Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2023 – 08:16 PM EDT

PDB ID	:	4KGQ
Title	:	Crystal structure of a human light loop mutant in complex with dcr3
Authors	:	Liu, W.; Zhan, C.; Bonanno, J.B.; Sampathkumar, P.; Toro, R.; Nathenson, S.G.; Almo, S.C.; New York Structural Genomics Research Consortium (NYSGRC); Atoms-to-Animals: The Immune Function Network (IFN)
Deposited on	:	2013-04-29
Resolution	:	2.27 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:

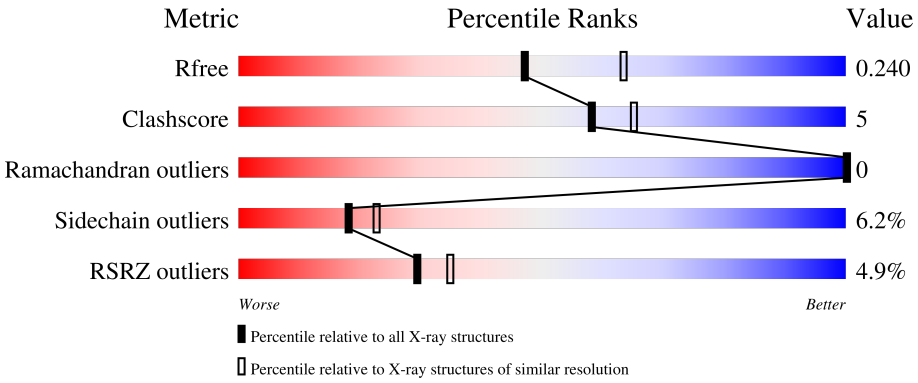
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.27 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	C	174	81% 13%
1	D	174	13% 78% 13% 6%
2	A	158	75% 13% 12%
2	B	158	3% 77% 9% 12%
3	E	4	75% 25%

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Mol	Chain	Length	Quality of chain
4	F	2	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4865 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 Tumor necrosis factor receptor superfamily member 6B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	167	Total	C	N	O	S	0	0	0
			1264	765	243	238	18			
1	D	164	Total	C	N	O	S	0	0	0
			1242	752	236	236	18			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	196	THR	-	expression tag	UNP O95407
C	197	GLY	-	expression tag	UNP O95407
C	198	HIS	-	expression tag	UNP O95407
C	199	HIS	-	expression tag	UNP O95407
C	200	HIS	-	expression tag	UNP O95407
C	201	HIS	-	expression tag	UNP O95407
C	202	HIS	-	expression tag	UNP O95407
C	203	HIS	-	expression tag	UNP O95407
D	196	THR	-	expression tag	UNP O95407
D	197	GLY	-	expression tag	UNP O95407
D	198	HIS	-	expression tag	UNP O95407
D	199	HIS	-	expression tag	UNP O95407
D	200	HIS	-	expression tag	UNP O95407
D	201	HIS	-	expression tag	UNP O95407
D	202	HIS	-	expression tag	UNP O95407
D	203	HIS	-	expression tag	UNP O95407

- Molecule 2 is a protein called Tumor necrosis factor ligand superfamily member 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	139	Total	C	N	O	S	0	0	0
			1076	690	181	202	3			
2	B	139	Total	C	N	O	S	0	0	0
			1076	690	181	202	3			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	214	GLU	LYS	variant	UNP O43557
A	226	ASP	ARG	engineered mutation	UNP O43557
A	227	TYR	LEU	engineered mutation	UNP O43557
A	228	THR	ARG	engineered mutation	UNP O43557
A	229	LYS	ASP	engineered mutation	UNP O43557
A	230	GLU	GLY	engineered mutation	UNP O43557
A	231	ASP	THR	engineered mutation	UNP O43557
B	214	GLU	LYS	variant	UNP O43557
B	226	ASP	ARG	engineered mutation	UNP O43557
B	227	TYR	LEU	engineered mutation	UNP O43557
B	228	THR	ARG	engineered mutation	UNP O43557
B	229	LYS	ASP	engineered mutation	UNP O43557
B	230	GLU	GLY	engineered mutation	UNP O43557
B	231	ASP	THR	engineered mutation	UNP O43557

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	4	50	28	2	20	0	0	0

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

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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Mg 1 1	0	0
5	D	1	Total Mg 1 1	0	0

- Molecule 6 is water.

