Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 10:56 AM EDT

PDB ID	:	2QKI
Title	:	Human C3c in complex with the inhibitor compstatin
Authors	:	Janssen, B.J.C.; Halff, E.F.; Lambris, J.D.; Gros, P.
Deposited on	:	2007-07-11
Resolution	:	2.40 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 (i) 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 (i)) were used in the production of this report:

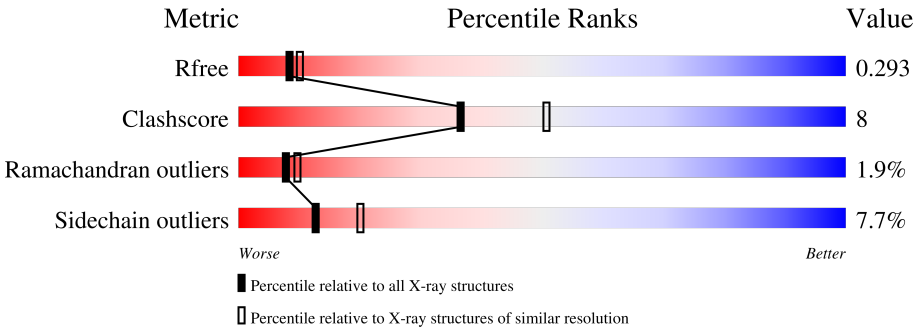
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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%

Mol	Chain	Length	Quality of chain
1	A	643	74% 20%
1	D	643	73% 21%
2	B	188	78% 18%
2	E	188	81% 15%
3	C	343	68% 15% 15%
3	F	343	73% 12% 14%
4	G	15	93% 7%

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Mol	Chain	Length	Quality of chain
4	H	15	47% 40% 13%
5	I	2	100%
5	J	2	50% 50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	J	1	X	-	-	-
8	GOL	A	809	-	-	X	-
8	GOL	E	916	-	-	X	-
8	GOL	F	840	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 18480 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 Complement C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	631	Total	C	N	O	S	0	0	0
			4912	3131	831	935	15			
1	D	632	Total	C	N	O	S	0	0	0
			4919	3137	829	938	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	292	LEU	PRO	SEE REMARK 999	UNP P01024
D	292	LEU	PRO	SEE REMARK 999	UNP P01024

- Molecule 2 is a protein called Complement C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	184	Total	C	N	O	S	0	0	0
			1484	954	250	275	5			
2	E	186	Total	C	N	O	S	0	0	0
			1500	964	252	279	5			

- Molecule 3 is a protein called Complement C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	292	Total	C	N	O	S	0	0	0
			2372	1497	388	467	20			
3	F	295	Total	C	N	O	S	0	0	0
			2395	1510	392	473	20			

- Molecule 4 is a protein called compstatin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	15	Total	C	N	O	S	0	0	1
			113	71	22	18	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	15	Total	C	N	O	S	0	0	1
			113	71	22	18	2			

- Molecule 5 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
5	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	K	0	0
			1	1		
6	C	1	Total	K	0	0
			1	1		
6	D	2	Total	K	0	0
			2	2		
6	F	1	Total	K	0	0
			1	1		

- Molecule 7 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	8	Total	Br	0	0
			8	8		
7	B	3	Total	Br	0	0
			3	3		
7	C	1	Total	Br	0	0
			1	1		
7	D	15	Total	Br	0	0
			15	15		
7	E	3	Total	Br	0	0
			3	3		

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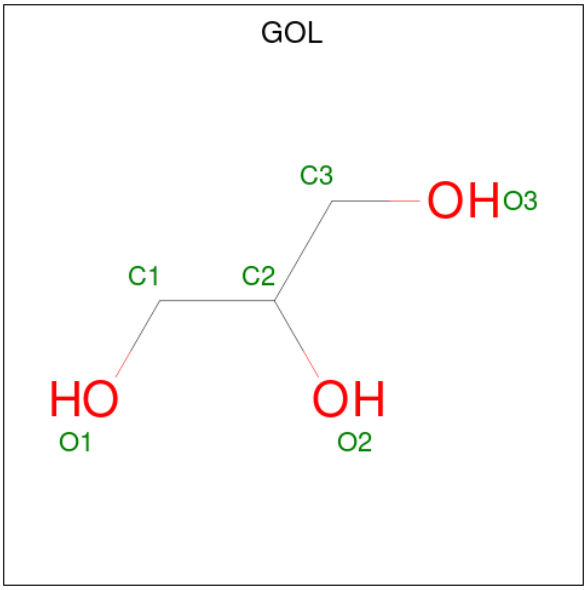
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	2	Total Br 2 2	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total C O 6 3 3	0	0
8	D	1	Total C O 6 3 3	0	0
8	D	1	Total C O 6 3 3	0	0
8	D	1	Total C O 6 3 3	0	0
8	E	1	Total C O 6 3 3	0	0
8	E	1	Total C O 6 3 3	0	0
8	F	1	Total C O 6 3 3	0	0
8	H	1	Total C O 6 3 3	0	0

- Molecule 9 is water.

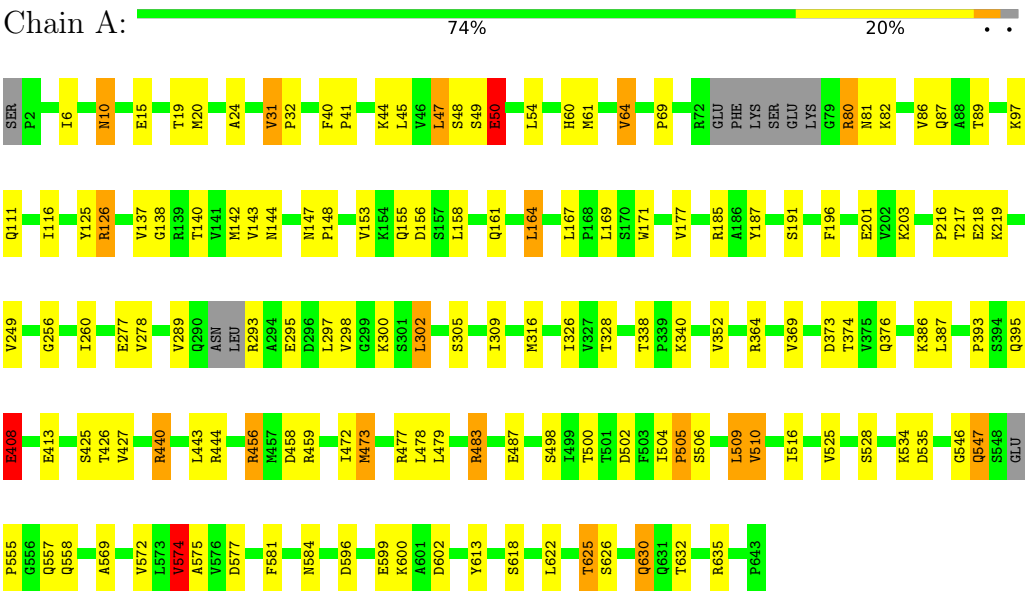
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	111	Total O 111 111	0	0
9	B	47	Total O 47 47	0	0
9	C	23	Total O 23 23	0	0
9	D	188	Total O 188 188	0	0
9	E	62	Total O 62 62	0	0
9	F	35	Total O 35 35	0	0
9	H	5	Total O 5 5	0	0

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. 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. 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.

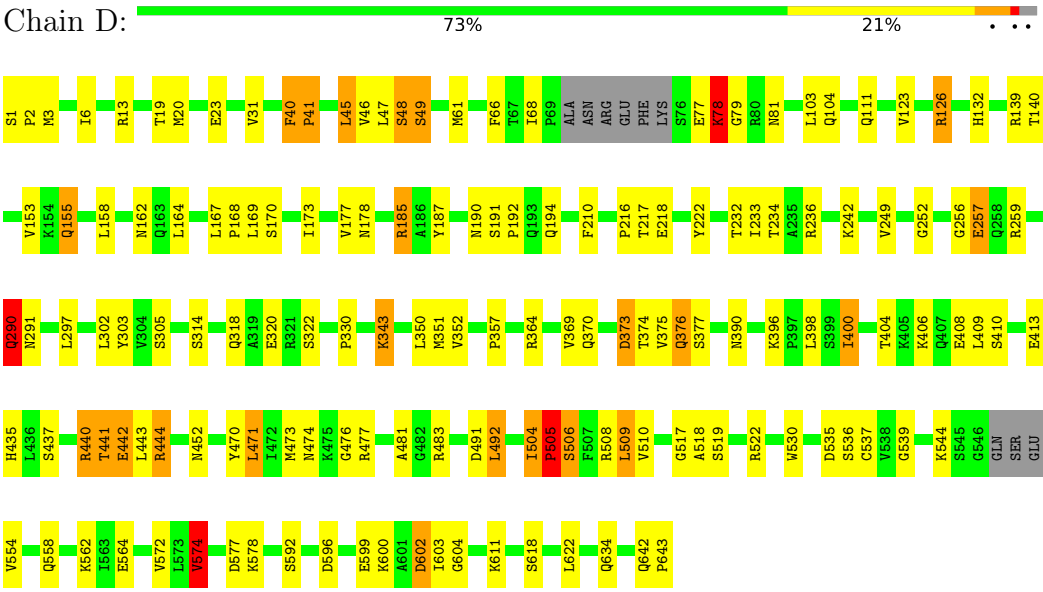
• Molecule 1: Complement C3

Chain A:



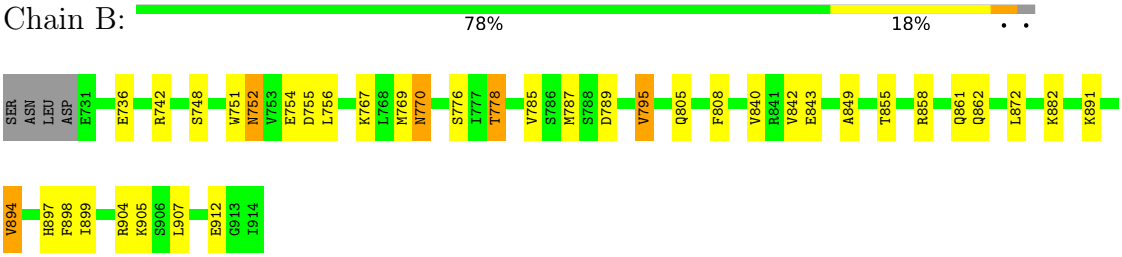
• Molecule 1: Complement C3

Chain D:



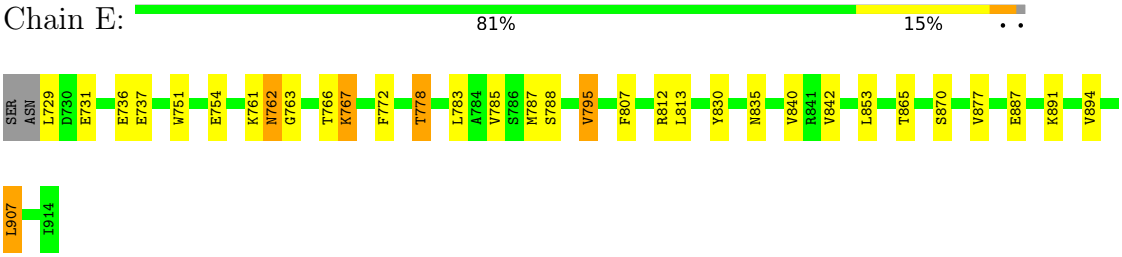
• Molecule 2: Complement C3

Chain B:



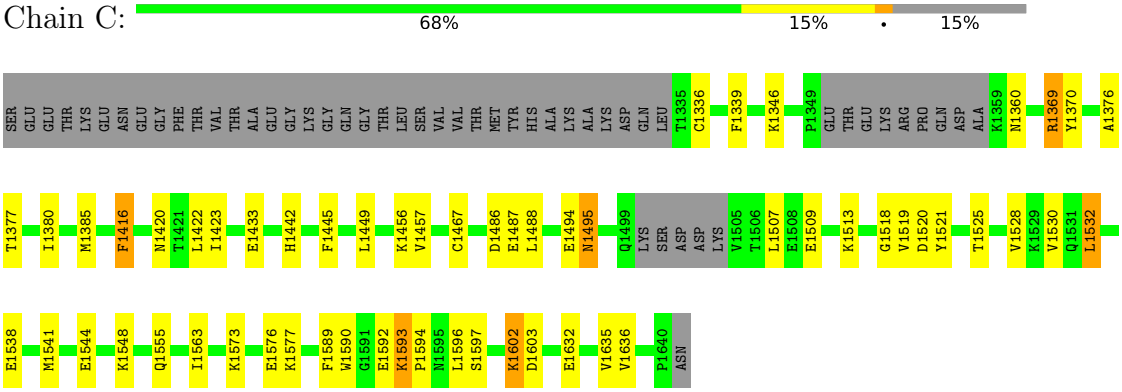
• Molecule 2: Complement C3

Chain E:



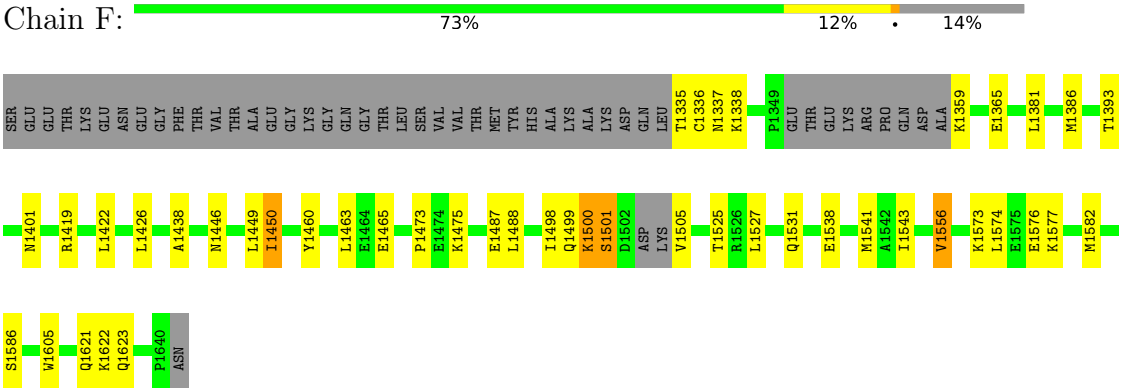
• Molecule 3: Complement C3

Chain C:



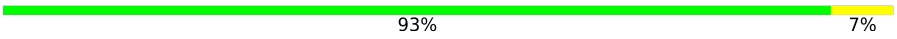
• Molecule 3: Complement C3

Chain F:



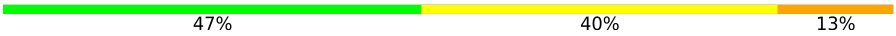
• Molecule 4: compstatin

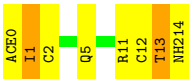
Chain G:



• Molecule 4: compstatin

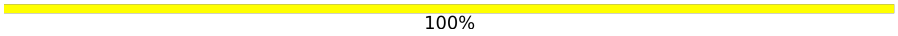
Chain H:





• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.81Å 124.75Å 127.37Å 90.00° 95.08° 90.00°	Depositor
Resolution (Å)	33.00 – 2.40 32.77 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.3 (33.00-2.40) 96.2 (32.77-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.3.0008	Depositor
R, R_{free}	0.213 , 0.281 0.268 , 0.293	Depositor DCC
R_{free} test set	5005 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	43.0	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 22.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	18480	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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: NAG, NH2, BR, K, ACE, 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	0.48	1/5009 (0.0%)	0.71	3/6804 (0.0%)
1	D	0.52	0/5017	0.70	3/6817 (0.0%)
2	B	0.47	0/1516	0.63	0/2060
2	E	0.52	0/1532	0.67	0/2082
3	C	0.85	10/2418 (0.4%)	0.63	3/3261 (0.1%)
3	F	0.45	0/2441	0.57	0/3291
4	G	0.39	0/114	0.56	0/156
4	H	0.56	0/114	0.82	0/156
All	All	0.55	11/18161 (0.1%)	0.67	9/24627 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	4
3	C	0	1
All	All	0	5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1495	ASN	CG-OD1	23.53	1.75	1.24
3	C	1520	ASP	CG-OD2	11.48	1.51	1.25
3	C	1495	ASN	CB-CG	10.92	1.76	1.51
3	C	1602	LYS	CE-NZ	8.22	1.69	1.49
3	C	1518	GLY	C-O	7.93	1.36	1.23
3	C	1632	GLU	CD-OE2	7.20	1.33	1.25
3	C	1603	ASP	CG-OD1	6.37	1.40	1.25
3	C	1519	VAL	CB-CG1	6.01	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1495	ASN	CG-ND2	-5.96	1.18	1.32
1	A	89	THR	C-O	5.52	1.33	1.23
3	C	1519	VAL	CB-CG2	5.17	1.63	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	504	ILE	C-N-CD	-21.38	73.56	120.60
1	A	504	ILE	C-N-CA	13.21	177.47	122.00
3	C	1495	ASN	CB-CG-ND2	7.48	134.66	116.70
3	C	1520	ASP	CB-CG-OD2	-7.36	111.68	118.30
1	A	574	VAL	CB-CA-C	-6.86	98.38	111.40
1	D	504	ILE	C-N-CD	-6.68	105.91	120.60
3	C	1495	ASN	OD1-CG-ND2	-6.38	107.23	121.90
1	D	509	LEU	CA-CB-CG	6.19	129.53	115.30
1	D	574	VAL	CB-CA-C	-5.59	100.79	111.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	1635	VAL	Mainchain
1	D	290	GLN	Peptide
1	D	40	PHE	Peptide
1	D	504	ILE	Peptide
1	D	505	PRO	Peptide

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	4912	0	4976	88	0
1	D	4919	0	4986	112	0
2	B	1484	0	1511	22	0
2	E	1500	0	1526	22	0
3	C	2372	0	2280	30	0
3	F	2395	0	2302	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	113	0	98	0	0
4	H	113	0	98	6	0
5	I	28	0	25	1	0
5	J	28	0	25	1	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
6	D	2	0	0	0	0
6	F	1	0	0	0	0
7	A	8	0	0	3	0
7	B	3	0	0	0	0
7	C	1	0	0	0	0
7	D	15	0	0	5	0
7	E	3	0	0	0	0
7	F	2	0	0	0	0
8	A	30	0	40	7	0
8	B	6	0	8	1	0
8	C	6	0	8	1	0
8	D	42	0	56	16	0
8	E	12	0	16	5	0
8	F	6	0	8	5	0
8	H	6	0	8	0	0
9	A	111	0	0	1	0
9	B	47	0	0	1	0
9	C	23	0	0	0	0
9	D	188	0	0	4	0
9	E	62	0	0	1	0
9	F	35	0	0	1	0
9	H	5	0	0	0	0
All	All	18480	0	17971	285	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 8.

