



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:46 AM UTC

PDB ID : 8TRQ / pdb_00008trq
Title : T cell recognition of citrullinated vimentin peptide presented by HLA-DR4
Authors : Loh, T.J.; Lim, J.J.; Reid, H.H.; Rossjohn, J.
Deposited on : 2023-08-10
Resolution : 2.75 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

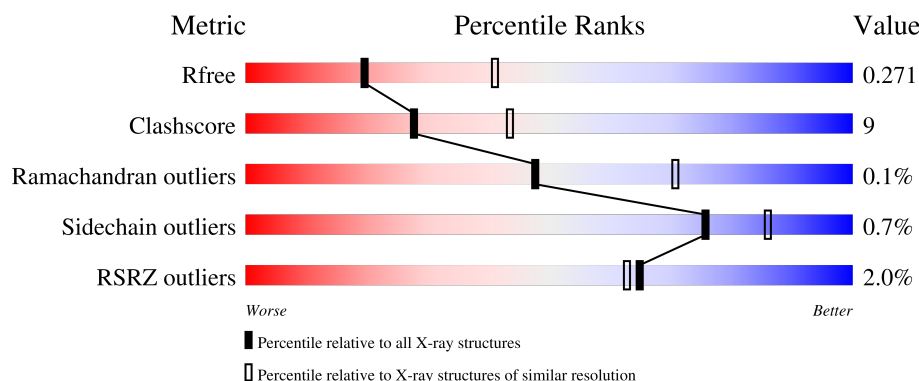
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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.



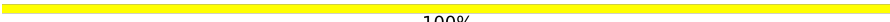
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	189	
2	B	199	
3	C	13	
4	D	209	
5	E	245	

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Mol	Chain	Length	Quality of chain
6	F	2	 100%

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
7	GOL	D	301	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6638 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	180	Total	C	N	O	S	0	0	0
			1458	944	234	275	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ILE	-	expression tag	UNP P01903
A	2	LYS	-	expression tag	UNP P01903
A	3	GLU	-	expression tag	UNP P01903
A	4	GLU	-	expression tag	UNP P01903
A	182	THR	-	expression tag	UNP P01903
A	183	SER	-	expression tag	UNP P01903
A	184	GLY	-	expression tag	UNP P01903
A	185	ASP	-	expression tag	UNP P01903
A	186	ASP	-	expression tag	UNP P01903
A	187	ASP	-	expression tag	UNP P01903
A	188	ASP	-	expression tag	UNP P01903
A	189	LYS	-	expression tag	UNP P01903

- Molecule 2 is a protein called HLA class II histocompatibility antigen, DRB1 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	190	Total	C	N	O	S	0	0	0
			1546	979	273	289	5			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	9	GLU	TRP	variant	UNP P01911
B	11	VAL	PRO	variant	UNP P01911
B	13	HIS	ARG	variant	UNP P01911
B	33	HIS	ASN	variant	UNP P01911

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Chain	Residue	Modelled	Actual	Comment	Reference
B	37	TYR	SER	variant	UNP P01911
B	47	TYR	PHE	variant	UNP P01911
B	67	LEU	ILE	variant	UNP P01911
B	71	LYS	ALA	variant	UNP P01911
B	86	GLY	VAL	variant	UNP P01911
B	96	TYR	GLN	variant	UNP P01911
B	98	GLU	LYS	variant	UNP P01911
B	104	ALA	SER	variant	UNP P01911
B	120	ASN	SER	variant	UNP P01911
B	133	ARG	LEU	variant	UNP P01911
B	140	THR	ALA	variant	UNP P01911
B	142	VAL	MET	variant	UNP P01911
B	180	LEU	VAL	variant	UNP P01911
B	191	GLY	-	expression tag	UNP P01911
B	192	SER	-	expression tag	UNP P01911
B	193	GLY	-	expression tag	UNP P01911
B	194	LEU	-	expression tag	UNP P01911
B	195	GLU	-	expression tag	UNP P01911
B	196	VAL	-	expression tag	UNP P01911
B	197	LEU	-	expression tag	UNP P01911
B	198	PHE	-	expression tag	UNP P01911
B	199	GLN	-	expression tag	UNP P01911

- Molecule 3 is a protein called Vimentin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	0	0	0
			94	58	18	18			

- Molecule 4 is a protein called A07 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	205	Total	C	N	O	S	0	0	0
			1533	960	248	317	8			

- Molecule 5 is a protein called A07 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	243	Total	C	N	O	S	0	0	0
			1882	1187	326	362	7			

