Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 07:35 PM EDT

PDB ID	:	3BL8
Title	:	Crystal structure of the extracellular domain of neuroligin 2A from mouse
Authors	:	Jin, X.; Koehnke, J.; Shapiro, L.
Deposited on	:	2007-12-10
Resolution	:	3.30 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:

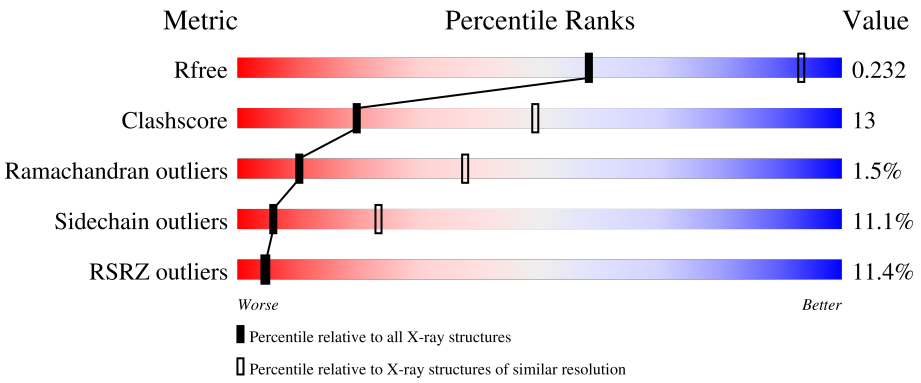
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	580	4%; 59%; 31%; 6%; •
1	B	580	9%; 64%; 24%; 6%; 6%
1	C	580	8%; 66%; 25%; •; 6%
1	D	580	22%; 65%; 24%; •; 7%
2	E	3	100%

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Mol	Chain	Length	Quality of chain
3	F	7	71% 29%

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	MAN	E	3	X	-	-	-
3	MAN	F	5	-	-	-	X
4	NAG	A	710	-	-	-	X
4	NAG	B	810	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 17374 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 Neuroligin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	556	4358	2782	744	814	18	0	0	0
1	B	546	4283	2737	731	797	18	0	0	0
1	C	545	4282	2736	732	796	18	0	0	0
1	D	541	4249	2714	726	791	18	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	GLN	-	expression tag	UNP Q69ZK9
A	41	LYS	-	expression tag	UNP Q69ZK9
A	613	HIS	-	expression tag	UNP Q69ZK9
A	614	HIS	-	expression tag	UNP Q69ZK9
A	615	HIS	-	expression tag	UNP Q69ZK9
A	616	HIS	-	expression tag	UNP Q69ZK9
A	617	HIS	-	expression tag	UNP Q69ZK9
A	618	HIS	-	expression tag	UNP Q69ZK9
A	619	HIS	-	expression tag	UNP Q69ZK9
B	40	GLN	-	expression tag	UNP Q69ZK9
B	41	LYS	-	expression tag	UNP Q69ZK9
B	613	HIS	-	expression tag	UNP Q69ZK9
B	614	HIS	-	expression tag	UNP Q69ZK9
B	615	HIS	-	expression tag	UNP Q69ZK9
B	616	HIS	-	expression tag	UNP Q69ZK9
B	617	HIS	-	expression tag	UNP Q69ZK9
B	618	HIS	-	expression tag	UNP Q69ZK9
B	619	HIS	-	expression tag	UNP Q69ZK9
C	40	GLN	-	expression tag	UNP Q69ZK9
C	41	LYS	-	expression tag	UNP Q69ZK9
C	613	HIS	-	expression tag	UNP Q69ZK9

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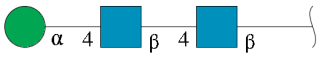
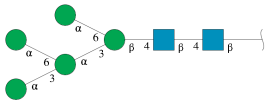
Chain	Residue	Modelled	Actual	Comment	Reference
C	614	HIS	-	expression tag	UNP Q69ZK9
C	615	HIS	-	expression tag	UNP Q69ZK9
C	616	HIS	-	expression tag	UNP Q69ZK9
C	617	HIS	-	expression tag	UNP Q69ZK9
C	618	HIS	-	expression tag	UNP Q69ZK9
C	619	HIS	-	expression tag	UNP Q69ZK9
D	40	GLN	-	expression tag	UNP Q69ZK9
D	41	LYS	-	expression tag	UNP Q69ZK9
D	613	HIS	-	expression tag	UNP Q69ZK9
D	614	HIS	-	expression tag	UNP Q69ZK9
D	615	HIS	-	expression tag	UNP Q69ZK9
D	616	HIS	-	expression tag	UNP Q69ZK9
D	617	HIS	-	expression tag	UNP Q69ZK9
D	618	HIS	-	expression tag	UNP Q69ZK9
D	619	HIS	-	expression tag	UNP Q69ZK9

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



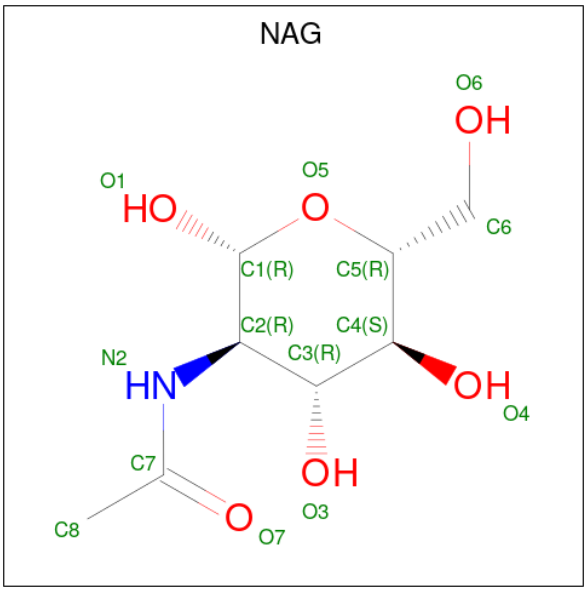
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	3	39	22	2	15	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
			Total	C	N	O			
3	F	7	83	46	2	35	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is water.

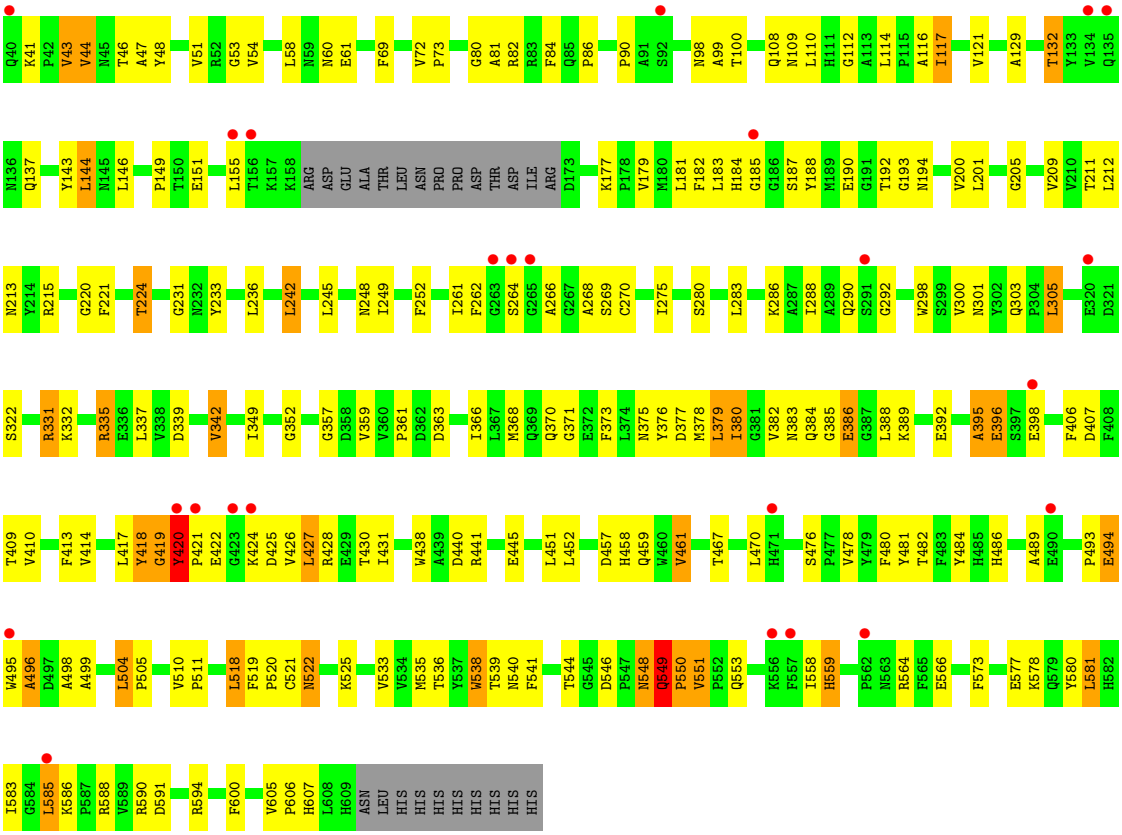
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	31	31	31	0	0
			Total	O		
5	B	11	11	11	0	0
			Total	O		
5	C	5	5	5	0	0
			Total	O		
5	D	5	5	5	0	0

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 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.

