Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 06:57 AM BST

PDB ID	:	6IAA
Title	:	hRobo2 ectodomain
Authors	:	Barak, R.; Isupov, N.M.; Opatowsky, Y.
Deposited on	:	2018-11-26
Resolution	:	3.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

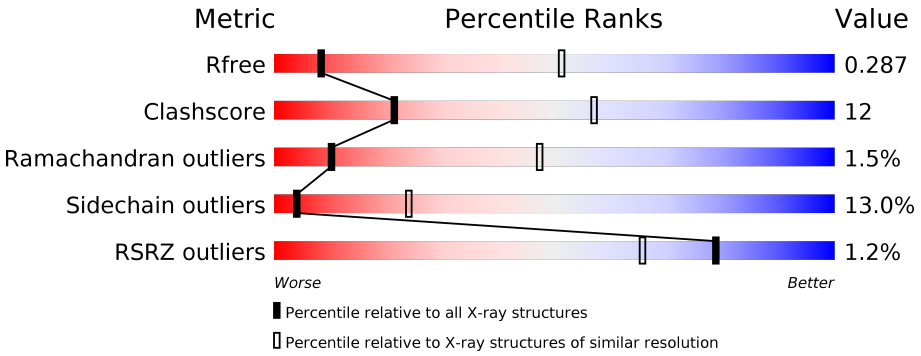
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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 on 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	A	859	% 63% 27% 5% 5%
1	B	859	% 63% 26% 5% 5%
1	C	859	% 63% 27% • 5%
2	D	2	100%
2	F	2	100%
2	H	2	50% 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	5	80% 20%
3	G	5	60% 40%
3	I	5	80% 20%

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
2	NAG	F	2	-	-	-	X
3	MAN	E	4	-	-	-	X
3	MAN	I	4	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19296 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 Roundabout homolog 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	815	Total	C	N	O	S	Se	0	0	0
			6343	3969	1125	1226	12	11			
1	B	815	Total	C	N	O	S	Se	0	0	0
			6343	3969	1125	1226	12	11			
1	C	815	Total	C	N	O	S	Se	0	0	0
			6343	3969	1125	1226	12	11			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	ASP	-	expression tag	UNP Q9HCK4
A	12	TYR	-	expression tag	UNP Q9HCK4
A	13	LYS	-	expression tag	UNP Q9HCK4
A	14	ASP	-	expression tag	UNP Q9HCK4
A	15	ASP	-	expression tag	UNP Q9HCK4
A	16	ASP	-	expression tag	UNP Q9HCK4
A	17	ASP	-	expression tag	UNP Q9HCK4
A	18	LYS	-	expression tag	UNP Q9HCK4
A	19	ARG	-	expression tag	UNP Q9HCK4
A	20	PRO	-	expression tag	UNP Q9HCK4
A	21	HIS	-	expression tag	UNP Q9HCK4
A	860	LYS	-	expression tag	UNP Q9HCK4
A	861	LEU	-	expression tag	UNP Q9HCK4
A	862	GLY	-	expression tag	UNP Q9HCK4
A	863	SER	-	expression tag	UNP Q9HCK4
A	864	HIS	-	expression tag	UNP Q9HCK4
A	865	HIS	-	expression tag	UNP Q9HCK4
A	866	HIS	-	expression tag	UNP Q9HCK4
A	867	HIS	-	expression tag	UNP Q9HCK4
A	868	HIS	-	expression tag	UNP Q9HCK4
A	869	HIS	-	expression tag	UNP Q9HCK4
B	11	ASP	-	expression tag	UNP Q9HCK4
B	12	TYR	-	expression tag	UNP Q9HCK4

Continued on next page...

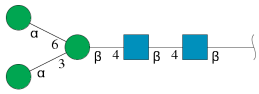
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	13	LYS	-	expression tag	UNP Q9HCK4
B	14	ASP	-	expression tag	UNP Q9HCK4
B	15	ASP	-	expression tag	UNP Q9HCK4
B	16	ASP	-	expression tag	UNP Q9HCK4
B	17	ASP	-	expression tag	UNP Q9HCK4
B	18	LYS	-	expression tag	UNP Q9HCK4
B	19	ARG	-	expression tag	UNP Q9HCK4
B	20	PRO	-	expression tag	UNP Q9HCK4
B	21	HIS	-	expression tag	UNP Q9HCK4
B	860	LYS	-	expression tag	UNP Q9HCK4
B	861	LEU	-	expression tag	UNP Q9HCK4
B	862	GLY	-	expression tag	UNP Q9HCK4
B	863	SER	-	expression tag	UNP Q9HCK4
B	864	HIS	-	expression tag	UNP Q9HCK4
B	865	HIS	-	expression tag	UNP Q9HCK4
B	866	HIS	-	expression tag	UNP Q9HCK4
B	867	HIS	-	expression tag	UNP Q9HCK4
B	868	HIS	-	expression tag	UNP Q9HCK4
B	869	HIS	-	expression tag	UNP Q9HCK4
C	11	ASP	-	expression tag	UNP Q9HCK4
C	12	TYR	-	expression tag	UNP Q9HCK4
C	13	LYS	-	expression tag	UNP Q9HCK4
C	14	ASP	-	expression tag	UNP Q9HCK4
C	15	ASP	-	expression tag	UNP Q9HCK4
C	16	ASP	-	expression tag	UNP Q9HCK4
C	17	ASP	-	expression tag	UNP Q9HCK4
C	18	LYS	-	expression tag	UNP Q9HCK4
C	19	ARG	-	expression tag	UNP Q9HCK4
C	20	PRO	-	expression tag	UNP Q9HCK4
C	21	HIS	-	expression tag	UNP Q9HCK4
C	860	LYS	-	expression tag	UNP Q9HCK4
C	861	LEU	-	expression tag	UNP Q9HCK4
C	862	GLY	-	expression tag	UNP Q9HCK4
C	863	SER	-	expression tag	UNP Q9HCK4
C	864	HIS	-	expression tag	UNP Q9HCK4
C	865	HIS	-	expression tag	UNP Q9HCK4
C	866	HIS	-	expression tag	UNP Q9HCK4
C	867	HIS	-	expression tag	UNP Q9HCK4
C	868	HIS	-	expression tag	UNP Q9HCK4
C	869	HIS	-	expression tag	UNP Q9HCK4

- Molecule 2 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
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



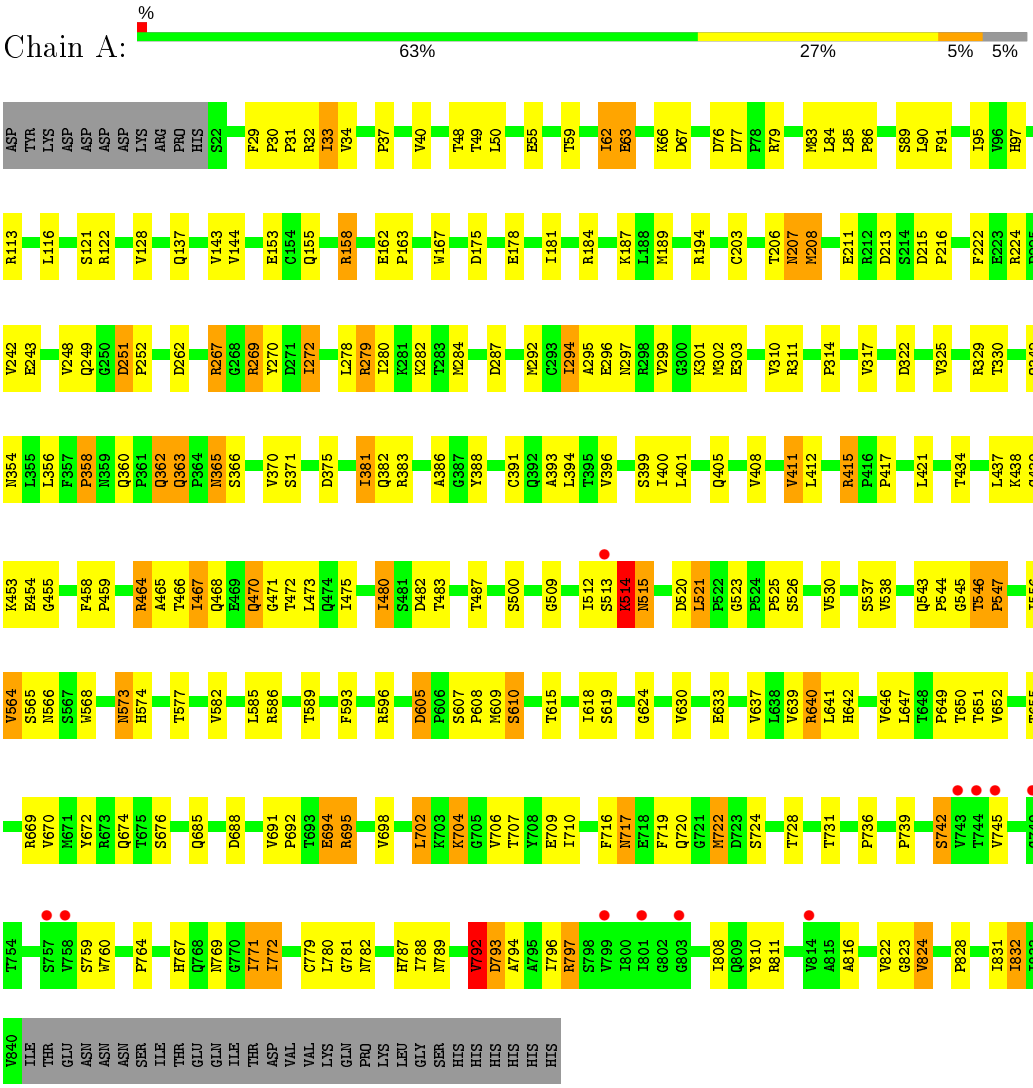
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	G	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	I	5	Total	C	N	O	0	0	0
			61	34	2	25			

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.

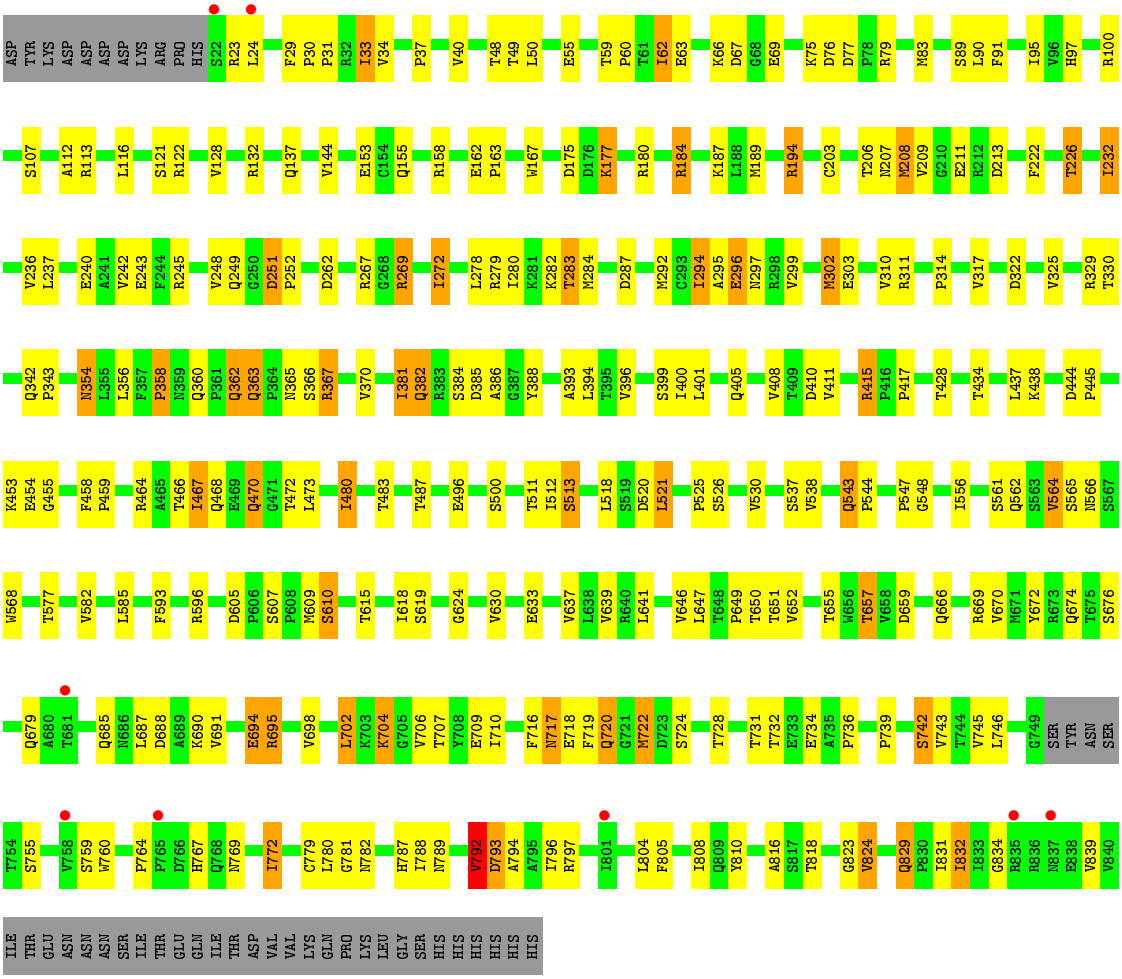
- Molecule 1: Roundabout homolog 2

Chain A:



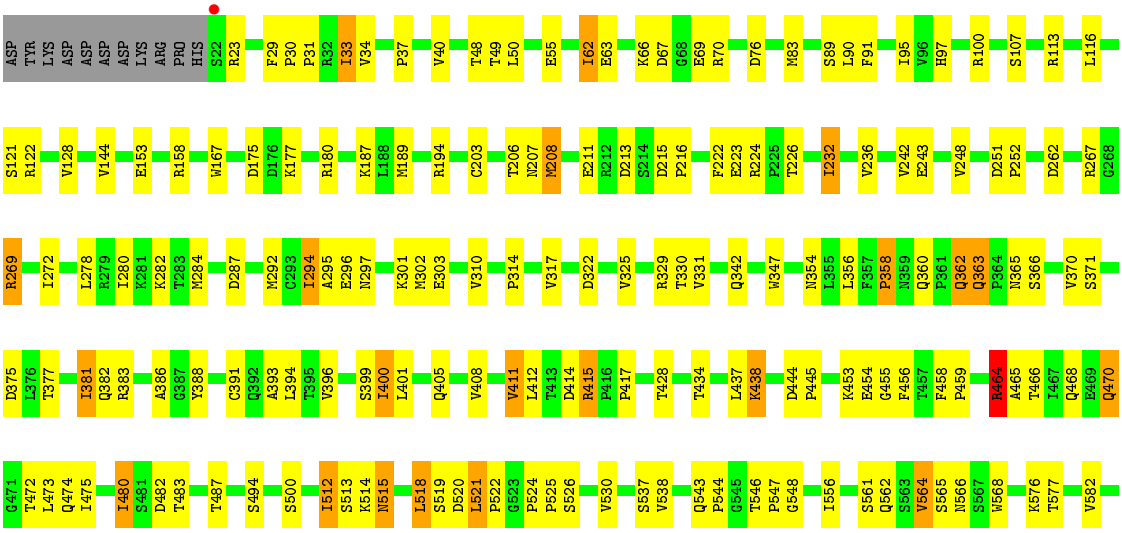
- Molecule 1: Roundabout homolog 2

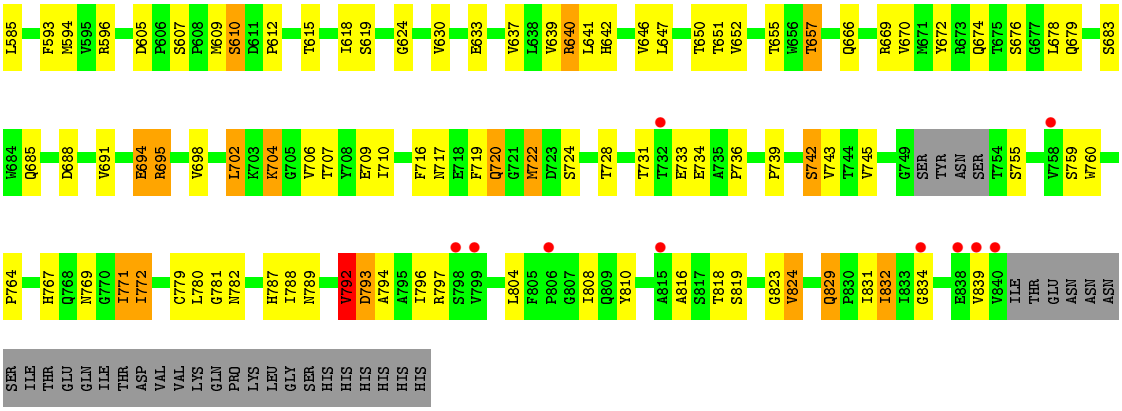
Chain B:



• Molecule 1: Roundabout homolog 2

Chain C:





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

Chain D:

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

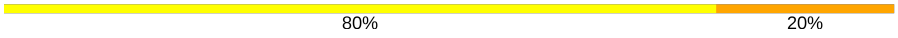
Chain F:

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

Chain H:

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

Chain E:

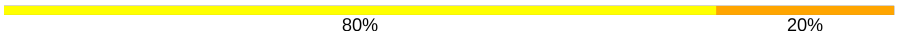


• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

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

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	290.77Å 81.57Å 158.66Å 90.00° 94.00° 90.00°	Depositor
Resolution (Å)	78.65 – 3.60 78.52 – 3.60	Depositor EDS
% Data completeness (in resolution range)	85.1 (78.65-3.60) 85.1 (78.52-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.75 (at 3.58Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.222 , 0.287 0.223 , 0.287	Depositor DCC
R_{free} test set	1909 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å^2)	95.0	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 65.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	19296	wwPDB-VP
Average B, all atoms (Å^2)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.90 % 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 1.6991e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

5.1 Standard geometry

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

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	0.52	4/6472 (0.1%)	0.85	10/8806 (0.1%)
1	B	0.42	2/6472 (0.0%)	0.76	7/8806 (0.1%)
1	C	0.48	2/6472 (0.0%)	0.79	10/8806 (0.1%)
All	All	0.48	8/19416 (0.0%)	0.80	27/26418 (0.1%)

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	A	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	GLU	CD-OE2	-18.27	1.05	1.25
1	C	63	GLU	CD-OE2	14.98	1.42	1.25
1	A	63	GLU	CG-CD	12.69	1.71	1.51
1	A	63	GLU	CD-OE1	11.60	1.38	1.25
1	B	113	ARG	CZ-NH2	10.88	1.47	1.33
1	B	63	GLU	CD-OE2	9.65	1.36	1.25
1	A	113	ARG	CZ-NH2	9.08	1.44	1.33
1	C	113	ARG	CZ-NH2	8.99	1.44	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	63	GLU	OE1-CD-OE2	28.42	157.41	123.30
1	A	63	GLU	CG-CD-OE2	-14.50	89.30	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	63	GLU	CG-CD-OE1	-9.36	99.58	118.30
1	C	722	MSE	CG-SE-CE	9.24	119.23	98.90
1	B	302	MSE	CG-SE-CE	8.96	118.61	98.90
1	A	722	MSE	CG-SE-CE	8.52	117.64	98.90
1	A	83	MSE	CG-SE-CE	8.09	116.69	98.90
1	B	189	MSE	CG-SE-CE	7.89	116.26	98.90
1	A	113	ARG	NE-CZ-NH1	-7.71	116.44	120.30
1	C	83	MSE	CG-SE-CE	7.70	115.85	98.90
1	C	189	MSE	CG-SE-CE	7.20	114.74	98.90
1	C	113	ARG	NE-CZ-NH1	-7.02	116.79	120.30
1	C	594	MSE	CG-SE-CE	6.99	114.28	98.90
1	B	722	MSE	CG-SE-CE	6.66	113.56	98.90
1	A	189	MSE	CG-SE-CE	6.55	113.31	98.90
1	B	83	MSE	CG-SE-CE	6.42	113.02	98.90
1	A	158	ARG	CB-CA-C	6.21	122.81	110.40
1	B	208	MSE	CG-SE-CE	6.13	112.39	98.90
1	C	208	MSE	CG-SE-CE	5.95	111.98	98.90
1	B	63	GLU	OE1-CD-OE2	5.90	130.38	123.30
1	C	284	MSE	CG-SE-CE	5.37	110.70	98.90
1	B	284	MSE	CG-SE-CE	5.26	110.47	98.90
1	C	63	GLU	OE1-CD-OE2	5.26	129.61	123.30
1	C	464	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	A	208	MSE	CG-SE-CE	5.06	110.04	98.90
1	C	722	MSE	CB-CG-SE	-5.05	97.56	112.70
1	A	284	MSE	CG-SE-CE	5.03	109.96	98.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	63	GLU	Sidechain

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	6343	0	6309	163	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	6343	0	6309	144	0
1	C	6343	0	6309	150	0
2	D	28	0	25	1	0
2	F	28	0	25	0	0
2	H	28	0	25	2	0
3	E	61	0	52	1	0
3	G	61	0	52	1	0
3	I	61	0	52	1	0
All	All	19296	0	19158	462	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 12.

