



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:36 AM UTC

PDB ID : 3EHU / pdb_00003ehu
Title : Crystal structure of the extracellular domain of human corticotropin releasing factor receptor type 1 (CRFR1) in complex with CRF
Authors : Pioszak, A.A.; Xu, H.E.
Deposited on : 2008-09-14
Resolution : 1.96 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:

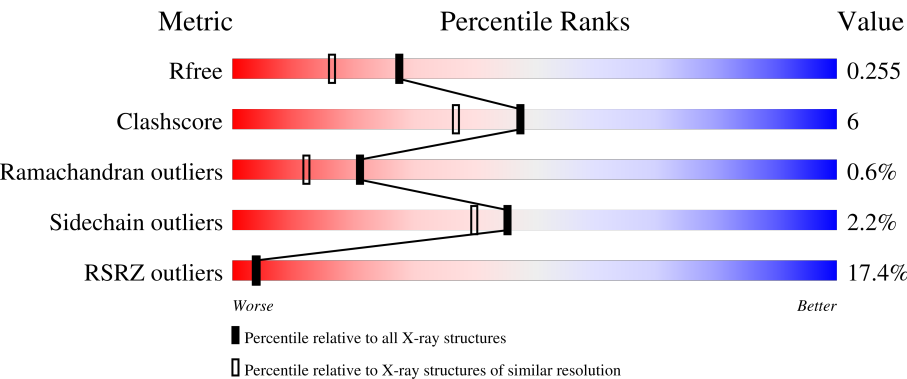
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	476	18% 83% 8% 7%
1	B	476	12% 81% 10% 7%
2	C	21	43% 62% 14% 5% 19%
2	D	21	33% 76% 5% 19%
3	E	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	2	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7584 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 FUSION PROTEIN OF CRFR1 EXTRACELLULAR DOMAIN AND MBP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	0	0
			3399	2173	561	654	11			
1	B	441	Total	C	N	O	S	0	0	0
			3399	2173	561	654	11			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-350	MET	-	initiating methionine	UNP P0AEX9
A	-25	GLU	ALA	engineered mutation	UNP P0AEX9
A	18	ASN	-	linker	UNP P0AEX9
A	19	ALA	-	linker	UNP P0AEX9
A	20	ALA	-	linker	UNP P0AEX9
A	21	ALA	-	linker	UNP P0AEX9
A	22	GLU	-	linker	UNP P0AEX9
A	23	PHE	-	linker	UNP P0AEX9
A	120	HIS	-	expression tag	UNP P34998
A	121	HIS	-	expression tag	UNP P34998
A	122	HIS	-	expression tag	UNP P34998
A	123	HIS	-	expression tag	UNP P34998
A	124	HIS	-	expression tag	UNP P34998
A	125	HIS	-	expression tag	UNP P34998
B	-350	MET	-	initiating methionine	UNP P0AEX9
B	-25	GLU	ALA	engineered mutation	UNP P0AEX9
B	18	ASN	-	linker	UNP P0AEX9
B	19	ALA	-	linker	UNP P0AEX9
B	20	ALA	-	linker	UNP P0AEX9
B	21	ALA	-	linker	UNP P0AEX9
B	22	GLU	-	linker	UNP P0AEX9
B	23	PHE	-	linker	UNP P0AEX9
B	120	HIS	-	expression tag	UNP P34998
B	121	HIS	-	expression tag	UNP P34998

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	122	HIS	-	expression tag	UNP P34998
B	123	HIS	-	expression tag	UNP P34998
B	124	HIS	-	expression tag	UNP P34998
B	125	HIS	-	expression tag	UNP P34998

- Molecule 2 is a protein called Corticoliberin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	17	Total 123	C 76	N 25	O 21	S 1	0	0	1
2	D	17	Total 123	C 76	N 25	O 21	S 1	0	0	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	42	NH2	-	amidation	UNP P06850
D	42	NH2	-	amidation	UNP P06850

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

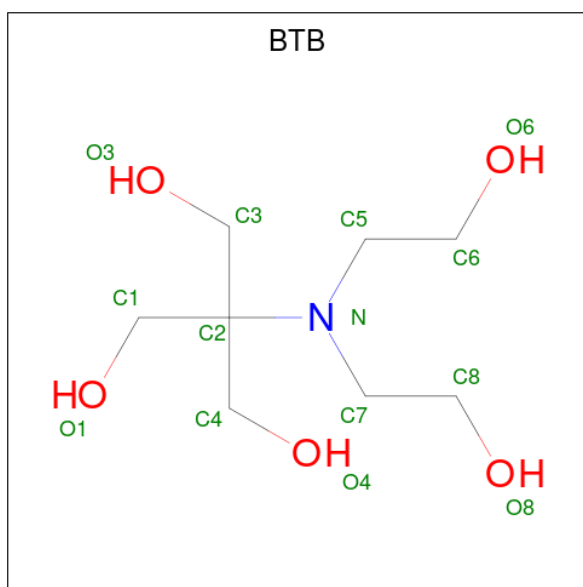


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	E	2	Total	C	O	0	0	0
			23	12	11			
3	F	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

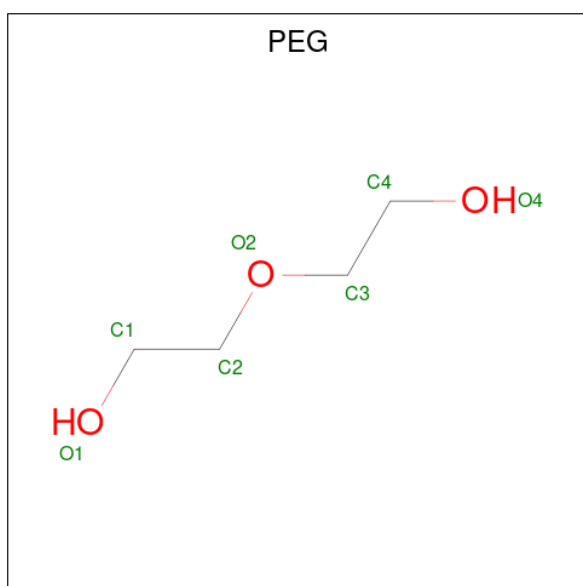
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: C₈H₁₉NO₅).