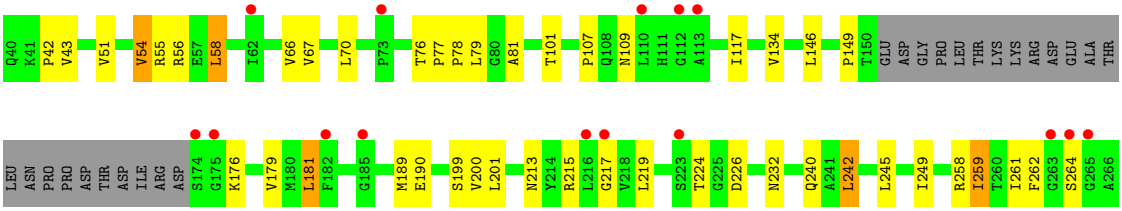
• Molecule 1: Neuroligin-2

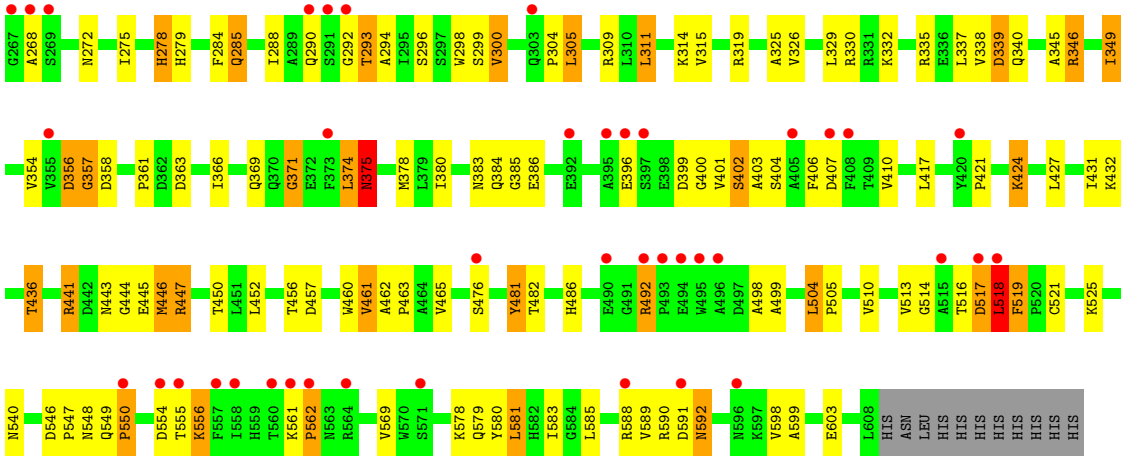
Chain A:



• Molecule 1: Neuroligin-2

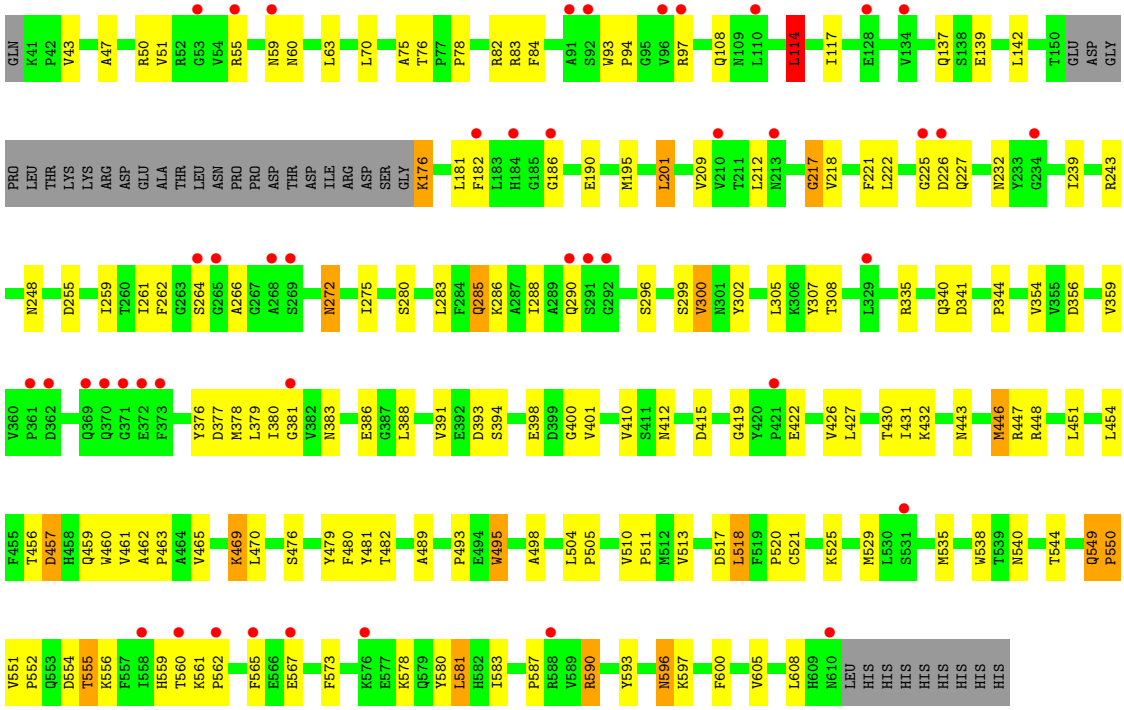
Chain B:





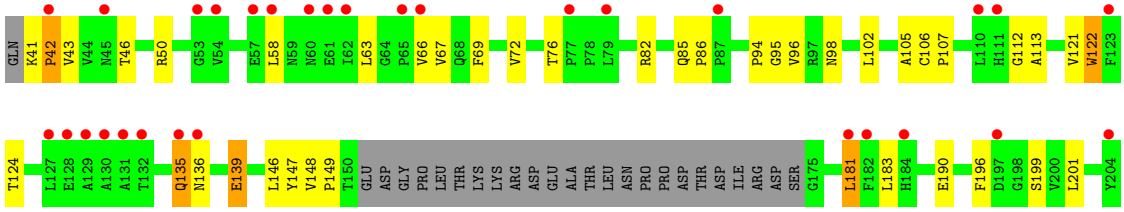
• Molecule 1: Neuroligin-2

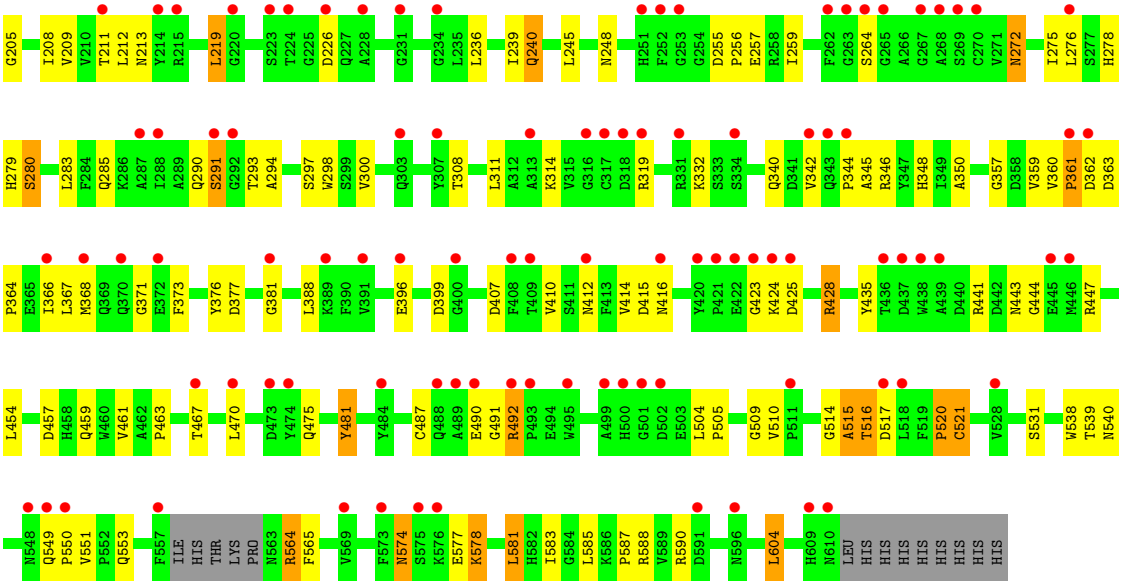
Chain C:



• Molecule 1: Neuroligin-2

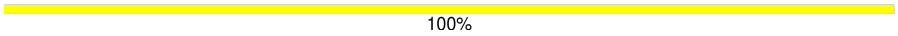
Chain D:





• Molecule 2: alpha-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)]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 F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	214.72Å 92.57Å 188.41Å 90.00° 98.36° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 29.74 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.5 (20.00-3.30) 98.5 (29.74-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 3.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.219 , 0.262 0.230 , 0.232	Depositor DCC
R_{free} test set	2760 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	108.0	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 135.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17374	wwPDB-VP
Average B, all atoms (Å^2)	125.0	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: BMA, MAN, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	A	0.44	0/4478	0.65	6/6101 (0.1%)
1	B	0.36	0/4401	0.60	5/5996 (0.1%)
1	C	0.38	0/4401	0.57	4/5998 (0.1%)
1	D	0.34	0/4365	0.61	12/5945 (0.2%)
All	All	0.38	0/17645	0.61	27/24040 (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	5
1	B	0	4
1	C	0	1
1	D	0	3
All	All	0	13