All (462) 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:B:526:SER:OG	1:B:543:GLN:HG2	1.54	1.06
1:C:438:LYS:HA	1:C:472:THR:HG22	1.39	1.04
1:C:232:ILE:HD12	1:C:232:ILE:H	1.33	0.91
1:B:394:LEU:HD13	1:B:399:SER:HB3	1.53	0.91
1:B:232:ILE:HD12	1:B:232:ILE:H	1.36	0.88
1:A:564:VAL:HG23	1:A:586:ARG:HH11	1.38	0.88
1:A:676:SER:HB2	1:A:706:VAL:HG13	1.57	0.85
1:A:394:LEU:HD13	1:A:399:SER:HB3	1.59	0.84
1:C:394:LEU:HD13	1:C:399:SER:HB3	1.60	0.84
1:B:676:SER:HB2	1:B:706:VAL:HG13	1.59	0.84
1:C:676:SER:HB2	1:C:706:VAL:HG13	1.60	0.84
1:A:694:GLU:O	1:A:695:ARG:NH1	2.13	0.82
1:C:296:GLU:HG3	1:C:301:LYS:HB3	1.62	0.80
1:A:545:GLY:C	1:A:547:PRO:HD3	2.02	0.79
1:A:296:GLU:HG3	1:A:301:LYS:HB3	1.65	0.78
1:B:704:LYS:HD3	1:B:704:LYS:H	1.48	0.77
1:A:564:VAL:HG23	1:A:586:ARG:NH1	1.99	0.77
1:A:704:LYS:HD3	1:A:704:LYS:H	1.50	0.76
1:C:704:LYS:HD3	1:C:704:LYS:H	1.49	0.76
1:A:582:VAL:HG12	1:A:585:LEU:HD11	1.68	0.75
1:A:468:GLN:HB2	1:A:472:THR:O	1.86	0.75
1:B:582:VAL:HG12	1:B:585:LEU:HD11	1.67	0.75
1:B:206:THR:HG22	1:B:211:GLU:HB3	1.68	0.74
1:C:582:VAL:HG12	1:C:585:LEU:HD11	1.69	0.74
1:A:206:THR:HG22	1:A:211:GLU:HB3	1.70	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:LYS:HA	1:A:472:THR:HG22	1.71	0.73
1:C:733:GLU:CG	1:C:819:SER:HB3	2.19	0.73
1:C:175:ASP:OD1	1:C:177:LYS:HB2	1.89	0.73
1:B:694:GLU:O	1:B:695:ARG:NH2	2.23	0.72
1:C:206:THR:HG22	1:C:211:GLU:HB3	1.71	0.72
1:C:733:GLU:HG3	1:C:819:SER:HB3	1.71	0.71
1:A:573:ASN:HD22	1:A:574:HIS:H	1.38	0.71
1:A:467:ILE:H	1:A:467:ILE:HD13	1.56	0.71
1:B:792:VAL:HB	1:B:796:ILE:HG13	1.73	0.71
1:B:556:ILE:HG23	1:B:596:ARG:HB2	1.73	0.70
1:C:694:GLU:O	1:C:695:ARG:NH2	2.25	0.70
1:A:672:TYR:HB3	1:A:710:ILE:CD1	2.22	0.70
1:C:672:TYR:HB3	1:C:710:ILE:CD1	2.21	0.70
1:A:779:CYS:HB2	1:A:788:ILE:HB	1.73	0.70
1:C:153:GLU:HG3	1:C:187:LYS:HG3	1.74	0.70
1:B:760:TRP:HE1	1:B:797:ARG:HH11	1.39	0.69
1:A:243:GLU:HB3	1:A:279:ARG:HG2	1.74	0.69
1:A:782:ASN:HB3	1:A:808:ILE:HG23	1.73	0.69
1:A:792:VAL:HB	1:A:796:ILE:HG13	1.73	0.69
1:A:556:ILE:HG23	1:A:596:ARG:HB2	1.74	0.69
1:A:672:TYR:HB3	1:A:710:ILE:HD13	1.74	0.69
1:B:782:ASN:HB3	1:B:808:ILE:HG23	1.74	0.69
1:C:760:TRP:HE1	1:C:797:ARG:HH11	1.39	0.69
1:B:672:TYR:HB3	1:B:710:ILE:CD1	2.21	0.69
1:C:782:ASN:HB3	1:C:808:ILE:HG23	1.74	0.68
1:A:760:TRP:HE1	1:A:797:ARG:HH21	1.39	0.68
1:B:672:TYR:HB3	1:B:710:ILE:HD13	1.73	0.68
1:B:779:CYS:HB2	1:B:788:ILE:HB	1.74	0.68
1:C:438:LYS:HA	1:C:472:THR:CG2	2.20	0.68
1:A:153:GLU:HG3	1:A:187:LYS:HG3	1.76	0.68
1:B:669:ARG:HH21	1:B:720:GLN:NE2	1.92	0.68
1:A:672:TYR:CE1	1:A:685:GLN:HB2	2.28	0.68
1:B:672:TYR:CE1	1:B:685:GLN:HB2	2.29	0.68
1:C:672:TYR:HB3	1:C:710:ILE:HD13	1.74	0.68
1:C:792:VAL:HB	1:C:796:ILE:HG13	1.75	0.68
1:B:132:ARG:HH21	1:B:158:ARG:HD2	1.59	0.67
1:C:733:GLU:OE1	1:C:771:ILE:HD11	1.95	0.67
1:C:779:CYS:HB2	1:C:788:ILE:HB	1.76	0.67
1:B:184:ARG:HB3	1:B:184:ARG:HH11	1.60	0.67
1:B:153:GLU:HG3	1:B:187:LYS:HG3	1.77	0.66
1:C:707:THR:HG22	1:C:728:THR:HG22	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:THR:HG22	1:A:728:THR:HG22	1.76	0.66
1:C:556:ILE:HG23	1:C:596:ARG:HB2	1.76	0.66
1:C:672:TYR:CE1	1:C:685:GLN:HB2	2.31	0.66
1:A:704:LYS:HE3	1:A:769:ASN:HA	1.79	0.65
1:C:314:PRO:HB2	1:C:400:ILE:HG12	1.78	0.65
1:A:437:LEU:O	1:A:472:THR:HA	1.96	0.65
1:A:363:GLN:NE2	1:A:363:GLN:H	1.95	0.65
1:B:363:GLN:NE2	1:B:363:GLN:H	1.95	0.64
1:B:669:ARG:HH21	1:B:720:GLN:HE22	1.43	0.64
1:B:314:PRO:HB2	1:B:400:ILE:HG12	1.81	0.63
1:B:707:THR:HG22	1:B:728:THR:HG22	1.79	0.63
1:C:363:GLN:H	1:C:363:GLN:NE2	1.96	0.63
1:C:232:ILE:HD12	1:C:232:ILE:N	2.12	0.63
1:A:97:HIS:CE1	1:A:128:VAL:HG21	2.34	0.63
1:A:546:THR:N	1:A:547:PRO:HD3	2.14	0.63
1:B:248:VAL:HG11	1:B:295:ALA:HB2	1.81	0.63
1:A:33:ILE:H	1:A:33:ILE:HD12	1.65	0.62
1:C:666:GLN:NE2	1:C:716:PHE:O	2.32	0.62
1:B:458:PHE:CG	1:B:459:PRO:HA	2.36	0.61
1:B:467:ILE:H	1:B:467:ILE:HD12	1.66	0.61
1:C:97:HIS:CE1	1:C:128:VAL:HG21	2.36	0.61
1:C:33:ILE:HD12	1:C:33:ILE:H	1.65	0.61
1:A:248:VAL:HG11	1:A:295:ALA:HB2	1.82	0.61
1:C:415:ARG:NH1	1:C:445:PRO:HD3	2.15	0.61
1:C:70:ARG:HB3	1:C:70:ARG:CZ	2.29	0.61
1:B:232:ILE:HD12	1:B:232:ILE:N	2.14	0.61
1:B:666:GLN:HB2	1:B:716:PHE:O	2.01	0.61
1:B:33:ILE:HD12	1:B:33:ILE:H	1.65	0.61
1:B:394:LEU:HD13	1:B:399:SER:CB	2.30	0.61
1:B:194:ARG:HB3	1:B:194:ARG:NH2	2.16	0.61
1:A:666:GLN:NE2	1:A:716:PHE:O	2.33	0.60
1:A:314:PRO:HB2	1:A:400:ILE:HG12	1.83	0.60
1:B:194:ARG:HB3	1:B:194:ARG:HH21	1.66	0.60
1:A:458:PHE:CG	1:A:459:PRO:HA	2.36	0.60
1:C:593:PHE:H	1:C:610:SER:HB3	1.66	0.60
1:C:733:GLU:CB	1:C:819:SER:HB3	2.32	0.60
1:B:97:HIS:CE1	1:B:128:VAL:HG21	2.37	0.60
1:A:267:ARG:HA	1:A:270:TYR:CE2	2.37	0.60
1:C:415:ARG:HD3	1:C:494:SER:HB3	1.84	0.60
1:C:669:ARG:HH21	1:C:720:GLN:NE2	2.00	0.59
1:A:468:GLN:HB3	1:A:470:GLN:OE1	2.01	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:666:GLN:NE2	1:B:716:PHE:O	2.35	0.59
1:A:657:THR:HA	1:A:695:ARG:HD2	1.85	0.59
1:C:248:VAL:HG11	1:C:295:ALA:HB2	1.85	0.59
1:A:417:PRO:HG2	1:A:568:TRP:CD1	2.38	0.59
1:A:480:ILE:O	1:A:483:THR:HG22	2.03	0.59
1:B:468:GLN:HB2	1:B:472:THR:O	2.03	0.58
1:A:294:ILE:HG23	1:A:303:GLU:HB3	1.85	0.58
1:B:243:GLU:HA	1:B:278:LEU:O	2.04	0.58
1:B:417:PRO:HG2	1:B:568:TRP:CD1	2.37	0.58
1:B:657:THR:HA	1:B:695:ARG:HD2	1.86	0.58
1:C:294:ILE:HG23	1:C:303:GLU:HB3	1.85	0.58
1:C:458:PHE:CG	1:C:459:PRO:HA	2.38	0.58
1:C:480:ILE:O	1:C:483:THR:HG22	2.02	0.58
2:H:1:NAG:HN2	2:H:1:NAG:H5	1.68	0.58
1:C:526:SER:HB2	1:C:543:GLN:H	1.67	0.58
1:A:243:GLU:HA	1:A:278:LEU:O	2.03	0.58
1:C:243:GLU:HA	1:C:278:LEU:O	2.04	0.58
1:A:394:LEU:HD13	1:A:399:SER:CB	2.33	0.57
1:C:329:ARG:HG2	1:C:330:THR:H	1.68	0.57
1:A:329:ARG:HG2	1:A:330:THR:H	1.69	0.57
1:B:294:ILE:HG23	1:B:303:GLU:HB3	1.87	0.57
1:C:657:THR:HA	1:C:695:ARG:HD2	1.87	0.57
1:A:394:LEU:CD1	1:A:399:SER:HB3	2.33	0.57
1:A:647:LEU:HB3	1:A:651:THR:HB	1.87	0.57
1:B:480:ILE:O	1:B:483:THR:HG22	2.04	0.57
1:B:526:SER:HB2	1:B:543:GLN:H	1.70	0.57
1:A:556:ILE:CG2	1:A:596:ARG:HB2	2.34	0.56
1:B:647:LEU:HB3	1:B:651:THR:HB	1.86	0.56
1:A:666:GLN:HB2	1:A:716:PHE:O	2.05	0.56
1:B:556:ILE:CG2	1:B:596:ARG:HB2	2.35	0.56
1:C:647:LEU:HB3	1:C:651:THR:HB	1.87	0.56
1:A:525:PRO:HD2	1:A:607:SER:HB2	1.88	0.56
1:B:437:LEU:HD12	1:B:473:LEU:HD23	1.87	0.56
1:C:180:ARG:NH1	1:C:194:ARG:HE	2.04	0.56
1:B:394:LEU:CD1	1:B:399:SER:HB3	2.31	0.56
1:A:546:THR:N	1:A:547:PRO:CD	2.69	0.56
1:C:576:LYS:HE3	3:I:5:MAN:H62	1.88	0.55
1:A:487:THR:HG23	1:A:500:SER:HB3	1.88	0.55
1:C:394:LEU:HD13	1:C:399:SER:CB	2.34	0.55
1:A:439:CYS:O	1:A:471:GLY:HA3	2.06	0.55
1:C:417:PRO:HG2	1:C:568:TRP:CD1	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:GLU:HB3	1:A:279:ARG:CG	2.36	0.55
1:C:512:ILE:O	1:C:512:ILE:HG22	2.06	0.55
1:A:269:ARG:NH1	1:A:287:ASP:OD1	2.39	0.55
1:A:48:THR:CG2	1:A:95:ILE:HD11	2.37	0.55
1:B:401:LEU:HD23	1:B:624:GLY:HA2	1.88	0.54
1:C:666:GLN:HB2	1:C:716:PHE:O	2.07	0.54
1:C:401:LEU:HD23	1:C:624:GLY:HA2	1.88	0.54
1:A:674:GLN:HE21	1:A:706:VAL:HG11	1.72	0.54
1:C:394:LEU:CD1	1:C:399:SER:HB3	2.35	0.54
1:C:522:PRO:HA	1:C:546:THR:O	2.07	0.54
1:C:487:THR:HG23	1:C:500:SER:HB3	1.90	0.54
1:C:674:GLN:HE21	1:C:706:VAL:HG11	1.73	0.54
1:B:487:THR:HG23	1:B:500:SER:HB3	1.89	0.54
1:B:649:PRO:HG3	1:B:732:THR:OG1	2.08	0.54
1:A:526:SER:HB2	1:A:543:GLN:H	1.73	0.54
1:B:354:ASN:ND2	1:B:354:ASN:H	2.06	0.53
1:A:412:LEU:HB3	1:A:415:ARG:HG2	1.91	0.53
1:C:48:THR:CG2	1:C:95:ILE:HD11	2.38	0.53
2:D:1:NAG:H3	2:D:2:NAG:HN2	1.73	0.53
1:A:401:LEU:HD23	1:A:624:GLY:HA2	1.90	0.53
1:A:437:LEU:HD12	1:A:473:LEU:HD23	1.90	0.53
1:A:417:PRO:HG2	1:A:568:TRP:NE1	2.24	0.53
1:C:556:ILE:CG2	1:C:596:ARG:HB2	2.38	0.53
1:A:573:ASN:ND2	1:A:574:HIS:H	2.05	0.53
1:B:184:ARG:HB3	1:B:184:ARG:NH1	2.23	0.53
1:C:672:TYR:CD1	1:C:685:GLN:HB2	2.44	0.53
1:B:593:PHE:H	1:B:610:SER:HB3	1.74	0.52
1:C:269:ARG:HG2	1:C:282:LYS:HB3	1.90	0.52
1:A:607:SER:OG	1:A:608:PRO:CD	2.57	0.52
1:C:29:PHE:C	1:C:116:LEU:HD13	2.30	0.52
1:A:672:TYR:CD1	1:A:685:GLN:HB2	2.44	0.52
1:B:48:THR:CG2	1:B:95:ILE:HD11	2.40	0.52
1:B:672:TYR:CD1	1:B:685:GLN:HB2	2.44	0.52
1:C:362:GLN:HE21	1:C:366:SER:HB3	1.75	0.52
1:A:593:PHE:H	1:A:610:SER:HB3	1.74	0.52
1:A:29:PHE:C	1:A:116:LEU:HD13	2.31	0.51
1:A:607:SER:OG	1:A:608:PRO:HD2	2.10	0.51
1:B:242:VAL:HG12	1:B:280:ILE:HB	1.91	0.51
1:B:417:PRO:HG2	1:B:568:TRP:NE1	2.25	0.51
1:A:672:TYR:CE1	1:A:685:GLN:CB	2.94	0.51
1:B:362:GLN:HE21	1:B:366:SER:HB3	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:VAL:O	1:A:310:VAL:HA	2.11	0.51
1:B:674:GLN:HE21	1:B:706:VAL:HG11	1.76	0.51
1:C:48:THR:HG22	1:C:95:ILE:HD11	1.93	0.51
1:C:354:ASN:HD22	1:C:354:ASN:H	1.56	0.51
1:A:242:VAL:HG12	1:A:280:ILE:HB	1.93	0.50
1:A:48:THR:HG22	1:A:95:ILE:HD11	1.92	0.50
1:C:354:ASN:ND2	1:C:354:ASN:H	2.09	0.50
1:A:781:GLY:HA3	1:A:810:TYR:HA	1.93	0.50
1:A:739:PRO:HB3	1:A:824:VAL:HG23	1.93	0.50
1:B:388:TYR:CE1	1:B:405:GLN:HB2	2.46	0.50
1:C:342:GLN:OE1	1:C:342:GLN:HA	2.11	0.50
1:C:325:VAL:HG13	1:C:381:ILE:HD13	1.94	0.50
1:A:358:PRO:HA	1:A:370:VAL:HB	1.93	0.50
1:C:236:VAL:O	1:C:310:VAL:HA	2.11	0.50
1:A:342:GLN:HA	1:A:342:GLN:OE1	2.12	0.50
1:A:672:TYR:CB	1:A:710:ILE:HD13	2.42	0.50
1:B:236:VAL:O	1:B:310:VAL:HA	2.11	0.50
1:B:358:PRO:HA	1:B:370:VAL:HB	1.94	0.50
1:C:415:ARG:HH11	1:C:445:PRO:HD3	1.77	0.50
1:B:363:GLN:HG2	1:B:365:ASN:HD22	1.76	0.49
1:B:672:TYR:CE1	1:B:685:GLN:CB	2.93	0.49
1:A:354:ASN:HD22	1:A:354:ASN:H	1.58	0.49
1:A:640:ARG:HH22	1:A:642:HIS:HD2	1.58	0.49
1:B:29:PHE:C	1:B:116:LEU:HD13	2.32	0.49
1:C:37:PRO:HD2	1:C:121:SER:OG	2.12	0.49
1:C:672:TYR:CE1	1:C:685:GLN:CB	2.95	0.49
1:A:354:ASN:H	1:A:354:ASN:ND2	2.11	0.49
1:B:342:GLN:HA	1:B:342:GLN:OE1	2.11	0.49
1:B:453:LYS:O	1:B:455:GLY:N	2.44	0.49
1:B:816:ALA:O	1:B:823:GLY:HA3	2.13	0.49
1:C:66:LYS:HA	1:C:107:SER:O	2.12	0.49
1:A:30:PRO:HG3	1:A:116:LEU:HB3	1.94	0.49
1:A:388:TYR:CE1	1:A:405:GLN:HB2	2.47	0.49
1:A:467:ILE:O	1:A:467:ILE:HG12	2.12	0.49
1:C:781:GLY:HA3	1:C:810:TYR:HA	1.95	0.49
1:A:267:ARG:HA	1:A:270:TYR:HE2	1.78	0.49
1:A:573:ASN:HD22	1:A:574:HIS:N	2.06	0.49
1:B:207:ASN:ND2	1:B:209:VAL:HG23	2.28	0.49
1:B:207:ASN:HD22	1:B:209:VAL:HG23	1.77	0.49
1:B:764:PRO:HB2	1:B:767:HIS:HB2	1.95	0.49
1:C:363:GLN:HG2	1:C:365:ASN:HD22	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:412:LEU:HD13	1:C:415:ARG:HG2	1.95	0.49