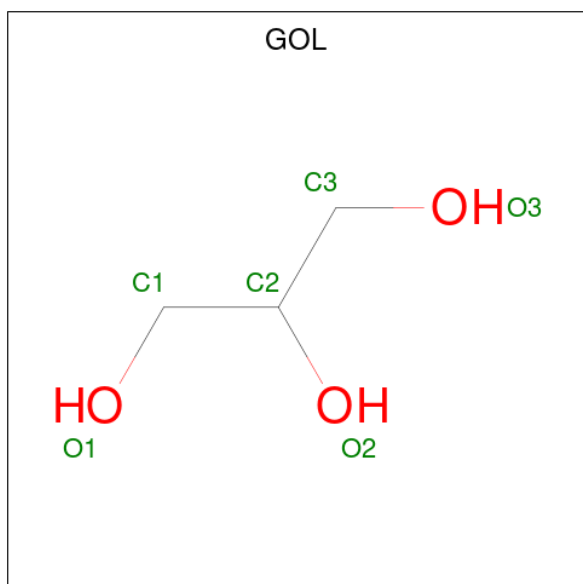
- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	E	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		

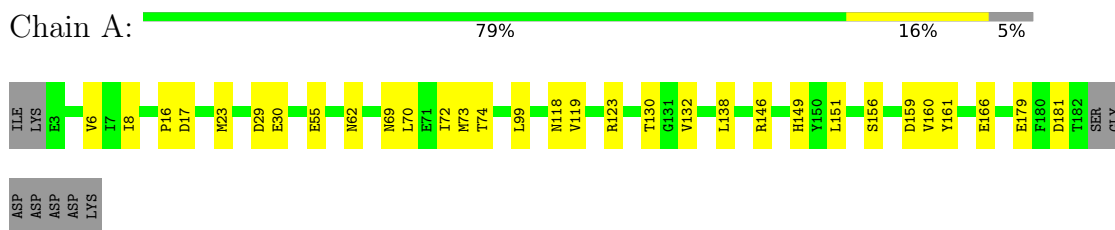
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	16	Total	O	0	0
			16	16		
8	B	10	Total	O	0	0
			10	10		
8	D	3	Total	O	0	0
			3	3		
8	E	8	Total	O	0	0
			8	8		

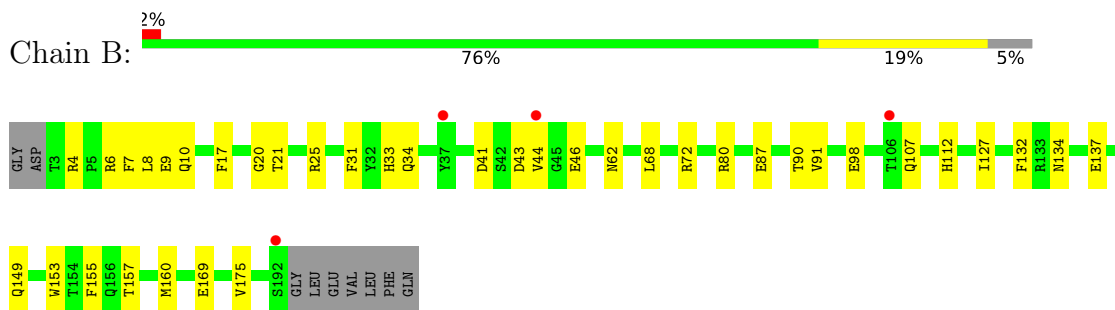
3 Residue-property plots

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.

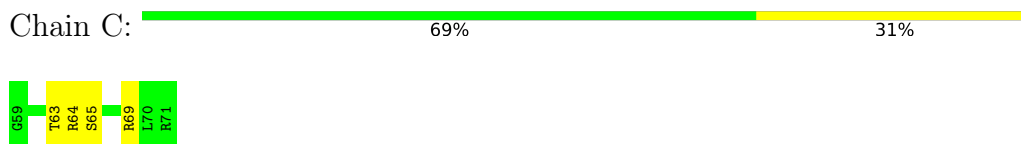
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain



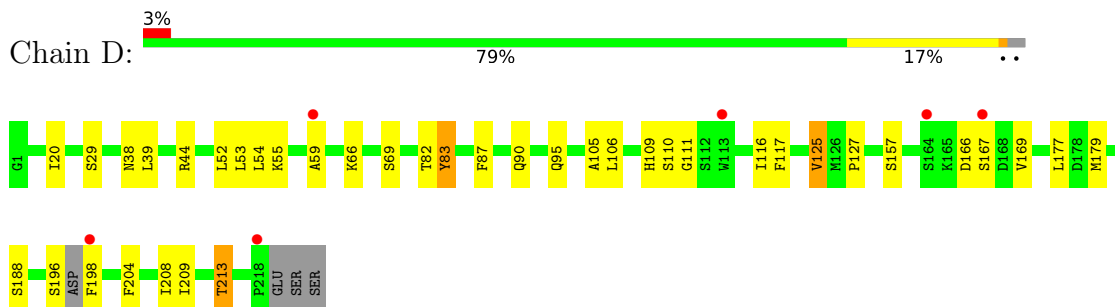
- Molecule 2: HLA class II histocompatibility antigen, DRB1 beta chain