All (285) 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)
3:C:1602:LYS:NZ	3:C:1602:LYS:CE	1.69	1.53
3:C:1495:ASN:CG	3:C:1495:ASN:CB	1.76	1.49
3:C:1495:ASN:CG	3:C:1495:ASN:OD1	1.75	1.24
1:D:139:ARG:HD2	8:D:807:GOL:H31	1.47	0.95
1:D:574:VAL:HG13	2:E:751:TRP:HE3	1.33	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:ARG:HB3	8:D:807:GOL:H2	1.48	0.93
2:E:795:VAL:HG22	8:E:916:GOL:H31	1.50	0.91
2:E:795:VAL:CG2	8:E:916:GOL:H31	2.01	0.89
3:F:1338:LYS:H	8:F:840:GOL:H12	1.38	0.88
1:D:3:MET:HE3	1:D:522:ARG:HG2	1.60	0.82
1:D:111:GLN:OE1	1:D:126:ARG:HD3	1.81	0.81
1:D:574:VAL:HG13	2:E:751:TRP:CE3	2.16	0.81
1:D:539:GLY:O	8:D:811:GOL:H2	1.82	0.79
1:D:604:GLY:O	8:D:824:GOL:H32	1.83	0.79
1:A:80:ARG:HG3	1:A:81:ASN:H	1.48	0.78
1:A:158:LEU:HD11	1:A:169:LEU:HD21	1.66	0.77
1:D:510:VAL:HG11	1:D:622:LEU:CD1	2.15	0.77
1:D:77:GLU:O	1:D:78:LYS:HB2	1.85	0.76
1:D:350:LEU:HD21	1:D:400:ILE:HG12	1.67	0.76
3:F:1465:GLU:HB3	8:F:840:GOL:H32	1.66	0.76
1:D:242:LYS:H	8:D:818:GOL:H11	1.52	0.76
1:A:577:ASP:OD1	2:B:778:THR:HG21	1.87	0.75
3:C:1369:ARG:HH11	3:C:1369:ARG:HG3	1.52	0.73
4:H:5:GLN:O	4:H:11:ARG:HG3	1.89	0.73
1:A:505:PRO:HD2	1:A:506:SER:H	1.53	0.71
9:D:3040:HOH:O	2:E:788:SER:HB2	1.91	0.71
1:D:168:PRO:O	1:D:169:LEU:HD23	1.91	0.71
1:D:510:VAL:HG11	1:D:622:LEU:HD12	1.72	0.71
1:A:574:VAL:HG13	2:B:751:TRP:HE3	1.56	0.70
1:A:427:VAL:HG23	8:A:809:GOL:H2	1.74	0.70
1:A:158:LEU:CD1	1:A:169:LEU:HD21	2.23	0.69
1:A:40:PHE:HB3	1:A:41:PRO:HD3	1.74	0.69
7:D:720:BR:BR	9:D:3183:HOH:O	2.66	0.68
1:D:190:ASN:OD1	8:D:807:GOL:H32	1.94	0.68
3:C:1544:GLU:HG2	8:C:819:GOL:H32	1.77	0.67
1:A:111:GLN:OE1	1:A:126:ARG:HD3	1.94	0.66
1:D:46:VAL:HG11	1:D:68:ILE:HG12	1.76	0.66
1:D:256:GLY:O	1:D:257:GLU:HB2	1.96	0.65
3:C:1530:VAL:HG12	3:C:1532:LEU:HD13	1.79	0.65
3:C:1602:LYS:NZ	3:C:1602:LYS:CD	2.57	0.64
1:A:249:VAL:HG11	1:A:278:VAL:HG11	1.80	0.64
1:D:3:MET:CE	1:D:522:ARG:HG2	2.27	0.63
3:F:1336:CYS:HA	8:F:840:GOL:H11	1.80	0.63
1:A:369:VAL:O	1:A:373:ASP:HA	1.98	0.63
1:D:322:SER:H	8:D:825:GOL:H2	1.63	0.63
1:D:404:THR:HG22	1:D:414:GLN:OE1	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:736:GLU:HG2	2:B:891:LYS:HD2	1.82	0.62
1:D:508:ARG:NH1	1:D:602:ASP:OD2	2.25	0.61
1:A:393:PRO:HB3	1:A:456:ARG:NH2	2.15	0.61
1:D:437:SER:HB3	1:D:452:ASN:HB2	1.82	0.61
3:C:1589:PHE:HD1	3:C:1596:LEU:HD11	1.64	0.61
3:F:1525:THR:HB	3:F:1541:MET:HE3	1.82	0.61
1:D:373:ASP:O	1:D:375:VAL:N	2.35	0.60
1:D:123:VAL:HG23	1:D:173:ILE:HD11	1.84	0.60
1:A:50:GLU:HB3	1:A:64:VAL:HG22	1.83	0.60
1:D:375:VAL:HG23	1:D:376:GLN:N	2.15	0.60
1:A:302:LEU:HD13	1:A:326:ILE:HD11	1.84	0.60
2:B:862:GLN:HG3	9:B:204:HOH:O	2.03	0.59
3:C:1593:LYS:HA	3:C:1596:LEU:HB2	1.84	0.59
1:A:10:ASN:OD1	1:A:635:ARG:HD2	2.02	0.59
1:A:547:GLN:HA	1:D:408:GLU:HB3	1.85	0.58
3:C:1495:ASN:CG	3:C:1495:ASN:CA	2.66	0.58
1:D:78:LYS:HE2	1:D:79:GLY:H	1.67	0.58
1:D:6:ILE:HG21	1:D:20:MET:HE2	1.85	0.58
2:E:736:GLU:HG2	2:E:891:LYS:HD2	1.85	0.58
1:A:50:GLU:HB3	1:A:64:VAL:CG2	2.33	0.58
1:D:126:ARG:CZ	1:D:572:VAL:HB	2.33	0.58
1:D:1:SER:N	1:D:2:PRO:HD3	2.18	0.57
1:A:535:ASP:HB3	7:A:708:BR:BR	2.58	0.57
1:A:293:ARG:HH21	1:A:295:GLU:HB2	1.68	0.57
1:D:162:ASN:HA	7:D:725:BR:BR	2.60	0.57
1:D:290:GLN:HA	1:D:290:GLN:NE2	2.19	0.57
1:A:393:PRO:HB3	1:A:456:ARG:HH22	1.70	0.57
2:E:795:VAL:HG22	8:E:916:GOL:C3	2.29	0.57
1:A:596:ASP:O	1:A:600:LYS:HG2	2.04	0.57
1:D:132:HIS:HB2	8:D:823:GOL:H2	1.86	0.57
3:F:1386:MET:HB3	3:F:1450:ILE:HD12	1.86	0.57
1:D:6:ILE:CG2	1:D:20:MET:HE2	2.36	0.56
1:D:242:LYS:HD2	8:D:818:GOL:H12	1.86	0.56
1:D:505:PRO:HD2	1:D:506:SER:N	2.20	0.56
1:D:471:LEU:HB2	1:D:510:VAL:HG13	1.87	0.56
1:A:546:GLY:O	1:A:547:GLN:HG2	2.06	0.56
1:D:564:GLU:HG2	2:E:766:THR:HG23	1.88	0.56
1:A:444:ARG:HH12	1:A:534:LYS:HE2	1.71	0.55
3:C:1530:VAL:HG23	3:C:1576:GLU:HG3	1.87	0.55
1:D:305:SER:OG	1:D:318:GLN:NE2	2.39	0.55
2:E:783:LEU:HD11	8:E:916:GOL:H12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:THR:HG21	5:I:1:NAG:H82	1.88	0.55
1:A:20:MET:HB3	1:A:64:VAL:HG12	1.90	0.55
3:C:1525:THR:HB	3:C:1541:MET:HE3	1.89	0.54
1:D:440:ARG:N	1:D:440:ARG:HD2	2.23	0.54
3:F:1525:THR:HB	3:F:1541:MET:CE	2.38	0.54
1:D:642:GLN:HG3	1:D:643:PRO:HD2	1.90	0.53
1:D:19:THR:HG21	5:J:1:NAG:H82	1.90	0.53
1:D:233:ILE:HD13	1:D:269:ILE:HD11	1.90	0.53
1:D:147:ASN:HB2	1:D:148:PRO:CD	2.39	0.53
1:A:338:THR:O	1:A:340:LYS:NZ	2.40	0.53
2:B:855:THR:OG1	2:B:858:ARG:HB3	2.09	0.53
3:F:1500:LYS:O	3:F:1501:SER:HB2	2.09	0.52
1:A:61:MET:SD	1:A:483:ARG:HG2	2.49	0.52
1:A:426:THR:HA	8:A:809:GOL:H31	1.91	0.52
1:A:574:VAL:HG13	2:B:751:TRP:CE3	2.40	0.52
1:A:80:ARG:CG	1:A:81:ASN:H	2.19	0.52
1:D:111:GLN:OE1	1:D:126:ARG:CD	2.56	0.52
1:D:505:PRO:CD	1:D:506:SER:N	2.73	0.52
3:F:1576:GLU:O	3:F:1577:LYS:HB2	2.08	0.52
1:A:554:VAL:HG22	1:A:555:PRO:HD2	1.92	0.52
1:D:259:ARG:NH1	1:D:320:GLU:OE2	2.29	0.52
1:D:577:ASP:OD1	2:E:778:THR:HG21	2.09	0.52
3:F:1621:GLN:O	3:F:1623:GLN:N	2.40	0.52
1:A:144:ASN:OD1	1:A:155:GLN:HG3	2.10	0.52
1:D:375:VAL:CG2	1:D:376:GLN:N	2.72	0.51
1:A:309:ILE:HG12	1:A:316:MET:HG3	1.91	0.51
1:D:473:MET:CE	1:D:603:ILE:HD11	2.39	0.51
3:C:1592:GLU:O	3:C:1593:LYS:HB2	2.10	0.51
3:F:1365:GLU:HG3	3:F:1438:ALA:HB2	1.93	0.51
1:A:505:PRO:CD	1:A:506:SER:H	2.22	0.51
3:C:1525:THR:OG1	3:C:1541:MET:HE2	2.11	0.50
1:D:351:MET:HG3	1:D:440:ARG:CG	2.41	0.50
1:A:626:SER:OG	1:A:630:GLN:HG2	2.11	0.50
1:D:1:SER:N	1:D:2:PRO:CD	2.74	0.50
1:D:506:SER:OG	1:D:530:TRP:NE1	2.44	0.50
3:C:1416:PHE:HZ	3:C:1442:HIS:HB2	1.77	0.49
1:D:252:GLY:HA3	1:D:303:TYR:CZ	2.48	0.49
1:A:404:THR:HG22	1:A:406:LYS:H	1.74	0.49
1:D:375:VAL:CG2	1:D:376:GLN:H	2.26	0.49
1:D:78:LYS:HE2	1:D:79:GLY:N	2.27	0.49
1:D:510:VAL:HG11	1:D:622:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1590:TRP:HB3	3:C:1597:SER:HB2	1.94	0.49
3:F:1386:MET:HB3	3:F:1450:ILE:CD1	2.43	0.49
1:D:474:ASN:HD21	1:D:505:PRO:HD3	1.77	0.49
1:D:452:ASN:HB3	1:D:492:LEU:HD21	1.95	0.48
1:A:97:LYS:HD3	1:A:625:THR:OG1	2.13	0.48
1:D:558:GLN:HB2	2:E:772:PHE:CE2	2.48	0.48
3:F:1475:LYS:NZ	9:F:570:HOH:O	2.47	0.48
3:C:1380:ILE:O	3:C:1457:VAL:HA	2.13	0.48
3:C:1509:GLU:HB3	3:C:1513:LYS:NZ	2.28	0.48
1:D:406:LYS:HB3	1:D:409:LEU:HD22	1.96	0.48
1:D:476:GLY:HA2	7:D:703:BR:BR	2.67	0.48
1:A:613:TYR:HB3	8:A:809:GOL:O2	2.14	0.48
1:A:425:SER:O	8:A:809:GOL:H11	2.13	0.48
1:D:330:PRO:O	1:D:357:PRO:HD3	2.12	0.48
1:A:472:ILE:HD13	1:A:509:LEU:HD22	1.95	0.48
3:C:1380:ILE:HG23	3:C:1423:ILE:HG23	1.96	0.48
2:E:853:LEU:HD22	3:F:1449:LEU:HD12	1.96	0.48
1:A:153:VAL:HG11	1:A:171:TRP:CZ2	2.49	0.47