1:A:325:VAL:HG13	1:A:381:ILE:HD13	1.95	0.49
1:B:226:THR:HG23	1:B:249:GLN:HB3	1.95	0.49
1:C:453:LYS:O	1:C:455:GLY:N	2.45	0.49
1:C:707:THR:CG2	1:C:728:THR:HG22	2.43	0.49
1:C:764:PRO:HB2	1:C:767:HIS:HB2	1.95	0.49
1:A:453:LYS:O	1:A:455:GLY:N	2.45	0.48
1:B:367:ARG:NH2	1:B:385:ASP:OD2	2.46	0.48
1:C:417:PRO:HG2	1:C:568:TRP:NE1	2.28	0.48
3:G:2:NAG:H62	3:G:3:BMA:C1	2.44	0.48
1:C:526:SER:CB	1:C:543:GLN:H	2.27	0.48
1:C:755:SER:HA	1:C:804:LEU:HD22	1.94	0.48
1:A:178:GLU:HG3	1:A:181:ILE:HD12	1.94	0.48
1:A:49:THR:HG23	1:A:91:PHE:HB2	1.96	0.48
1:B:652:VAL:HG23	1:B:702:LEU:HD11	1.95	0.48
1:C:222:PHE:HB3	1:C:251:ASP:O	2.14	0.48
1:C:388:TYR:CE1	1:C:405:GLN:HB2	2.49	0.48
1:C:739:PRO:HB3	1:C:824:VAL:HG23	1.95	0.48
1:C:816:ALA:O	1:C:823:GLY:HA3	2.14	0.48
1:A:37:PRO:HD2	1:A:121:SER:OG	2.13	0.48
1:B:511:THR:C	1:B:513:SER:H	2.17	0.48
1:C:437:LEU:HD12	1:C:473:LEU:HD23	1.95	0.48
1:A:467:ILE:CD1	1:A:467:ILE:H	2.26	0.48
1:A:362:GLN:HE21	1:A:366:SER:HB3	1.78	0.48
1:B:325:VAL:HG13	1:B:381:ILE:HD13	1.96	0.48
1:C:358:PRO:HA	1:C:370:VAL:HB	1.96	0.48
1:B:37:PRO:HD2	1:B:121:SER:OG	2.13	0.48
1:A:652:VAL:HG23	1:A:702:LEU:HD11	1.95	0.48
1:A:772:ILE:HD13	1:A:794:ALA:HB1	1.96	0.48
3:E:1:NAG:H3	3:E:1:NAG:O7	2.13	0.48
1:B:66:LYS:HA	1:B:107:SER:O	2.14	0.47
1:B:781:GLY:HA3	1:B:810:TYR:HA	1.96	0.47
1:A:764:PRO:HB2	1:A:767:HIS:HB2	1.95	0.47
1:B:739:PRO:HB3	1:B:824:VAL:HG23	1.96	0.47
1:C:242:VAL:HG12	1:C:280:ILE:HB	1.95	0.47
1:C:49:THR:HG23	1:C:91:PHE:HB2	1.94	0.47
1:A:834:GLY:HA3	1:A:839:VAL:HA	1.96	0.47
1:A:835:ARG:HB3	1:A:835:ARG:CZ	2.44	0.47
1:B:672:TYR:CB	1:B:710:ILE:HD13	2.42	0.47
1:A:226:THR:HG23	1:A:249:GLN:HB3	1.97	0.47
1:B:269:ARG:NH2	1:B:287:ASP:OD1	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:470:GLN:H	1:C:470:GLN:CD	2.18	0.47
1:C:269:ARG:NH2	1:C:287:ASP:OD1	2.48	0.47
1:C:772:ILE:HD13	1:C:794:ALA:HB1	1.96	0.47
1:A:816:ALA:O	1:A:823:GLY:HA3	2.15	0.47
1:C:672:TYR:CB	1:C:710:ILE:HD13	2.42	0.47
1:B:48:THR:HG22	1:B:95:ILE:HD11	1.97	0.47
1:B:707:THR:CG2	1:B:728:THR:HG22	2.45	0.47
1:B:525:PRO:HD2	1:B:607:SER:HB3	1.97	0.46
1:C:30:PRO:HG3	1:C:116:LEU:HB3	1.96	0.46
1:A:672:TYR:HA	1:A:709:GLU:O	2.15	0.46
1:B:386:ALA:HB2	1:B:408:VAL:HG23	1.98	0.46
1:B:672:TYR:HA	1:B:709:GLU:O	2.15	0.46
1:B:49:THR:HG23	1:B:91:PHE:HB2	1.96	0.46
1:A:393:ALA:HB3	1:A:400:ILE:HG13	1.97	0.46
1:A:641:LEU:HD12	1:A:655:THR:O	2.16	0.46
1:A:77:ASP:OD1	1:A:79:ARG:HG2	2.15	0.46
1:B:77:ASP:OD1	1:B:79:ARG:HG2	2.15	0.46
1:C:652:VAL:HG23	1:C:702:LEU:HD11	1.97	0.46
1:C:525:PRO:HD2	1:C:607:SER:HB3	1.96	0.46
1:C:640:ARG:HH22	1:C:642:HIS:HD2	1.63	0.46
1:C:641:LEU:HD12	1:C:655:THR:O	2.16	0.46
1:A:252:PRO:HG2	1:A:297:ASN:HB2	1.98	0.46
1:B:526:SER:CB	1:B:543:GLN:H	2.28	0.46
1:A:386:ALA:HB2	1:A:408:VAL:HG23	1.97	0.46
1:A:526:SER:CB	1:A:543:GLN:H	2.29	0.46
1:A:66:LYS:HA	1:A:107:SER:O	2.16	0.46
1:B:269:ARG:HG2	1:B:282:LYS:HB3	1.98	0.46
1:B:30:PRO:HG3	1:B:116:LEU:HB3	1.98	0.46
1:B:329:ARG:HG2	1:B:330:THR:H	1.81	0.46
1:C:524:PRO:HD3	1:C:605:ASP:HB2	1.97	0.46
1:C:672:TYR:HA	1:C:709:GLU:O	2.16	0.46
1:A:556:ILE:O	1:A:556:ILE:HG23	2.16	0.45
1:A:707:THR:CG2	1:A:728:THR:HG22	2.43	0.45
1:C:745:VAL:HG21	1:C:831:ILE:HG21	1.97	0.45
1:B:415:ARG:HB2	1:B:415:ARG:CZ	2.43	0.45
1:B:755:SER:HA	1:B:804:LEU:HD22	1.97	0.45
1:B:793:ASP:CG	1:B:794:ALA:N	2.70	0.45
1:A:269:ARG:HG2	1:A:282:LYS:HB3	1.97	0.45
1:B:31:PRO:HA	1:B:55:GLU:O	2.17	0.45
1:B:393:ALA:HB3	1:B:400:ILE:HG13	1.99	0.45
1:B:704:LYS:HG3	1:B:734:GLU:HB2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:716:PHE:HB3	1:C:719:PHE:HB2	1.98	0.45
1:A:31:PRO:HA	1:A:55:GLU:O	2.15	0.45
1:A:480:ILE:HG13	1:A:480:ILE:H	1.48	0.45
1:A:793:ASP:CG	1:A:794:ALA:N	2.70	0.45
1:C:386:ALA:HB2	1:C:408:VAL:HG23	1.99	0.45
1:B:381:ILE:HG13	1:B:381:ILE:H	1.34	0.45
1:B:834:GLY:HA3	1:B:839:VAL:HA	1.99	0.45
1:C:561:SER:HB3	1:C:564:VAL:HG12	1.99	0.45
1:C:669:ARG:HA	1:C:688:ASP:HB3	1.99	0.45
1:B:743:VAL:HB	1:B:829:GLN:HG3	1.98	0.44
1:B:704:LYS:HE3	1:B:769:ASN:HA	1.99	0.44
1:A:421:LEU:O	1:A:596:ARG:NH2	2.50	0.44
1:A:716:PHE:HB3	1:A:719:PHE:HB2	1.99	0.44
1:B:252:PRO:HG2	1:B:297:ASN:HB2	1.99	0.44
1:B:772:ILE:HD13	1:B:794:ALA:HB1	1.99	0.44
1:C:834:GLY:HA3	1:C:839:VAL:HA	1.99	0.44
1:A:514:LYS:O	1:A:515:ASN:O	2.36	0.44
1:B:745:VAL:HG21	1:B:831:ILE:HG21	1.99	0.44
1:A:669:ARG:HA	1:A:688:ASP:HB3	2.00	0.44
1:C:733:GLU:HG3	1:C:819:SER:CB	2.44	0.44
1:A:162:GLU:HA	1:A:163:PRO:HD3	1.86	0.44
1:B:243:GLU:HB3	1:B:279:ARG:HG2	2.00	0.44
1:C:371:SER:HB3	1:C:375:ASP:H	1.83	0.44
1:B:561:SER:HB3	1:B:564:VAL:HG12	2.00	0.44
1:C:793:ASP:CG	1:C:794:ALA:N	2.70	0.44
1:A:470:GLN:CD	1:A:470:GLN:H	2.21	0.44
1:A:640:ARG:NH2	1:A:642:HIS:HD2	2.15	0.44
1:B:415:ARG:NH1	1:B:415:ARG:H	2.16	0.44
1:B:641:LEU:HD12	1:B:655:THR:O	2.16	0.44
1:A:421:LEU:HB3	1:A:605:ASP:OD1	2.18	0.44
1:B:633:GLU:O	1:B:637:VAL:HG23	2.18	0.44
1:C:31:PRO:HA	1:C:55:GLU:O	2.18	0.44
1:C:50:LEU:HD12	1:C:90:LEU:HD23	2.00	0.44
1:A:50:LEU:HD12	1:A:90:LEU:HD23	2.00	0.43
1:C:393:ALA:HB3	1:C:400:ILE:HG13	1.99	0.43
1:C:678:LEU:HG	1:C:679:GLN:HE21	1.83	0.43
1:A:561:SER:HB3	1:A:564:VAL:HG12	2.00	0.43
1:B:787:HIS:HD2	1:B:789:ASN:HD21	1.66	0.43
1:C:639:VAL:O	1:C:724:SER:HB2	2.18	0.43
1:A:381:ILE:HG13	1:A:381:ILE:H	1.35	0.43
1:A:633:GLU:O	1:A:637:VAL:HG23	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:ILE:H	1:C:381:ILE:HG13	1.36	0.43
1:C:669:ARG:HH21	1:C:720:GLN:HE22	1.66	0.43
1:A:446:LEU:HG	1:A:447:PRO:HD2	2.00	0.43
1:A:523:GLY:H	1:A:547:PRO:HD2	1.83	0.43
1:A:521:LEU:H	1:A:521:LEU:HG	1.58	0.43
1:A:717:ASN:HD22	1:A:717:ASN:HA	1.70	0.43
1:B:639:VAL:O	1:B:724:SER:HB2	2.18	0.43
1:B:453:LYS:C	1:B:455:GLY:N	2.72	0.43
1:B:470:GLN:CD	1:B:470:GLN:H	2.21	0.43
1:C:453:LYS:C	1:C:455:GLY:N	2.70	0.43
1:C:512:ILE:HA	1:C:515:ASN:HD22	1.82	0.43
1:A:222:PHE:HB3	1:A:251:ASP:O	2.18	0.43
1:A:704:LYS:CD	1:A:704:LYS:H	2.26	0.43
1:B:342:GLN:HA	1:B:343:PRO:HD3	1.90	0.43
1:C:347:TRP:CE2	1:C:391:CYS:HB3	2.54	0.43
1:C:733:GLU:HB3	1:C:819:SER:HB3	2.01	0.43
1:B:237:LEU:N	1:B:237:LEU:HD12	2.34	0.43
1:C:521:LEU:H	1:C:521:LEU:HG	1.61	0.43
1:B:137:GLN:HB3	1:B:155:GLN:HB2	2.01	0.43
1:B:556:ILE:O	1:B:556:ILE:HG23	2.19	0.43
1:B:565:SER:OG	1:B:566:ASN:N	2.52	0.43
1:B:734:GLU:O	1:B:818:THR:HG21	2.19	0.43
1:C:771:ILE:HG13	1:C:771:ILE:H	1.57	0.43
1:A:371:SER:HB3	1:A:375:ASP:H	1.84	0.42
1:C:415:ARG:HG3	1:C:415:ARG:H	1.47	0.42
1:C:734:GLU:O	1:C:818:THR:CB	2.67	0.42
1:A:719:PHE:N	1:A:719:PHE:CD1	2.88	0.42
1:A:224:ARG:HG2	1:A:299:VAL:HG12	2.01	0.42
1:C:736:PRO:HA	1:C:769:ASN:HB2	2.01	0.42
1:A:736:PRO:HA	1:A:769:ASN:HB2	2.00	0.42
1:B:177:LYS:O	1:B:177:LYS:HE2	2.19	0.42
1:C:464:ARG:NH2	1:C:482:ASP:OD2	2.52	0.42
1:C:565:SER:OG	1:C:566:ASN:N	2.52	0.42
1:C:691:VAL:O	1:C:694:GLU:HB2	2.19	0.42
1:C:787:HIS:HD2	1:C:789:ASN:HD21	1.67	0.42
1:A:272:ILE:H	1:A:272:ILE:HG13	1.61	0.42
1:A:565:SER:OG	1:A:566:ASN:N	2.52	0.42
1:B:832:ILE:O	1:B:832:ILE:HG13	2.19	0.42
1:C:513:SER:O	1:C:514:LYS:HB2	2.19	0.42
1:C:633:GLU:O	1:C:637:VAL:HG23	2.20	0.42
1:C:167:TRP:CZ3	1:C:203:CYS:HB2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:787:HIS:HD2	1:A:789:ASN:HD21	1.66	0.42
1:B:272:ILE:HG13	1:B:272:ILE:H	1.62	0.42
1:B:444:ASP:HA	1:B:445:PRO:C	2.39	0.42
1:A:194:ARG:NH1	1:A:194:ARG:HB3	2.35	0.42
1:A:411:VAL:HG13	1:A:412:LEU:H	1.84	0.42
1:B:162:GLU:HA	1:B:163:PRO:HD3	1.85	0.42
1:B:521:LEU:HG	1:B:521:LEU:H	1.59	0.42
1:B:716:PHE:HB3	1:B:719:PHE:HB2	2.01	0.42
1:C:252:PRO:HG2	1:C:297:ASN:HB2	2.00	0.42
1:C:465:ALA:HB2	1:C:475:ILE:HG12	2.01	0.42
1:A:167:TRP:CZ3	1:A:203:CYS:HB2	2.55	0.42
1:A:363:GLN:HG2	1:A:365:ASN:HB3	2.02	0.42
1:A:513:SER:O	1:A:514:LYS:HB2	2.20	0.42
1:B:382:GLN:HB3	1:B:384:SER:H	1.85	0.42
1:C:743:VAL:HB	1:C:829:GLN:HG3	2.02	0.42
1:C:412:LEU:HD22	1:C:415:ARG:HB3	2.02	0.41
1:C:556:ILE:O	1:C:556:ILE:HG23	2.20	0.41
1:A:347:TRP:CE2	1:A:391:CYS:HB3	2.55	0.41
1:A:85:LEU:HB3	1:A:86:PRO:HD2	2.02	0.41
1:B:736:PRO:HA	1:B:769:ASN:HB2	2.02	0.41
1:A:639:VAL:O	1:A:724:SER:HB2	2.20	0.41
1:B:167:TRP:CZ3	1:B:203:CYS:HB2	2.55	0.41
1:B:29:PHE:HA	1:B:30:PRO:HD3	1.95	0.41
1:B:717:ASN:HA	1:B:717:ASN:HD22	1.70	0.41
1:C:215:ASP:HA	1:C:216:PRO:HD3	1.92	0.41
1:C:62:ILE:H	1:C:62:ILE:HD12	1.85	0.41
1:C:832:ILE:O	1:C:832:ILE:HG13	2.20	0.41
1:A:206:THR:HB	1:A:207:ASN:H	1.75	0.41
1:A:464:ARG:NH1	1:A:464:ARG:HB2	2.35	0.41
1:B:62:ILE:HD12	1:B:62:ILE:H	1.85	0.41
1:C:232:ILE:CD1	1:C:232:ILE:N	2.78	0.41
1:A:464:ARG:NH2	1:A:482:ASP:OD2	2.53	0.41
1:A:745:VAL:HG21	1:A:831:ILE:HG21	2.03	0.41
1:C:121:SER:OG	1:C:122:ARG:N	2.54	0.41
1:C:456:PHE:N	1:C:456:PHE:CD1	2.89	0.41
1:A:465:ALA:CB	1:A:475:ILE:HG12	2.51	0.41
1:A:771:ILE:H	1:A:771:ILE:HG13	1.57	0.41
1:B:60:PRO:HB2	1:B:112:ALA:HB1	2.03	0.41
1:C:347:TRP:CZ2	1:C:391:CYS:HB3	2.56	0.41
1:A:453:LYS:C	1:A:455:GLY:N	2.73	0.41
1:A:691:VAL:O	1:A:694:GLU:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:SER:OG	1:B:122:ARG:N	2.54	0.41
1:B:296:GLU:O	1:B:296:GLU:HG3	2.21	0.41
1:B:669:ARG:HA	1:B:688:ASP:HB3	2.02	0.41
1:C:518:LEU:HB3	1:C:519:SER:H	1.62	0.41
1:A:137:GLN:HB3	1:A:155:GLN:HB2	2.03	0.41
1:B:354:ASN:HD22	1:B:354:ASN:H	1.69	0.41
1:C:669:ARG:HA	1:C:688:ASP:CB	2.51	0.41
1:A:811:ARG:HD3	1:A:828:PRO:HB3	2.03	0.41
1:A:832:ILE:HG13	1:A:832:ILE:O	2.20	0.41
1:A:143:VAL:HG13	1:A:143:VAL:O	2.20	0.40
1:B:222:PHE:HB3	1:B:251:ASP:O	2.20	0.40
1:B:805:PHE:HB3	1:B:808:ILE:HD12	2.02	0.40
1:A:215:ASP:HA	1:A:216:PRO:HD3	1.93	0.40
1:A:691:VAL:HA	1:A:692:PRO:HD3	1.93	0.40
1:B:691:VAL:O	1:B:694:GLU:HB2	2.20	0.40
1:C:411:VAL:HG13	1:C:412:LEU:H	1.87	0.40
1:C:453:LYS:C	1:C:455:GLY:H	2.25	0.40
1:A:347:TRP:CZ2	1:A:391:CYS:HB3	2.55	0.40
1:B:299:VAL:O	1:B:299:VAL:HG12	2.22	0.40
1:B:240:GLU:O	1:B:283:THR:OG1	2.36	0.40
1:B:50:LEU:HD12	1:B:90:LEU:HD23	2.02	0.40
1:C:331:VAL:O	1:C:377:THR:HA	2.22	0.40
1:A:121:SER:OG	1:A:122:ARG:N	2.55	0.40
1:A:342:GLN:HA	1:A:343:PRO:HD3	1.86	0.40
1:A:62:ILE:HD12	1:A:62:ILE:H	1.85	0.40
1:C:444:ASP:HA	1:C:445:PRO:C	2.41	0.40
2:H:1:NAG:N2	2:H:1:NAG:H5	2.32	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	811/859 (94%)	721 (89%)	75 (9%)	15 (2%)	8 43
1	B	811/859 (94%)	724 (89%)	77 (10%)	10 (1%)	13 51
1	C	811/859 (94%)	722 (89%)	78 (10%)	11 (1%)	11 48
All	All	2433/2577 (94%)	2167 (89%)	230 (10%)	36 (2%)	10 47