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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		

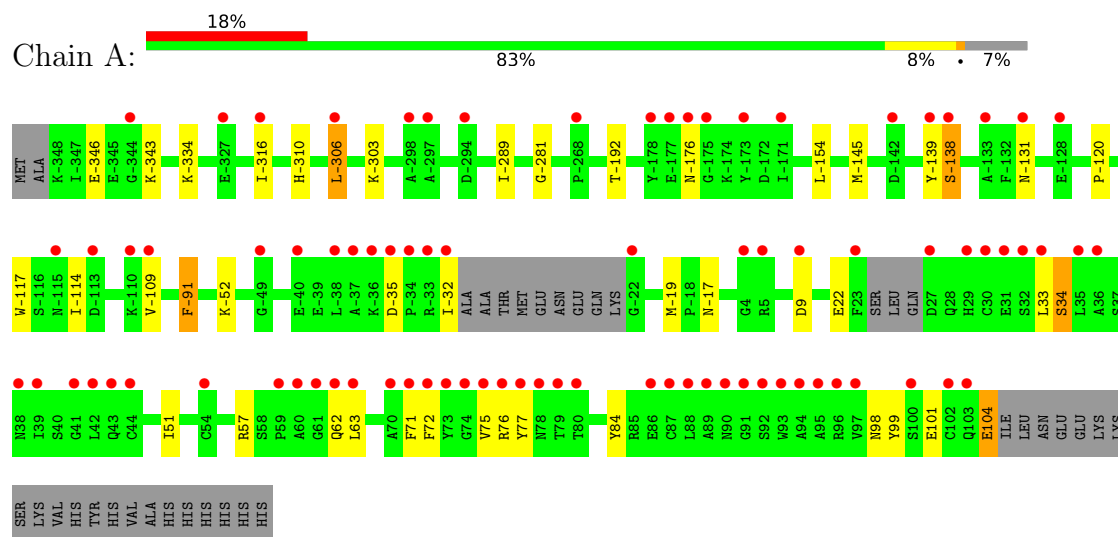
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	216	Total 216	O 216	0	0
7	B	225	Total 225	O 225	0	0
7	C	5	Total 5	O 5	0	0
7	D	4	Total 4	O 4	0	0

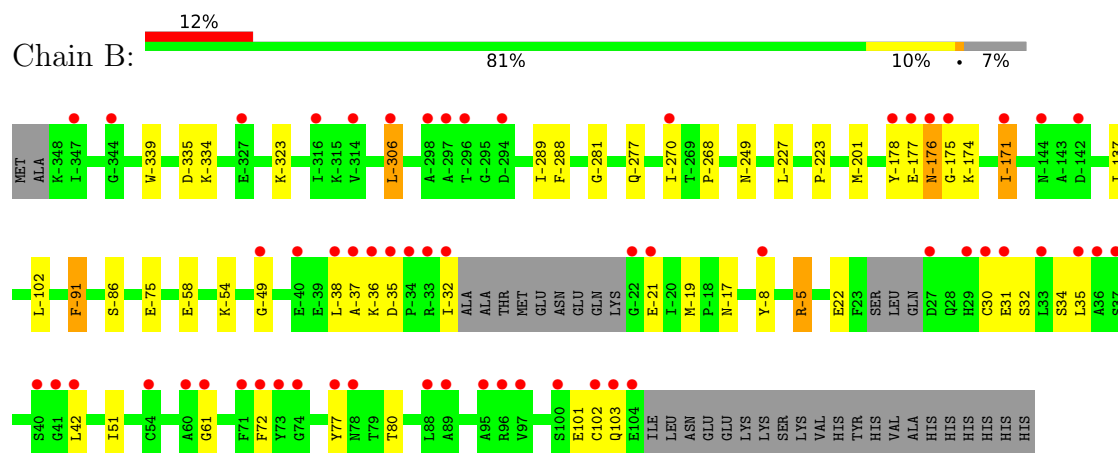
3 Residue-property plots

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.

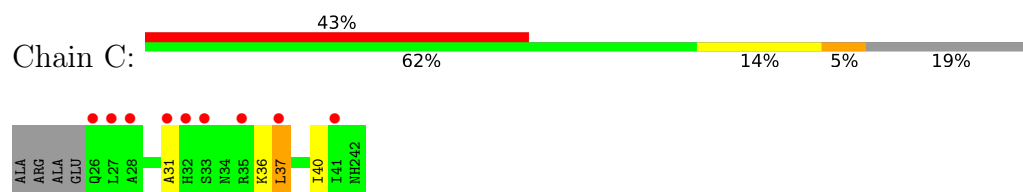
• Molecule 1: FUSION PROTEIN OF CRFR1 EXTRACELLULAR DOMAIN AND MBP



• Molecule 1: FUSION PROTEIN OF CRFR1 EXTRACELLULAR DOMAIN AND MBP

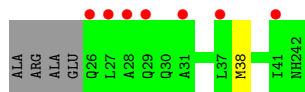


• Molecule 2: Corticoliberin

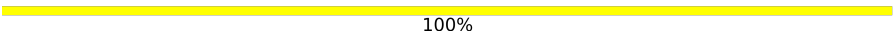


● Molecule 2: Corticoliberin

Chain D: 



● Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain E: 



● Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	49.20Å 63.48Å 85.88Å 99.75° 106.28° 101.67°	Depositor
Resolution (Å)	39.50 – 1.96 39.50 – 1.96	Depositor EDS
% Data completeness (in resolution range)	94.9 (39.50-1.96) 94.9 (39.50-1.96)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 1.95Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.209 , 0.256 0.209 , 0.255	Depositor DCC
R_{free} test set	3270 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtrriage
Anisotropy	0.465	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7584	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8890e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: BTB, GLC, NH2, CA, PEG

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	0.77	4/3480 (0.1%)	0.85	2/4729 (0.0%)
1	B	0.68	1/3480 (0.0%)	0.83	2/4729 (0.0%)
2	C	0.43	0/122	0.79	0/162
2	D	0.67	1/122 (0.8%)	0.91	0/162
All	All	0.72	6/7204 (0.1%)	0.84	4/9782 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	GLU	C-O	19.43	1.62	1.23
1	B	103	GLN	C-O	8.23	1.33	1.23
1	A	77	TYR	CG-CD1	6.70	1.53	1.39
1	A	76	ARG	C-N	6.60	1.42	1.33
1	A	77	TYR	CE2-CZ	6.47	1.53	1.38
2	D	38	MET	SD-CE	5.33	1.92	1.79

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	GLU	CA-C-O	-9.90	103.98	120.80
1	B	-102	LEU	CA-C-N	-5.36	115.22	120.52
1	B	-102	LEU	C-N-CA	-5.36	115.22	120.52
1	A	-109	VAL	N-CA-C	-5.05	103.06	109.58

There are no chirality outliers.

There are no planarity outliers.

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	3399	0	3314	37	0
1	B	3399	0	3314	38	0
2	C	123	0	124	3	0
2	D	123	0	124	0	0
3	E	23	0	21	0	0
3	F	23	0	21	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	14	0	15	5	0
5	B	14	0	15	3	0
6	A	7	0	10	0	0
6	B	7	0	10	1	0
7	A	216	0	0	11	0
7	B	225	0	0	13	0
7	C	5	0	0	0	0
7	D	4	0	0	0	0
All	All	7584	0	6968	79	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 6.

All (79) 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)
1:A:-52:LYS:HE2	7:A:555:HOH:O	1.61	1.00
1:B:101:GLU:HB3	7:B:711:HOH:O	1.71	0.90
1:B:-8:TYR:HD2	7:B:633:HOH:O	1.56	0.87
1:B:-339:TRP:HE3	7:B:718:HOH:O	1.63	0.81
1:A:101:GLU:HB3	7:A:600:HOH:O	1.82	0.80
1:B:-306:LEU:HB2	7:B:718:HOH:O	1.80	0.79
1:A:-334:LYS:NZ	7:A:718:HOH:O	2.16	0.78
1:A:-310:HIS:HE1	7:A:707:HOH:O	1.67	0.76
1:B:-339:TRP:CE3	7:B:718:HOH:O	2.40	0.70
1:A:-35:ASP:HB3	1:A:-32:ILE:HB	1.75	0.68
1:A:101:GLU:OE2	1:B:-5:ARG:NH2	2.28	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:SER:HB3	7:A:549:HOH:O	1.97	0.65
1:B:-35:ASP:HB3	1:B:-32:ILE:HD12	1.78	0.64
1:B:-201:MET:CE	1:B:-137:ILE:HG22	2.28	0.64
1:B:-171:ILE:HD12	1:B:22:GLU:OE2	1.97	0.64
1:A:-334:LYS:HE3	7:A:718:HOH:O	1.97	0.63
1:A:-334:LYS:CE	7:A:718:HOH:O	2.46	0.63
1:B:-201:MET:HE1	1:B:-137:ILE:HG22	1.80	0.63
1:B:101:GLU:HB2	7:B:580:HOH:O	1.98	0.63
1:A:-154:LEU:CD1	1:A:-145:MET:HE1	2.34	0.57
1:A:51:ILE:HD12	1:A:99:TYR:CE1	2.40	0.57
5:A:501:BTB:H11	7:A:701:HOH:O	2.03	0.57
1:B:-335:ASP:OD1	1:B:-334:LYS:NZ	2.37	0.57
1:A:-192:THR:HG23	7:A:703:HOH:O	2.04	0.57
1:A:-131:ASN:OD1	1:A:-114:ILE:HA	2.06	0.55
1:B:-306:LEU:HD13	7:B:718:HOH:O	2.07	0.55
1:B:-49:GLY:O	1:B:-32:ILE:HD13	2.07	0.54
1:A:-32:ILE:HG21	7:A:704:HOH:O	2.06	0.54
1:B:-281:GLY:HA3	1:B:-17:ASN:O	2.08	0.53
1:B:-5:ARG:NH1	7:B:588:HOH:O	2.32	0.52
5:B:501:BTB:H11	7:B:710:HOH:O	2.10	0.52
1:A:104:GLU:OE1	2:C:31:ALA:HB1	2.11	0.51
1:A:71:PHE:HA	1:A:75:VAL:O	2.11	0.51
1:B:-174:LYS:HG3	7:B:619:HOH:O	2.12	0.50
1:B:-306:LEU:C	1:B:-306:LEU:HD12	2.36	0.49
1:A:-154:LEU:HD12	1:A:-145:MET:HE1	1.95	0.49
1:A:-306:LEU:HD12	1:A:-306:LEU:C	2.37	0.49
1:B:-270:ILE:HD12	1:B:-268:PRO:HD3	1.95	0.48
5:A:501:BTB:H62	5:A:501:BTB:C1	2.44	0.48
1:A:33:LEU:O	1:A:34:SER:HB2	2.14	0.48
1:A:57:ARG:HH11	1:A:57:ARG:HG3	1.79	0.48
1:B:-323:LYS:HD2	6:B:502:PEG:H41	1.95	0.48
1:A:98:ASN:ND2	1:B:-8:TYR:OH	2.46	0.47
1:B:32:SER:HA	1:B:35:LEU:HG	1.97	0.46
1:A:-154:LEU:HD11	1:A:-145:MET:HE1	1.97	0.46
1:B:-75:GLU:HG2	7:B:713:HOH:O	2.14	0.46
1:B:72:PHE:HB3	1:B:77:TYR:CE1	2.50	0.46
1:A:63:LEU:HD11	1:A:84:TYR:HB3	1.98	0.46
1:B:-177:GLU:O	1:B:-176:ASN:C	2.58	0.45
1:B:72:PHE:HB3	1:B:77:TYR:HE1	1.80	0.45
2:C:36:LYS:HE2	2:C:40:ILE:HD11	1.99	0.45
1:A:-281:GLY:HA3	1:A:-17:ASN:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-303:LYS:NZ	7:A:619:HOH:O	2.48	0.44
1:B:-288:PHE:HA	1:B:-86:SER:O	2.17	0.44
1:B:-91:PHE:CG	1:B:-19:MET:HG2	2.53	0.44
1:A:-139:TYR:CG	1:A:-138:SER:N	2.86	0.44
1:A:-91:PHE:CG	1:A:-19:MET:HG2	2.53	0.43
1:B:30:CYS:C	1:B:32:SER:H	2.26	0.43
1:B:32:SER:C	1:B:34:SER:H	2.25	0.43
1:A:-139:TYR:CD1	5:A:501:BTB:H41	2.54	0.43
1:A:62:GLN:NE2	1:B:-277:GLN:OE1	2.47	0.43
5:A:501:BTB:H71	5:A:501:BTB:H32	1.57	0.43
1:A:22:GLU:HB2	1:B:61:GLY:HA2	2.01	0.43
1:A:72:PHE:HZ	2:C:37:LEU:HD23	1.83	0.43
5:B:501:BTB:H32	5:B:501:BTB:H71	1.78	0.43
1:B:-227:LEU:HD21	1:B:-223:PRO:HD3	2.01	0.42
1:A:33:LEU:O	1:A:34:SER:CB	2.67	0.42
1:A:-346:GLU:CD	1:A:-343:LYS:HD3	2.43	0.42
1:B:-58:GLU:HG3	1:B:-54:LYS:HE3	2.00	0.42
1:A:57:ARG:HG3	1:A:57:ARG:NH1	2.34	0.42
1:B:-38:LEU:C	1:B:-36:LYS:H	2.28	0.42
1:B:-21:GLU:HG2	7:B:604:HOH:O	2.20	0.42
1:B:-178:TYR:OH	1:B:-175:GLY:HA2	2.19	0.42
1:A:-343:LYS:HA	1:A:-316:ILE:HG23	2.03	0.41
5:A:501:BTB:H62	5:A:501:BTB:H12	2.02	0.41
5:B:501:BTB:H62	5:B:501:BTB:O1	2.20	0.41
1:A:-117:TRP:HA	1:A:-114:ILE:HD12	2.01	0.41
1:B:-8:TYR:CD2	7:B:633:HOH:O	2.46	0.41
1:A:-120:PRO:HA	1:A:-117:TRP:CE2	2.56	0.41