1:D:390:ASN:ND2	4:H:2:CYS:H	2.12	0.47
1:D:505:PRO:HD2	1:D:506:SER:H	1.79	0.47
1:A:97:LYS:NZ	1:A:632:THR:O	2.47	0.47
2:E:785:VAL:HG22	2:E:795:VAL:HB	1.97	0.47
4:H:12:CYS:O	4:H:14:NH2:N	2.48	0.47
1:D:77:GLU:O	1:D:78:LYS:CB	2.60	0.47
1:A:581:PHE:HA	1:A:584:ASN:O	2.15	0.47
2:B:843:GLU:HG3	2:B:861:GLN:HB3	1.95	0.47
3:C:1336:CYS:HB3	3:C:1339:PHE:O	2.15	0.47
1:D:40:PHE:CD2	1:D:41:PRO:HD2	2.50	0.47
1:D:314:SER:HB3	2:E:812:ARG:HG3	1.95	0.47
1:A:407:GLN:O	1:A:408:GLU:HB3	2.15	0.47
1:D:126:ARG:NH2	1:D:572:VAL:HB	2.30	0.47
1:D:409:LEU:HG	1:D:413:GLU:HB3	1.96	0.46
3:F:1527:LEU:CD2	3:F:1574:LEU:HB3	2.46	0.46
3:C:1495:ASN:OD1	3:C:1495:ASN:ND2	2.38	0.46
2:E:783:LEU:CD1	8:E:916:GOL:H12	2.45	0.46
1:A:147:ASN:HB2	1:A:148:PRO:HD2	1.97	0.46
1:A:196:PHE:HB3	8:A:802:GOL:H2	1.98	0.46
1:D:369:VAL:HG13	1:D:400:ILE:HD12	1.98	0.46
1:A:569:ALA:HB3	2:B:756:LEU:HD12	1.97	0.46
1:A:116:ILE:HD11	1:A:203:LYS:HD2	1.98	0.46
1:A:444:ARG:NH1	1:A:534:LYS:HG2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:894:VAL:HG22	2:B:897:HIS:HB2	1.98	0.46
1:A:386:LYS:HB3	1:A:440:ARG:HD2	1.97	0.45
4:H:0:ACE:H1	4:H:2:CYS:HB3	1.97	0.45
1:A:153:VAL:CG1	1:A:171:TRP:CZ2	2.99	0.45
1:D:599:GLU:O	1:D:602:ASP:HB2	2.16	0.45
1:A:426:THR:HA	8:A:809:GOL:H11	1.98	0.45
3:F:1393:THR:HG22	3:F:1419:ARG:HH12	1.82	0.45
1:A:558:GLN:NE2	2:B:770:ASN:OD1	2.46	0.45
2:B:751:TRP:C	2:B:752:ASN:HD22	2.20	0.45
1:A:147:ASN:HB2	1:A:148:PRO:CD	2.46	0.45
9:A:3061:HOH:O	2:B:770:ASN:ND2	2.50	0.45
1:A:472:ILE:CD1	1:A:509:LEU:HD22	2.46	0.45
1:D:537:CYS:H	8:D:811:GOL:H11	1.81	0.45
2:E:762:ASN:HB3	2:E:763:GLY:H	1.42	0.45
1:D:1:SER:H2	1:D:2:PRO:HD3	1.81	0.45
1:D:351:MET:HG3	1:D:440:ARG:HG2	1.98	0.45
1:A:297:LEU:HA	1:A:300:LYS:HD3	1.98	0.44
1:A:298:VAL:HG21	1:A:328:THR:HG23	1.98	0.44
2:B:785:VAL:HG22	2:B:795:VAL:HB	1.97	0.44
2:B:805:GLN:HE21	2:B:808:PHE:HB3	1.82	0.44
1:A:554:VAL:HG12	1:A:557:GLN:HB2	1.99	0.44
3:C:1538:GLU:HG2	3:C:1563:ILE:HG12	1.99	0.44
1:A:126:ARG:NH2	1:A:572:VAL:HB	2.33	0.44
1:D:123:VAL:CG2	1:D:173:ILE:HD11	2.47	0.44
3:F:1381:LEU:HG	3:F:1426:LEU:HD11	1.98	0.44
1:D:233:ILE:HD11	1:D:249:VAL:HG21	1.98	0.44
1:A:575:ALA:O	2:B:748:SER:HA	2.18	0.44
1:D:45:LEU:HD11	1:D:48:SER:HA	2.00	0.44
1:A:217:THR:HG23	1:A:230:GLU:O	2.18	0.44
1:A:407:GLN:O	1:A:408:GLU:CB	2.66	0.43
1:D:222:TYR:HB2	8:D:822:GOL:H11	1.99	0.43
3:C:1385:MET:HB3	3:C:1385:MET:HE2	1.88	0.43
3:F:1386:MET:SD	3:F:1473:PRO:HD3	2.58	0.43
1:A:24:ALA:HB3	1:A:60:HIS:HB3	1.99	0.43
1:A:473:MET:HE3	1:A:622:LEU:HD21	1.99	0.43
1:D:79:GLY:C	1:D:81:ASN:N	2.71	0.43
2:E:807:PHE:HA	2:E:830:TYR:O	2.18	0.43
3:F:1463:LEU:O	3:F:1463:LEU:HG	2.19	0.43
1:A:164:LEU:O	2:B:787:MET:HG2	2.18	0.43
1:A:233:ILE:HD11	1:A:249:VAL:HG21	2.01	0.43
1:D:517:GLY:O	1:D:519:SER:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:VAL:HG13	1:A:54:LEU:HB2	2.00	0.43
1:D:47:LEU:HD23	1:D:49:SER:H	1.82	0.43
1:D:178:ASN:HB2	7:D:704:BR:BR	2.74	0.43
2:E:887:GLU:HG3	9:E:269:HOH:O	2.19	0.43
3:C:1530:VAL:CG1	3:C:1532:LEU:HD13	2.48	0.43
1:D:442:GLU:HB3	1:D:444:ARG:NH1	2.34	0.43
1:A:126:ARG:CZ	1:A:572:VAL:HB	2.49	0.42
2:B:849:ALA:HA	2:B:882:LYS:HD2	2.01	0.42
3:C:1495:ASN:CG	3:C:1495:ASN:H	2.22	0.42
3:C:1495:ASN:CG	3:C:1495:ASN:N	2.72	0.42
1:D:330:PRO:HG3	8:D:822:GOL:H12	2.00	0.42
2:E:813:LEU:HD13	2:E:907:LEU:HG	2.01	0.42
1:D:146:GLU:OE1	1:D:185:ARG:HD2	2.19	0.42
2:B:756:LEU:HD23	2:B:767:LYS:HB2	2.00	0.42
1:A:505:PRO:HD2	1:A:506:SER:N	2.30	0.42
2:B:742:ARG:HG2	8:B:915:GOL:H2	2.01	0.42
3:C:1370:TYR:CD1	3:C:1376:ALA:HB2	2.54	0.42
3:C:1456:LYS:HA	3:C:1467:CYS:O	2.19	0.42
1:D:190:ASN:O	1:D:192:PRO:HD3	2.18	0.42
1:D:210:PHE:HB2	1:D:236:ARG:O	2.20	0.42
1:D:535:ASP:HB3	7:D:710:BR:BR	2.74	0.42
1:A:201:GLU:OE2	1:A:203:LYS:HE2	2.20	0.42
1:D:23:GLU:CG	1:D:61:MET:HG3	2.50	0.42
1:A:297:LEU:O	1:A:300:LYS:HB2	2.20	0.42
3:C:1576:GLU:O	3:C:1577:LYS:HB2	2.20	0.42
1:D:13:ARG:HD3	8:D:823:GOL:H11	2.02	0.42
1:D:470:TYR:O	1:D:481:ALA:HA	2.20	0.42
1:A:505:PRO:HB2	1:A:599:GLU:OE2	2.19	0.41
3:C:1521:TYR:HA	3:C:1548:LYS:O	2.20	0.41
2:E:754:GLU:HB3	2:E:767:LYS:HD3	2.01	0.41
1:A:458:ASP:HA	7:A:724:BR:BR	2.75	0.41
1:D:47:LEU:HD13	1:D:66:PHE:HB2	2.02	0.41
1:D:562:LYS:HE3	2:E:766:THR:HG21	2.02	0.41
2:E:761:LYS:O	2:E:762:ASN:CB	2.68	0.41
1:A:143:VAL:HG13	1:A:156:ASP:HB2	2.02	0.41
1:A:473:MET:HE1	1:A:478:LEU:HG	2.02	0.41
1:D:216:PRO:HB2	1:D:218:GLU:O	2.20	0.41
1:A:510:VAL:HB	1:A:528:SER:HB3	2.03	0.41
3:F:1336:CYS:CA	8:F:840:GOL:H11	2.49	0.41
1:A:48:SER:OG	1:A:49:SER:N	2.52	0.41
3:F:1531:GLN:HB2	3:F:1538:GLU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LEU:HB2	1:A:69:PRO:HD3	2.02	0.41
1:A:352:VAL:HG21	1:A:387:LEU:HD12	2.03	0.41
1:A:479:LEU:HD11	1:A:502:ASP:HB3	2.03	0.41
1:A:525:VAL:HA	8:A:809:GOL:O2	2.20	0.41
1:A:577:ASP:CG	2:B:778:THR:HG21	2.40	0.41
1:D:23:GLU:HG2	1:D:61:MET:HG3	2.02	0.41
1:D:390:ASN:OD1	4:H:1:ILE:N	2.54	0.41
1:D:440:ARG:NH2	1:D:530:TRP:O	2.46	0.41
1:D:473:MET:HE1	1:D:603:ILE:HD11	2.02	0.41
3:F:1582:MET:HA	3:F:1605:TRP:O	2.21	0.41
1:A:142:MET:HG3	1:A:187:TYR:CE1	2.56	0.41
1:A:500:THR:HA	7:A:717:BR:BR	2.76	0.41
1:D:217:THR:HG22	9:D:3107:HOH:O	2.20	0.41
1:D:536:SER:HB2	8:D:811:GOL:H12	2.03	0.41
3:F:1543:ILE:HG22	3:F:1556:VAL:HA	2.03	0.41
4:H:11:ARG:HE	4:H:11:ARG:HB2	1.68	0.41
1:A:31:VAL:HA	1:A:32:PRO:HD2	1.96	0.40
2:B:898:PHE:O	2:B:899:ILE:HD13	2.20	0.40
1:D:440:ARG:O	1:D:441:THR:HG23	2.21	0.40
1:D:602:ASP:HB3	8:D:824:GOL:H32	2.02	0.40
1:A:138:GLY:HA3	1:A:161:GLN:HA	2.02	0.40
1:A:216:PRO:HB2	1:A:218:GLU:O	2.21	0.40
1:D:234:THR:HG23	9:D:3106:HOH:O	2.19	0.40
1:D:505:PRO:CD	1:D:506:SER:H	2.33	0.40
2:B:754:GLU:HB3	2:B:767:LYS:HD3	2.03	0.40
1:D:104:GLN:HB2	1:D:194:GLN:HE21	1.86	0.40
1:D:322:SER:OG	8:D:825:GOL:H2	2.20	0.40
1:D:155:GLN:HE21	1:D:155:GLN:HB2	1.74	0.40
1:D:187:TYR:CD1	1:D:192:PRO:HA	2.56	0.40
3:F:1465:GLU:C	8:F:840:GOL:O2	2.60	0.40
1:A:108:LEU:HD12	1:A:196:PHE:CD1	2.57	0.40
1:D:343:LYS:NZ	1:D:435:HIS:ND1	2.66	0.40
1:D:398:LEU:O	1:D:420:GLN:HA	2.22	0.40
1:D:596:ASP:O	1:D:600:LYS:HG2	2.20	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	623/643 (97%)	583 (94%)	32 (5%)	8 (1%)	12 17
1	D	626/643 (97%)	587 (94%)	24 (4%)	15 (2%)	6 6
2	B	182/188 (97%)	172 (94%)	10 (6%)	0	100 100
2	E	184/188 (98%)	175 (95%)	7 (4%)	2 (1%)	14 20
3	C	286/343 (83%)	262 (92%)	16 (6%)	8 (3%)	5 4
3	F	289/343 (84%)	266 (92%)	17 (6%)	6 (2%)	7 8
4	G	13/15 (87%)	10 (77%)	2 (15%)	1 (8%)	1 0
4	H	13/15 (87%)	10 (77%)	2 (15%)	1 (8%)	1 0
All	All	2216/2378 (93%)	2065 (93%)	110 (5%)	41 (2%)	8 10