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	396	GLU	CB-CA-C	-9.49	91.41	110.40
1	A	395	ALA	CB-CA-C	-9.02	96.57	110.10
1	D	279	HIS	N-CA-C	9.01	135.33	111.00
1	D	279	HIS	CB-CA-C	-8.34	93.72	110.40
1	D	113	ALA	N-CA-CB	8.23	121.62	110.10
1	D	112	GLY	N-CA-C	8.09	133.32	113.10
1	B	345	ALA	CB-CA-C	7.43	121.24	110.10
1	D	564	ARG	CB-CA-C	-7.30	95.81	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	291	SER	N-CA-C	7.01	129.92	111.00
1	A	496	ALA	N-CA-C	-6.28	94.04	111.00
1	D	521	CYS	CB-CA-C	6.18	122.77	110.40
1	D	280	SER	N-CA-C	-6.12	94.49	111.00
1	C	498	ALA	N-CA-C	5.91	126.95	111.00
1	C	226	ASP	N-CA-C	5.87	126.85	111.00
1	D	565	PHE	N-CA-CB	5.86	121.15	110.60
1	D	280	SER	N-CA-CB	5.83	119.25	110.50
1	C	114	LEU	CA-CB-CG	5.82	128.69	115.30
1	B	345	ALA	N-CA-C	-5.69	95.63	111.00
1	C	227	GLN	N-CA-CB	5.49	120.49	110.60
1	D	113	ALA	N-CA-C	-5.45	96.30	111.00
1	A	496	ALA	CB-CA-C	5.42	118.23	110.10
1	B	384	GLN	CB-CA-C	-5.40	99.59	110.40
1	A	395	ALA	N-CA-C	5.19	125.01	111.00
1	B	384	GLN	N-CA-C	5.18	124.99	111.00
1	D	604	LEU	CA-CB-CG	5.12	127.08	115.30
1	A	518	LEU	CA-CB-CG	5.11	127.04	115.30
1	A	396	GLU	N-CA-CB	5.05	119.69	110.60

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	418	TYR	Peptide
1	A	419	GLY	Peptide
1	A	420	TYR	Peptide
1	A	494	GLU	Peptide
1	A	549	GLN	Peptide
1	B	402	SER	Peptide
1	B	517	ASP	Peptide
1	B	518	LEU	Peptide
1	B	78	PRO	Peptide
1	C	549	GLN	Peptide
1	D	371	GLY	Peptide
1	D	396	GLU	Peptide
1	D	549	GLN	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	4358	0	4194	157	0
1	B	4283	0	4129	102	0
1	C	4282	0	4123	91	0
1	D	4249	0	4091	80	0
2	E	39	0	34	0	0
3	F	83	0	70	4	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
5	A	31	0	0	0	0
5	B	11	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
All	All	17374	0	16667	433	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 13.