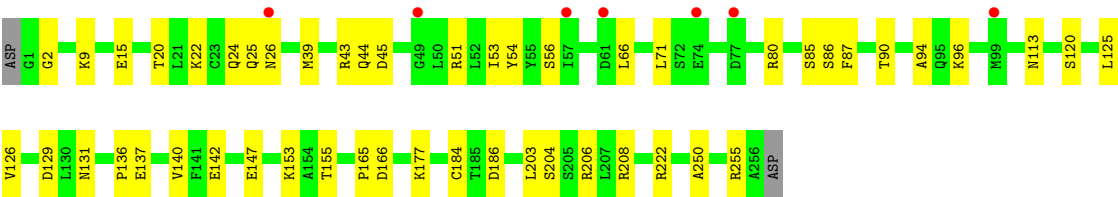
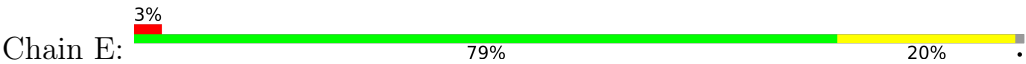
- Molecule 3: Vimentin



- Molecule 4: A07 TCR alpha chain



● Molecule 5: A07 TCR beta chain



● Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.60Å 76.62Å 224.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.55 – 2.75 46.55 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.55-2.75) 99.9 (46.55-2.75)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.216 , 0.264 0.224 , 0.271	Depositor DCC
R_{free} test set	1315 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	66.3	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 62.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6638	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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

5.1 Standard geometry

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

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	0.40	0/1503	0.59	0/2056
2	B	0.42	0/1590	0.61	0/2164
3	C	0.42	0/82	0.69	0/109
4	D	0.36	0/1566	0.53	0/2138
5	E	0.41	0/1928	0.60	0/2625
All	All	0.40	0/6669	0.59	0/9092

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
3	C	0	1
5	E	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	63	THR	Mainchain
5	E	222	ARG	Sidechain