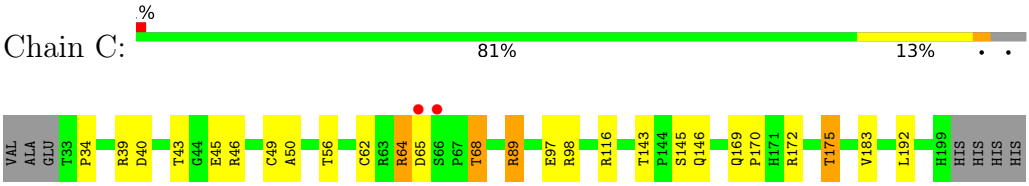
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	38	Total O 38 38	0	0
6	D	10	Total O 10 10	0	0
6	A	44	Total O 44 44	0	0
6	B	35	Total O 35 35	0	0

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.

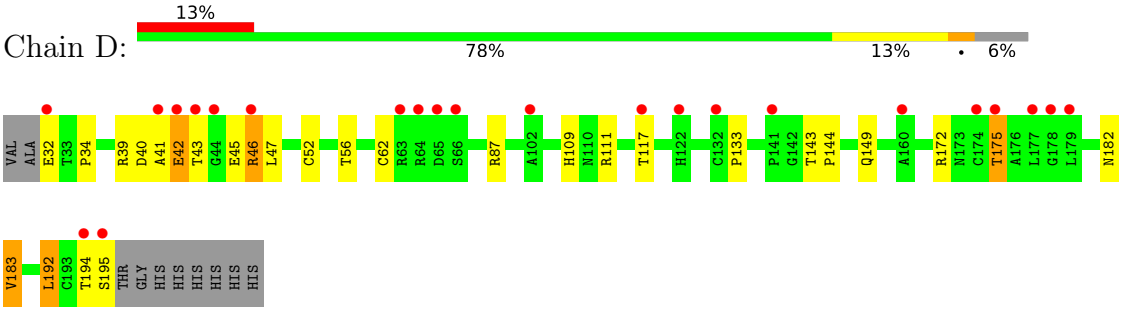
• Molecule 1: Tumor necrosis factor receptor superfamily member 6B

Chain C:



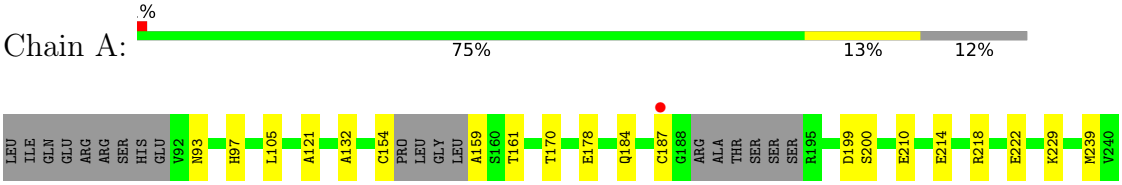
• Molecule 1: Tumor necrosis factor receptor superfamily member 6B

Chain D:



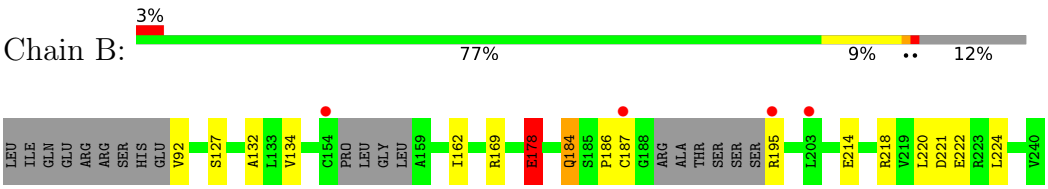
• Molecule 2: Tumor necrosis factor ligand superfamily member 14

Chain A:



• Molecule 2: Tumor necrosis factor ligand superfamily member 14

Chain B:

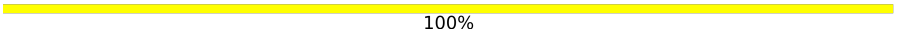


• Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

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

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	149.27Å 149.27Å 149.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.35 – 2.27 37.32 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.9 (37.35-2.27) 99.9 (37.32-2.27)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	4.50 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.195 , 0.238 0.201 , 0.240	Depositor DCC
R_{free} test set	2609 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	39.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4865	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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: BMA, MAN, MG, 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	C	1.12	1/1304 (0.1%)	1.11	8/1781 (0.4%)
1	D	0.91	0/1280	0.91	3/1748 (0.2%)
2	A	1.22	1/1101 (0.1%)	1.08	2/1493 (0.1%)
2	B	1.19	3/1101 (0.3%)	1.13	3/1493 (0.2%)
All	All	1.11	5/4786 (0.1%)	1.06	16/6515 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	210	GLU	CD-OE2	8.74	1.35	1.25
2	B	169	ARG	CD-NE	-5.55	1.37	1.46
1	C	56	THR	CB-CG2	5.13	1.69	1.52
2	B	178	GLU	CD-OE2	5.11	1.31	1.25
2	B	218	ARG	CZ-NH2	5.11	1.39	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	169	ARG	NE-CZ-NH2	-12.15	114.22	120.30
1	C	39	ARG	NE-CZ-NH1	8.77	124.69	120.30
1	C	172	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	C	172	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	D	172	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	C	89	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	D	111	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	C	46	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	C	46	ARG	NE-CZ-NH2	-6.33	117.14	120.30
2	B	218	ARG	NE-CZ-NH2	6.29	123.45	120.30
2	B	218	ARG	NE-CZ-NH1	-5.93	117.33	120.30
2	A	218	ARG	NE-CZ-NH2	5.93	123.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	199	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	C	89	ARG	NE-CZ-NH1	-5.71	117.45	120.30
1	D	111	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	C	65	ASP	CB-CG-OD1	5.06	122.85	118.30

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	C	1264	0	1147	13	0
1	D	1242	0	1129	21	0
2	A	1076	0	1047	6	0
2	B	1076	0	1047	8	0
3	E	50	0	43	2	0
4	F	28	0	25	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	44	0	0	1	0
6	B	35	0	0	2	0
6	C	38	0	0	0	0
6	D	10	0	0	0	0
All	All	4865	0	4438	44	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 (44) 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:178:GLU:HG2	6:B:328:HOH:O	1.53	1.05
2:B:186:PRO:HD2	6:B:335:HOH:O	1.78	0.84
1:C:43:THR:HG23	1:C:45:GLU:H	1.52	0.72
1:C:146:GLN:NE2	1:D:149:GLN:HE22	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:ALA:O	1:C:68:THR:HG21	1.98	0.63
1:D:41:ALA:O	1:D:42:GLU:HB2	1.99	0.62
1:D:40:ASP:HB2	1:D:47:LEU:HD11	1.82	0.61
1:C:40:ASP:OD2	1:C:64:ARG:HG2	2.05	0.56
1:D:42:GLU:HA	1:D:42:GLU:OE1	2.07	0.55
1:D:43:THR:HG22	1:D:45:GLU:H	1.71	0.55
1:D:40:ASP:HB3	1:D:43:THR:HB	1.89	0.54
2:B:162:ILE:HD11	2:B:224:LEU:HD13	1.89	0.54
1:D:183:VAL:HG13	1:D:192:LEU:HB2	1.89	0.53
1:C:34:PRO:HG3	1:D:175:THR:HB	1.90	0.53
1:D:43:THR:HG21	1:D:45:GLU:OE1	2.09	0.52
2:B:195:ARG:CZ	2:B:195:ARG:HB3	2.44	0.48
1:D:47:LEU:N	1:D:47:LEU:HD12	2.29	0.47
1:D:109:HIS:CE1	3:E:4:MAN:H2	2.49	0.47
2:A:132:ALA:HB1	2:A:214:GLU:HB3	1.98	0.46
1:C:62:CYS:HB3	1:C:68:THR:HG22	1.97	0.46
1:C:175:THR:HB	1:D:34:PRO:HB3	1.96	0.46
1:D:183:VAL:CG1	1:D:192:LEU:HB2	2.46	0.46
1:D:143:THR:HB	1:D:144:PRO:HD2	1.97	0.46
2:B:127:SER:HB2	2:B:134:VAL:HB	1.99	0.45
2:B:132:ALA:HB1	2:B:214:GLU:HB3	1.99	0.45
1:D:109:HIS:HE1	3:E:4:MAN:H2	1.82	0.45
1:C:49:CYS:HB3	1:C:68:THR:HG22	1.99	0.44
2:B:220:LEU:HA	2:B:221:ASP:HA	1.83	0.44
1:D:133:PRO:HG3	2:A:159:ALA:HB2	2.00	0.44
1:C:97:GLU:O	1:C:116:ARG:NH1	2.47	0.43
1:C:143:THR:OG1	1:C:146:GLN:HG2	2.19	0.43
1:D:182:ASN:HB2	1:D:194:THR:HG23	2.00	0.42
1:D:40:ASP:HB2	1:D:47:LEU:CD1	2.47	0.42
1:D:52:CYS:HB3	1:D:56:THR:OG1	2.20	0.42
2:A:97:HIS:O	2:A:121:ALA:HA	2.20	0.42
2:B:184:GLN:HE21	2:B:184:GLN:HB3	1.73	0.42
1:C:50:ALA:O	1:C:68:THR:CG2	2.67	0.41
1:D:143:THR:HB	1:D:144:PRO:CD	2.50	0.41
2:A:93:ASN:HD21	2:A:239:MET:HB3	1.86	0.41
2:A:105:LEU:HD22	2:A:222:GLU:HG2	2.03	0.41
1:D:46:ARG:HG2	1:D:46:ARG:O	2.21	0.41
1:C:169:GLN:HE21	1:C:170:PRO:HD3	1.85	0.40
2:A:178:GLU:HG2	6:A:310:HOH:O	2.20	0.40
1:C:64:ARG:HB2	1:C:64:ARG:CZ	2.52	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	C	165/174 (95%)	160 (97%)	5 (3%)	0	100	100
1	D	162/174 (93%)	156 (96%)	6 (4%)	0	100	100
2	A	133/158 (84%)	130 (98%)	3 (2%)	0	100	100
2	B	133/158 (84%)	131 (98%)	2 (2%)	0	100	100
All	All	593/664 (89%)	577 (97%)	16 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	C	140/146 (96%)	132 (94%)	8 (6%)	20	26
1	D	138/146 (94%)	127 (92%)	11 (8%)	12	14
2	A	113/130 (87%)	106 (94%)	7 (6%)	18	23
2	B	113/130 (87%)	108 (96%)	5 (4%)	28	37
All	All	504/552 (91%)	473 (94%)	31 (6%)	18	23