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	435/476 (91%)	426 (98%)	8 (2%)	1 (0%)	43	36
1	B	435/476 (91%)	420 (97%)	11 (2%)	4 (1%)	14	6
2	C	15/21 (71%)	15 (100%)	0	0	100	100
2	D	15/21 (71%)	15 (100%)	0	0	100	100
All	All	900/994 (90%)	876 (97%)	19 (2%)	5 (1%)	21	12

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	SER
1	B	-176	ASN
1	B	31	GLU
1	B	-37	ALA
1	B	102	CYS

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	352/386 (91%)	346 (98%)	6 (2%)	53	49
1	B	352/386 (91%)	343 (97%)	9 (3%)	40	33
2	C	12/16 (75%)	11 (92%)	1 (8%)	10	3
2	D	12/16 (75%)	12 (100%)	0	100	100
All	All	728/804 (90%)	712 (98%)	16 (2%)	45	40

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-306	LEU
1	A	-289	ILE
1	A	-176	ASN
1	A	-138	SER
1	A	-91	PHE
1	A	9	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	-306	LEU
1	B	-289	ILE
1	B	-249	ASN
1	B	-171	ILE
1	B	-91	PHE
1	B	-5	ARG
1	B	42	LEU
1	B	51	ILE
1	B	80	THR
2	C	37	LEU

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	-331	ASN
1	A	-176	ASN
1	A	-148	ASN
1	A	62	GLN
1	A	81	ASN
1	A	82	ASN
1	B	-277	GLN
1	B	-148	ASN
1	B	-115	ASN
1	B	0	ASN
1	B	6	GLN
1	B	38	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	$\# Z > 2$
3	GLC	E	1	3	12,12,12	0.59	0	17,17,17	1.51	3 (17%)
3	GLC	E	2	3	11,11,12	0.61	0	15,15,17	1.21	2 (13%)
3	GLC	F	1	3	12,12,12	0.56	0	17,17,17	1.05	0
3	GLC	F	2	3	11,11,12	0.52	0	15,15,17	1.10	1 (6%)

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	GLC	E	1	3	-	0/2/22/22	0/1/1/1
3	GLC	E	2	3	-	0/2/19/22	0/1/1/1
3	GLC	F	1	3	-	0/2/22/22	0/1/1/1
3	GLC	F	2	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	GLC	O5-C1-C2	4.03	117.38	110.30
3	F	2	GLC	C1-O5-C5	3.38	116.72	112.19
3	E	2	GLC	C1-O5-C5	3.25	116.54	112.19
3	E	1	GLC	C1-O5-C5	3.22	119.87	113.65
3	E	1	GLC	O3-C3-C2	-2.16	105.29	110.38
3	E	2	GLC	O4-C4-C3	-2.06	105.53	110.38

There are no chirality outliers.