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	515	ASN
1	A	546	THR
1	B	512	ILE
1	A	358	PRO
1	A	454	GLU
1	A	509	GLY
1	A	514	LYS
1	B	358	PRO
1	B	454	GLU
1	C	358	PRO
1	B	411	VAL
1	C	411	VAL
1	C	454	GLU
1	C	515	ASN
1	A	67	ASP
1	B	67	ASP
1	B	742	SER
1	C	67	ASP
1	A	547	PRO
1	A	742	SER
1	B	548	GLY
1	C	512	ILE
1	C	742	SER
1	A	411	VAL
1	B	547	PRO
1	C	547	PRO
1	C	548	GLY
1	A	649	PRO
1	A	822	VAL
1	A	512	ILE
1	A	544	PRO
1	A	792	VAL
1	B	544	PRO
1	B	792	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	544	PRO
1	C	792	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	715/747 (96%)	627 (88%)	88 (12%)	4 26
1	B	715/747 (96%)	613 (86%)	102 (14%)	3 21
1	C	715/747 (96%)	627 (88%)	88 (12%)	4 26
All	All	2145/2241 (96%)	1867 (87%)	278 (13%)	4 24

All (278) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	33	ILE
1	A	34	VAL
1	A	40	VAL
1	A	59	THR
1	A	62	ILE
1	A	76	ASP
1	A	84	LEU
1	A	89	SER
1	A	100	ARG
1	A	144	VAL
1	A	158	ARG
1	A	175	ASP
1	A	184	ARG
1	A	207	ASN
1	A	208	MSE
1	A	213	ASP
1	A	226	THR
1	A	251	ASP
1	A	262	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	267	ARG
1	A	269	ARG
1	A	272	ILE
1	A	279	ARG
1	A	292	MSE
1	A	294	ILE
1	A	302	MSE
1	A	311	ARG
1	A	317	VAL
1	A	322	ASP
1	A	356	LEU
1	A	360	GLN
1	A	362	GLN
1	A	363	GLN
1	A	365	ASN
1	A	381	ILE
1	A	382	GLN
1	A	383	ARG
1	A	396	VAL
1	A	415	ARG
1	A	434	THR
1	A	464	ARG
1	A	466	THR
1	A	467	ILE
1	A	470	GLN
1	A	480	ILE
1	A	514	LYS
1	A	520	ASP
1	A	521	LEU
1	A	530	VAL
1	A	537	SER
1	A	538	VAL
1	A	562	GLN
1	A	564	VAL
1	A	573	ASN
1	A	577	THR
1	A	589	THR
1	A	605	ASP
1	A	609	MSE
1	A	610	SER
1	A	615	THR
1	A	618	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	619	SER
1	A	630	VAL
1	A	640	ARG
1	A	646	VAL
1	A	650	THR
1	A	657	THR
1	A	670	VAL
1	A	694	GLU
1	A	695	ARG
1	A	698	VAL
1	A	702	LEU
1	A	704	LYS
1	A	717	ASN
1	A	720	GLN
1	A	722	MSE
1	A	731	THR
1	A	742	SER
1	A	759	SER
1	A	771	ILE
1	A	772	ILE
1	A	780	LEU
1	A	792	VAL
1	A	793	ASP
1	A	797	ARG
1	A	824	VAL
1	A	832	ILE
1	B	23	ARG
1	B	24	LEU
1	B	33	ILE
1	B	34	VAL
1	B	40	VAL
1	B	59	THR
1	B	62	ILE
1	B	69	GLU
1	B	75	LYS
1	B	76	ASP
1	B	89	SER
1	B	100	ARG
1	B	144	VAL
1	B	175	ASP
1	B	177	LYS
1	B	180	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	184	ARG
1	B	194	ARG
1	B	208	MSE
1	B	213	ASP
1	B	226	THR
1	B	232	ILE
1	B	245	ARG
1	B	251	ASP
1	B	262	ASP
1	B	267	ARG
1	B	269	ARG
1	B	272	ILE
1	B	283	THR
1	B	292	MSE
1	B	294	ILE
1	B	296	GLU
1	B	302	MSE
1	B	311	ARG
1	B	317	VAL
1	B	322	ASP
1	B	354	ASN
1	B	356	LEU
1	B	360	GLN
1	B	362	GLN
1	B	363	GLN
1	B	367	ARG
1	B	381	ILE
1	B	382	GLN
1	B	396	VAL
1	B	410	ASP
1	B	415	ARG
1	B	428	THR
1	B	434	THR
1	B	438	LYS
1	B	464	ARG
1	B	466	THR
1	B	467	ILE
1	B	470	GLN
1	B	480	ILE
1	B	496	GLU
1	B	513	SER
1	B	518	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	520	ASP
1	B	521	LEU
1	B	530	VAL
1	B	537	SER
1	B	538	VAL
1	B	543	GLN
1	B	562	GLN
1	B	564	VAL
1	B	577	THR
1	B	605	ASP
1	B	609	MSE
1	B	610	SER
1	B	615	THR
1	B	618	ILE
1	B	619	SER
1	B	630	VAL
1	B	646	VAL
1	B	650	THR
1	B	657	THR
1	B	659	ASP
1	B	670	VAL
1	B	679	GLN
1	B	687	LEU
1	B	690	LYS
1	B	694	GLU
1	B	695	ARG
1	B	698	VAL
1	B	702	LEU
1	B	704	LYS
1	B	717	ASN
1	B	718	GLU
1	B	720	GLN
1	B	722	MSE
1	B	731	THR
1	B	742	SER
1	B	746	LEU
1	B	759	SER
1	B	772	ILE
1	B	780	LEU
1	B	792	VAL
1	B	793	ASP
1	B	824	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	829	GLN
1	B	832	ILE
1	C	23	ARG
1	C	33	ILE
1	C	34	VAL
1	C	40	VAL
1	C	62	ILE
1	C	69	GLU
1	C	76	ASP
1	C	89	SER
1	C	100	ARG
1	C	144	VAL
1	C	158	ARG
1	C	207	ASN
1	C	208	MSE
1	C	213	ASP
1	C	223	GLU
1	C	224	ARG
1	C	226	THR
1	C	232	ILE
1	C	262	ASP
1	C	267	ARG
1	C	269	ARG
1	C	272	ILE
1	C	292	MSE
1	C	294	ILE
1	C	302	MSE
1	C	317	VAL
1	C	322	ASP
1	C	356	LEU
1	C	360	GLN
1	C	362	GLN
1	C	363	GLN
1	C	381	ILE
1	C	382	GLN
1	C	383	ARG
1	C	396	VAL
1	C	400	ILE
1	C	414	ASP
1	C	415	ARG
1	C	428	THR
1	C	434	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	438	LYS
1	C	464	ARG
1	C	466	THR
1	C	468	GLN
1	C	470	GLN
1	C	474	GLN
1	C	480	ILE
1	C	518	LEU
1	C	520	ASP
1	C	521	LEU
1	C	530	VAL
1	C	537	SER
1	C	538	VAL
1	C	562	GLN
1	C	564	VAL
1	C	577	THR
1	C	609	MSE
1	C	610	SER
1	C	612	PRO
1	C	615	THR
1	C	618	ILE
1	C	619	SER
1	C	630	VAL
1	C	640	ARG
1	C	646	VAL
1	C	650	THR
1	C	657	THR
1	C	670	VAL
1	C	683	SER
1	C	694	GLU
1	C	695	ARG
1	C	698	VAL
1	C	702	LEU
1	C	704	LYS
1	C	717	ASN
1	C	720	GLN
1	C	722	MSE
1	C	731	THR
1	C	742	SER
1	C	759	SER
1	C	771	ILE
1	C	772	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	780	LEU
1	C	792	VAL
1	C	793	ASP
1	C	824	VAL
1	C	829	GLN
1	C	832	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	253	GLN
1	A	354	ASN
1	A	362	GLN
1	A	363	GLN
1	A	365	ASN
1	A	529	GLN
1	A	573	ASN
1	A	642	HIS
1	A	643	ASN
1	A	663	GLN
1	A	666	GLN
1	A	674	GLN
1	A	717	ASN
1	A	769	ASN
1	A	773	GLN
1	A	787	HIS
1	A	809	GLN
1	B	207	ASN
1	B	253	GLN
1	B	354	ASN
1	B	362	GLN
1	B	363	GLN
1	B	365	ASN
1	B	599	ASN
1	B	643	ASN
1	B	663	GLN
1	B	674	GLN
1	B	717	ASN
1	B	720	GLN
1	B	769	ASN
1	B	773	GLN
1	B	787	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	809	GLN
1	C	253	GLN
1	C	354	ASN
1	C	362	GLN
1	C	363	GLN
1	C	365	ASN
1	C	529	GLN
1	C	642	HIS
1	C	643	ASN
1	C	663	GLN
1	C	666	GLN
1	C	674	GLN
1	C	679	GLN
1	C	717	ASN
1	C	720	GLN
1	C	769	ASN
1	C	773	GLN
1	C	787	HIS
1	C	809	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

21 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	$\#\|Z\|>2$
2	NAG	D	1	1,2	14,14,15	0.54	0	17,19,21	2.02	5 (29%)
2	NAG	D	2	2	14,14,15	0.66	0	17,19,21	1.37	2 (11%)
3	NAG	E	1	1,3	14,14,15	0.63	0	17,19,21	1.61	2 (11%)
3	NAG	E	2	3	14,14,15	1.00	1 (7%)	17,19,21	2.34	8 (47%)
3	BMA	E	3	3	11,11,12	1.02	1 (9%)	15,15,17	1.91	4 (26%)
3	MAN	E	4	3	11,11,12	0.38	0	15,15,17	1.36	3 (20%)
3	MAN	E	5	3	11,11,12	0.78	0	15,15,17	2.38	4 (26%)
2	NAG	F	1	1,2	14,14,15	0.63	0	17,19,21	2.46	5 (29%)
2	NAG	F	2	2	14,14,15	0.62	0	17,19,21	1.47	3 (17%)
3	NAG	G	1	1,3	14,14,15	0.52	0	17,19,21	2.52	5 (29%)
3	NAG	G	2	3	14,14,15	0.55	0	17,19,21	1.24	3 (17%)
3	BMA	G	3	3	11,11,12	1.29	1 (9%)	15,15,17	2.98	6 (40%)
3	MAN	G	4	3	11,11,12	0.72	0	15,15,17	1.91	5 (33%)
3	MAN	G	5	3	11,11,12	0.42	0	15,15,17	1.12	2 (13%)
2	NAG	H	1	1,2	14,14,15	0.74	0	17,19,21	1.55	3 (17%)
2	NAG	H	2	2	14,14,15	0.91	1 (7%)	17,19,21	1.52	3 (17%)
3	NAG	I	1	1,3	14,14,15	0.62	0	17,19,21	2.14	4 (23%)
3	NAG	I	2	3	14,14,15	0.84	0	17,19,21	2.89	9 (52%)
3	BMA	I	3	3	11,11,12	0.70	0	15,15,17	1.58	3 (20%)
3	MAN	I	4	3	11,11,12	0.70	0	15,15,17	1.92	5 (33%)
3	MAN	I	5	3	11,11,12	0.66	0	15,15,17	0.88	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
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1
3	BMA	E	3	3	-	2/2/19/22	0/1/1/1
3	MAN	E	4	3	-	1/2/19/22	0/1/1/1
3	MAN	E	5	3	-	0/2/19/22	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	6/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	BMA	G	3	3	-	2/2/19/22	0/1/1/1
3	MAN	G	4	3	-	1/2/19/22	0/1/1/1
3	MAN	G	5	3	-	2/2/19/22	1/1/1/1
2	NAG	H	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	H	2	2	-	3/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	BMA	I	3	3	-	2/2/19/22	1/1/1/1
3	MAN	I	4	3	-	2/2/19/22	0/1/1/1
3	MAN	I	5	3	-	1/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	3	BMA	C2-C3	3.46	1.57	1.52
2	H	2	NAG	C1-C2	2.31	1.55	1.52
3	E	2	NAG	C1-C2	2.06	1.55	1.52
3	E	3	BMA	C1-C2	2.05	1.56	1.52

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	2	NAG	C4-C3-C2	-7.15	100.54	111.02
3	G	3	BMA	C1-C2-C3	6.31	117.42	109.67
2	F	1	NAG	C1-O5-C5	6.06	120.40	112.19
3	G	1	NAG	O5-C5-C6	5.50	115.83	107.20
3	E	5	MAN	C1-O5-C5	5.20	119.24	112.19
3	G	3	BMA	C3-C4-C5	-5.12	101.10	110.24
3	G	1	NAG	C1-O5-C5	5.11	119.11	112.19
3	I	1	NAG	C1-O5-C5	4.97	118.93	112.19
3	G	4	MAN	C1-C2-C3	4.93	115.73	109.67
3	G	1	NAG	C4-C3-C2	4.85	118.13	111.02
3	E	1	NAG	C2-N2-C7	4.73	129.64	122.90
3	G	3	BMA	O5-C5-C6	4.66	114.51	107.20
3	E	2	NAG	C1-O5-C5	4.66	118.50	112.19
3	E	3	BMA	O5-C5-C6	4.61	114.44	107.20
3	E	5	MAN	O5-C1-C2	4.55	117.79	110.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1	NAG	C3-C4-C5	4.54	118.33	110.24
3	E	2	NAG	C4-C3-C2	4.53	117.65	111.02
3	E	5	MAN	C1-C2-C3	4.45	115.13	109.67
2	F	1	NAG	O5-C1-C2	4.44	118.30	111.29
3	E	3	BMA	C1-C2-C3	4.24	114.88	109.67
3	I	2	NAG	O5-C1-C2	-4.06	104.87	111.29
3	G	3	BMA	C1-O5-C5	-4.05	106.70	112.19
2	D	1	NAG	C1-O5-C5	4.01	117.63	112.19
2	H	2	NAG	C2-N2-C7	3.99	128.59	122.90
2	D	2	NAG	C2-N2-C7	3.97	128.56	122.90
3	I	1	NAG	O3-C3-C2	3.89	117.52	109.47
3	E	2	NAG	O4-C4-C3	-3.84	101.47	110.35
3	I	4	MAN	C1-C2-C3	3.83	114.38	109.67
3	I	2	NAG	C1-C2-N2	3.72	116.85	110.49
3	I	1	NAG	O5-C5-C6	3.70	113.01	107.20
2	F	2	NAG	C2-N2-C7	3.66	128.11	122.90
3	I	2	NAG	C2-N2-C7	-3.59	117.78	122.90
3	I	2	NAG	C8-C7-N2	3.41	121.87	116.10
2	D	1	NAG	O5-C1-C2	3.29	116.49	111.29
3	I	1	NAG	C1-C2-N2	-3.28	104.88	110.49
2	F	1	NAG	C4-C3-C2	3.22	115.74	111.02
2	H	2	NAG	C1-O5-C5	3.19	116.52	112.19
3	I	3	BMA	O2-C2-C1	3.17	115.64	109.15
2	D	2	NAG	C4-C3-C2	3.14	115.63	111.02
3	E	4	MAN	C1-O5-C5	3.12	116.42	112.19
2	D	1	NAG	C8-C7-N2	3.07	121.30	116.10
2	D	1	NAG	C2-N2-C7	3.07	127.27	122.90
3	I	4	MAN	O5-C5-C6	3.06	112.00	107.20
2	H	1	NAG	C2-N2-C7	3.05	127.24	122.90
3	I	4	MAN	O5-C1-C2	3.04	115.47	110.77
3	G	4	MAN	C1-O5-C5	2.93	116.16	112.19
3	E	1	NAG	C4-C3-C2	2.73	115.03	111.02
3	E	5	MAN	O5-C5-C6	2.73	111.48	107.20
3	G	3	BMA	O3-C3-C2	2.68	115.12	109.99
3	I	3	BMA	O5-C1-C2	-2.67	106.65	110.77
2	H	1	NAG	O4-C4-C5	2.65	115.88	109.30
2	D	1	NAG	C4-C3-C2	2.63	114.87	111.02
3	G	2	NAG	O5-C1-C2	-2.60	107.19	111.29
3	E	3	BMA	C1-O5-C5	-2.59	108.68	112.19
3	E	4	MAN	O5-C5-C6	2.58	111.25	107.20
3	I	4	MAN	C1-O5-C5	2.55	115.64	112.19
2	H	1	NAG	O3-C3-C4	-2.53	104.49	110.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	2	NAG	O5-C5-C6	2.52	111.16	107.20
3	E	4	MAN	C1-C2-C3	2.52	112.76	109.67
3	I	2	NAG	C1-O5-C5	2.51	115.59	112.19
3	E	2	NAG	C3-C4-C5	2.51	114.71	110.24
2	F	1	NAG	C8-C7-N2	2.50	120.34	116.10
3	G	3	BMA	O5-C5-C4	-2.45	104.87	110.83
3	I	2	NAG	O4-C4-C3	2.45	116.01	110.35
3	G	5	MAN	C1-O5-C5	2.44	115.50	112.19
3	E	2	NAG	O7-C7-C8	-2.38	117.64	122.06
3	E	3	BMA	O2-C2-C1	2.37	113.99	109.15
3	G	2	NAG	O4-C4-C5	2.35	115.14	109.30
2	F	2	NAG	C4-C3-C2	2.34	114.45	111.02
2	H	2	NAG	O5-C1-C2	2.34	114.97	111.29
3	G	1	NAG	C3-C4-C5	2.31	114.36	110.24
3	G	5	MAN	O5-C5-C6	2.30	110.80	107.20
3	E	2	NAG	O5-C5-C4	2.29	116.39	110.83
3	G	4	MAN	O5-C5-C6	2.28	110.77	107.20
3	I	5	MAN	C1-C2-C3	2.25	112.43	109.67
3	G	4	MAN	C2-C3-C4	2.25	114.78	110.89
3	G	2	NAG	C3-C4-C5	-2.23	106.25	110.24
3	I	3	BMA	C2-C3-C4	-2.22	107.06	110.89
3	E	2	NAG	C8-C7-N2	2.21	119.84	116.10
3	G	4	MAN	C3-C4-C5	2.16	114.09	110.24
3	I	4	MAN	C3-C4-C5	-2.13	106.44	110.24
3	I	2	NAG	O4-C4-C5	2.13	114.58	109.30
3	G	1	NAG	O3-C3-C2	-2.05	105.22	109.47
3	I	2	NAG	C3-C4-C5	2.05	113.89	110.24
3	E	2	NAG	O4-C4-C5	2.04	114.36	109.30