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	1458	0	1365	24	0
2	B	1546	0	1438	28	0
3	C	94	0	89	6	0
4	D	1533	0	1403	33	0
5	E	1882	0	1769	39	0
6	F	28	0	25	2	0
7	A	30	0	37	3	0
7	B	12	0	16	2	0
7	D	6	0	8	4	0
7	E	12	0	15	3	0
8	A	16	0	0	0	0
8	B	10	0	0	0	0
8	D	3	0	0	0	0
8	E	8	0	0	2	0
All	All	6638	0	6165	115	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (115) 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)
5:E:15:GLU:HG2	5:E:96:LYS:HE2	1.68	0.75
4:D:44:ARG:NH1	5:E:44:GLN:OE1	2.20	0.74
4:D:59:ALA:HA	4:D:83:TYR:CD2	2.23	0.73
5:E:26:ASN:HB3	8:E:401:HOH:O	1.91	0.69
2:B:25:ARG:NH2	2:B:43:ASP:OD2	2.25	0.69
1:A:138:LEU:HB2	1:A:146:ARG:HG3	1.75	0.68
2:B:134:ASN:HD21	2:B:169:GLU:HG2	1.59	0.67
4:D:117:PHE:H	7:D:301:GOL:H12	1.59	0.66
2:B:98:GLU:OE1	7:B:201:GOL:O3	2.14	0.65
2:B:41:ASP:HB3	2:B:44:VAL:HG22	1.80	0.64
5:E:137:GLU:HG2	7:E:302:GOL:H11	1.82	0.61
5:E:142:GLU:OE2	5:E:255:ARG:NH2	2.33	0.61
2:B:21:THR:O	2:B:80:ARG:NH1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:PHE:HA	2:B:33:HIS:HE1	1.65	0.61
2:B:25:ARG:CZ	2:B:43:ASP:OD2	2.49	0.60
7:D:301:GOL:H31	5:E:51:ARG:HA	1.84	0.59
5:E:136:PRO:O	7:E:302:GOL:H12	2.03	0.59
5:E:15:GLU:HG2	5:E:96:LYS:HG3	1.84	0.58
4:D:179:MET:HE1	5:E:153:LYS:HD3	1.86	0.58
4:D:39:LEU:HD12	4:D:83:TYR:CD1	2.39	0.57
5:E:166:ASP:OD1	5:E:166:ASP:N	2.34	0.57
4:D:166:ASP:HB3	4:D:169:VAL:HG12	1.85	0.57
1:A:73:MET:HB2	3:C:69:ARG:HH12	1.69	0.56
4:D:66:LYS:HB2	4:D:82:THR:HG22	1.88	0.56
4:D:54:LEU:HD12	4:D:69:SER:HB3	1.87	0.56
1:A:123:ARG:NH1	1:A:161:TYR:OH	2.39	0.56
4:D:59:ALA:HA	4:D:83:TYR:HD2	1.70	0.56
5:E:56:SER:O	5:E:80:ARG:NH1	2.39	0.56
1:A:69:ASN:CG	3:C:69:ARG:HG2	2.30	0.55
2:B:10:GLN:HB2	2:B:31:PHE:HB2	1.88	0.55
4:D:177:LEU:HB3	5:E:184:CYS:HB2	1.88	0.55
5:E:25:GLN:HG2	5:E:39:MET:HE3	1.89	0.55
4:D:53:LEU:HG	4:D:54:LEU:HD13	1.89	0.55
5:E:54:TYR:OH	5:E:71:LEU:HD13	2.07	0.55
4:D:59:ALA:HA	4:D:83:TYR:CE2	2.43	0.54
4:D:117:PHE:N	7:D:301:GOL:H12	2.22	0.54
1:A:73:MET:HE2	3:C:69:ARG:NH1	2.22	0.54
4:D:196:SER:O	4:D:198:PHE:N	2.41	0.54
4:D:209:ILE:O	4:D:213:THR:HG22	2.08	0.54
4:D:39:LEU:HD13	4:D:87:PHE:HB2	1.91	0.53
1:A:72:ILE:HD12	3:C:69:ARG:HB2	1.91	0.53
4:D:95:GLN:O	4:D:125:VAL:HG11	2.09	0.52
4:D:111:GLY:HA2	5:E:113:ASN:OD1	2.10	0.52
7:A:304:GOL:H11	2:B:149:GLN:H	1.75	0.51
2:B:87:GLU:HA	2:B:91:VAL:HG12	1.92	0.51
1:A:118:ASN:HB2	1:A:166:GLU:HB2	1.91	0.51
4:D:52:LEU:HD21	4:D:55:LYS:HE2	1.94	0.50
5:E:22:LYS:NZ	5:E:86:SER:HB3	2.26	0.50
1:A:16:PRO:HG3	2:B:4:ARG:HD2	1.94	0.50
5:E:43:ARG:HB2	5:E:53:ILE:HD11	1.92	0.50
1:A:99:LEU:H	1:A:99:LEU:HD12	1.77	0.50
5:E:20:THR:HA	5:E:90:THR:HG22	1.94	0.50
5:E:22:LYS:HE3	5:E:86:SER:HB3	1.94	0.49
4:D:20:ILE:HG12	4:D:90:GLN:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLU:HG3	4:D:29:SER:HB2	1.93	0.48
5:E:204:SER:OG	5:E:206:ARG:NH2	2.47	0.48
4:D:53:LEU:HG	4:D:54:LEU:CD1	2.43	0.48