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	505	PRO
3	C	1593	LYS
1	D	41	PRO
1	D	78	LYS
1	D	290	GLN
1	D	291	ASN
1	D	373	ASP
1	D	374	THR
1	D	441	THR
1	D	505	PRO
2	E	762	ASN
3	F	1501	SER
1	A	47	LEU
1	A	256	GLY
3	C	1416	PHE
1	D	45	LEU
1	D	49	SER

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Mol	Chain	Res	Type
3	F	1499	GLN
4	H	13	THR
1	A	15	GLU
1	A	408	GLU
3	C	1377	THR
3	C	1449	LEU
1	D	257	GLU
1	D	376	GLN
1	D	518	ALA
3	F	1500	LYS
3	F	1622	LYS
1	A	374	THR
3	C	1494	GLU
1	D	442	GLU
2	E	731	GLU
3	F	1556	VAL
4	G	13	THR
1	A	45	LEU
3	C	1486	ASP
3	C	1594	PRO
1	D	506	SER
1	A	50	GLU
3	F	1498	ILE
3	C	1636	VAL

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	A	555/567 (98%)	504 (91%)	51 (9%)	9 13
1	D	557/567 (98%)	512 (92%)	45 (8%)	11 18
2	B	171/175 (98%)	155 (91%)	16 (9%)	8 13
2	E	173/175 (99%)	159 (92%)	14 (8%)	11 18
3	C	266/309 (86%)	252 (95%)	14 (5%)	22 37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	F	269/309 (87%)	256 (95%)	13 (5%)	25 41
4	G	11/11 (100%)	11 (100%)	0	100 100
4	H	11/11 (100%)	9 (82%)	2 (18%)	1 2
All	All	2013/2124 (95%)	1858 (92%)	155 (8%)	13 20