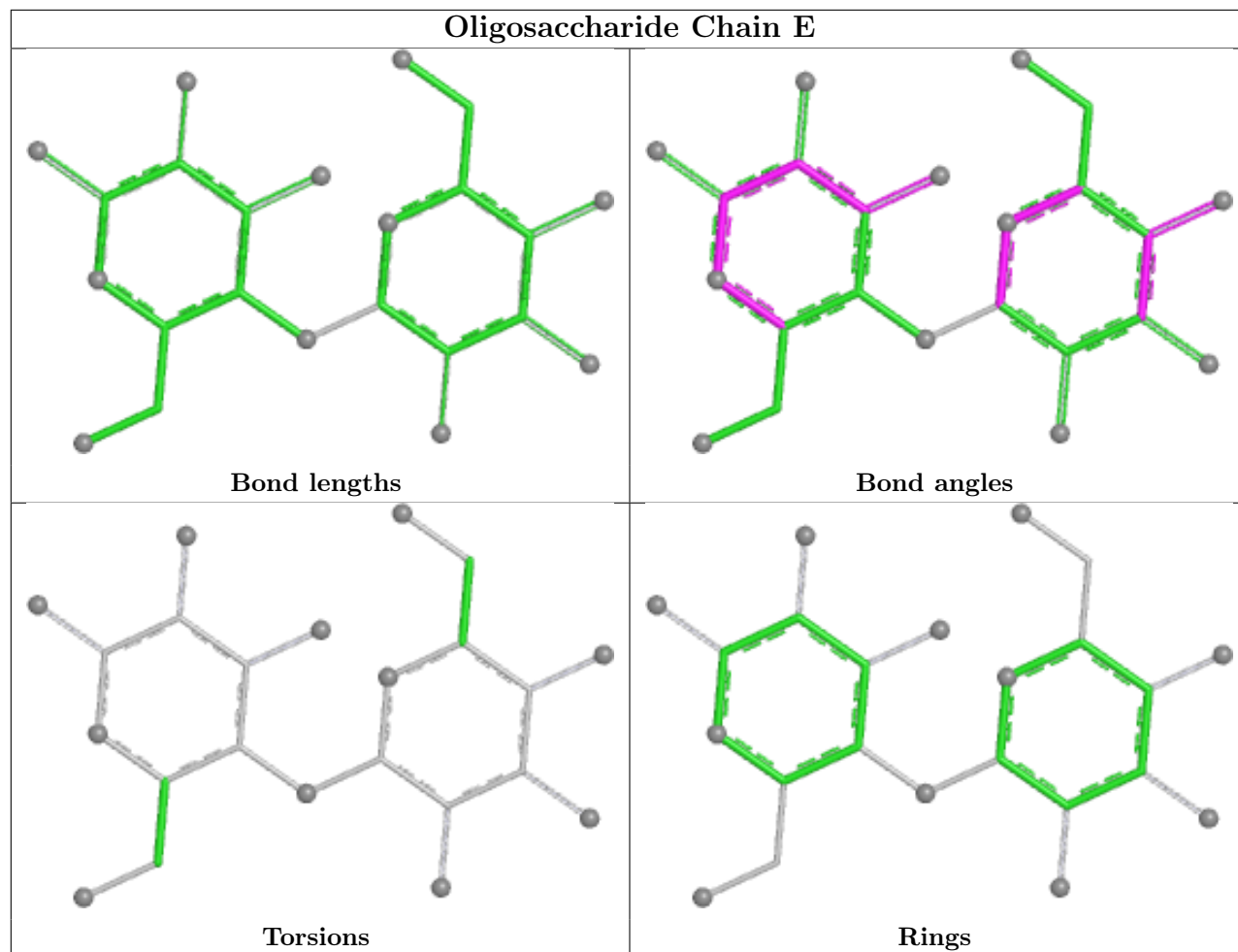
There are no torsion outliers.