1:A:23:MET:HE2	1:A:30:GLU:HG3	1.95	0.48
2:B:87:GLU:HG3	2:B:91:VAL:CG1	2.44	0.47
1:A:119:VAL:HB	1:A:149:HIS:CE1	2.49	0.47
5:E:147:GLU:OE2	5:E:155:THR:OG1	2.33	0.47
2:B:46:GLU:HB2	2:B:62:ASN:OD1	2.14	0.47
1:A:70:LEU:HB2	2:B:9:GLU:HB2	1.94	0.47
5:E:129:ASP:OD2	5:E:131:ASN:HB3	2.14	0.47
1:A:17:ASP:OD1	2:B:6:ARG:NH1	2.37	0.46
2:B:157:THR:HG21	7:B:202:GOL:O3	2.15	0.46
5:E:24:GLN:HA	5:E:85:SER:O	2.16	0.46
4:D:166:ASP:HB3	4:D:169:VAL:CG1	2.46	0.46
2:B:33:HIS:O	2:B:34:GLN:HG2	2.16	0.46
4:D:105:ALA:HA	4:D:116:ILE:O	2.16	0.45
4:D:188:SER:OG	5:E:206:ARG:HD2	2.17	0.45
2:B:25:ARG:NE	2:B:43:ASP:OD2	2.49	0.45
4:D:38:ASN:HD21	4:D:109:HIS:HD2	1.64	0.45
1:A:70:LEU:O	1:A:74:THR:HG23	2.17	0.45
1:A:156:SER:HB3	1:A:159:ASP:HB2	1.98	0.45
1:A:29:ASP:HB3	2:B:153:TRP:CE2	2.52	0.44
2:B:8:LEU:H	2:B:33:HIS:CE1	2.35	0.44
1:A:62:ASN:HD21	3:C:65:SER:HA	1.82	0.44
6:F:1:NAG:H61	6:F:2:NAG:O5	2.18	0.44
5:E:66:LEU:HD12	5:E:66:LEU:HA	1.82	0.43
2:B:107:GLN:NE2	2:B:112:HIS:O	2.49	0.43
5:E:94:ALA:HB1	5:E:126:VAL:HG21	2.00	0.43
5:E:22:LYS:CE	5:E:86:SER:HB3	2.48	0.42
3:C:65:SER:HB3	4:D:110:SER:O	2.20	0.42
5:E:186:ASP:HB2	5:E:203:LEU:HD12	2.02	0.42
2:B:68:LEU:O	2:B:72:ARG:HG3	2.19	0.42
4:D:39:LEU:HB3	4:D:87:PHE:CD2	2.55	0.42
1:A:160:VAL:HG22	1:A:179:GLU:HG2	1.99	0.42
5:E:39:MET:SD	5:E:87:PHE:HB2	2.60	0.42
2:B:149:GLN:HG2	2:B:155:PHE:CE2	2.55	0.42
4:D:166:ASP:OD1	4:D:167:SER:N	2.53	0.42
5:E:43:ARG:NE	5:E:45:ASP:OD1	2.51	0.42
5:E:80:ARG:HG3	5:E:86:SER:O	2.19	0.42
5:E:140:VAL:HG23	5:E:250:ALA:HB3	2.02	0.42
5:E:9:LYS:HE3	5:E:120:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:THR:OG1	7:A:303:GOL:O3	2.20	0.42
2:B:127:ILE:HD11	2:B:175:VAL:HG13	2.02	0.42
4:D:179:MET:HE2	5:E:208:ARG:HD3	2.01	0.42
5:E:2:GLY:HA2	8:E:401:HOH:O	2.19	0.42
5:E:136:PRO:O	7:E:302:GOL:H32	2.20	0.42
4:D:117:PHE:H	7:D:301:GOL:C1	2.31	0.42
6:F:1:NAG:H4	6:F:2:NAG:H2	1.79	0.42
5:E:177:LYS:O	5:E:177:LYS:HG3	2.19	0.41
2:B:90:THR:OG1	2:B:91:VAL:N	2.53	0.41
1:A:6:VAL:HG12	1:A:8:ILE:HG13	2.00	0.41
1:A:8:ILE:HD12	7:A:301:GOL:H11	2.03	0.41
1:A:132:VAL:HG22	1:A:151:LEU:HD13	2.02	0.41
2:B:132:PHE:CE2	2:B:137:GLU:HB2	2.55	0.41
4:D:204:PHE:O	4:D:208:ILE:HB	2.21	0.41
2:B:134:ASN:ND2	2:B:169:GLU:HG2	2.33	0.41
1:A:123:ARG:HG3	1:A:161:TYR:CE1	2.56	0.40
2:B:17:PHE:HB3	2:B:20:GLY:O	2.20	0.40
5:E:15:GLU:CG	5:E:96:LYS:HG3	2.49	0.40
5:E:125:LEU:HD13	5:E:165:PRO:HB3	2.03	0.40
4:D:127:PRO:O	4:D:157:SER:OG	2.34	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	178/189 (94%)	172 (97%)	6 (3%)	0	100	100
2	B	188/199 (94%)	183 (97%)	5 (3%)	0	100	100
3	C	10/13 (77%)	10 (100%)	0	0	100	100
4	D	201/209 (96%)	191 (95%)	9 (4%)	1 (0%)	24	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	241/245 (98%)	223 (92%)	18 (8%)	0	100	100
All	All	818/855 (96%)	779 (95%)	38 (5%)	1 (0%)	48	71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	83	TYR