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	10	ASN
1	A	31	VAL
1	A	44	LYS
1	A	50	GLU
1	A	64	VAL
1	A	80	ARG
1	A	82	LYS
1	A	86	VAL
1	A	87	GLN
1	A	103	LEU
1	A	125	TYR
1	A	126	ARG
1	A	137	VAL
1	A	140	THR
1	A	164	LEU
1	A	167	LEU
1	A	177	VAL
1	A	185	ARG
1	A	191	SER
1	A	219	LYS
1	A	232	THR
1	A	260	ILE
1	A	277	GLU
1	A	289	VAL
1	A	302	LEU
1	A	305	SER
1	A	364	ARG
1	A	376	GLN
1	A	395	GLN
1	A	407	GLN
1	A	408	GLU
1	A	413	GLU

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Mol	Chain	Res	Type
1	A	440	ARG
1	A	443	LEU
1	A	456	ARG
1	A	459	ARG
1	A	473	MET
1	A	477	ARG
1	A	483	ARG
1	A	487	GLU
1	A	498	SER
1	A	509	LEU
1	A	510	VAL
1	A	516	ILE
1	A	547	GLN
1	A	574	VAL
1	A	602	ASP
1	A	618	SER
1	A	625	THR
1	A	630	GLN
2	B	752	ASN
2	B	755	ASP
2	B	769	MET
2	B	770	ASN
2	B	776	SER
2	B	778	THR
2	B	789	ASP
2	B	795	VAL
2	B	840	VAL
2	B	842	VAL
2	B	872	LEU
2	B	894	VAL
2	B	904	ARG
2	B	905	LYS
2	B	907	LEU
2	B	912	GLU
3	C	1346	LYS
3	C	1360	ASN
3	C	1369	ARG
3	C	1420	ASN
3	C	1422	LEU
3	C	1433	GLU
3	C	1445	PHE
3	C	1487	GLU

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Mol	Chain	Res	Type
3	C	1488	LEU
3	C	1507	LEU
3	C	1528	VAL
3	C	1532	LEU
3	C	1555	GLN
3	C	1573	LYS
1	D	31	VAL
1	D	48	SER
1	D	78	LYS
1	D	103	LEU
1	D	126	ARG
1	D	140	THR
1	D	153	VAL
1	D	155	GLN
1	D	158	LEU
1	D	164	LEU
1	D	167	LEU
1	D	170	SER
1	D	177	VAL
1	D	185	ARG
1	D	191	SER
1	D	232	THR
1	D	275	SER
1	D	297	LEU
1	D	302	LEU
1	D	343	LYS
1	D	352	VAL
1	D	364	ARG
1	D	370	GLN
1	D	377	SER
1	D	396	LYS
1	D	400	ILE
1	D	410	SER
1	D	440	ARG
1	D	443	LEU
1	D	444	ARG
1	D	471	LEU
1	D	477	ARG
1	D	483	ARG
1	D	491	ASP
1	D	492	LEU
1	D	509	LEU

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Mol	Chain	Res	Type
1	D	544	LYS
1	D	554	VAL
1	D	574	VAL
1	D	578	LYS
1	D	592	SER
1	D	602	ASP
1	D	611	LYS
1	D	618	SER
1	D	634	GLN
2	E	729	LEU
2	E	737	GLU
2	E	767	LYS
2	E	778	THR
2	E	787	MET
2	E	795	VAL
2	E	835	ASN
2	E	840	VAL
2	E	842	VAL
2	E	865	THR
2	E	870	SER
2	E	877	VAL
2	E	894	VAL
2	E	907	LEU
3	F	1335	THR
3	F	1337	ASN
3	F	1359	LYS
3	F	1401	ASN
3	F	1422	LEU
3	F	1446	ASN
3	F	1450	ILE
3	F	1460	TYR
3	F	1487	GLU
3	F	1488	LEU
3	F	1505	VAL
3	F	1573	LYS
3	F	1586	SER
4	H	1	ILE
4	H	13	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	181	GLN
1	A	376	GLN
1	A	407	GLN
1	A	587	ASN
2	B	752	ASN
2	B	805	GLN
3	C	1401	ASN
3	C	1431	HIS
3	C	1531	GLN
3	C	1555	GLN
1	D	155	GLN
1	D	318	GLN
1	D	332	GLN
1	D	370	GLN
1	D	431	ASN
1	D	630	GLN
1	D	642	GLN
3	F	1495	ASN
3	F	1545	GLN
3	F	1608	HIS
3	F	1620	ASN
4	H	10	HIS

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	$\#\|Z\| > 2$
5	NAG	I	1	1,5	14,14,15	0.54	0	17,19,21	0.94	0
5	NAG	I	2	5	14,14,15	0.60	0	17,19,21	1.65	3 (17%)
5	NAG	J	1	1,5	14,14,15	0.60	0	17,19,21	1.11	2 (11%)
5	NAG	J	2	5	14,14,15	0.70	0	17,19,21	1.51	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	I	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
5	NAG	J	1	1,5	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	2	NAG	C1-O5-C5	4.77	118.66	112.19
5	J	2	NAG	C4-C3-C2	4.33	117.36	111.02
5	I	2	NAG	O5-C1-C2	3.62	117.01	111.29
5	J	2	NAG	C3-C4-C5	3.29	116.11	110.24
5	J	1	NAG	O5-C1-C2	-2.76	106.93	111.29
5	J	1	NAG	O5-C5-C6	2.10	110.50	107.20
5	I	2	NAG	C4-C3-C2	2.03	113.99	111.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	J	1	NAG	C1

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	I	2	NAG	O7-C7-N2-C2
5	J	2	NAG	O7-C7-N2-C2
5	J	2	NAG	C8-C7-N2-C2
5	I	1	NAG	O5-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
5	J	2	NAG	C4-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6

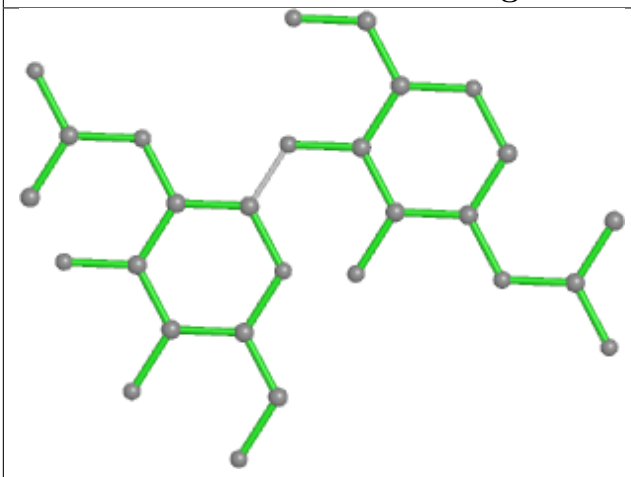
There are no ring outliers.

2 monomers are involved in 2 short contacts:

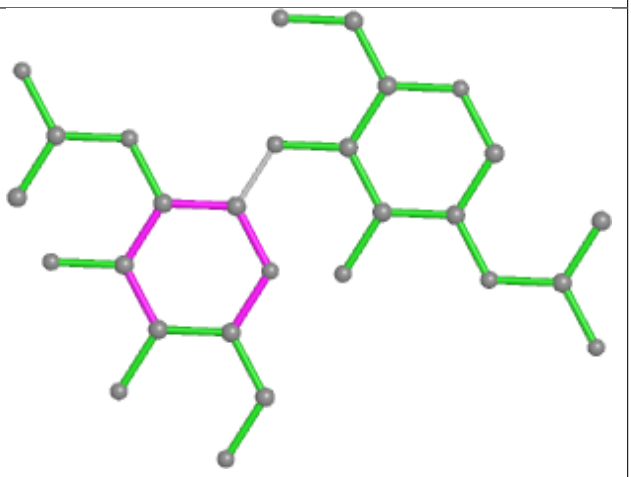
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	1	NAG	1	0
5	I	1	NAG	1	0