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	64	ARG
1	C	68	THR

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Mol	Chain	Res	Type
1	C	89	ARG
1	C	98	ARG
1	C	145	SER
1	C	175	THR
1	C	183	VAL
1	C	192	LEU
1	D	32	GLU
1	D	39	ARG
1	D	42	GLU
1	D	46	ARG
1	D	62	CYS
1	D	87	ARG
1	D	117	THR
1	D	175	THR
1	D	183	VAL
1	D	192	LEU
1	D	195	SER
2	A	154	CYS
2	A	161	THR
2	A	170	THR
2	A	184	GLN
2	A	187	CYS
2	A	200	SER
2	A	229	LYS
2	B	92	VAL
2	B	178	GLU
2	B	184	GLN
2	B	187	CYS
2	B	222	GLU

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

Mol	Chain	Res	Type
1	C	146	GLN
1	C	167	GLN
1	C	169	GLN
1	C	198	HIS
1	D	109	HIS
1	D	169	GLN
2	A	93	ASN
2	B	93	ASN
2	B	184	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

6 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	$\#\|Z\| > 2$
3	NAG	E	1	1,3	14,14,15	1.83	5 (35%)	17,19,21	2.67	10 (58%)
3	NAG	E	2	3	14,14,15	0.88	0	17,19,21	2.25	3 (17%)
3	BMA	E	3	3	11,11,12	1.18	0	15,15,17	2.36	6 (40%)
3	MAN	E	4	3	11,11,12	1.04	1 (9%)	15,15,17	2.33	5 (33%)
4	NAG	F	1	4,1	14,14,15	0.91	1 (7%)	17,19,21	3.15	7 (41%)
4	NAG	F	2	4	14,14,15	0.71	0	17,19,21	1.60	3 (17%)

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	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	1/2/19/22	0/1/1/1
4	NAG	F	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	NAG	O5-C1	-3.71	1.37	1.43
3	E	1	NAG	C1-C2	2.88	1.56	1.52
3	E	4	MAN	C2-C3	2.62	1.56	1.52
3	E	1	NAG	C4-C5	2.48	1.58	1.53
3	E	1	NAG	C6-C5	2.47	1.60	1.51
4	F	1	NAG	C6-C5	2.14	1.59	1.51
3	E	1	NAG	C2-N2	2.01	1.49	1.46