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	160/173 (92%)	159 (99%)	1 (1%)	78	88
2	B	165/178 (93%)	164 (99%)	1 (1%)	78	88
3	C	8/9 (89%)	8 (100%)	0	100	100
4	D	169/186 (91%)	166 (98%)	3 (2%)	51	71
5	E	199/213 (93%)	199 (100%)	0	100	100
All	All	701/759 (92%)	696 (99%)	5 (1%)	76	86

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

Mol	Chain	Res	Type
1	A	181	ASP
2	B	160	MET
4	D	106	LEU
4	D	125	VAL
4	D	213	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN

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Mol	Chain	Res	Type
2	B	33	HIS
2	B	70	GLN
2	B	111	HIS
2	B	120	ASN
2	B	150	ASN
2	B	156	GLN
4	D	109	HIS
4	D	163	GLN
4	D	206	ASN
5	E	14	GLN
5	E	150	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
3	CIR	C	64	3	9,10,11	3.24	3 (33%)	6,11,13	1.14	1 (16%)

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
3	CIR	C	64	3	-	2/8/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	64	CIR	C7-N6	7.58	1.45	1.34
3	C	64	CIR	C7-N8	4.65	1.45	1.33
3	C	64	CIR	O7-C7	-3.40	1.19	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	64	CIR	O7-C7-N8	-2.26	118.63	123.18

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	64	CIR	C4-C5-N6-C7
3	C	64	CIR	CA-C3-C4-C5

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

2 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	F	1	1,6	14,14,15	0.34	0	17,19,21	0.65	0
6	NAG	F	2	6	14,14,15	0.32	0	17,19,21	0.86	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	F	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	F	2	6	-	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.

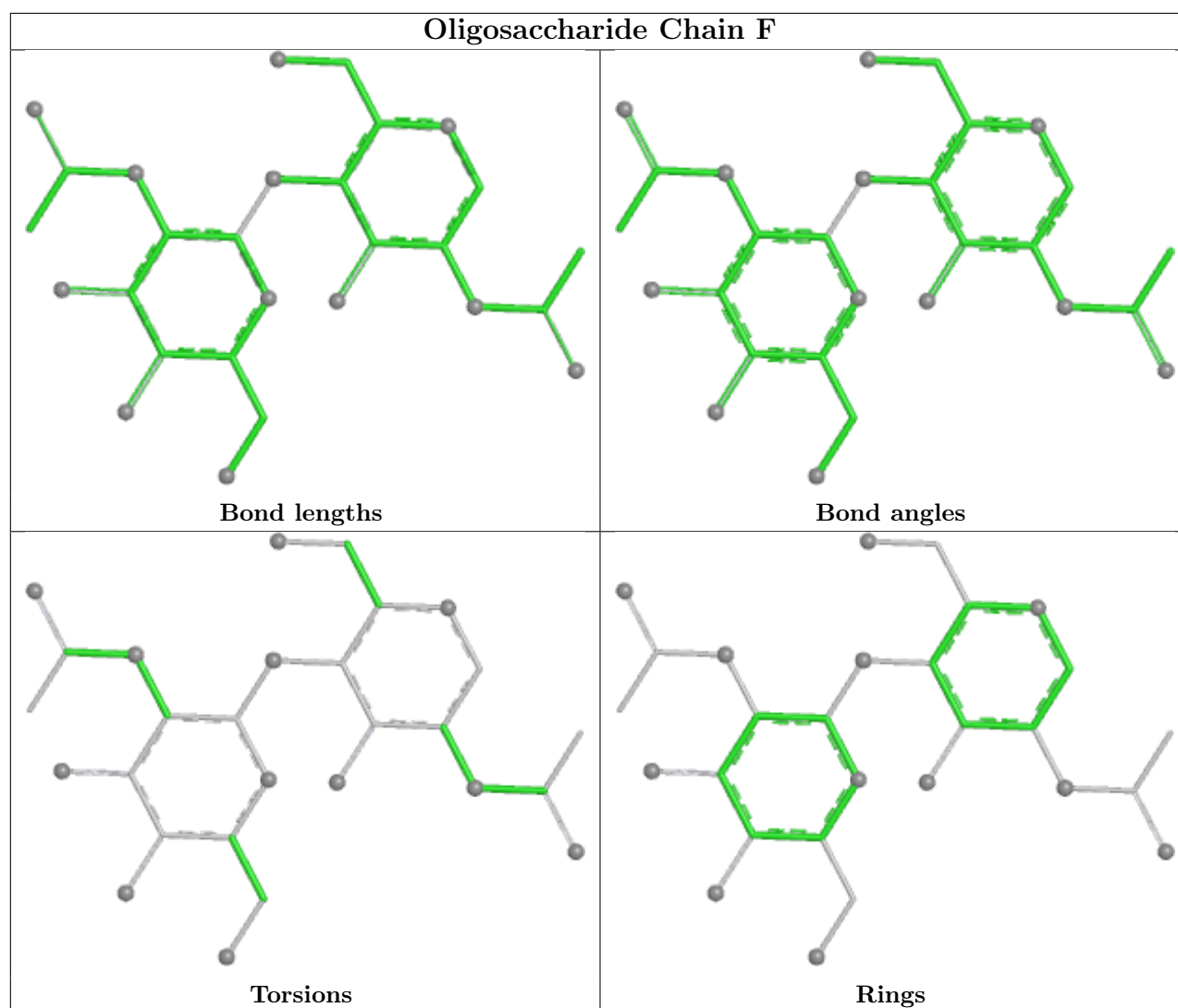
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	1	NAG	2	0
6	F	2	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.