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
3	I	1	NAG	C8-C7-N2-C2
3	I	1	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
3	E	1	NAG	C3-C2-N2-C7
2	D	1	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	O7-C7-N2-C2
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
2	H	2	NAG	C8-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	E	1	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	G	3	BMA	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	I	4	MAN	O5-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
3	G	2	NAG	C8-C7-N2-C2
2	H	1	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
3	I	3	BMA	O5-C5-C6-O6
3	I	4	MAN	C4-C5-C6-O6
3	E	3	BMA	C4-C5-C6-O6
3	G	2	NAG	O7-C7-N2-C2
3	G	5	MAN	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	G	4	MAN	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
3	I	5	MAN	O5-C5-C6-O6
3	G	1	NAG	C1-C2-N2-C7
3	G	5	MAN	C4-C5-C6-O6
3	G	1	NAG	C3-C2-N2-C7
3	I	3	BMA	C4-C5-C6-O6
3	E	4	MAN	C4-C5-C6-O6

All (2) ring outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms

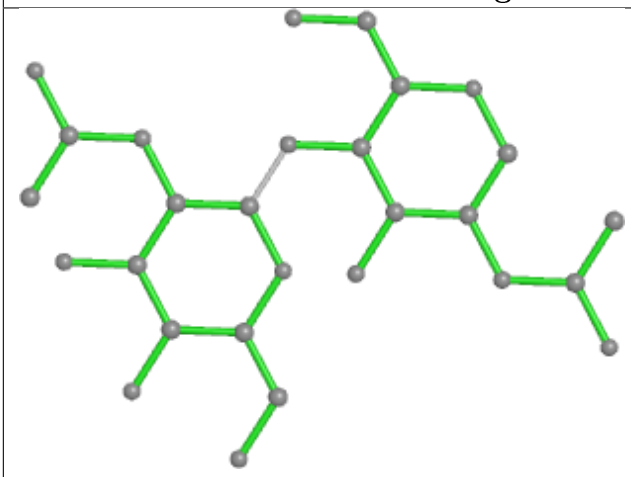
Mol	Chain	Res	Type	Atoms
3	G	5	MAN	C1-C2-C3-C4-C5-O5
3	I	3	BMA	C1-C2-C3-C4-C5-O5

7 monomers are involved in 6 short contacts:

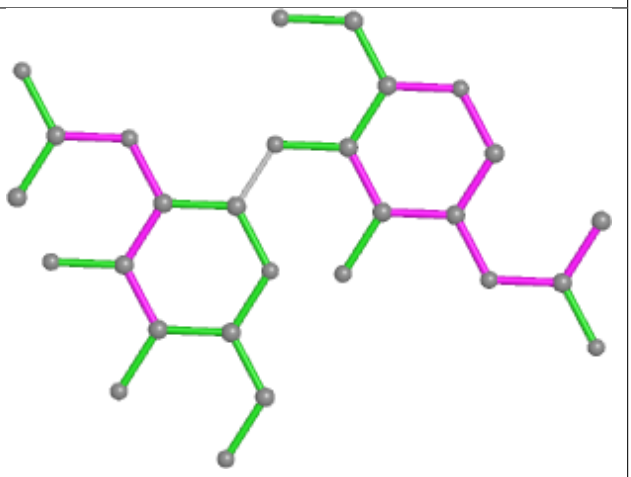
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	NAG	1	0
2	H	1	NAG	2	0
3	I	5	MAN	1	0
3	G	2	NAG	1	0
3	E	1	NAG	1	0
2	D	1	NAG	1	0
3	G	3	BMA	1	0