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	1	NAG	C1-O5-C5	7.29	122.07	112.19
3	E	2	NAG	C1-O5-C5	6.97	121.63	112.19
4	F	1	NAG	O5-C5-C6	6.48	117.36	107.20
3	E	4	MAN	C1-O5-C5	5.76	120.00	112.19
3	E	3	BMA	O5-C5-C6	4.86	114.83	107.20
3	E	1	NAG	C3-C4-C5	4.77	118.74	110.24
4	F	1	NAG	C3-C4-C5	4.25	117.83	110.24
4	F	1	NAG	O7-C7-C8	-4.24	114.18	122.06
4	F	2	NAG	C2-N2-C7	4.15	128.81	122.90
3	E	1	NAG	O7-C7-N2	3.95	129.21	121.95
3	E	1	NAG	O5-C5-C4	-3.78	101.62	110.83
3	E	3	BMA	C1-O5-C5	3.68	117.18	112.19
3	E	4	MAN	O3-C3-C2	3.67	117.02	109.99
3	E	3	BMA	O3-C3-C4	3.62	118.71	110.35
3	E	2	NAG	O3-C3-C2	-3.62	101.98	109.47
3	E	1	NAG	O7-C7-C8	-3.54	115.48	122.06
3	E	4	MAN	C1-C2-C3	3.42	113.87	109.67
4	F	1	NAG	O6-C6-C5	3.30	122.60	111.29
3	E	4	MAN	O2-C2-C1	3.23	115.75	109.15
3	E	1	NAG	O6-C6-C5	3.22	122.35	111.29
3	E	1	NAG	C1-O5-C5	3.05	116.32	112.19
3	E	3	BMA	O2-C2-C3	2.89	115.92	110.14
3	E	1	NAG	O3-C3-C4	2.81	116.84	110.35
3	E	1	NAG	C6-C5-C4	2.72	119.38	113.00
4	F	1	NAG	C1-C2-N2	2.51	114.78	110.49
4	F	2	NAG	O7-C7-C8	-2.49	117.43	122.06
4	F	1	NAG	C8-C7-N2	2.47	120.29	116.10
3	E	3	BMA	O3-C3-C2	2.41	114.61	109.99
3	E	4	MAN	O5-C5-C6	2.32	110.84	107.20
3	E	1	NAG	C2-N2-C7	2.30	126.17	122.90
3	E	1	NAG	O4-C4-C5	2.29	114.97	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	3	BMA	O5-C5-C4	-2.11	105.69	110.83
4	F	2	NAG	C1-O5-C5	2.03	114.94	112.19
3	E	2	NAG	C4-C3-C2	2.03	113.99	111.02

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	1	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	E	4	MAN	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6

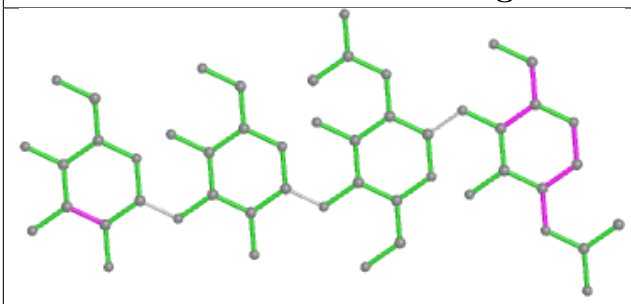
There are no ring outliers.

1 monomer is involved in 2 short contacts:

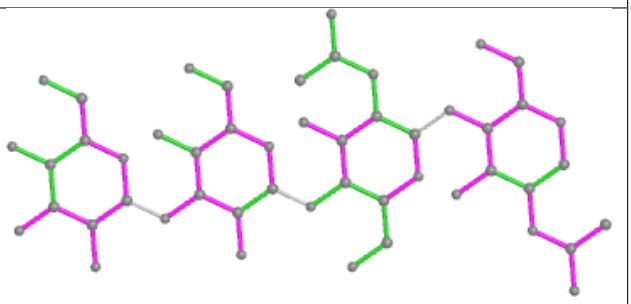
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	4	MAN	2	0