All (433) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:TYR:H	1:A:421:PRO:HA	1.02	1.17
1:B:561:LYS:HG3	1:B:562:PRO:HD2	1.20	1.11
1:C:540:ASN:HD21	1:C:551:VAL:HG12	1.18	1.03
1:A:420:TYR:H	1:A:421:PRO:CA	1.77	0.98
1:A:421:PRO:O	1:A:424:LYS:N	1.97	0.97
1:B:561:LYS:CG	1:B:562:PRO:HD2	2.00	0.92
1:A:286:LYS:HG2	1:A:377:ASP:HB2	1.51	0.91
1:A:420:TYR:N	1:A:421:PRO:HA	1.86	0.90
1:A:457:ASP:HA	1:A:461:VAL:HG13	1.54	0.88
1:A:335:ARG:O	1:A:339:ASP:OD2	1.91	0.87
1:B:518:LEU:C	1:B:518:LEU:HD22	1.96	0.87
1:B:581:LEU:HD13	1:B:583:ILE:HG12	1.56	0.86
1:B:66:VAL:HG12	1:B:149:PRO:HA	1.58	0.85
1:A:493:PRO:O	1:A:496:ALA:CB	2.26	0.83
1:A:486:HIS:CE1	1:A:496:ALA:O	2.34	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:PRO:O	1:A:496:ALA:HB2	1.81	0.80
1:B:400:GLY:C	1:B:401:VAL:HG22	2.02	0.79
1:B:548:ASN:O	1:B:549:GLN:HG2	1.81	0.78
1:A:80:GLY:C	1:A:82:ARG:H	1.86	0.78
1:B:346:ARG:H	1:B:346:ARG:HD2	1.47	0.77
1:A:201:LEU:HA	1:A:535:MET:CE	2.13	0.77
1:A:236:LEU:HD21	1:A:359:VAL:HG11	1.66	0.76
1:A:395:ALA:O	1:A:495:TRP:CH2	2.38	0.76
1:D:514:GLY:O	1:D:515:ALA:HB3	1.85	0.75
1:A:201:LEU:HA	1:A:535:MET:HE3	1.68	0.75
1:B:403:ALA:HA	1:B:406:PHE:HB3	1.70	0.74
1:C:431:ILE:HG22	1:C:600:PHE:HZ	1.53	0.74
1:B:70:LEU:HB3	1:B:101:THR:O	1.87	0.73
1:B:375:ASN:HB2	1:B:476:SER:HB3	1.71	0.73
1:D:492:ARG:H	1:D:492:ARG:HE	1.36	0.73
1:A:420:TYR:N	1:A:421:PRO:CA	2.48	0.73
1:D:444:GLY:HA2	1:D:447:ARG:HB2	1.72	0.72
1:A:421:PRO:O	1:A:424:LYS:CB	2.37	0.72
1:D:121:VAL:HA	1:D:124:THR:HG22	1.70	0.72
1:A:108:GLN:HG2	1:A:137:GLN:NE2	2.05	0.72
1:A:41:LYS:HE2	1:A:54:VAL:HG12	1.72	0.71
1:C:286:LYS:HG2	1:C:377:ASP:HB2	1.72	0.70
1:A:73:PRO:HA	1:A:143:TYR:HD2	1.55	0.70
1:D:564:ARG:O	1:D:587:PRO:HG2	1.91	0.70
1:B:457:ASP:HA	1:B:461:VAL:HG22	1.73	0.69
1:C:431:ILE:HG22	1:C:600:PHE:CZ	2.27	0.69
1:A:201:LEU:HB3	1:A:209:VAL:HG21	1.74	0.69
1:A:268:ALA:HB3	1:A:292:GLY:HA3	1.75	0.69
1:B:400:GLY:C	1:B:401:VAL:CG2	2.61	0.69
1:A:44:VAL:HG11	1:A:252:PHE:CE2	2.28	0.69
1:D:551:VAL:HG13	1:D:551:VAL:O	1.94	0.68
1:A:378:MET:HB2	1:A:478:VAL:HA	1.74	0.68
1:C:540:ASN:ND2	1:C:551:VAL:HG12	2.02	0.68
1:D:581:LEU:HD12	1:D:583:ILE:HG13	1.74	0.67
1:D:514:GLY:O	1:D:515:ALA:CB	2.42	0.67
1:A:489:ALA:HA	1:A:521:CYS:HB3	1.77	0.67
1:B:268:ALA:HB3	1:B:292:GLY:HA3	1.75	0.67
1:A:349:ILE:HD12	1:A:352:GLY:HA3	1.77	0.66
1:B:518:LEU:HD13	1:B:518:LEU:H	1.61	0.65
1:B:518:LEU:HD22	1:B:518:LEU:O	1.96	0.65
1:B:407:ASP:HA	1:B:410:VAL:HG12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:THR:OG1	1:A:549:GLN:HB3	1.97	0.65
1:B:432:LYS:O	1:B:436:THR:HG22	1.96	0.65
1:A:109:ASN:HB2	1:A:339:ASP:HB3	1.78	0.65
1:A:414:VAL:HG21	1:A:428:ARG:HB2	1.79	0.64
1:B:259:ILE:HD11	1:B:284:PHE:HB3	1.77	0.64
1:B:357:GLY:HA2	1:B:361:PRO:HA	1.80	0.64
1:B:77:PRO:HB2	1:B:79:LEU:HG	1.79	0.63
1:B:518:LEU:C	1:B:518:LEU:CD2	2.66	0.63
1:C:412:ASN:HA	1:C:415:ASP:HB2	1.79	0.63
1:D:106:CYS:HB3	1:D:107:PRO:HD2	1.81	0.63
1:D:236:LEU:HA	1:D:239:ILE:HG22	1.80	0.63
1:A:205:GLY:HA3	1:A:539:THR:HG21	1.79	0.63
1:C:461:VAL:O	1:C:465:VAL:HG12	1.98	0.63
1:C:114:LEU:HD22	1:C:114:LEU:H	1.63	0.63
1:D:291:SER:O	1:D:291:SER:OG	2.15	0.63
1:B:304:PRO:HG3	1:B:354:VAL:HG11	1.80	0.63
1:B:402:SER:O	1:B:404:SER:N	2.32	0.62
1:A:342:VAL:O	1:A:342:VAL:CG2	2.47	0.62
1:B:400:GLY:O	1:B:401:VAL:CG2	2.47	0.62
1:B:446:MET:H	1:B:446:MET:HE2	1.64	0.62
1:C:559:HIS:HD2	1:C:561:LYS:HB2	1.65	0.62
1:B:486:HIS:HB3	1:B:498:ALA:HA	1.82	0.62
1:A:493:PRO:O	1:A:496:ALA:HB3	1.98	0.61
1:B:581:LEU:CD1	1:B:583:ILE:HG12	2.27	0.61
1:A:264:SER:HA	1:A:290:GLN:O	1.99	0.61
1:C:378:MET:HE3	1:C:380:ILE:HD11	1.82	0.61
1:A:41:LYS:HG2	1:A:54:VAL:HA	1.83	0.61
1:C:427:LEU:HD21	1:C:605:VAL:HG13	1.82	0.61
1:D:46:THR:HB	1:D:248:ASN:HD22	1.66	0.61
1:A:548:ASN:ND2	1:A:548:ASN:H	1.99	0.61
1:B:181:LEU:HD12	1:B:242:LEU:HD13	1.81	0.61
1:D:314:LYS:HB3	1:D:340:GLN:HE22	1.66	0.60
1:D:490:GLU:CD	1:D:520:PRO:O	2.40	0.60
1:C:529:MET:HG2	1:C:555:THR:HG21	1.83	0.60
1:A:406:PHE:O	1:A:410:VAL:HG23	2.02	0.60
1:C:426:VAL:O	1:C:430:THR:HG22	2.02	0.60
1:B:374:LEU:HD12	1:B:374:LEU:H	1.67	0.59
1:B:518:LEU:O	1:B:518:LEU:CD2	2.51	0.59
1:D:490:GLU:OE1	1:D:520:PRO:O	2.20	0.59
1:D:510:VAL:HG12	1:D:515:ALA:HA	1.85	0.59
1:D:50:ARG:HD3	1:D:96:VAL:HG22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:ASP:OD2	1:C:359:VAL:HG12	2.03	0.58
1:A:80:GLY:C	1:A:82:ARG:N	2.57	0.58
1:B:181:LEU:HD12	1:B:242:LEU:CD1	2.33	0.58
1:D:357:GLY:HA2	1:D:361:PRO:HA	1.85	0.58
1:C:186:GLY:H	1:C:266:ALA:HB3	1.69	0.58
1:A:121:VAL:HG22	1:A:389:LYS:HE2	1.84	0.58
1:B:514:GLY:O	1:B:516:THR:HG23	2.03	0.58
1:A:505:PRO:HG3	1:A:519:PHE:CD2	2.38	0.58
1:A:546:ASP:OD1	1:A:548:ASN:ND2	2.37	0.58
1:B:278:HIS:ND1	1:B:278:HIS:N	2.51	0.57
1:C:427:LEU:O	1:C:431:ILE:HG23	2.03	0.57
1:A:368:MET:SD	1:A:467:THR:HG23	2.44	0.57
1:A:426:VAL:O	1:A:430:THR:HG22	2.04	0.57
1:D:509:GLY:HA2	1:D:531:SER:OG	2.05	0.57
1:B:579:GLN:HA	1:B:591:ASP:HA	1.86	0.57
3:F:2:NAG:H4	3:F:3:BMA:O2	2.03	0.57
1:C:391:VAL:HG12	1:C:394:SER:HB3	1.85	0.57
1:D:280:SER:HB2	1:D:283:LEU:HB2	1.87	0.57
1:A:538:TRP:O	1:A:541:PHE:HB3	2.04	0.57
1:C:540:ASN:ND2	1:C:550:PRO:HD2	2.18	0.57
3:F:2:NAG:O3	3:F:3:BMA:H2	2.05	0.56
1:D:362:ASP:H	1:D:367:LEU:HD21	1.70	0.56
1:A:185:GLY:O	1:A:266:ALA:HB3	2.05	0.56
1:B:58:LEU:HD21	1:B:199:SER:HB3	1.87	0.56
1:C:381:GLY:HA3	1:C:481:TYR:CD2	2.41	0.56
1:B:400:GLY:O	1:B:401:VAL:HG23	2.06	0.56
1:D:41:LYS:HB3	1:D:42:PRO:HD2	1.88	0.56
1:D:275:ILE:HG23	1:D:376:TYR:HD2	1.71	0.55
1:A:47:ALA:H	1:A:248:ASN:ND2	2.04	0.55
1:B:356:ASP:O	1:B:358:ASP:N	2.40	0.55
1:C:465:VAL:O	1:C:469:LYS:HB2	2.07	0.55
1:C:554:ASP:OD1	1:C:556:LYS:HE2	2.07	0.55
1:B:403:ALA:CA	1:B:406:PHE:HB3	2.36	0.55
1:B:561:LYS:O	1:B:562:PRO:C	2.45	0.55
1:A:98:ASN:HB3	1:A:100:THR:HG22	1.88	0.55
1:C:550:PRO:O	1:C:552:PRO:HD3	2.07	0.55
1:A:427:LEU:O	1:A:431:ILE:HG23	2.07	0.55
1:B:561:LYS:HG3	1:B:562:PRO:CD	2.13	0.55
1:A:540:ASN:OD1	1:A:551:VAL:HG13	2.07	0.54
1:A:224:THR:HG21	1:A:322:SER:HB2	1.89	0.54
1:A:431:ILE:HG22	1:A:600:PHE:HZ	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:GLY:H	1:C:221:PHE:HD2	1.54	0.54
1:C:83:ARG:HD3	1:C:139:GLU:OE1	2.08	0.54
1:B:232:ASN:HD21	1:B:354:VAL:H	1.56	0.54
1:C:264:SER:HA	1:C:290:GLN:O	2.08	0.54
1:D:205:GLY:HA3	1:D:539:THR:HG21	1.89	0.54
1:A:395:ALA:O	1:A:495:TRP:CZ2	2.61	0.54
1:D:272:ASN:HA	1:D:275:ILE:HD12	1.90	0.54
1:B:109:ASN:HB2	1:B:339:ASP:HB3	1.90	0.53