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

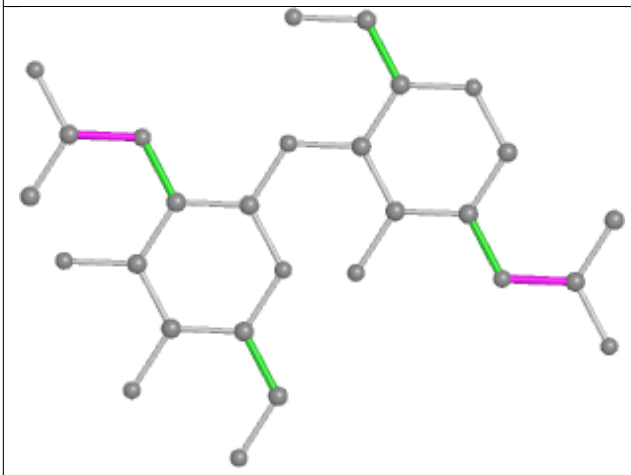
Oligosaccharide Chain D



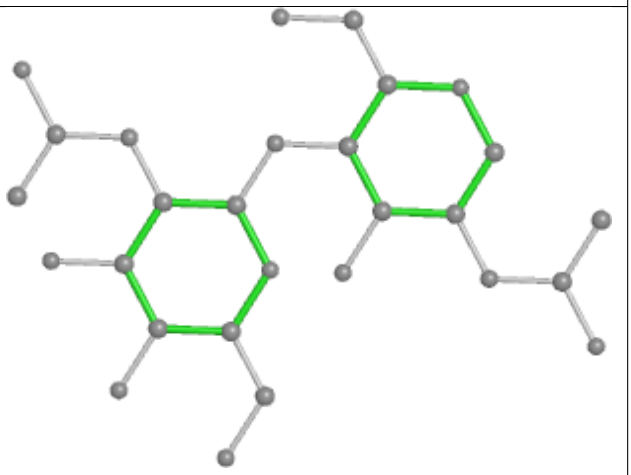
Bond lengths



Bond angles

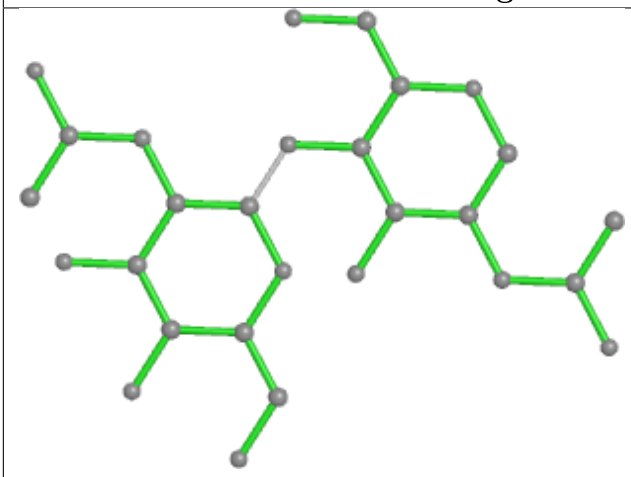


Torsions

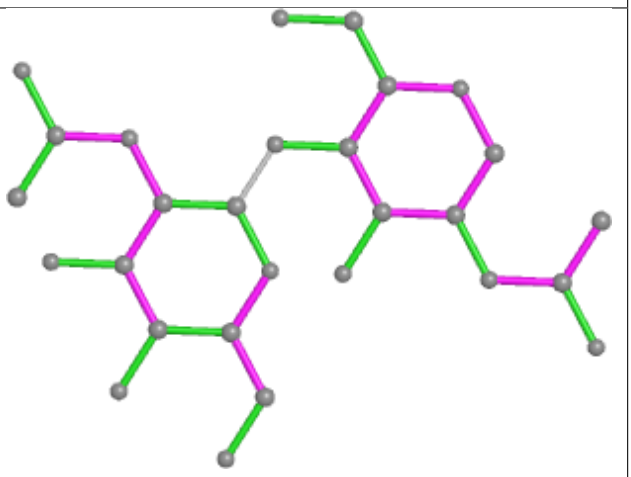


Rings

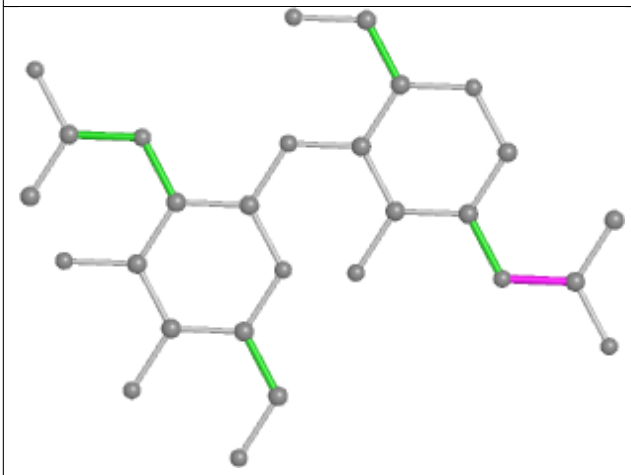
Oligosaccharide Chain F



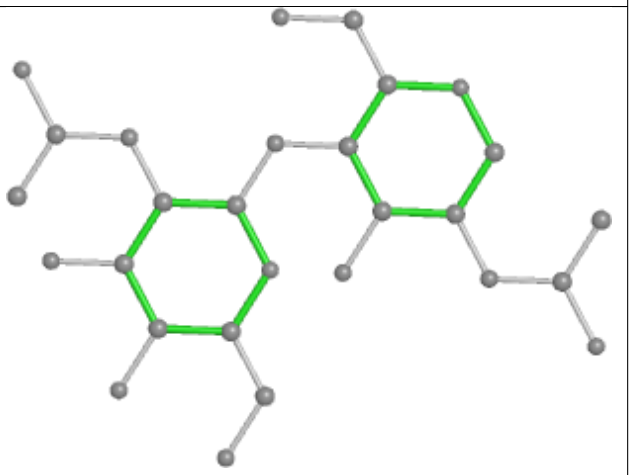
Bond lengths



Bond angles

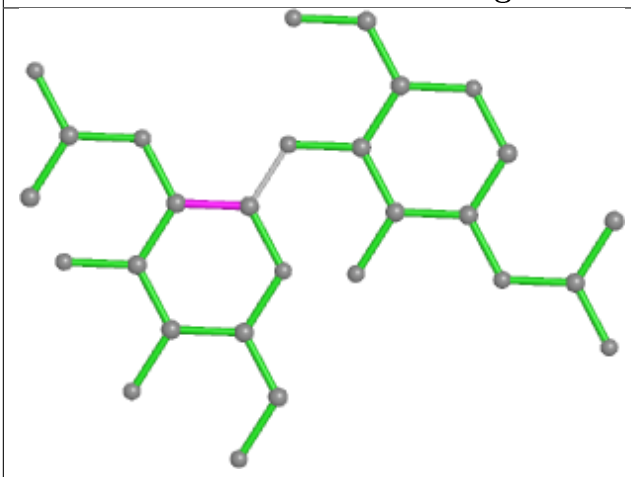


Torsions

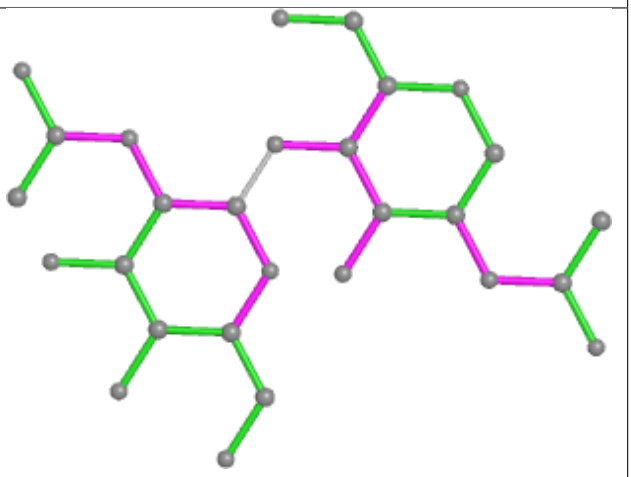


Rings

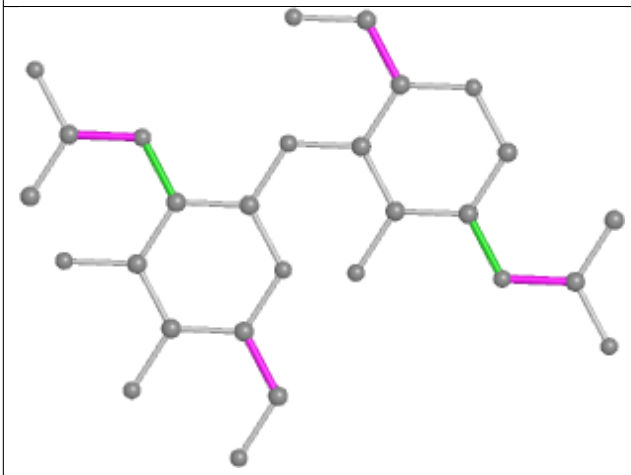
Oligosaccharide Chain H



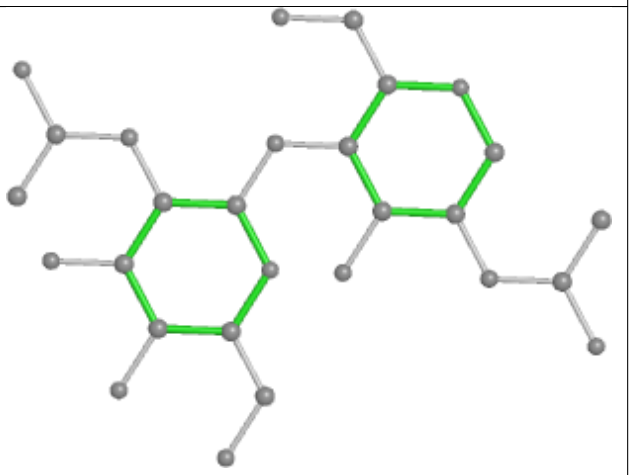
Bond lengths



Bond angles

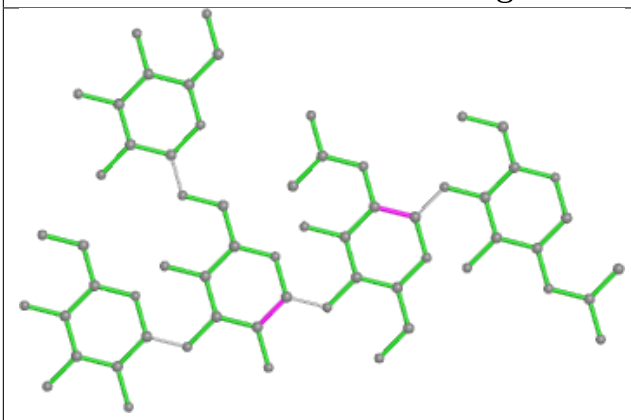


Torsions

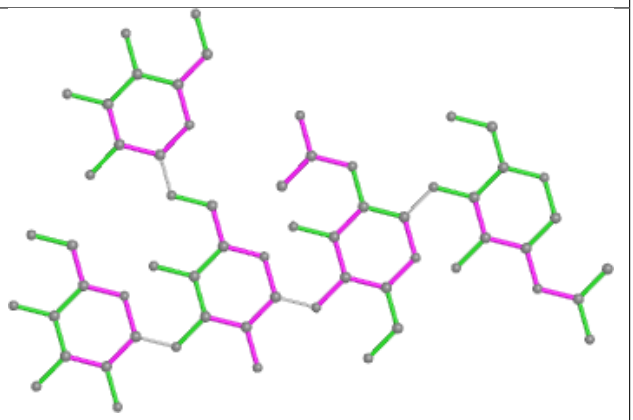


Rings

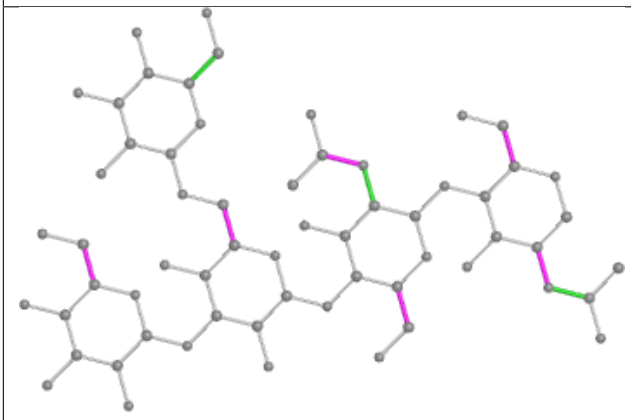
Oligosaccharide Chain E



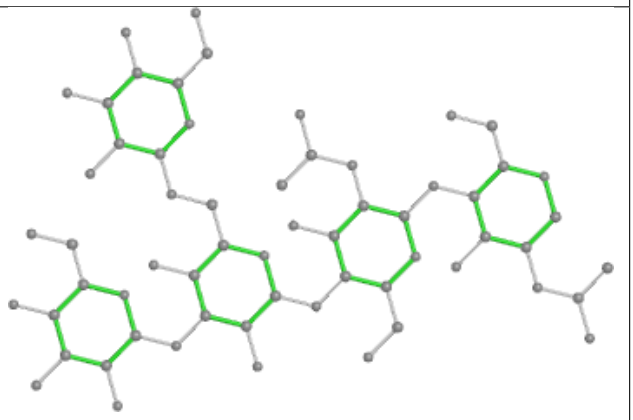
Bond lengths



Bond angles

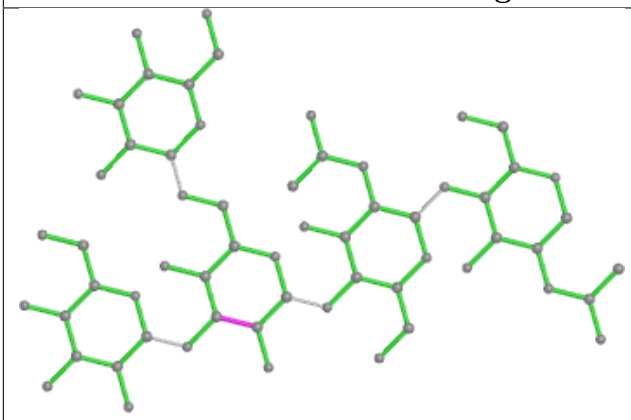


Torsions

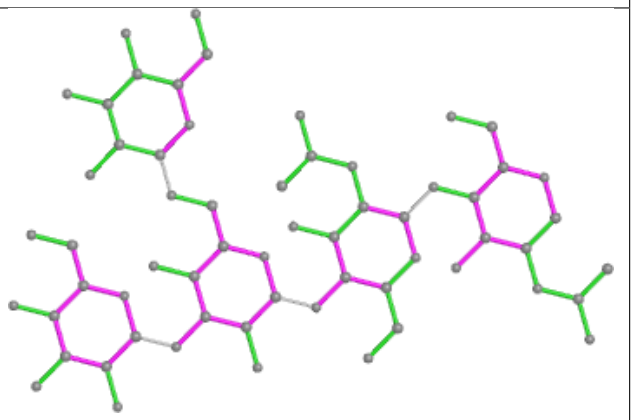


Rings

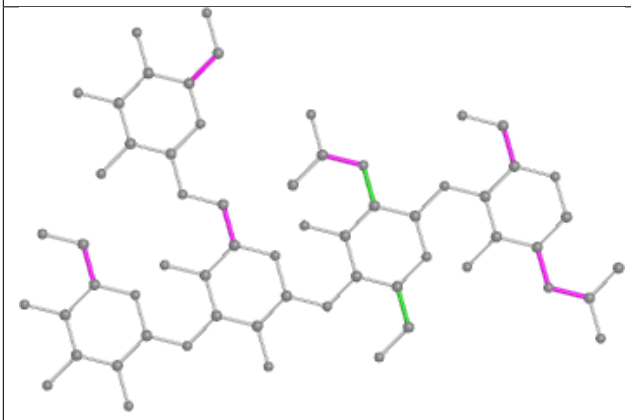
Oligosaccharide Chain G



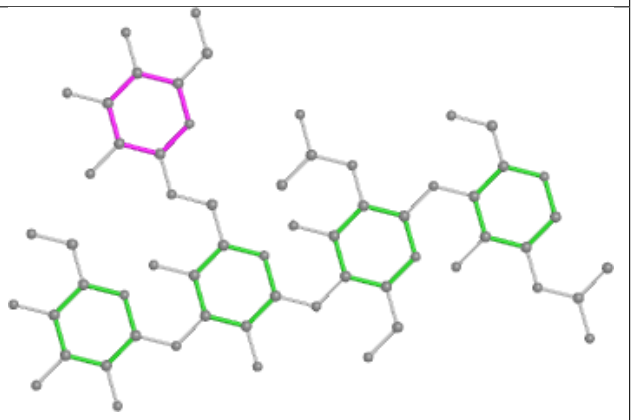
Bond lengths



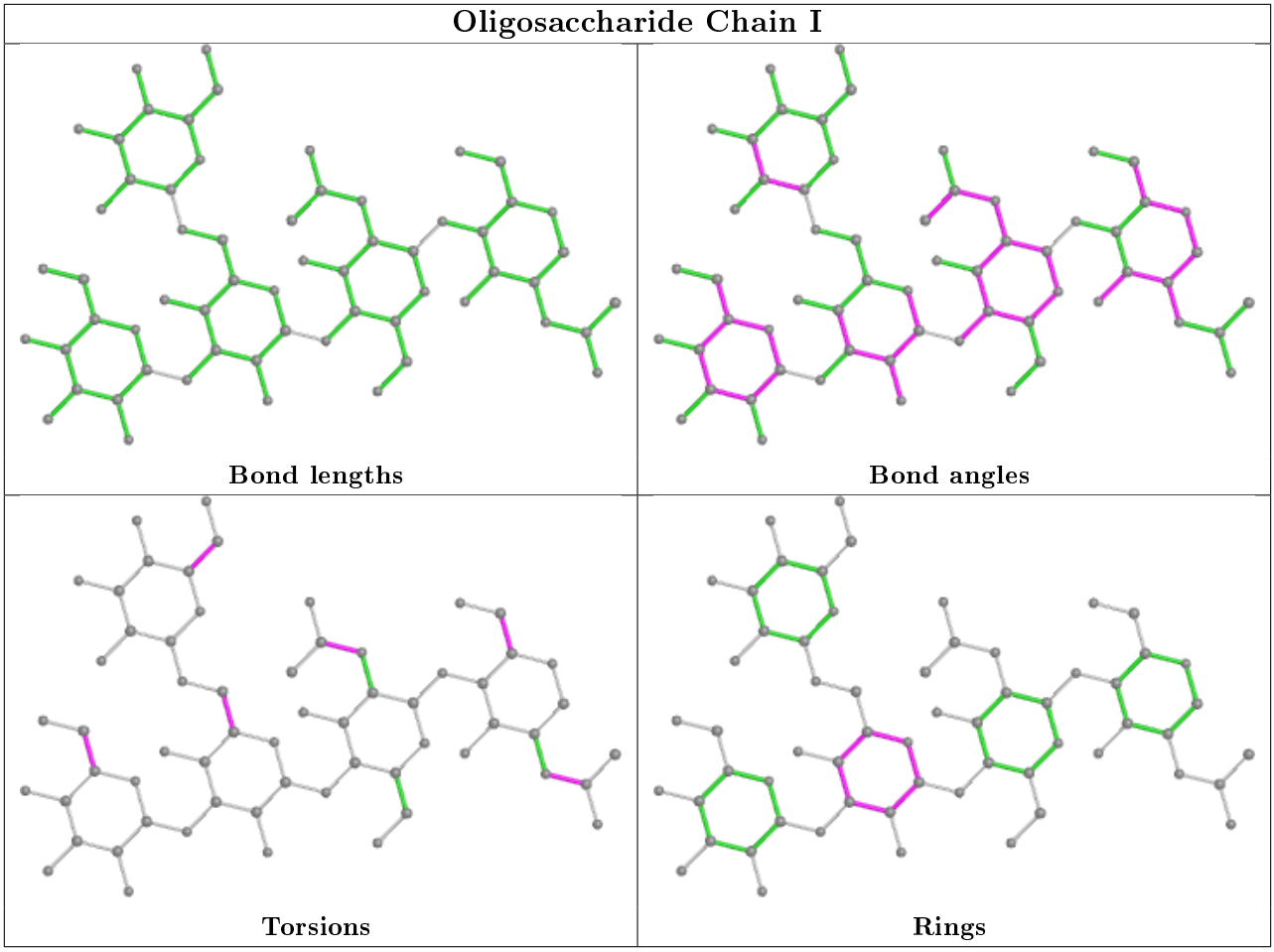
Bond angles



Torsions



Rings



5.6 Ligand geometry

There are no ligands in this entry.

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	A	804/859 (93%)	-0.28	11 (1%)	75	61	38, 104, 211, 282	0
1	B	804/859 (93%)	-0.24	8 (0%)	82	70	53, 114, 248, 348	0
1	C	804/859 (93%)	-0.28	11 (1%)	75	61	40, 84, 234, 308	0
All	All	2412/2577 (93%)	-0.27	30 (1%)	79	66	38, 101, 234, 348	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	799	VAL	6.4
1	B	22	SER	5.1
1	A	757	SER	4.5
1	C	840	VAL	4.0
1	C	798	SER	3.5
1	A	758	VAL	3.4
1	C	838	GLU	3.0
1	C	815	ALA	3.0
1	B	835	ARG	2.9
1	A	799	VAL	2.8
1	B	801	ILE	2.8
1	A	749	GLY	2.7
1	B	765	PRO	2.7
1	A	744	THR	2.5
1	C	834	GLY	2.5
1	A	743	VAL	2.4
1	B	758	VAL	2.4
1	A	803	GLY	2.3
1	C	732	THR	2.3
1	C	839	VAL	2.3
1	A	513	SER	2.3
1	A	814	VAL	2.3
1	C	758	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	745	VAL	2.1
1	B	837	ASN	2.1
1	B	681	THR	2.1
1	B	24	LEU	2.1
1	C	806	PRO	2.1
1	C	22	SER	2.1
1	A	801	ILE	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)

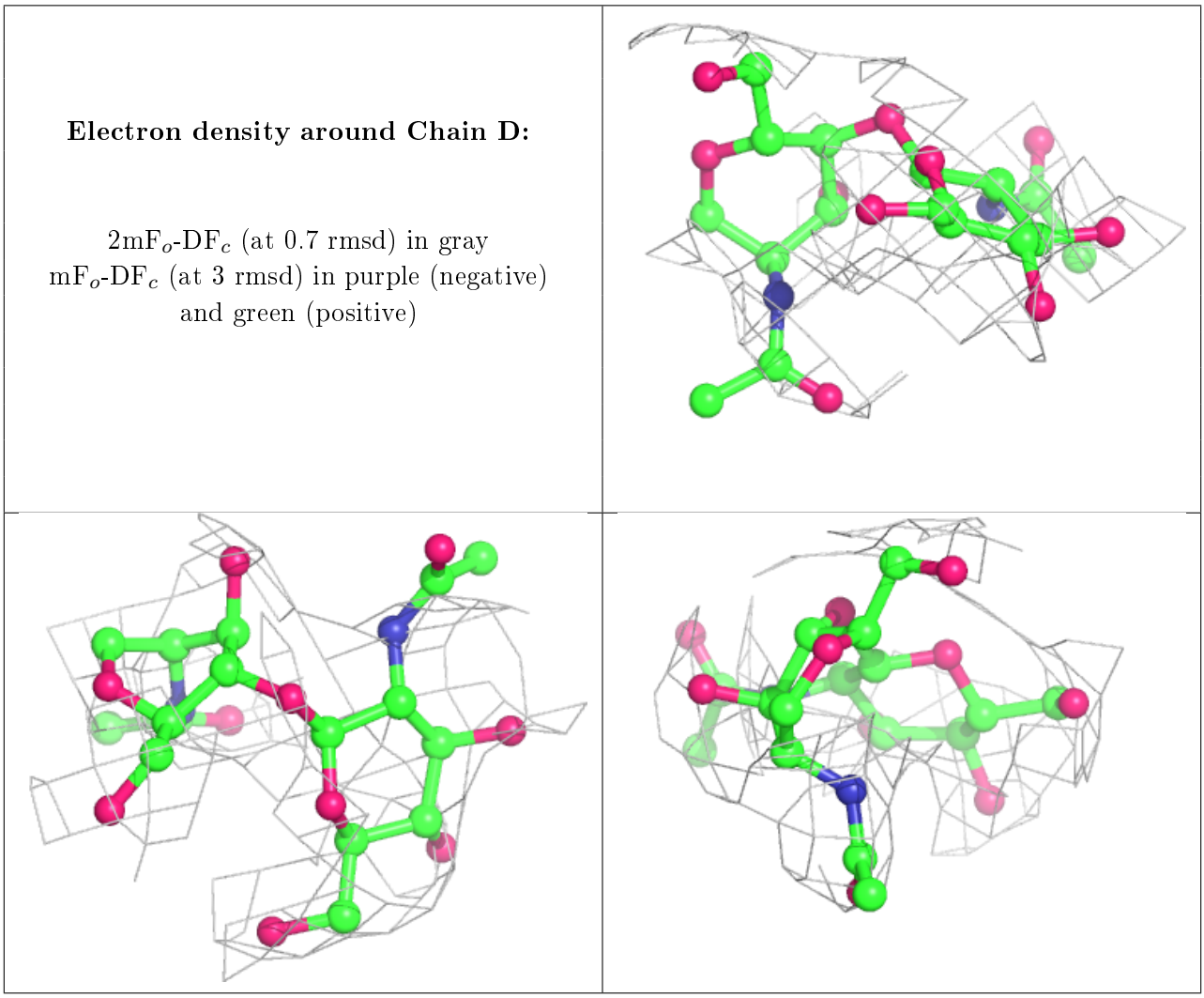
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	NAG	D	2	14/15	0.67	0.32	158,189,205,208	0
3	MAN	E	4	11/12	0.68	0.51	192,207,212,216	0
2	NAG	F	1	14/15	0.73	0.24	113,155,162,179	0
3	BMA	E	3	11/12	0.73	0.24	173,178,185,200	0
3	MAN	I	4	11/12	0.74	0.41	166,198,220,224	0
2	NAG	F	2	14/15	0.77	0.46	169,178,184,187	0
3	MAN	I	5	11/12	0.79	0.39	152,165,184,185	0
3	BMA	I	3	11/12	0.80	0.23	153,159,171,189	0
2	NAG	H	2	14/15	0.80	0.28	147,174,181,187	0
2	NAG	D	1	14/15	0.82	0.20	133,144,150,160	0
3	NAG	E	2	14/15	0.83	0.22	110,156,174,174	0
3	MAN	E	5	11/12	0.83	0.32	145,162,169,174	0
3	MAN	G	5	11/12	0.86	0.34	151,165,174,176	0
2	NAG	H	1	14/15	0.87	0.19	107,124,131,143	0
3	BMA	G	3	11/12	0.88	0.14	133,147,164,171	0
3	MAN	G	4	11/12	0.89	0.43	152,168,175,183	0
3	NAG	G	1	14/15	0.91	0.15	106,129,142,146	0
3	NAG	I	2	14/15	0.91	0.19	99,118,136,156	0
3	NAG	G	2	14/15	0.92	0.17	110,129,156,158	0
3	NAG	E	1	14/15	0.93	0.19	124,128,165,174	0
3	NAG	I	1	14/15	0.95	0.19	92,104,115,132	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.