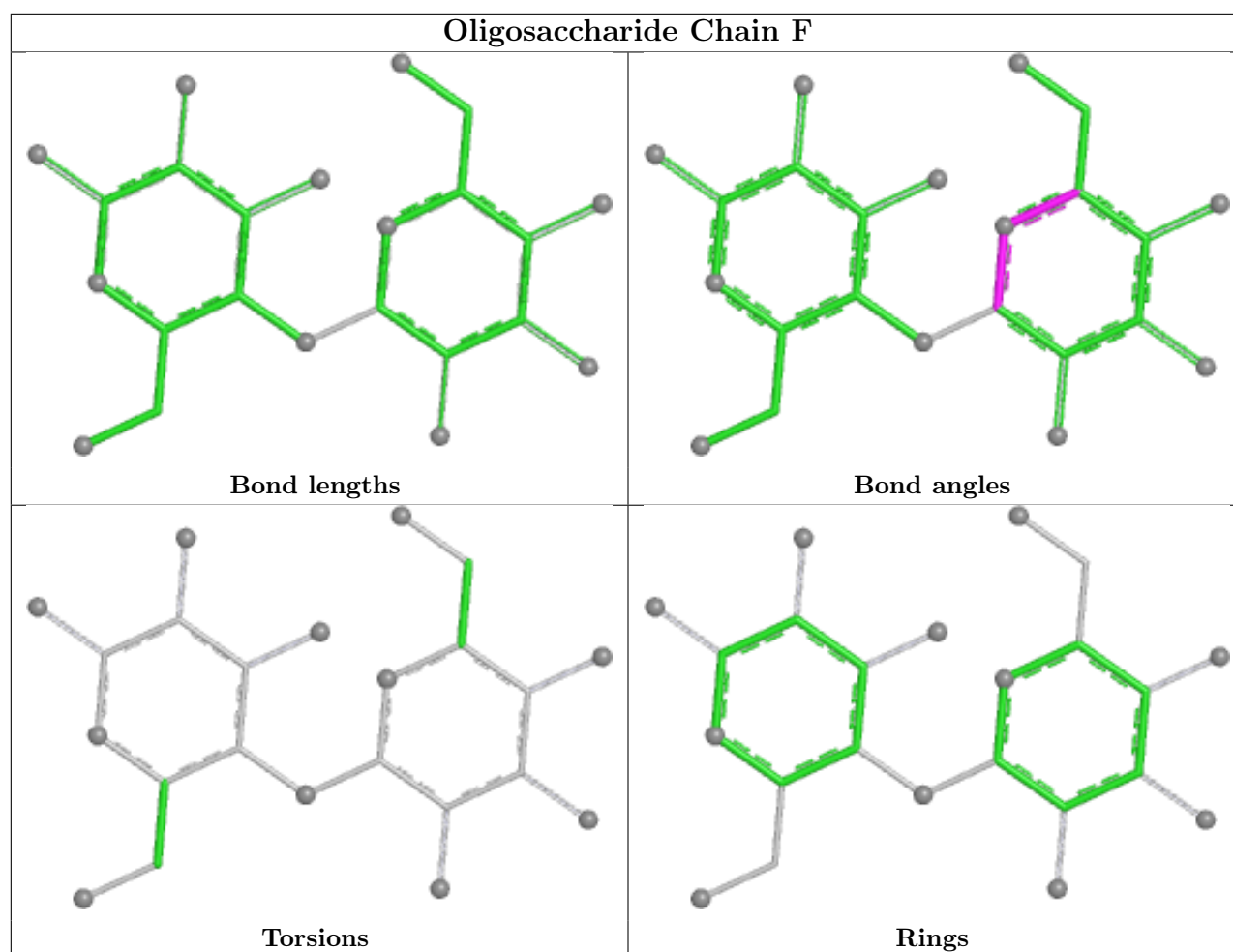
There are no ring outliers.

No monomer is involved in short contacts.

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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	PEG	B	502	-	6,6,6	0.47	0	5,5,5	0.19	0
5	BTB	B	501	4	13,13,13	0.40	0	7,16,16	0.86	0
6	PEG	A	502	-	6,6,6	0.41	0	5,5,5	0.33	0
5	BTB	A	501	4	13,13,13	0.69	0	7,16,16	1.23	1 (14%)

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	PEG	B	502	-	-	3/4/4/4	-
5	BTB	B	501	4	-	4/21/21/21	-
6	PEG	A	502	-	-	2/4/4/4	-
5	BTB	A	501	4	-	3/21/21/21	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	BTB	O3-C3-C2	2.34	116.90	111.40

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	BTB	C3-C2-N-C7
6	A	502	PEG	O2-C3-C4-O4
6	B	502	PEG	O2-C3-C4-O4
5	B	501	BTB	O1-C1-C2-C3
5	B	501	BTB	C8-C7-N-C5
5	A	501	BTB	C6-C5-N-C2
5	B	501	BTB	C6-C5-N-C2
5	B	501	BTB	C3-C2-N-C7
6	B	502	PEG	C4-C3-O2-C2
6	A	502	PEG	C4-C3-O2-C2
6	B	502	PEG	O1-C1-C2-O2
5	A	501	BTB	C1-C2-N-C5