1:C:272:ASN:HA	1:C:275:ILE:HD12	1.91	0.53
1:B:314:LYS:HB3	1:B:340:GLN:NE2	2.24	0.53
1:C:573:PHE:CE2	1:C:578:LYS:HB2	2.43	0.53
1:B:349:ILE:HD13	1:B:349:ILE:H	1.74	0.53
1:C:296:SER:HB3	1:C:299:SER:OG	2.07	0.53
1:C:462:ALA:HB3	1:C:463:PRO:HD3	1.90	0.53
1:B:375:ASN:HB2	1:B:476:SER:CB	2.37	0.53
1:C:78:PRO:HD3	1:C:142:LEU:HD12	1.91	0.53
1:C:93:TRP:CD1	1:C:97:ARG:HG3	2.44	0.53
1:C:513:VAL:HG13	1:C:513:VAL:O	2.09	0.52
1:C:443:ASN:OD1	1:C:446:MET:HB2	2.09	0.52
1:A:395:ALA:O	1:A:495:TRP:HH2	1.90	0.52
1:D:264:SER:HA	1:D:290:GLN:O	2.10	0.52
1:D:540:ASN:OD1	1:D:551:VAL:HG12	2.10	0.52
1:C:381:GLY:HA3	1:C:481:TYR:CE2	2.45	0.52
1:A:144:LEU:HA	1:A:212:LEU:HA	1.91	0.52
1:A:540:ASN:ND2	1:A:549:GLN:O	2.43	0.52
1:C:201:LEU:HB3	1:C:209:VAL:HG21	1.92	0.52
1:A:549:GLN:HB3	1:A:550:PRO:HD2	1.91	0.52
1:D:368:MET:HE2	1:D:470:LEU:HD12	1.92	0.52
1:B:378:MET:HG2	1:B:380:ILE:HG13	1.92	0.52
1:A:459:GLN:HA	1:A:459:GLN:NE2	2.24	0.51
1:B:232:ASN:ND2	1:B:354:VAL:H	2.08	0.51
1:D:58:LEU:HD11	1:D:66:VAL:HG22	1.92	0.51
1:A:236:LEU:CD2	1:A:359:VAL:HG11	2.37	0.51
1:D:381:GLY:HA3	1:D:481:TYR:CE2	2.44	0.51
1:D:412:ASN:O	1:D:416:ASN:ND2	2.44	0.51
1:A:363:ASP:HB3	1:A:366:ILE:HD12	1.93	0.51
1:B:134:VAL:HG12	1:B:134:VAL:O	2.11	0.51
1:A:414:VAL:O	1:A:419:GLY:N	2.44	0.51
1:C:201:LEU:HA	1:C:535:MET:HE3	1.93	0.50
1:D:147:TYR:HE2	1:D:211:THR:HG22	1.76	0.50
1:D:181:LEU:HD23	1:D:245:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:407:ASP:HA	1:D:410:VAL:HG12	1.93	0.50
1:A:46:THR:HB	1:A:248:ASN:HD22	1.74	0.50
1:A:421:PRO:O	1:A:424:LYS:HB3	2.11	0.50
1:A:540:ASN:ND2	1:A:551:VAL:O	2.36	0.50
1:D:66:VAL:HG12	1:D:149:PRO:HA	1.93	0.50
1:C:596:ASN:HD22	1:C:596:ASN:H	1.58	0.50
1:B:107:PRO:HB2	1:B:338:VAL:HG21	1.93	0.50
1:A:342:VAL:O	1:A:342:VAL:HG23	2.11	0.50
1:A:385:GLY:O	1:A:499:ALA:HA	2.11	0.50
1:B:578:LYS:HG3	1:B:592:ASN:HD21	1.77	0.50
1:D:510:VAL:CG1	1:D:515:ALA:HA	2.42	0.50
1:B:385:GLY:HA2	1:B:452:LEU:HD21	1.94	0.50
1:C:551:VAL:HG13	1:C:551:VAL:O	2.12	0.50
1:A:417:LEU:HD13	1:A:458:HIS:CD2	2.47	0.49
1:A:558:ILE:HG22	1:A:559:HIS:HD2	1.77	0.49
1:A:181:LEU:HD12	1:A:183:LEU:HD13	1.93	0.49
1:A:236:LEU:HD21	1:A:359:VAL:CG1	2.40	0.49
1:A:580:TYR:CE1	1:A:590:ARG:HB2	2.47	0.49
1:A:486:HIS:HB3	1:A:498:ALA:HA	1.95	0.49
1:C:181:LEU:HB3	1:C:261:ILE:HG22	1.95	0.49
1:C:340:GLN:O	1:C:341:ASP:HB3	2.13	0.49
1:A:117:ILE:HD12	1:A:117:ILE:H	1.78	0.49
1:A:376:TYR:O	1:A:476:SER:HB3	2.12	0.49
1:A:431:ILE:HG22	1:A:600:PHE:CZ	2.47	0.49
1:B:580:TYR:CZ	1:B:590:ARG:HB3	2.48	0.49
1:D:297:SER:HB3	1:D:459:GLN:HE22	1.78	0.49
1:B:441:ARG:HH22	1:D:578:LYS:HZ2	1.60	0.48
1:C:401:VAL:HG21	1:C:451:LEU:HD12	1.94	0.48
1:C:60:ASN:HD22	1:C:63:LEU:HG	1.77	0.48
1:C:580:TYR:CE1	1:C:590:ARG:HB2	2.48	0.48
1:A:427:LEU:HD21	1:A:605:VAL:HG13	1.94	0.48
1:C:47:ALA:H	1:C:248:ASN:ND2	2.11	0.48
1:A:332:LYS:HB2	1:A:337:LEU:HD13	1.96	0.48
1:A:600:PHE:O	1:A:605:VAL:HG23	2.14	0.48
1:C:108:GLN:H	1:C:137:GLN:HE22	1.59	0.48
1:B:54:VAL:HB	1:B:56:ARG:HD3	1.95	0.48
1:A:221:PHE:HB3	1:A:352:GLY:O	2.14	0.48
1:A:383:ASN:O	1:A:386:GLU:HG2	2.14	0.48
1:A:457:ASP:OD1	1:A:594:ARG:NH2	2.47	0.48
1:A:533:VAL:HA	1:A:553:GLN:HE22	1.79	0.48
1:B:179:VAL:HG21	1:B:249:ILE:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:VAL:HG11	1:A:461:VAL:HA	1.95	0.47
1:D:551:VAL:O	1:D:551:VAL:CG1	2.60	0.47
1:B:314:LYS:HB3	1:B:340:GLN:HE21	1.79	0.47
1:A:290:GLN:HB3	1:A:481:TYR:OH	2.14	0.47
1:A:301:ASN:ND2	1:A:303:GLN:H	2.11	0.47
1:A:368:MET:HB3	1:A:470:LEU:HD13	1.96	0.47
1:A:421:PRO:O	1:A:424:LYS:HB2	2.12	0.47
1:A:183:LEU:HD23	1:A:270:CYS:HB2	1.96	0.47
1:D:105:ALA:HA	1:D:213:ASN:HD21	1.79	0.47
1:A:414:VAL:O	1:A:418:TYR:HB2	2.14	0.47
1:A:438:TRP:HZ3	1:A:441:ARG:HH11	1.61	0.47
1:A:564:ARG:HH12	1:A:586:LYS:HE3	1.79	0.47
1:B:421:PRO:HA	1:B:424:LYS:HB2	1.97	0.47
1:B:305:LEU:HD12	1:B:305:LEU:H	1.79	0.47
1:D:435:TYR:CE2	1:D:454:LEU:HA	2.50	0.47
1:D:574:ASN:HB3	1:D:577:GLU:H	1.79	0.47
1:D:201:LEU:HB3	1:D:209:VAL:HG21	1.96	0.47
1:C:379:LEU:HD12	1:C:479:TYR:HB2	1.97	0.47
1:A:179:VAL:HG21	1:A:249:ILE:HG12	1.96	0.46
1:C:391:VAL:HG11	1:C:448:ARG:HG3	1.97	0.46
1:A:108:GLN:HG2	1:A:137:GLN:HE21	1.76	0.46
1:B:293:THR:OG1	1:B:294:ALA:N	2.49	0.46
1:A:149:PRO:HG2	1:A:177:LYS:HE3	1.96	0.46
1:B:319:ARG:HB2	1:B:325:ALA:HB2	1.98	0.46
1:D:364:PRO:O	1:D:368:MET:HG2	2.16	0.46
1:A:548:ASN:H	1:A:548:ASN:HD22	1.62	0.46
1:D:69:PHE:HB2	1:D:146:LEU:HB2	1.97	0.46
1:D:107:PRO:HG3	1:D:219:LEU:HD13	1.97	0.46
1:A:184:HIS:CE1	1:A:192:THR:HA	2.50	0.46
1:A:418:TYR:O	1:A:420:TYR:HB3	2.16	0.46
1:A:84:PHE:HA	1:A:233:TYR:CE2	2.50	0.46
1:A:114:LEU:C	1:A:116:ALA:H	2.19	0.46
1:B:465:VAL:HG11	1:B:598:VAL:HG11	1.98	0.46
1:B:518:LEU:HD21	1:B:519:PHE:CE1	2.51	0.46
1:D:196:PHE:HE1	1:D:504:LEU:HD11	1.80	0.46
1:A:129:ALA:O	1:A:132:THR:HG22	2.16	0.45
1:A:181:LEU:HD12	1:A:183:LEU:CD1	2.46	0.45
1:A:224:THR:HG22	1:A:305:LEU:HD12	1.97	0.45
1:B:42:PRO:HG2	1:B:67:VAL:HG11	1.98	0.45
1:C:493:PRO:HB3	1:C:495:TRP:CE2	2.50	0.45
1:A:181:LEU:HD11	1:A:212:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:LYS:HG3	1:B:592:ASN:ND2	2.31	0.45
1:C:422:GLU:O	1:C:426:VAL:HB	2.17	0.45
1:D:139:GLU:OE1	1:D:219:LEU:HD21	2.16	0.45
1:A:357:GLY:HA2	1:A:361:PRO:HA	1.99	0.45
1:A:413:PHE:CE1	1:A:417:LEU:HD12	2.52	0.45
1:B:599:ALA:O	1:B:603:GLU:HB2	2.16	0.45
1:C:243:ARG:HG2	1:C:283:LEU:HD21	1.98	0.45
1:D:346:ARG:HG2	1:D:416:ASN:ND2	2.31	0.45
1:A:69:PHE:HB2	1:A:146:LEU:HB2	1.97	0.45
1:B:581:LEU:HD13	1:B:583:ILE:CG1	2.39	0.45
1:C:457:ASP:OD1	1:C:597:LYS:HB3	2.17	0.45
1:C:460:TRP:C	1:C:463:PRO:HD2	2.36	0.45
1:B:444:GLY:O	1:B:447:ARG:HB2	2.17	0.45
1:D:67:VAL:HB	1:D:148:VAL:HG23	1.99	0.45
1:D:587:PRO:O	1:D:588:ARG:HG3	2.17	0.45
1:B:264:SER:HB2	1:B:290:GLN:HB2	1.99	0.45
1:C:217:GLY:HA2	1:C:221:PHE:HB2	1.99	0.45
1:D:148:VAL:HG12	1:D:208:ILE:HG12	1.98	0.45
1:A:262:PHE:HB2	1:A:288:ILE:HB	1.99	0.45
1:D:359:VAL:HG13	1:D:360:VAL:HG23	1.99	0.45
1:A:510:VAL:N	1:A:511:PRO:CD	2.80	0.45
1:D:516:THR:HG22	1:D:517:ASP:H	1.81	0.45
1:C:93:TRP:HA	1:C:94:PRO:HD3	1.86	0.44
1:A:53:GLY:HA2	1:A:99:ALA:O	2.17	0.44
1:B:300:VAL:C	1:B:349:ILE:HD11	2.38	0.44
1:B:585:LEU:H	1:B:585:LEU:HD22	1.82	0.44
1:C:75:ALA:HB3	1:C:142:LEU:HD13	2.00	0.44
1:D:122:TRP:CD1	1:D:122:TRP:C	2.91	0.44
1:C:51:VAL:HG12	1:C:97:ARG:HB2	1.98	0.44
1:C:83:ARG:HG2	1:C:84:PHE:CD2	2.53	0.44
1:C:300:VAL:HG13	1:C:302:TYR:HE2	1.81	0.44
1:C:489:ALA:HA	1:C:521:CYS:HB3	1.98	0.44