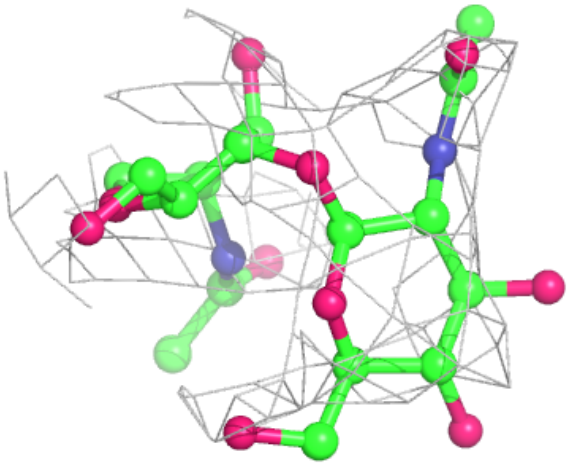
Electron density around Chain D:

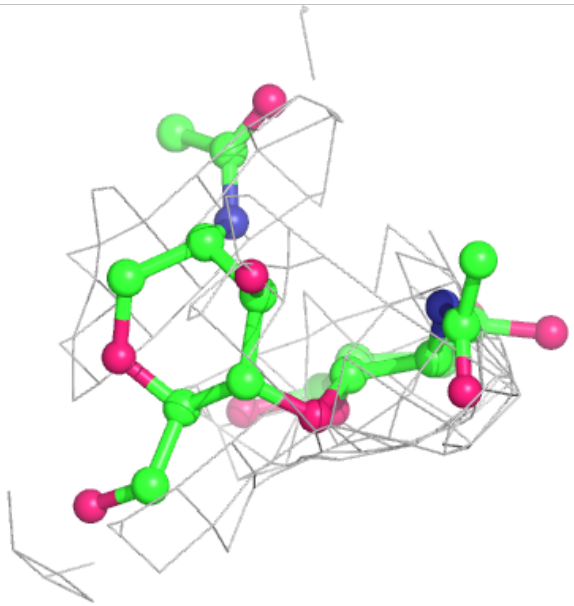
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

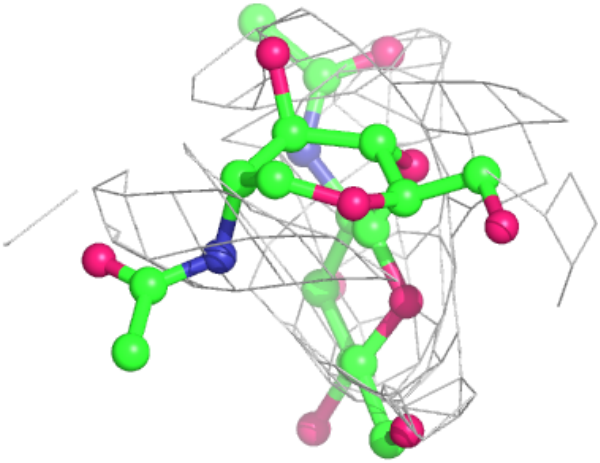


Electron density around Chain F:

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

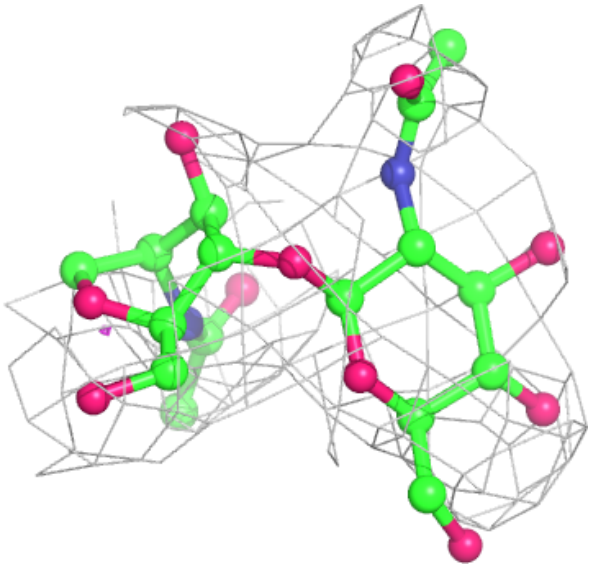


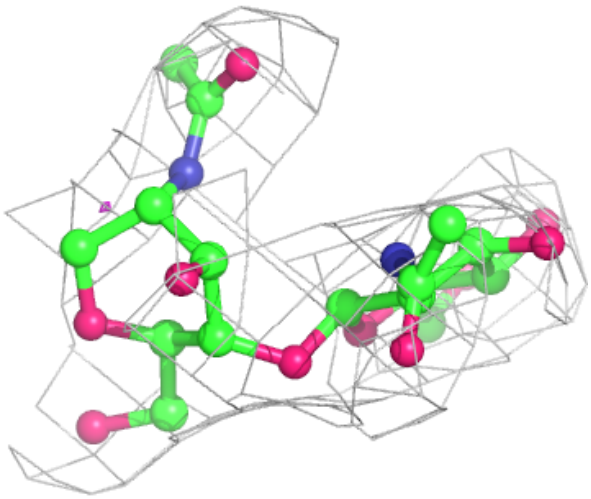


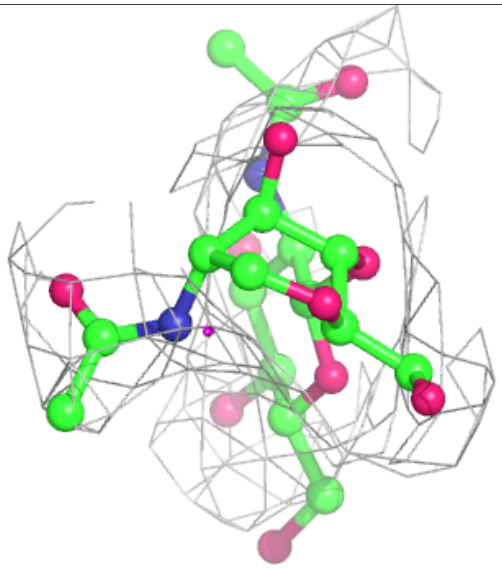


Electron density around Chain H:

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

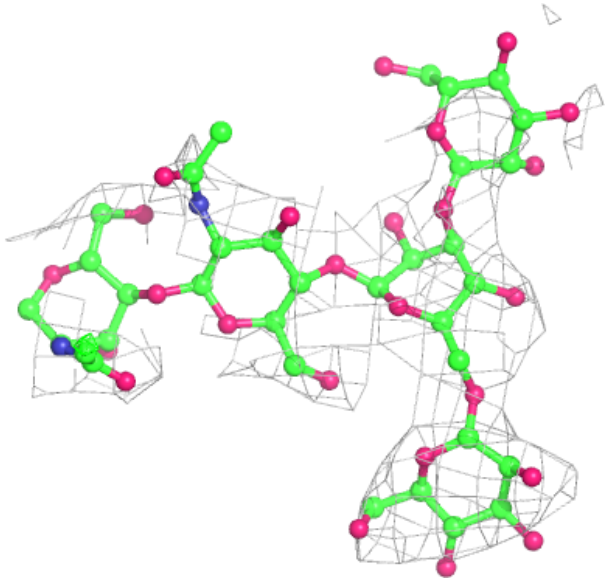


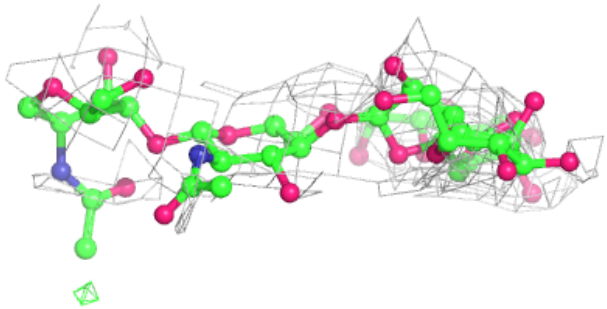


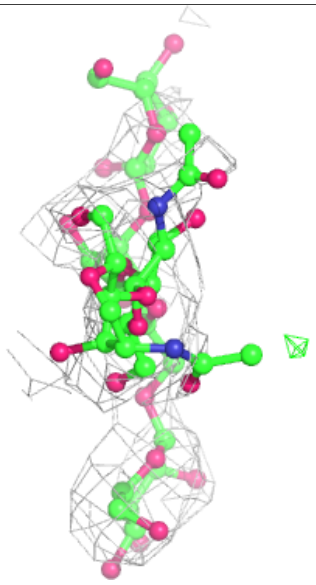


Electron density around Chain E:

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

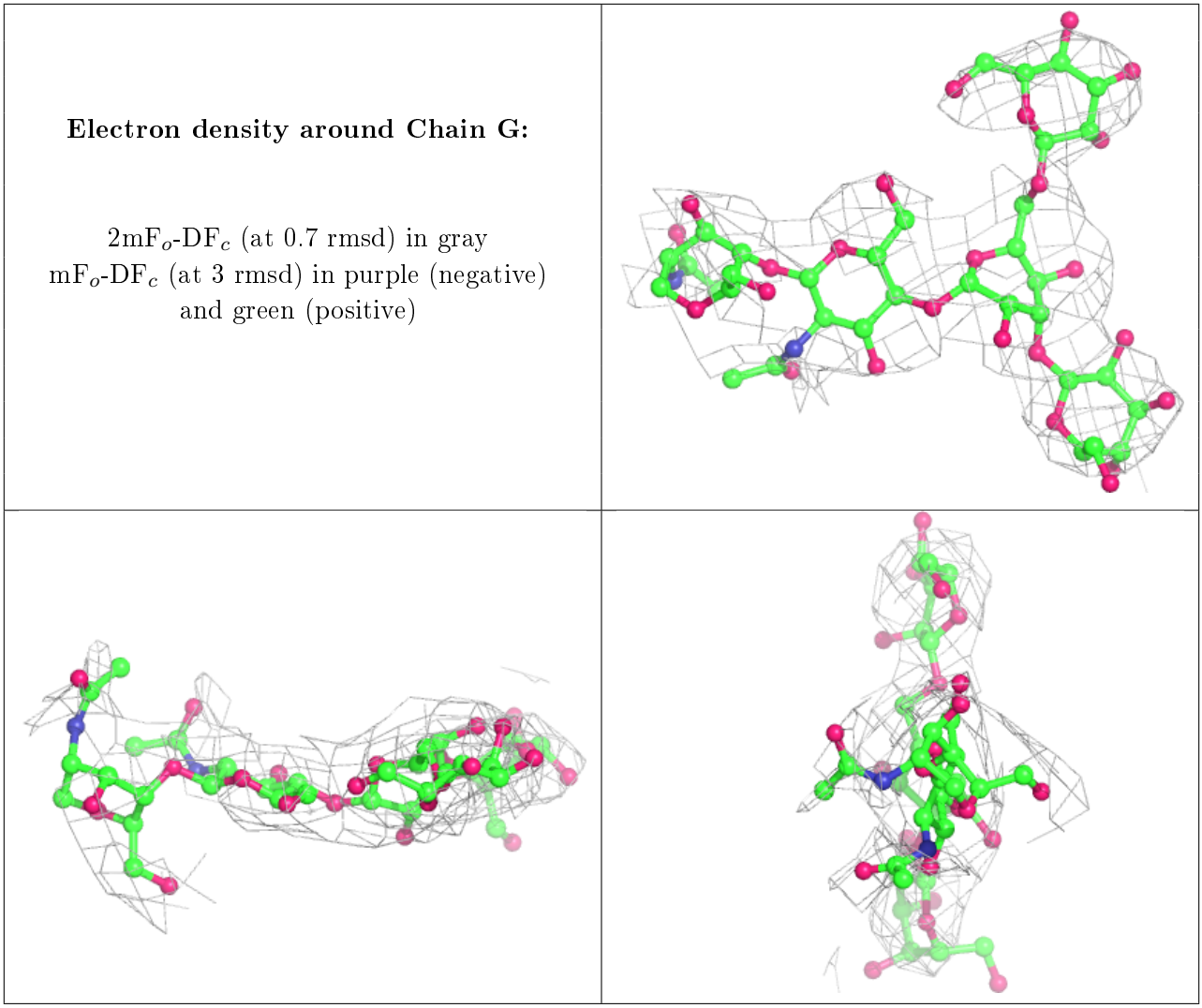






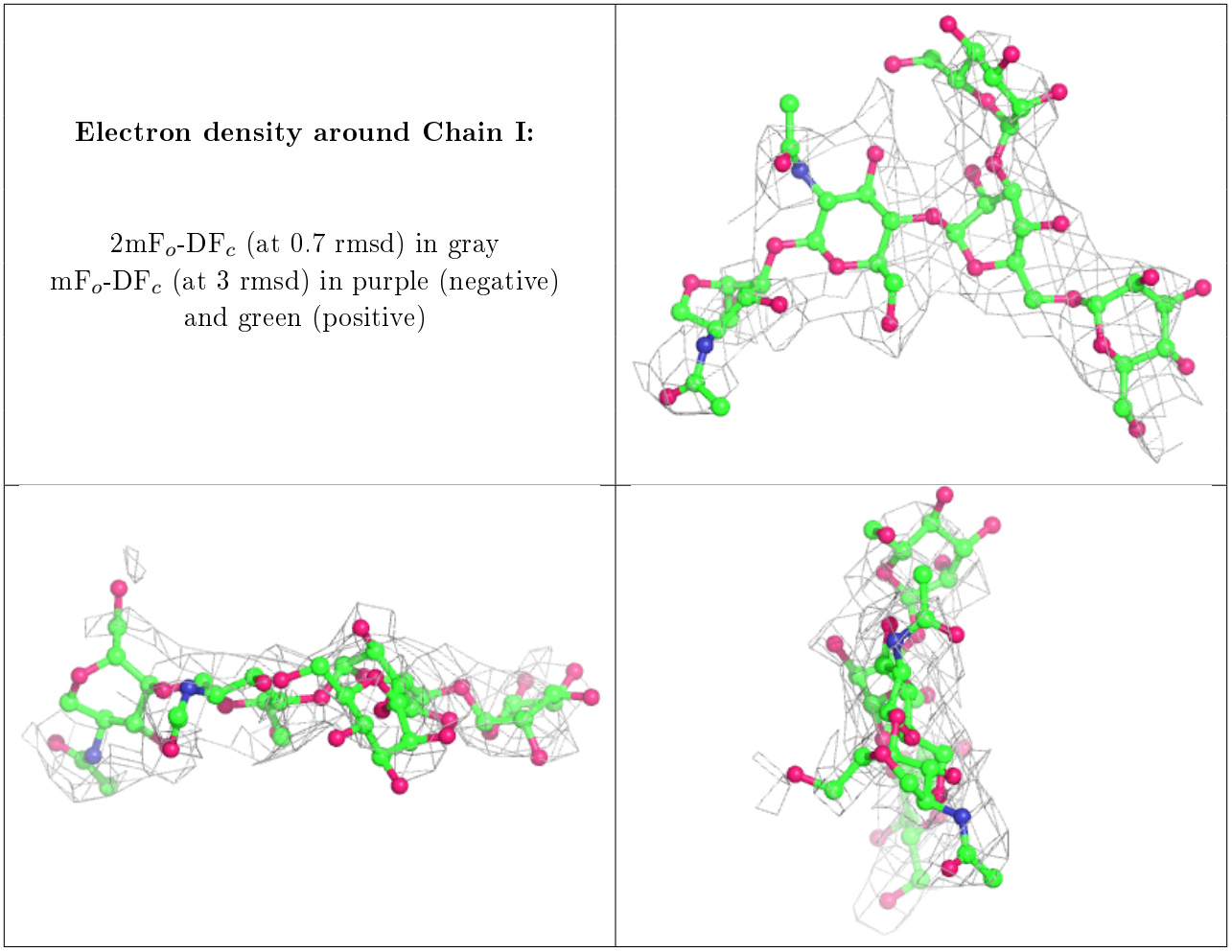
Electron density around Chain G:

$2mF_o$-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 I:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.