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

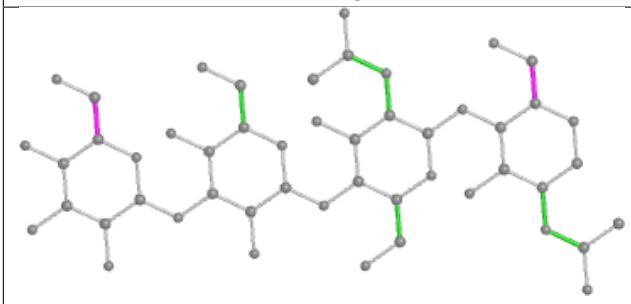
Oligosaccharide Chain E



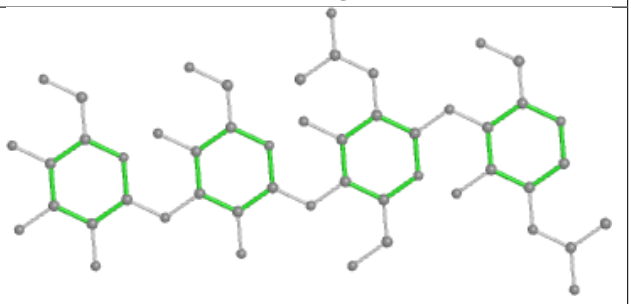
Bond lengths



Bond angles

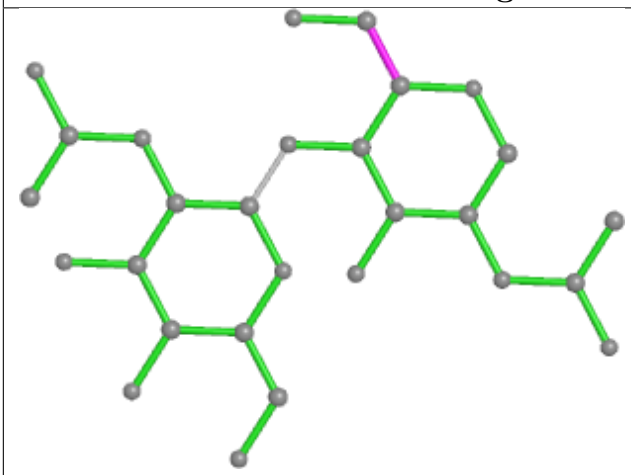


Torsions

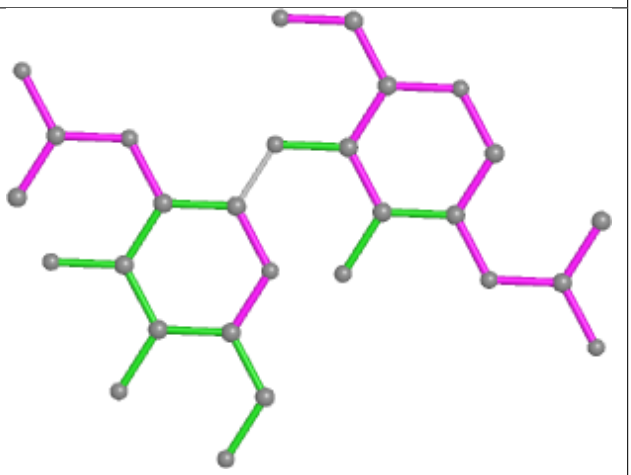


Rings

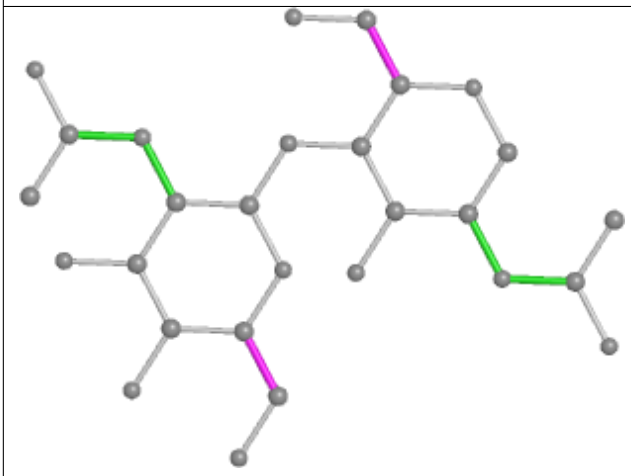
Oligosaccharide Chain F



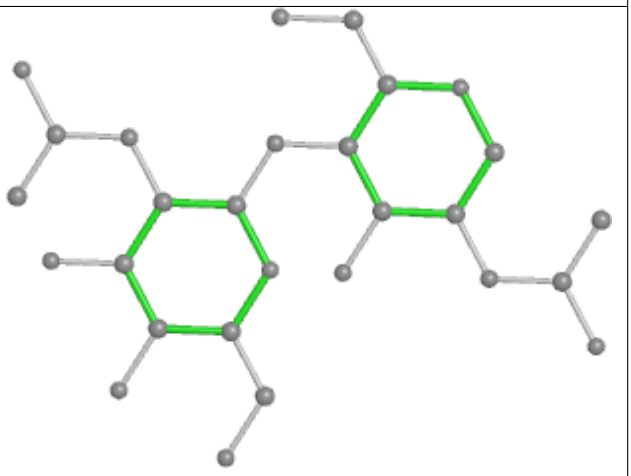
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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

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, 95^{th} 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	C	167/174 (95%)	-0.21	2 (1%) 79 82	26, 44, 64, 97	0
1	D	164/174 (94%)	0.72	23 (14%) 2 3	32, 59, 96, 128	0
2	A	139/158 (87%)	0.06	1 (0%) 87 90	18, 30, 70, 102	0
2	B	139/158 (87%)	-0.00	4 (2%) 51 57	21, 33, 69, 104	0
All	All	609/664 (91%)	0.15	30 (4%) 29 35	18, 43, 82, 128	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	64	ARG	7.6
1	D	195	SER	4.9
1	D	179	LEU	4.7
1	D	65	ASP	4.7