1:A:86:PRO:HB3	1:A:236:LEU:HD13	1.98	0.44
1:A:548:ASN:ND2	1:A:548:ASN:N	2.65	0.44
1:C:398:GLU:C	1:C:400:GLY:H	2.21	0.44
1:D:293:THR:OG1	1:D:294:ALA:N	2.50	0.44
1:C:114:LEU:H	1:C:114:LEU:CD2	2.31	0.44
1:D:256:PRO:HA	1:D:259:ILE:HD11	2.00	0.44
1:D:585:LEU:HD22	1:D:585:LEU:H	1.82	0.44
1:A:181:LEU:HD13	1:A:182:PHE:N	2.32	0.44
1:A:187:SER:O	1:A:188:TYR:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ARG:HB3	1:A:220:GLY:CA	2.48	0.44
1:A:384:GLN:HB2	1:A:484:TYR:CD1	2.53	0.44
1:A:406:PHE:CE1	1:A:451:LEU:HG	2.52	0.44
1:A:581:LEU:CD1	1:A:583:ILE:HG12	2.48	0.44
1:C:518:LEU:O	1:C:520:PRO:HD3	2.18	0.44
1:A:371:GLY:HA2	1:A:373:PHE:CE2	2.52	0.44
1:B:338:VAL:HG12	1:B:339:ASP:N	2.33	0.44
1:B:462:ALA:HB3	1:B:463:PRO:HD3	2.00	0.44
1:C:482:THR:HG21	1:C:593:TYR:CE1	2.53	0.44
1:A:144:LEU:H	1:A:144:LEU:HG	1.64	0.43
1:B:55:ARG:O	1:B:56:ARG:HD2	2.17	0.43
1:C:280:SER:HA	1:C:283:LEU:HD13	1.99	0.43
1:C:376:TYR:O	1:C:476:SER:OG	2.33	0.43
1:C:410:VAL:HG11	1:C:432:LYS:HG2	2.00	0.43
1:A:151:GLU:HG3	1:A:155:LEU:HD11	2.01	0.43
1:B:176:LYS:O	1:B:258:ARG:NH2	2.51	0.43
1:B:259:ILE:H	1:B:285:GLN:NE2	2.16	0.43
1:B:445:GLU:HB2	1:B:446:MET:HE1	2.00	0.43
1:B:461:VAL:CG2	1:B:462:ALA:N	2.81	0.43
1:C:383:ASN:HB2	1:C:386:GLU:HG2	2.00	0.43
1:D:102:LEU:HD12	1:D:102:LEU:H	1.83	0.43
1:A:181:LEU:HB3	1:A:261:ILE:HG22	2.00	0.43
1:A:379:LEU:CD2	1:A:481:TYR:HD2	2.31	0.43
1:B:369:GLN:C	1:B:371:GLY:H	2.22	0.43
1:C:510:VAL:N	1:C:511:PRO:CD	2.81	0.43
1:D:381:GLY:HA3	1:D:481:TYR:CD2	2.54	0.43
3:F:2:NAG:H4	3:F:3:BMA:HO2	1.83	0.43
1:A:144:LEU:HD22	1:A:245:LEU:HD11	2.00	0.43
1:B:554:ASP:O	1:B:556:LYS:N	2.50	0.43
1:D:255:ASP:C	1:D:257:GLU:H	2.22	0.43
1:D:564:ARG:HB3	1:D:587:PRO:HG2	2.01	0.43
1:A:215:ARG:HB3	1:A:220:GLY:HA2	2.00	0.43
1:B:278:HIS:CE1	1:B:361:PRO:HG3	2.54	0.43
1:C:504:LEU:N	1:C:505:PRO:HD2	2.34	0.43
1:A:301:ASN:HB2	1:A:349:ILE:HG13	2.01	0.43
1:A:573:PHE:CZ	1:A:578:LYS:HG2	2.54	0.43
1:B:383:ASN:HB2	1:B:386:GLU:HG2	2.00	0.43
1:C:232:ASN:HD21	1:C:354:VAL:H	1.65	0.43
1:D:46:THR:HB	1:D:248:ASN:ND2	2.33	0.43
1:A:421:PRO:O	1:A:424:LYS:CA	2.64	0.43
1:B:481:TYR:CD1	1:B:481:TYR:C	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:VAL:O	1:A:413:PHE:HB3	2.19	0.43
1:A:193:GLY:H	1:A:213:ASN:ND2	2.16	0.43
1:C:430:THR:HG21	1:C:608:LEU:HD13	2.01	0.43
1:D:457:ASP:HA	1:D:461:VAL:HB	2.00	0.43
1:A:566:GLU:OE2	1:A:566:GLU:HA	2.19	0.42
1:A:388:LEU:HA	1:A:452:LEU:HD11	2.01	0.42
1:A:605:VAL:N	1:A:606:PRO:HD2	2.34	0.42
1:B:272:ASN:HA	1:B:275:ILE:HD12	2.02	0.42
1:C:264:SER:HB2	1:C:290:GLN:HE21	1.83	0.42
1:A:378:MET:HE2	1:A:380:ILE:HD11	2.01	0.42
1:B:81:ALA:HA	1:B:330:ARG:HD3	2.00	0.42
1:B:514:GLY:O	1:B:516:THR:CG2	2.68	0.42
1:C:288:ILE:HD13	1:C:538:TRP:CD1	2.54	0.42
1:D:278:HIS:HB2	1:D:361:PRO:HG3	2.01	0.42
1:A:504:LEU:O	1:A:505:PRO:C	2.57	0.42
1:B:262:PHE:HB2	1:B:288:ILE:HB	2.02	0.42
1:C:93:TRP:CE2	1:C:97:ARG:HD2	2.54	0.42
1:D:540:ASN:HD21	1:D:551:VAL:HG12	1.84	0.42
1:A:242:LEU:HD12	1:A:242:LEU:HA	1.94	0.42
1:D:280:SER:HA	1:D:283:LEU:HD13	2.01	0.42
1:A:44:VAL:HG12	1:A:69:PHE:CZ	2.55	0.42
1:A:375:ASN:HA	1:A:476:SER:OG	2.18	0.42
1:C:565:PHE:CE2	1:C:587:PRO:HB3	2.54	0.42
1:A:414:VAL:HG23	1:A:424:LYS:HE2	2.02	0.42
1:C:84:PHE:HE1	1:C:222:LEU:HB3	1.84	0.42
3:F:2:NAG:O3	3:F:3:BMA:C2	2.68	0.42
1:A:262:PHE:CB	1:A:288:ILE:HB	2.50	0.42
1:D:135:GLN:HG3	1:D:136:ASN:HD22	1.84	0.42
1:D:414:VAL:HG21	1:D:428:ARG:HG2	2.02	0.42
1:C:559:HIS:CD2	1:C:561:LYS:HB2	2.49	0.42
1:D:585:LEU:O	1:D:587:PRO:HD3	2.20	0.42
1:C:176:LYS:HB3	1:C:255:ASP:HB2	2.02	0.41
1:A:380:ILE:O	1:A:480:PHE:HA	2.20	0.41
1:A:420:TYR:O	1:A:420:TYR:CD1	2.73	0.41
1:B:363:ASP:HB2	1:B:366:ILE:HD12	2.01	0.41
1:C:459:GLN:O	1:C:463:PRO:HG2	2.20	0.41
1:C:581:LEU:HD12	1:C:583:ILE:HG12	2.02	0.41
1:D:344:PRO:HB3	1:D:350:ALA:N	2.35	0.41
1:B:79:LEU:HD23	1:B:79:LEU:HA	1.94	0.41
1:A:266:ALA:O	1:A:269:SER:HB2	2.20	0.41
1:B:546:ASP:HA	1:B:547:PRO:HD3	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:PHE:CE1	1:D:504:LEU:HD11	2.55	0.41
1:D:345:ALA:HB3	1:D:348:HIS:HB2	2.02	0.41
1:D:363:ASP:HB3	1:D:366:ILE:HD12	2.03	0.41
1:D:364:PRO:HA	1:D:367:LEU:HD12	2.03	0.41
1:B:326:VAL:HA	1:B:329:LEU:HD12	2.03	0.41
1:B:385:GLY:O	1:B:499:ALA:HA	2.21	0.41
1:C:580:TYR:CZ	1:C:590:ARG:HB2	2.56	0.41
1:A:182:PHE:HB3	1:A:211:THR:HG22	2.02	0.41
1:A:525:LYS:HD2	1:A:559:HIS:NE2	2.36	0.41
1:B:504:LEU:N	1:B:505:PRO:HD2	2.36	0.41
1:C:78:PRO:HA	1:C:82:ARG:HB2	2.03	0.41
1:D:236:LEU:O	1:D:240:GLN:HB2	2.19	0.41
1:A:192:THR:C	1:A:194:ASN:N	2.73	0.41
1:A:275:ILE:HA	1:A:376:TYR:HE2	1.86	0.41
1:A:522:ASN:HD22	1:A:522:ASN:HA	1.56	0.41
1:B:492:ARG:H	1:B:492:ARG:HG2	1.74	0.41
1:C:93:TRP:CD2	1:C:97:ARG:HD2	2.56	0.41
1:C:288:ILE:HG21	1:C:538:TRP:NE1	2.35	0.41
1:C:556:LYS:HB2	1:C:560:THR:HG22	2.02	0.41
1:D:275:ILE:HG23	1:D:376:TYR:CD2	2.52	0.41
1:A:60:ASN:OD1	1:A:61:GLU:N	2.54	0.41
1:A:458:HIS:CD2	1:A:459:GLN:NE2	2.89	0.41
1:B:549:GLN:HA	1:B:550:PRO:HA	1.71	0.41
1:C:43:VAL:HA	1:C:51:VAL:O	2.21	0.41
1:C:182:PHE:HB2	1:C:262:PHE:CE2	2.56	0.41
1:C:259:ILE:H	1:C:285:GLN:NE2	2.19	0.41
1:A:43:VAL:HA	1:A:51:VAL:O	2.21	0.41
1:A:188:TYR:CE2	1:A:349:ILE:HD13	2.56	0.41
1:A:585:LEU:HD12	1:A:585:LEU:HA	1.81	0.41
1:D:85:GLN:HG3	1:D:86:PRO:HD2	2.02	0.41
1:A:231:GLY:HA2	1:A:233:TYR:CE2	2.56	0.40
1:B:311:LEU:HD22	1:B:340:GLN:HG2	2.03	0.40
1:B:456:THR:HA	1:B:460:TRP:CE3	2.56	0.40
1:C:380:ILE:O	1:C:480:PHE:HA	2.22	0.40
1:A:44:VAL:HG11	1:A:252:PHE:CD2	2.56	0.40
1:A:540:ASN:HB3	1:A:549:GLN:O	2.22	0.40
1:B:293:THR:HG23	1:B:296:SER:OG	2.21	0.40
1:B:315:VAL:O	1:B:332:LYS:NZ	2.55	0.40
1:C:307:TYR:CE2	1:C:344:PRO:HA	2.55	0.40
1:D:504:LEU:N	1:D:505:PRO:HD2	2.37	0.40
1:B:58:LEU:HD13	1:B:58:LEU:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:TYR:CZ	1:A:90:PRO:HD2	2.57	0.40
1:A:200:VAL:HG12	1:A:535:MET:HE1	2.03	0.40
1:A:331:ARG:HE	1:A:331:ARG:HB2	1.70	0.40
1:A:392:GLU:HA	1:A:395:ALA:HB2	2.04	0.40
1:B:293:THR:O	1:B:299:SER:OG	2.38	0.40
1:B:513:VAL:CG1	1:B:514:GLY:N	2.85	0.40
1:C:456:THR:HA	1:C:460:TRP:HE3	1.86	0.40
1:D:293:THR:HG21	1:D:463:PRO:CB	2.51	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	552/580 (95%)	490 (89%)	56 (10%)	6 (1%)	14	45
1	B	542/580 (93%)	467 (86%)	66 (12%)	9 (2%)	9	35
1	C	541/580 (93%)	469 (87%)	67 (12%)	5 (1%)	17	48
1	D	535/580 (92%)	456 (85%)	67 (12%)	12 (2%)	6	30
All	All	2170/2320 (94%)	1882 (87%)	256 (12%)	32 (2%)	10	38