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

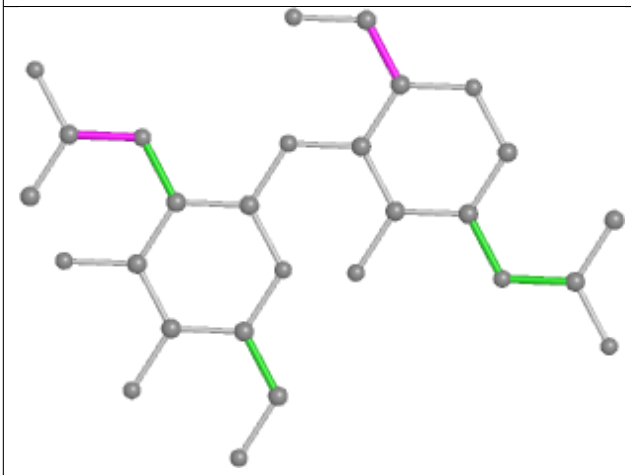
Oligosaccharide Chain I



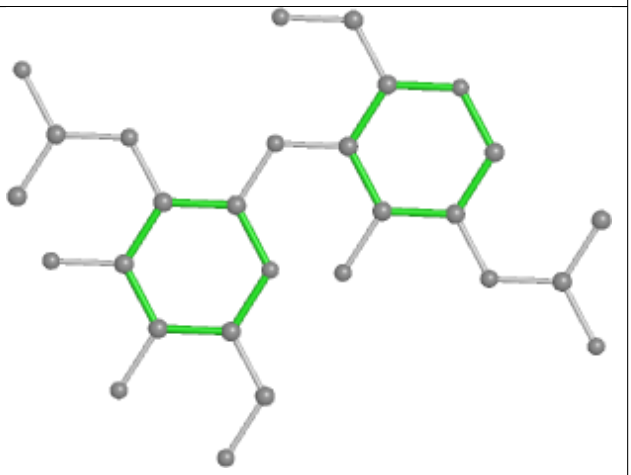
Bond lengths



Bond angles

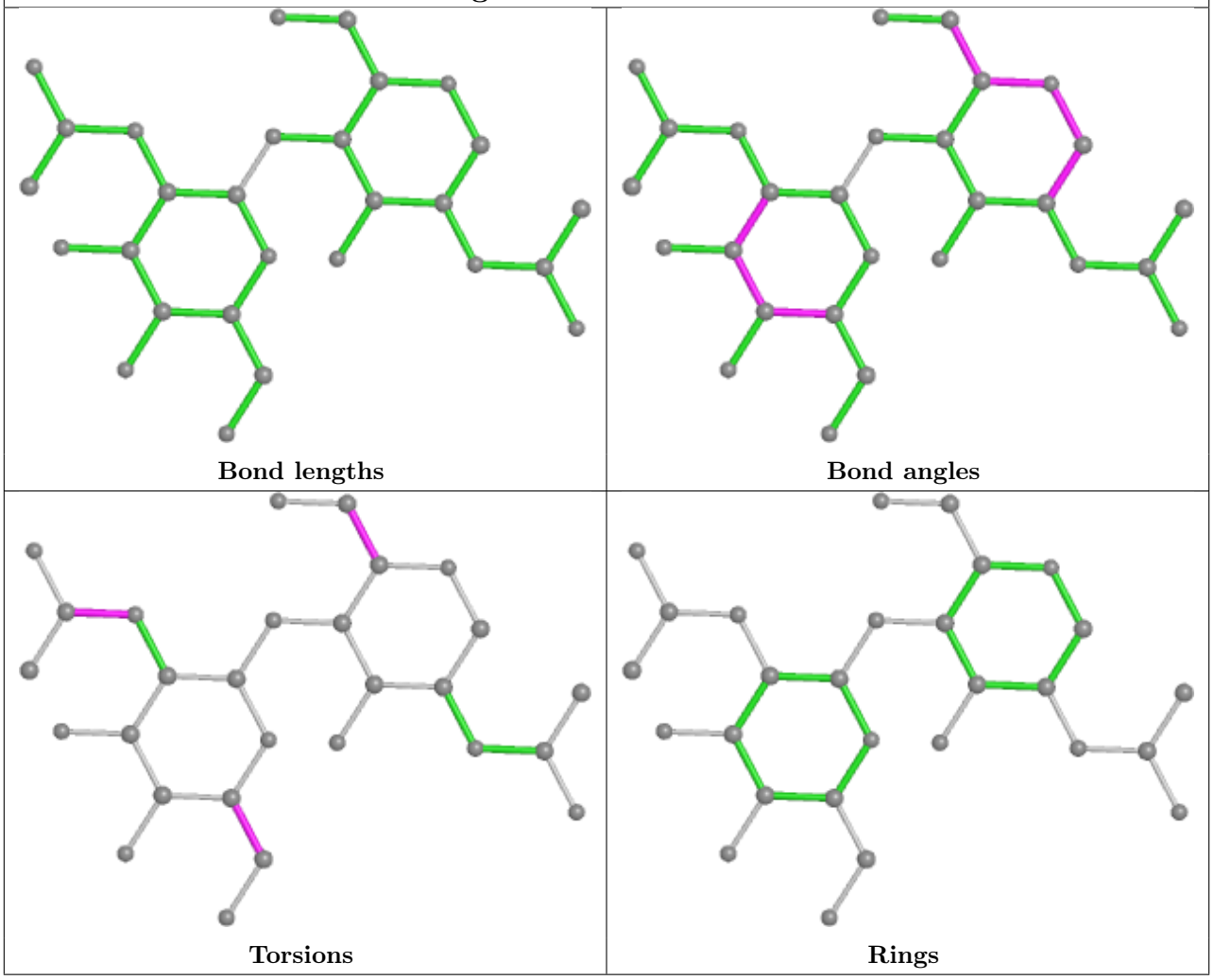


Torsions



Rings

Oligosaccharide Chain J



5.6 Ligand geometry (i)

Of 55 ligands modelled in this entry, 37 are monoatomic - leaving 18 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	$\#\|Z\| > 2$
8	GOL	A	816	-	5,5,5	0.46	0	5,5,5	0.56	0
8	GOL	E	916	-	5,5,5	0.32	0	5,5,5	0.56	0
8	GOL	H	820	-	5,5,5	0.29	0	5,5,5	0.45	0
8	GOL	D	823	-	5,5,5	0.44	0	5,5,5	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	GOL	D	825	-	5,5,5	0.42	0	5,5,5	0.29	0
8	GOL	D	811	-	5,5,5	0.32	0	5,5,5	0.37	0
8	GOL	E	915	-	5,5,5	0.34	0	5,5,5	0.15	0
8	GOL	B	915	-	5,5,5	0.35	0	5,5,5	0.55	0
8	GOL	D	822	-	5,5,5	0.33	0	5,5,5	0.63	0
8	GOL	F	840	-	5,5,5	0.42	0	5,5,5	0.48	0
8	GOL	A	802	-	5,5,5	0.52	0	5,5,5	0.67	0
8	GOL	A	821	-	5,5,5	0.37	0	5,5,5	0.32	0
8	GOL	D	818	-	5,5,5	0.41	0	5,5,5	0.33	0
8	GOL	C	819	-	5,5,5	0.36	0	5,5,5	0.19	0
8	GOL	D	807	-	5,5,5	0.47	0	5,5,5	0.34	0
8	GOL	A	809	-	5,5,5	0.55	0	5,5,5	0.41	0
8	GOL	D	824	-	5,5,5	0.38	0	5,5,5	0.41	0
8	GOL	A	845	-	5,5,5	0.45	0	5,5,5	0.27	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
8	GOL	A	816	-	-	4/4/4/4	-
8	GOL	E	916	-	-	2/4/4/4	-
8	GOL	H	820	-	-	4/4/4/4	-
8	GOL	D	823	-	-	4/4/4/4	-
8	GOL	D	825	-	-	4/4/4/4	-
8	GOL	D	811	-	-	2/4/4/4	-
8	GOL	E	915	-	-	2/4/4/4	-
8	GOL	B	915	-	-	4/4/4/4	-
8	GOL	D	822	-	-	4/4/4/4	-
8	GOL	F	840	-	-	4/4/4/4	-
8	GOL	A	802	-	-	2/4/4/4	-
8	GOL	A	821	-	-	2/4/4/4	-
8	GOL	D	818	-	-	2/4/4/4	-
8	GOL	C	819	-	-	2/4/4/4	-
8	GOL	D	807	-	-	4/4/4/4	-
8	GOL	A	809	-	-	4/4/4/4	-
8	GOL	D	824	-	-	4/4/4/4	-
8	GOL	A	845	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	802	GOL	O1-C1-C2-C3
8	A	809	GOL	O1-C1-C2-C3
8	A	809	GOL	C1-C2-C3-O3
8	A	816	GOL	C1-C2-C3-O3
8	A	821	GOL	O1-C1-C2-C3
8	A	845	GOL	O1-C1-C2-C3
8	B	915	GOL	O1-C1-C2-C3
8	B	915	GOL	C1-C2-C3-O3
8	B	915	GOL	O2-C2-C3-O3
8	C	819	GOL	C1-C2-C3-O3
8	D	807	GOL	C1-C2-C3-O3
8	D	811	GOL	C1-C2-C3-O3
8	D	818	GOL	O1-C1-C2-C3
8	D	822	GOL	C1-C2-C3-O3
8	D	822	GOL	O2-C2-C3-O3
8	D	823	GOL	O1-C1-C2-O2
8	D	823	GOL	O1-C1-C2-C3
8	D	823	GOL	C1-C2-C3-O3
8	D	823	GOL	O2-C2-C3-O3
8	D	824	GOL	O1-C1-C2-C3
8	D	824	GOL	C1-C2-C3-O3
8	D	825	GOL	O1-C1-C2-C3
8	E	916	GOL	C1-C2-C3-O3
8	F	840	GOL	O1-C1-C2-C3
8	F	840	GOL	C1-C2-C3-O3
8	H	820	GOL	C1-C2-C3-O3
8	A	809	GOL	O1-C1-C2-O2
8	A	816	GOL	O1-C1-C2-O2
8	D	818	GOL	O1-C1-C2-O2
8	A	816	GOL	O1-C1-C2-C3
8	D	807	GOL	O1-C1-C2-C3
8	D	825	GOL	C1-C2-C3-O3
8	E	915	GOL	C1-C2-C3-O3
8	A	809	GOL	O2-C2-C3-O3
8	A	816	GOL	O2-C2-C3-O3
8	A	821	GOL	O1-C1-C2-O2
8	A	845	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
8	B	915	GOL	O1-C1-C2-O2
8	C	819	GOL	O2-C2-C3-O3
8	D	811	GOL	O2-C2-C3-O3
8	D	824	GOL	O1-C1-C2-O2
8	D	824	GOL	O2-C2-C3-O3
8	D	825	GOL	O2-C2-C3-O3
8	F	840	GOL	O2-C2-C3-O3
8	H	820	GOL	O2-C2-C3-O3
8	A	802	GOL	O1-C1-C2-O2
8	D	807	GOL	O2-C2-C3-O3
8	F	840	GOL	O1-C1-C2-O2
8	D	822	GOL	O1-C1-C2-C3
8	E	916	GOL	O2-C2-C3-O3
8	D	822	GOL	O1-C1-C2-O2
8	H	820	GOL	O1-C1-C2-O2
8	D	825	GOL	O1-C1-C2-O2
8	D	807	GOL	O1-C1-C2-O2
8	H	820	GOL	O1-C1-C2-C3
8	E	915	GOL	O2-C2-C3-O3

There are no ring outliers.