5.6 Ligand geometry [i](#)

10 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	GOL	A	301	-	5,5,5	1.47	1 (20%)	5,5,5	1.26	1 (20%)
7	GOL	E	301	-	5,5,5	1.14	0	5,5,5	0.88	0
7	GOL	A	304	-	5,5,5	0.89	0	5,5,5	1.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	E	302	-	5,5,5	1.24	1 (20%)	5,5,5	0.83	0
7	GOL	B	201	-	5,5,5	1.01	0	5,5,5	1.13	0
7	GOL	A	305	-	5,5,5	1.46	1 (20%)	5,5,5	1.18	0
7	GOL	A	303	-	5,5,5	0.87	0	5,5,5	1.30	0
7	GOL	B	202	-	5,5,5	1.10	0	5,5,5	1.03	0
7	GOL	A	302	-	5,5,5	1.02	0	5,5,5	1.07	0
7	GOL	D	301	-	5,5,5	0.69	0	5,5,5	1.31	1 (20%)

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	GOL	A	301	-	-	2/4/4/4	-
7	GOL	E	301	-	-	0/4/4/4	-
7	GOL	A	304	-	-	1/4/4/4	-
7	GOL	E	302	-	-	3/4/4/4	-
7	GOL	B	201	-	-	3/4/4/4	-
7	GOL	A	305	-	-	4/4/4/4	-
7	GOL	A	303	-	-	4/4/4/4	-
7	GOL	B	202	-	-	0/4/4/4	-
7	GOL	A	302	-	-	0/4/4/4	-
7	GOL	D	301	-	-	3/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	305	GOL	O2-C2	-2.77	1.35	1.43
7	A	301	GOL	O2-C2	-2.57	1.35	1.43
7	E	302	GOL	O2-C2	-2.29	1.36	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	301	GOL	C3-C2-C1	-2.74	101.75	111.80
7	A	301	GOL	C3-C2-C1	-2.08	104.15	111.80

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	303	GOL	O1-C1-C2-C3
7	A	303	GOL	C1-C2-C3-O3
7	B	201	GOL	O1-C1-C2-C3
7	E	302	GOL	C1-C2-C3-O3
7	E	302	GOL	O2-C2-C3-O3
7	A	301	GOL	C1-C2-C3-O3
7	A	305	GOL	O1-C1-C2-C3
7	A	305	GOL	C1-C2-C3-O3
7	D	301	GOL	O1-C1-C2-C3
7	A	301	GOL	O2-C2-C3-O3
7	A	303	GOL	O1-C1-C2-O2
7	A	305	GOL	O1-C1-C2-O2
7	B	201	GOL	O1-C1-C2-O2
7	A	303	GOL	O2-C2-C3-O3
7	D	301	GOL	O1-C1-C2-O2
7	B	201	GOL	O2-C2-C3-O3
7	A	304	GOL	O2-C2-C3-O3
7	A	305	GOL	O2-C2-C3-O3
7	E	302	GOL	O1-C1-C2-O2
7	D	301	GOL	O2-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	301	GOL	1	0
7	A	304	GOL	1	0
7	E	302	GOL	3	0
7	B	201	GOL	1	0
7	A	303	GOL	1	0
7	B	202	GOL	1	0
7	D	301	GOL	4	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	180/189 (95%)	0.12	0 100 100	50, 71, 91, 106	0
2	B	190/199 (95%)	0.16	4 (2%) 63 61	49, 63, 88, 118	0
3	C	12/13 (92%)	0.15	0 100 100	54, 58, 75, 82	0
4	D	205/209 (98%)	0.36	6 (2%) 53 52	54, 75, 102, 111	0
5	E	243/245 (99%)	0.34	7 (2%) 53 52	47, 70, 97, 106	0
All	All	830/855 (97%)	0.25	17 (2%) 65 63	47, 70, 97, 118	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	167	SER	4.7
5	E	99	MET	3.3
4	D	113	TRP	3.2
5	E	61	ASP	3.1
5	E	74	GLU	3.1
2	B	44	VAL	3.1
5	E	57	ILE	2.9
4	D	218	PRO	2.8
2	B	192	SER	2.7
5	E	26	ASN	2.7
4	D	164	SER	2.5
4	D	198	PHE	2.4
5	E	77	ASP	2.3
2	B	37	TYR	2.2
4	D	59	ALA	2.2
5	E	49	GLY	2.2
2	B	106	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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.