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	550	PRO
1	B	357	GLY
1	C	550	PRO
1	D	94	PRO
1	D	550	PRO
1	B	217	GLY
1	B	279	HIS

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Mol	Chain	Res	Type
1	B	371	GLY
1	B	399	ASP
1	B	562	PRO
1	D	42	PRO
1	D	491	GLY
1	D	515	ALA
1	A	420	TYR
1	C	562	PRO
1	D	361	PRO
1	A	386	GLU
1	A	520	PRO
1	B	375	ASN
1	B	550	PRO
1	B	555	THR
1	C	419	GLY
1	D	441	ARG
1	D	475	GLN
1	D	95	GLY
1	A	81	ALA
1	C	217	GLY
1	D	423	GLY
1	C	225	GLY
1	A	112	GLY
1	D	43	VAL
1	D	520	PRO

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	462/488 (95%)	413 (89%)	49 (11%)	6 25
1	B	454/488 (93%)	388 (86%)	66 (14%)	3 14
1	C	454/488 (93%)	415 (91%)	39 (9%)	10 35
1	D	450/488 (92%)	402 (89%)	48 (11%)	6 25
All	All	1820/1952 (93%)	1618 (89%)	202 (11%)	6 23

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	VAL
1	A	44	VAL
1	A	58	LEU
1	A	72	VAL
1	A	110	LEU
1	A	117	ILE
1	A	132	THR
1	A	144	LEU
1	A	190	GLU
1	A	224	THR
1	A	242	LEU
1	A	280	SER
1	A	283	LEU
1	A	298	TRP
1	A	300	VAL
1	A	305	LEU
1	A	331	ARG
1	A	335	ARG
1	A	342	VAL
1	A	370	GLN
1	A	379	LEU
1	A	380	ILE
1	A	396	GLU
1	A	398	GLU
1	A	407	ASP
1	A	409	THR
1	A	422	GLU
1	A	425	ASP
1	A	427	LEU
1	A	440	ASP
1	A	445	GLU
1	A	461	VAL
1	A	482	THR
1	A	494	GLU
1	A	504	LEU
1	A	518	LEU
1	A	522	ASN
1	A	536	THR
1	A	538	TRP
1	A	548	ASN
1	A	549	GLN
1	A	551	VAL

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Mol	Chain	Res	Type
1	A	559	HIS
1	A	577	GLU
1	A	581	LEU
1	A	585	LEU
1	A	588	ARG
1	A	591	ASP
1	A	607	HIS
1	B	43	VAL
1	B	51	VAL
1	B	54	VAL
1	B	58	LEU
1	B	76	THR
1	B	117	ILE
1	B	146	LEU
1	B	181	LEU
1	B	189	MET
1	B	190	GLU
1	B	200	VAL
1	B	201	LEU
1	B	213	ASN
1	B	215	ARG
1	B	219	LEU
1	B	224	THR
1	B	226	ASP
1	B	240	GLN
1	B	242	LEU
1	B	245	LEU
1	B	259	ILE
1	B	261	ILE
1	B	278	HIS
1	B	285	GLN
1	B	293	THR
1	B	298	TRP
1	B	300	VAL
1	B	305	LEU
1	B	309	ARG
1	B	311	LEU
1	B	335	ARG
1	B	337	LEU
1	B	339	ASP
1	B	346	ARG
1	B	349	ILE

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Mol	Chain	Res	Type
1	B	356	ASP
1	B	374	LEU
1	B	375	ASN
1	B	417	LEU
1	B	424	LYS
1	B	427	LEU
1	B	431	ILE
1	B	436	THR
1	B	441	ARG
1	B	443	ASN
1	B	446	MET
1	B	447	ARG
1	B	450	THR
1	B	461	VAL
1	B	481	TYR
1	B	482	THR
1	B	492	ARG
1	B	504	LEU
1	B	510	VAL
1	B	517	ASP
1	B	518	LEU
1	B	519	PHE
1	B	521	CYS
1	B	525	LYS
1	B	540	ASN
1	B	556	LYS
1	B	569	VAL
1	B	581	LEU
1	B	588	ARG
1	B	589	VAL
1	B	592	ASN
1	C	50	ARG
1	C	55	ARG
1	C	59	ASN
1	C	70	LEU
1	C	76	THR
1	C	114	LEU
1	C	117	ILE
1	C	176	LYS
1	C	190	GLU
1	C	195	MET
1	C	201	LEU

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Mol	Chain	Res	Type
1	C	212	LEU
1	C	218	VAL
1	C	239	ILE
1	C	272	ASN
1	C	285	GLN
1	C	300	VAL
1	C	305	LEU
1	C	308	THR
1	C	335	ARG
1	C	388	LEU
1	C	393	ASP
1	C	446	MET
1	C	447	ARG
1	C	454	LEU
1	C	457	ASP
1	C	469	LYS
1	C	470	LEU
1	C	495	TRP
1	C	517	ASP
1	C	518	LEU
1	C	525	LYS
1	C	544	THR
1	C	549	GLN
1	C	555	THR
1	C	567	GLU
1	C	581	LEU
1	C	590	ARG
1	C	596	ASN
1	D	63	LEU
1	D	72	VAL
1	D	76	THR
1	D	82	ARG
1	D	98	ASN
1	D	122	TRP
1	D	135	GLN
1	D	139	GLU
1	D	181	LEU
1	D	183	LEU
1	D	190	GLU
1	D	199	SER
1	D	212	LEU
1	D	219	LEU

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Mol	Chain	Res	Type
1	D	226	ASP
1	D	240	GLN
1	D	272	ASN
1	D	276	LEU
1	D	285	GLN
1	D	298	TRP
1	D	300	VAL
1	D	308	THR
1	D	311	LEU
1	D	319	ARG
1	D	332	LYS
1	D	342	VAL
1	D	373	PHE
1	D	377	ASP
1	D	388	LEU
1	D	399	ASP
1	D	415	ASP
1	D	424	LYS
1	D	425	ASP
1	D	428	ARG
1	D	443	ASN
1	D	467	THR
1	D	481	TYR
1	D	487	CYS
1	D	492	ARG
1	D	516	THR
1	D	521	CYS
1	D	538	TRP
1	D	553	GLN
1	D	574	ASN
1	D	578	LYS
1	D	581	LEU
1	D	590	ARG
1	D	604	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	184	HIS
1	A	213	ASN
1	A	248	ASN

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Mol	Chain	Res	Type
1	A	272	ASN
1	A	303	GLN
1	A	340	GLN
1	A	384	GLN
1	A	412	ASN
1	A	416	ASN
1	A	458	HIS
1	A	459	GLN
1	A	471	HIS
1	A	522	ASN
1	A	553	GLN
1	A	559	HIS
1	B	68	GLN
1	B	206	ASN
1	B	227	GLN
1	B	232	ASN
1	B	272	ASN
1	B	285	GLN
1	B	303	GLN
1	B	340	GLN
1	B	375	ASN
1	B	384	GLN
1	B	459	GLN
1	B	540	ASN
1	B	559	HIS
1	B	592	ASN
1	C	59	ASN
1	C	60	ASN
1	C	136	ASN
1	C	137	GLN
1	C	238	GLN
1	C	248	ASN
1	C	279	HIS
1	C	285	GLN
1	C	340	GLN
1	C	348	HIS
1	C	384	GLN
1	C	458	HIS
1	C	540	ASN
1	C	553	GLN
1	C	559	HIS
1	C	563	ASN

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Mol	Chain	Res	Type
1	C	596	ASN
1	D	68	GLN
1	D	98	ASN
1	D	136	ASN
1	D	248	ASN
1	D	285	GLN
1	D	340	GLN
1	D	369	GLN
1	D	416	ASN
1	D	458	HIS
1	D	459	GLN
1	D	553	GLN
1	D	574	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

10 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	E	1	1,2	14,14,15	0.63	0	17,19,21	1.24	2 (11%)
2	NAG	E	2	2	14,14,15	0.55	0	17,19,21	1.25	3 (17%)
2	MAN	E	3	2	11,11,12	0.67	0	15,15,17	0.76	1 (6%)
3	NAG	F	1	1,3	14,14,15	1.16	1 (7%)	17,19,21	1.16	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	F	2	3	14,14,15	0.51	0	17,19,21	1.48	3 (17%)
3	BMA	F	3	3	11,11,12	0.91	0	15,15,17	1.92	2 (13%)
3	MAN	F	4	3	11,11,12	0.68	0	15,15,17	2.56	6 (40%)
3	MAN	F	5	3	11,11,12	0.58	0	15,15,17	2.09	1 (6%)
3	MAN	F	6	3	11,11,12	0.63	0	15,15,17	1.78	3 (20%)
3	MAN	F	7	3	11,11,12	0.85	0	15,15,17	2.45	4 (26%)