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	502	PEG	1	0
5	B	501	BTB	3	0
5	A	501	BTB	5	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	441/476 (92%)	1.11	84 (19%) 3 3	20, 28, 40, 58	0
1	B	441/476 (92%)	1.01	59 (13%) 7 8	21, 28, 40, 61	0
2	C	16/21 (76%)	2.23	9 (56%) 0 0	27, 38, 40, 41	0
2	D	16/21 (76%)	2.04	7 (43%) 0 0	26, 32, 36, 36	0
All	All	914/994 (91%)	1.10	159 (17%) 4 4	20, 28, 40, 61	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-37	ALA	5.9
1	B	-175	GLY	5.1
1	A	-178	TYR	4.7
1	B	33	LEU	4.3
1	A	42	LEU	4.3
1	A	61	GLY	4.2
1	B	-178	TYR	4.2
1	A	74	GLY	4.2
1	B	-37	ALA	4.1
1	B	73	TYR	4.1
2	C	31	ALA	4.1
1	A	76	ARG	4.0
1	A	35	LEU	4.0
1	A	73	TYR	3.9
1	A	39	ILE	3.9
1	A	78	ASN	3.9
1	B	-176	ASN	3.8
2	C	28	ALA	3.8
1	A	89	ALA	3.8
1	B	-32	ILE	3.8
1	B	29	HIS	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	-34	PRO	3.6
1	B	72	PHE	3.6
1	A	72	PHE	3.5
1	A	33	LEU	3.5
1	A	-38	LEU	3.5
2	C	27	LEU	3.5
2	D	31	ALA	3.4
2	D	37	LEU	3.4
1	A	-40	GLU	3.4
1	B	103	GLN	3.4
1	B	89	ALA	3.4
2	D	41	ILE	3.3
1	A	-32	ILE	3.2
1	A	95	ALA	3.2
1	B	-38	LEU	3.2
1	A	103	GLN	3.2
1	B	-33	ARG	3.2
1	A	88	LEU	3.2
2	D	28	ALA	3.1
1	A	41	GLY	3.1
1	A	9	ASP	3.1
1	A	60	ALA	3.1
1	B	54	CYS	3.1
1	B	-22	GLY	3.1
1	A	71	PHE	3.0
1	A	32	SER	3.0
1	A	-316	ILE	3.0
1	A	63	LEU	3.0
1	B	104	GLU	3.0
1	A	-113	ASP	3.0
1	B	-36	LYS	3.0
1	A	27	ASP	2.9
1	A	-175	GLY	2.9
1	A	54	CYS	2.9
2	C	37	LEU	2.9
1	A	-139	TYR	2.9
1	A	-176	ASN	2.9
1	A	-306	LEU	2.9
1	A	-109	VAL	2.9
1	B	27	ASP	2.9
1	B	42	LEU	2.9
1	B	71	PHE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	-142	ASP	2.8
1	B	74	GLY	2.8
1	A	-34	PRO	2.8
1	A	75	VAL	2.8
1	B	61	GLY	2.8
1	A	-36	LYS	2.8
1	B	100	SER	2.8
1	B	-297	ALA	2.8
1	B	30	CYS	2.8
1	B	-327	GLU	2.8
1	A	96	ARG	2.7
1	B	31	GLU	2.7
1	A	5	ARG	2.7
1	A	-33	ARG	2.6
1	B	-306	LEU	2.6
1	A	102	CYS	2.6
1	B	35	LEU	2.6
1	A	-35	ASP	2.6
2	C	32	HIS	2.5
1	A	43	GLN	2.5
1	A	-22	GLY	2.5
1	A	70	ALA	2.5
1	A	94	ALA	2.5
1	A	-110	LYS	2.5
1	B	-49	GLY	2.5
1	A	-171	ILE	2.5
1	A	36	ALA	2.5
1	A	-177	GLU	2.5
1	A	38	ASN	2.5
2	C	35	ARG	2.5
1	B	-21	GLU	2.5
1	B	36	ALA	2.5
1	B	95	ALA	2.5
1	A	30	CYS	2.4
1	B	41	GLY	2.4
1	A	-173	TYR	2.4
1	A	-138	SER	2.4
1	A	90	ASN	2.4
1	A	100	SER	2.4
2	C	33	SER	2.4
1	B	-347	ILE	2.4
1	A	59	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	26	GLN	2.4
1	A	-49	GLY	2.4
1	B	-316	ILE	2.4
2	C	41	ILE	2.4
1	B	60	ALA	2.4
1	A	-268	PRO	2.4
1	A	29	HIS	2.4
1	A	87	CYS	2.4
1	B	-35	ASP	2.3
1	A	80	THR	2.3
1	A	-298	ALA	2.3
2	D	27	LEU	2.3
1	A	-131	ASN	2.3
1	B	37	SER	2.3
2	D	26	GLN	2.3
1	A	91	GLY	2.3
1	A	92	SER	2.3
1	B	78	ASN	2.3
1	A	-297	ALA	2.2
1	A	-133	ALA	2.2
1	B	-40	GLU	2.2
1	B	40	SER	2.2
1	A	-294	ASP	2.2
1	B	-314	VAL	2.2
1	A	-142	ASP	2.2
1	B	-344	GLY	2.2
1	B	-270	ILE	2.2
1	A	-327	GLU	2.2
1	A	-128	GLU	2.2
1	A	86	GLU	2.2
1	A	79	THR	2.2
1	A	97	VAL	2.1
1	B	97	VAL	2.1
1	A	4	GLY	2.1
2	D	29	GLN	2.1
1	B	-171	ILE	2.1
1	B	-294	ASP	2.1
1	A	93	TRP	2.1
1	B	96	ARG	2.1
1	A	31	GLU	2.1
1	A	44	CYS	2.1
1	B	-144	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	77	TYR	2.1
1	B	-8	TYR	2.1
1	A	-115	ASN	2.1
1	B	88	LEU	2.1
1	A	23	PHE	2.0
1	B	77	TYR	2.0
1	A	62	GLN	2.0
1	B	102	CYS	2.0
1	B	-298	ALA	2.0
1	B	-177	GLU	2.0
1	A	-344	GLY	2.0
1	B	-296	THR	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](#)

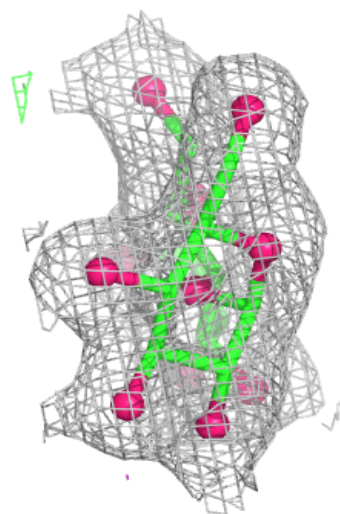
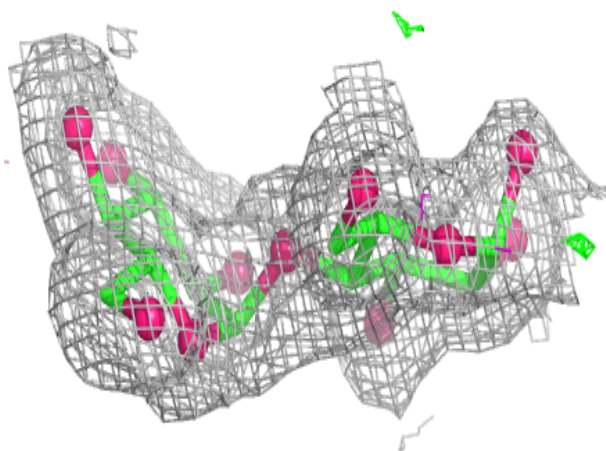
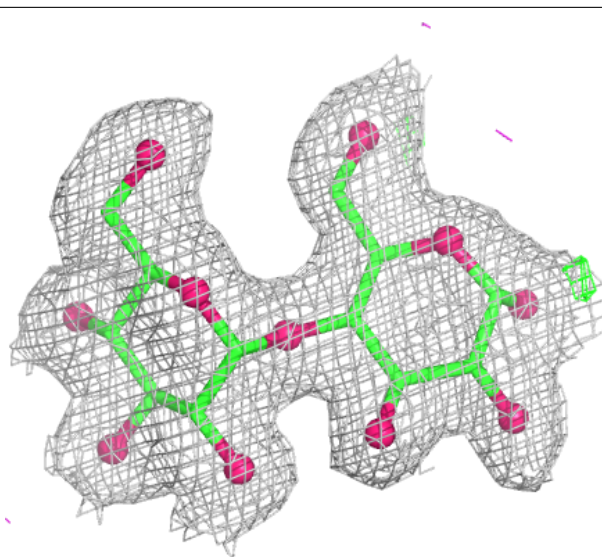
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