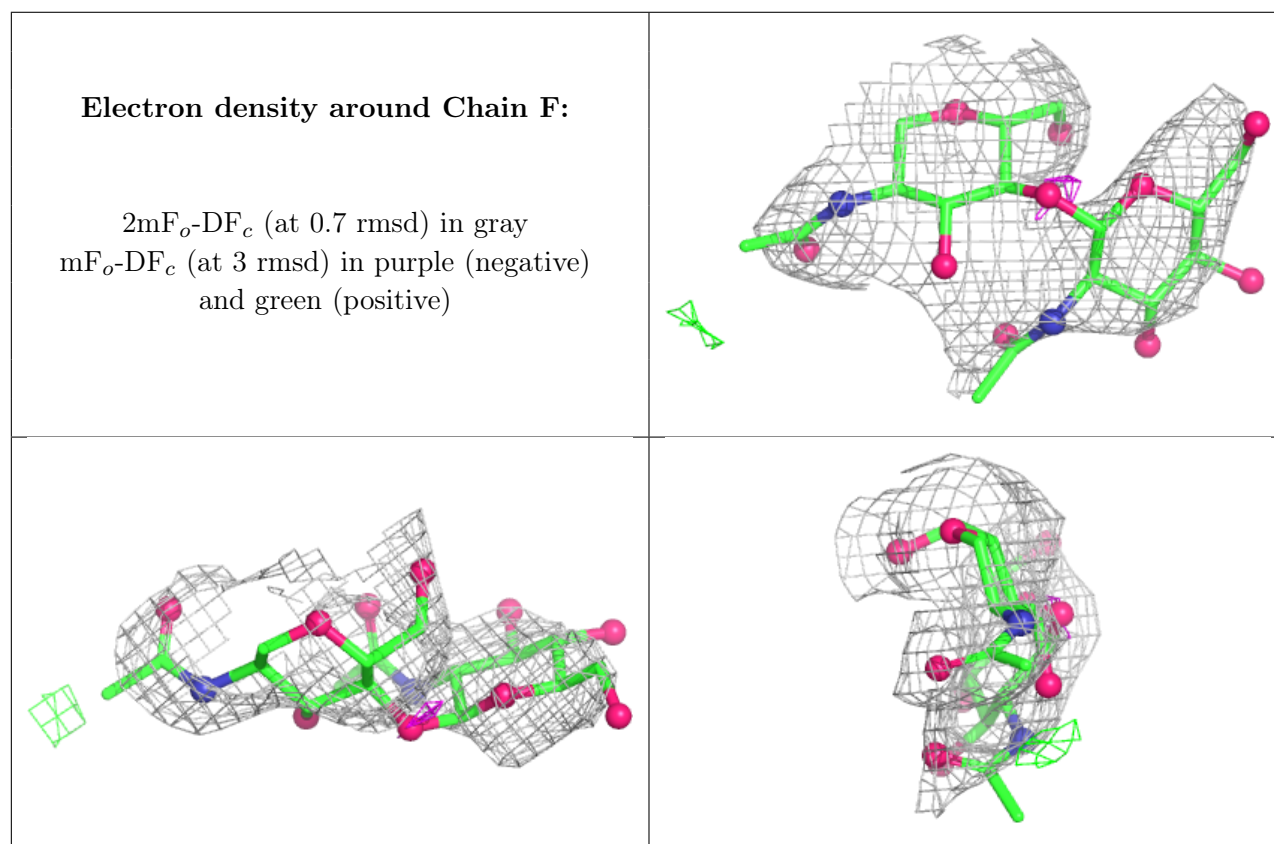
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CIR	C	64	11/12	0.95	0.09	52,55,59,59	0

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	F	2	14/15	0.56	0.13	116,127,130,130	0
6	NAG	F	1	14/15	0.72	0.14	86,102,123,135	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
7	GOL	A	302	6/6	0.69	0.14	96,100,101,105	0
7	GOL	A	303	6/6	0.73	0.18	78,82,87,92	0
7	GOL	E	301	6/6	0.73	0.14	76,79,80,80	0
7	GOL	B	202	6/6	0.76	0.22	62,71,74,99	0
7	GOL	A	305	6/6	0.80	0.15	60,70,84,91	0
7	GOL	A	301	6/6	0.82	0.14	63,66,71,73	0
7	GOL	E	302	6/6	0.83	0.22	49,57,74,98	0
7	GOL	A	304	6/6	0.84	0.18	61,65,65,71	0
7	GOL	D	301	6/6	0.85	0.11	67,71,81,101	0
7	GOL	B	201	6/6	0.91	0.15	59,75,82,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.