1	D	46	ARG	4.0
1	D	177	LEU	3.6
1	D	63	ARG	3.1
1	D	43	THR	3.1
1	D	174	CYS	3.0
1	D	66	SER	2.9
1	D	175	THR	2.9
1	D	41	ALA	2.9
1	D	194	THR	2.9
1	D	44	GLY	2.8
1	C	66	SER	2.7
1	D	117	THR	2.6
1	D	102	ALA	2.6
2	B	203	LEU	2.6
1	D	32	GLU	2.4
1	C	65	ASP	2.4
1	D	42	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	178	GLY	2.3
2	B	195	ARG	2.3
1	D	132	CYS	2.2
1	D	160	ALA	2.2
2	B	154	CYS	2.2
1	D	122	HIS	2.2
1	D	141	PRO	2.1
2	B	187	CYS	2.1
2	A	187	CYS	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)

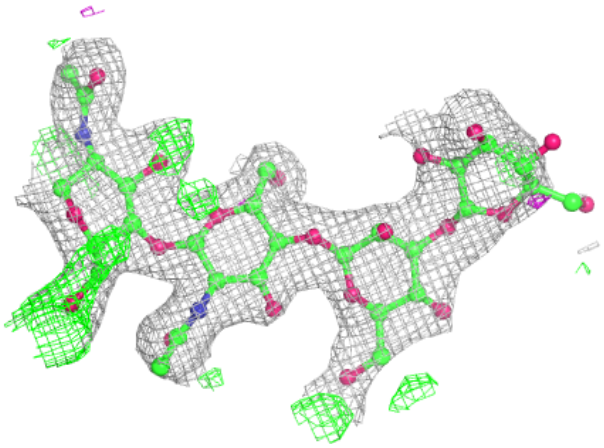
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

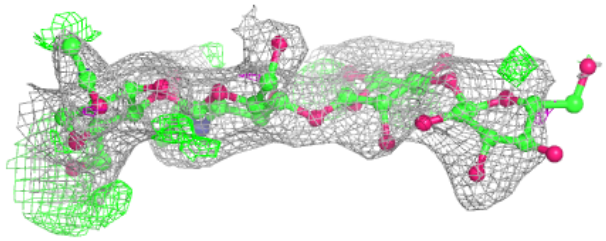
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MAN	E	4	11/12	0.81	0.26	75,91,107,108	0
4	NAG	F	2	14/15	0.81	0.36	75,86,95,97	0
4	NAG	F	1	14/15	0.87	0.15	55,70,77,78	0
3	BMA	E	3	11/12	0.88	0.25	59,71,76,78	0
3	NAG	E	1	14/15	0.90	0.11	39,49,57,59	0
3	NAG	E	2	14/15	0.92	0.20	47,58,63,65	0

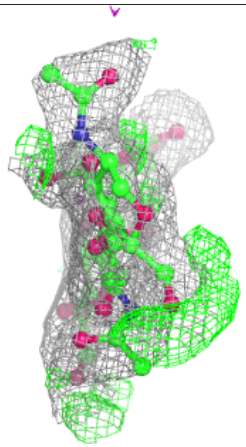
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