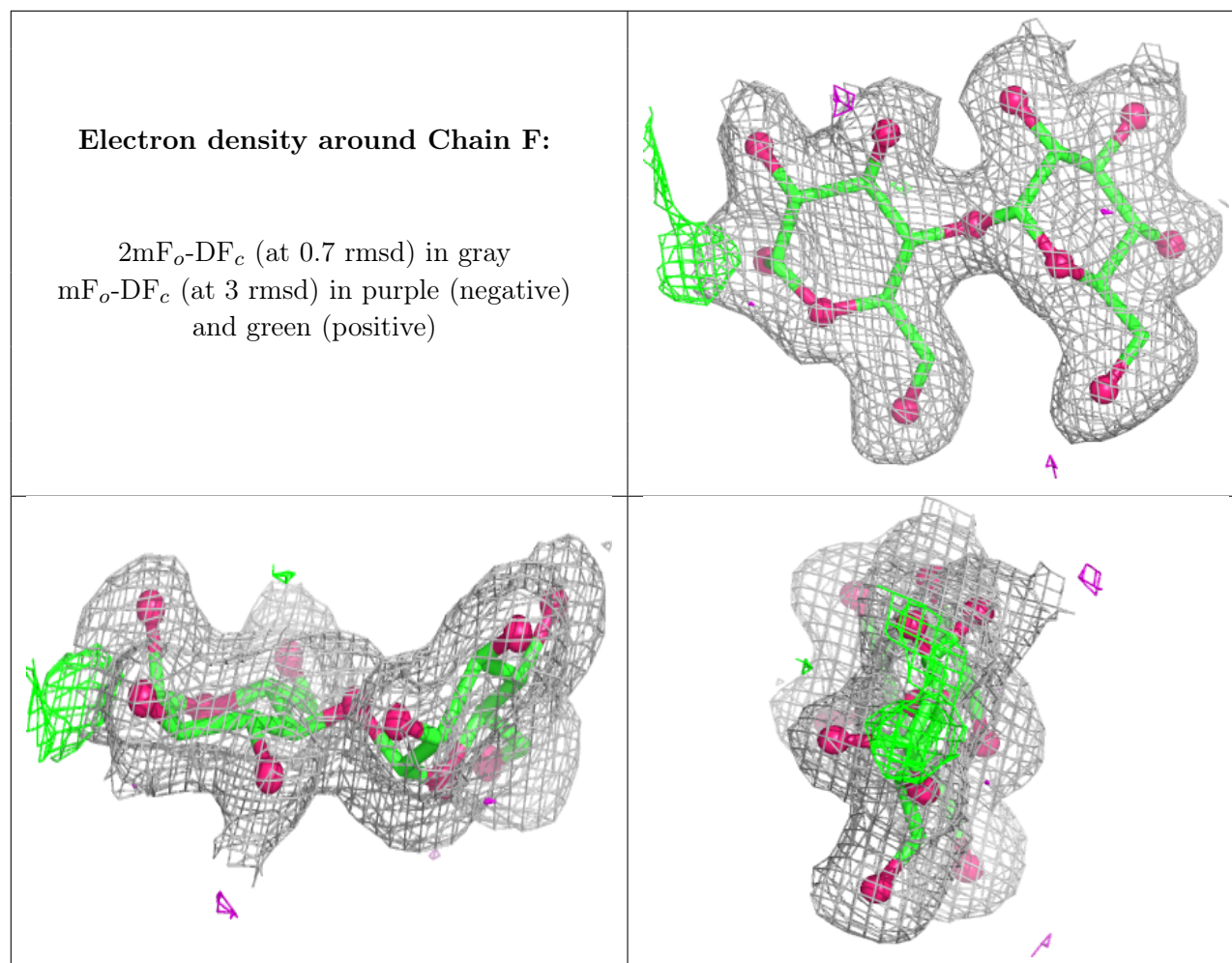
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GLC	E	1	12/12	0.94	0.10	27,30,35,37	0
3	GLC	F	1	12/12	0.94	0.09	28,31,34,39	0
3	GLC	E	2	11/12	0.96	0.06	25,25,27,27	0
3	GLC	F	2	11/12	0.96	0.06	23,25,27,27	0

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)





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
5	BTB	A	501	14/14	0.83	0.15	21,26,28,33	0
6	PEG	A	502	7/7	0.85	0.14	36,38,39,41	0
6	PEG	B	502	7/7	0.87	0.13	38,40,44,45	0
5	BTB	B	501	14/14	0.88	0.12	14,22,25,31	0
4	CA	A	500	1/1	0.98	0.14	18,18,18,18	0
4	CA	B	500	1/1	0.99	0.17	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.