	0.23	7 (3%) 47 41	38, 55, 94, 115	0
4	D	244/255 (95%)	-0.01	3 (1%) 76 73	33, 48, 80, 120	0
5	P	20/22 (90%)	0.62	4 (20%) 3 2	37, 50, 86, 101	0
All	All	815/937 (86%)	0.12	23 (2%) 55 49	33, 51, 91, 120	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	169	GLU	3.7
3	C	2	GLN	3.5
5	P	12	GLY	3.2
2	B	4	ARG	3.1
3	C	201	PRO	3.0
2	B	133	ARG	3.0
4	D	182	ALA	3.0
1	A	83	ALA	2.9
3	C	150	SER	2.8
5	P	-4	PRO	2.7
3	C	65	LYS	2.7
5	P	16	VAL	2.7
2	B	164	VAL	2.5
3	C	189	ASN	2.5
4	D	221	ASP	2.5
4	D	176	PRO	2.4
5	P	10	GLY	2.3
1	A	1	ILE	2.3
3	C	179	SER	2.3
1	A	168	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	148	LYS	2.1
2	B	165	PRO	2.1
2	B	186	VAL	2.0

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

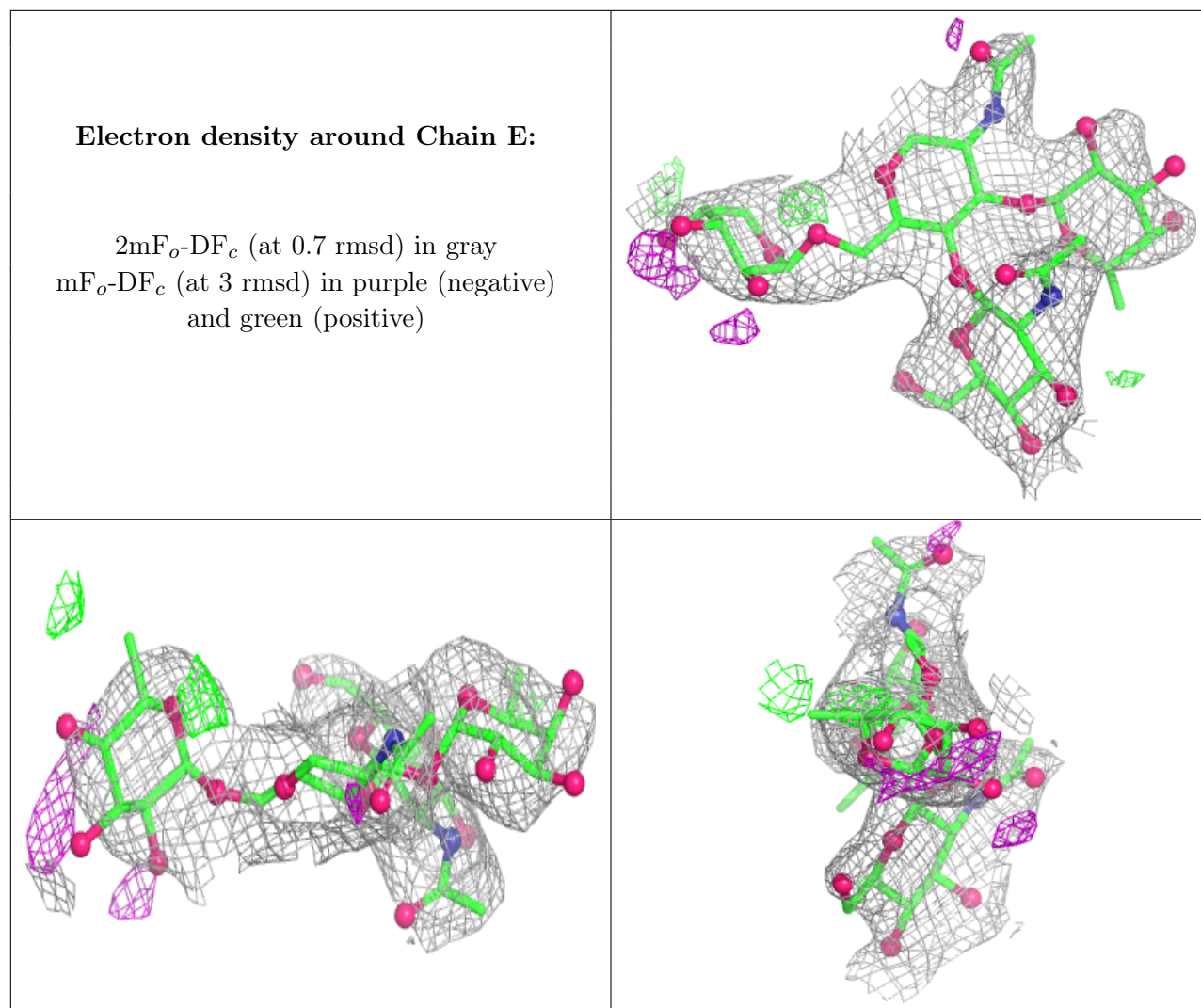
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	NAG	E	1	14/15	-	-	82,93,102,104	0
6	FUC	E	2	10/11	-	-	100,104,107,110	0
6	NAG	E	3	14/15	-	-	93,97,101,106	0
6	FUC	E	4	10/11	-	-	77,87,94,100	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($\text{\AA}^2$)	Q<0.9
7	NAG	A	901	14/15	0.63	0.15	83,96,103,105	0
7	NAG	C	902	14/15	0.65	0.15	82,89,98,99	0
7	NAG	C	901	14/15	0.81	0.12	63,79,91,93	0

6.5 Other polymers [i](#)

There are no such residues in this entry.