13 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	916	GOL	5	0
8	D	823	GOL	2	0
8	D	825	GOL	2	0
8	D	811	GOL	3	0
8	B	915	GOL	1	0
8	D	822	GOL	2	0
8	F	840	GOL	5	0
8	A	802	GOL	1	0
8	D	818	GOL	2	0
8	C	819	GOL	1	0
8	D	807	GOL	3	0
8	A	809	GOL	6	0
8	D	824	GOL	2	0

5.7 Other polymers

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

Unable to reproduce the depositors R factor - this section is therefore empty.

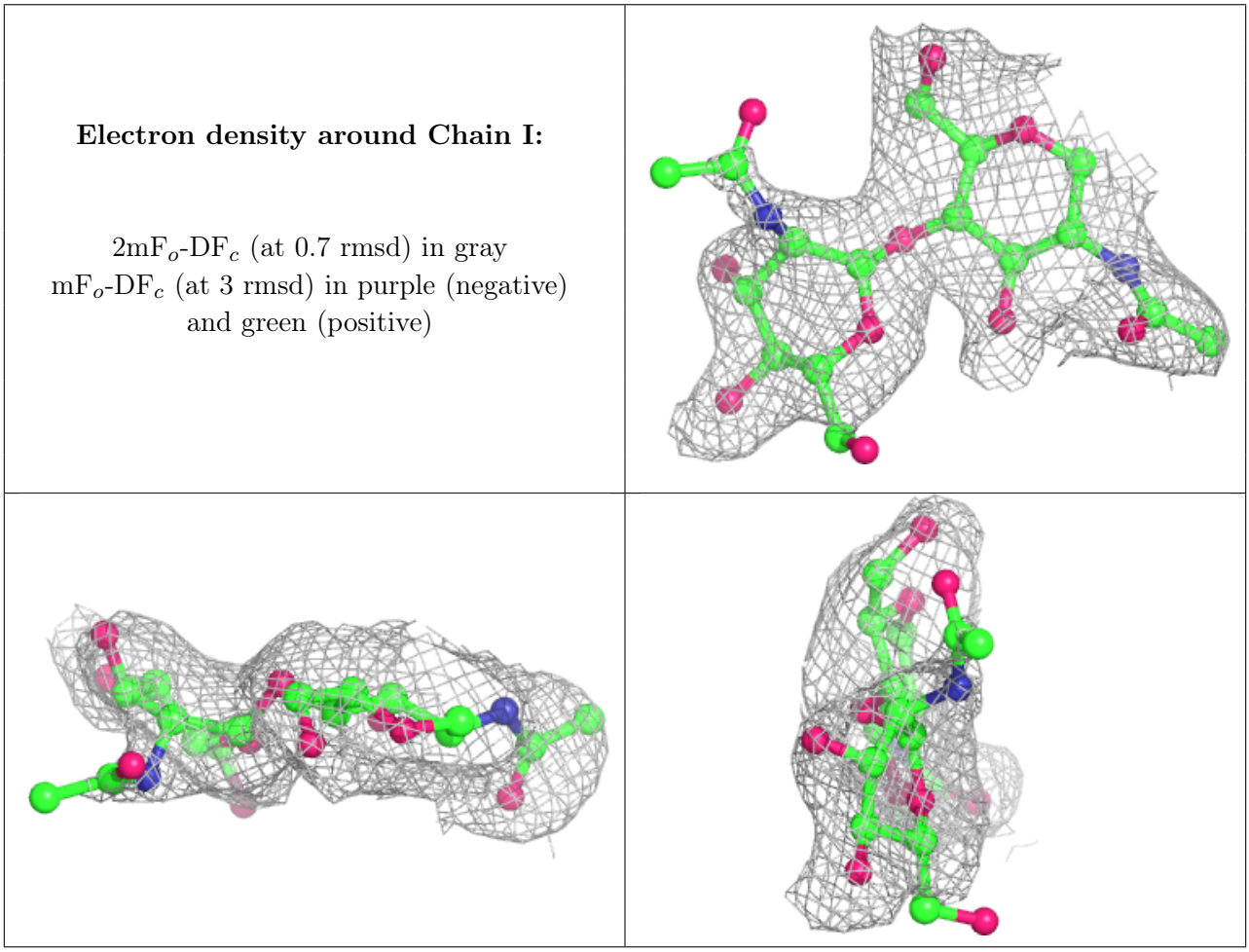
6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

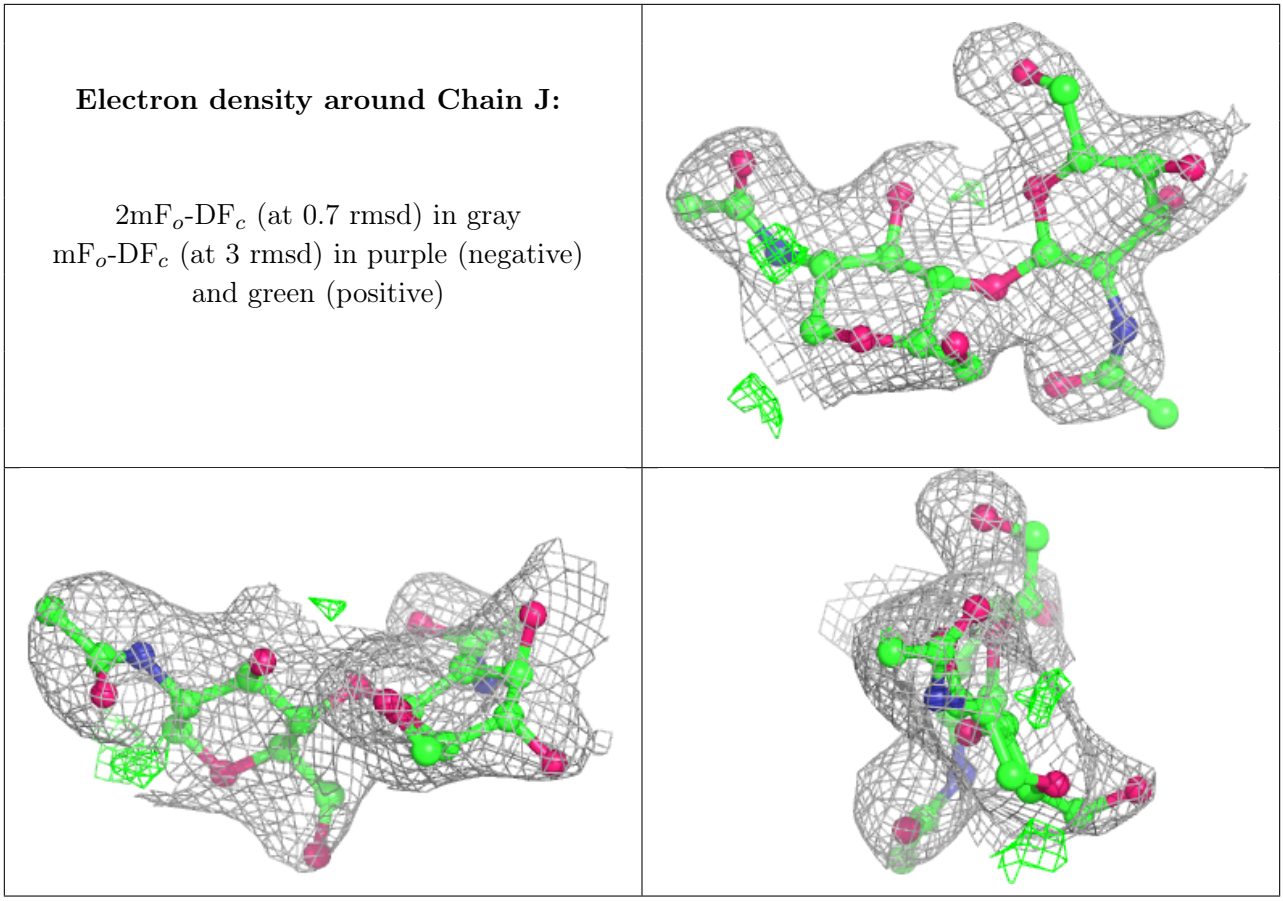
Unable to reproduce the depositors R factor - this section is therefore empty.

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 J:

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



6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.