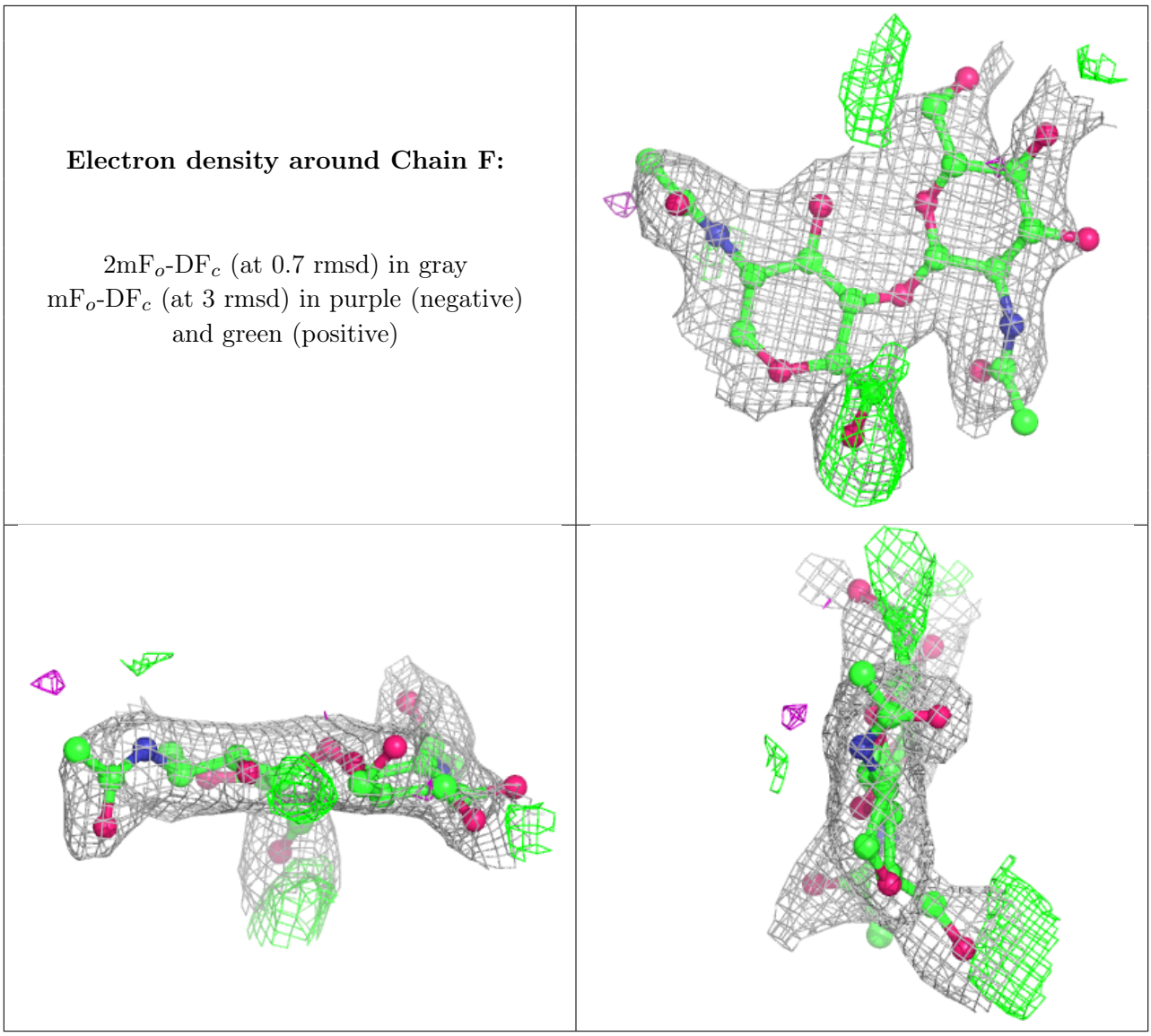






Electron density around Chain F:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.4 Ligands

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, 95^{th} 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	MG	C	301	1/1	0.98	0.13	47,47,47,47	0
5	MG	D	301	1/1	0.99	0.20	55,55,55,55	0

6.5 Other polymers

There are no such residues in this entry.