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	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
2	MAN	E	3	2	1/1/4/5	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	MAN	F	5	3	-	2/2/19/22	0/1/1/1
3	MAN	F	6	3	-	0/2/19/22	0/1/1/1
3	MAN	F	7	3	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	NAG	O5-C1	-3.94	1.37	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	5	MAN	C1-O5-C5	7.10	121.71	112.19
3	F	4	MAN	C1-O5-C5	6.18	120.47	112.19
3	F	7	MAN	C3-C4-C5	5.70	120.57	110.23
3	F	3	BMA	C3-C4-C5	-5.70	99.90	110.23
3	F	6	MAN	C1-O5-C5	5.48	119.54	112.19
3	F	7	MAN	C1-C2-C3	-4.80	102.65	109.64
3	F	4	MAN	C1-C2-C3	3.71	115.04	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	7	MAN	O4-C4-C3	-3.58	101.93	110.38
3	F	4	MAN	C3-C4-C5	3.56	116.68	110.23
3	F	4	MAN	O3-C3-C2	-3.49	102.93	110.05
3	F	7	MAN	C1-O5-C5	3.14	116.39	112.19
3	F	2	NAG	O3-C3-C2	-3.11	102.95	109.40
3	F	3	BMA	O6-C6-C5	-3.07	100.88	111.33
2	E	1	NAG	C4-C3-C2	2.89	115.25	111.02
3	F	2	NAG	C1-O5-C5	2.88	116.05	112.19
3	F	2	NAG	C4-C3-C2	2.87	115.22	111.02
3	F	4	MAN	O5-C1-C2	2.76	117.37	110.79
3	F	1	NAG	C1-O5-C5	2.70	115.81	112.19
3	F	6	MAN	O5-C5-C6	2.58	112.69	107.66
2	E	2	NAG	O5-C1-C2	-2.49	107.44	111.29
3	F	4	MAN	O5-C5-C6	2.30	112.14	107.66
2	E	2	NAG	C1-C2-N2	2.26	114.00	110.43
2	E	2	NAG	C4-C3-C2	-2.23	107.75	111.02
2	E	1	NAG	O4-C4-C3	-2.18	105.24	110.38
2	E	3	MAN	O5-C5-C6	2.05	111.66	107.66
3	F	6	MAN	C3-C4-C5	2.00	113.86	110.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	3	MAN	C1

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	E	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
3	F	5	MAN	C4-C5-C6-O6
3	F	5	MAN	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	F	7	MAN	C4-C5-C6-O6
3	F	2	NAG	C8-C7-N2-C2
3	F	7	MAN	O5-C5-C6-O6
3	F	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2

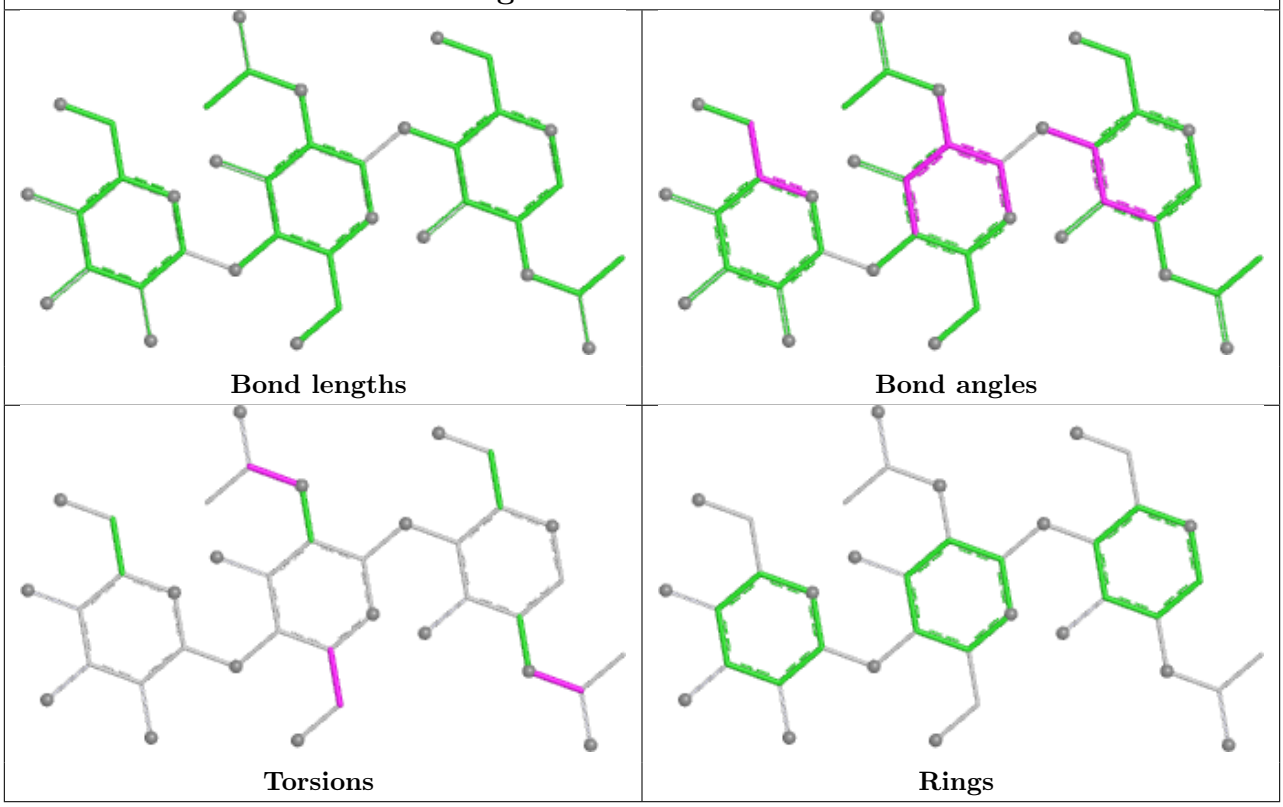
There are no ring outliers.

2 monomers are involved in 4 short contacts:

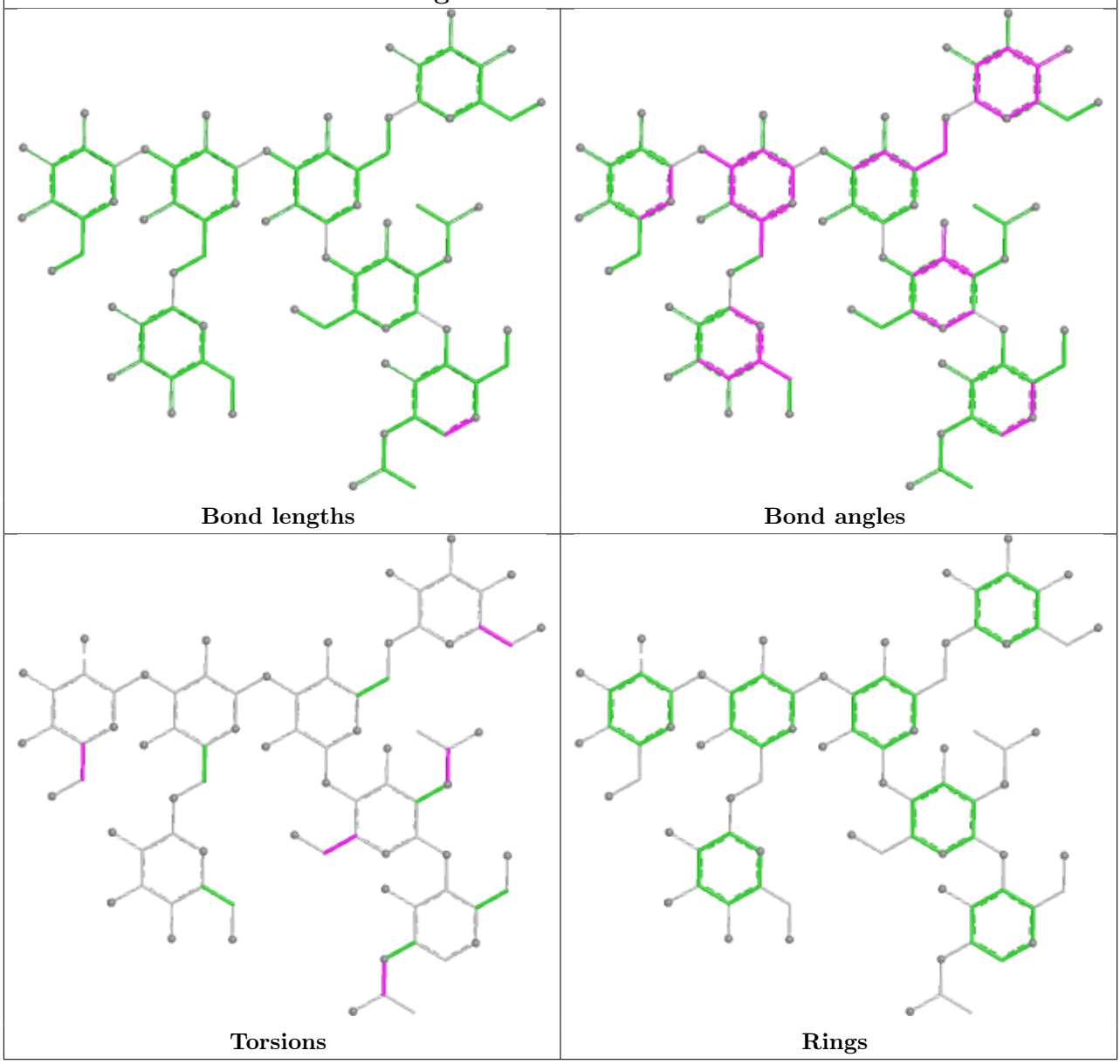
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	3	BMA	4	0
3	F	2	NAG	4	0

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

Oligosaccharide Chain E



Oligosaccharide Chain F



5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	710	-	14,14,15	0.69	0	17,19,21	1.29	1 (5%)
4	NAG	B	810	1	14,14,15	0.71	0	17,19,21	1.40	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
4	NAG	A	710	-	-	4/6/23/26	0/1/1/1
4	NAG	B	810	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	810	NAG	C4-C3-C2	4.42	117.50	111.02
4	A	710	NAG	C4-C3-C2	3.98	116.85	111.02
4	B	810	NAG	C3-C4-C5	2.59	114.94	110.23

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	710	NAG	C8-C7-N2-C2
4	A	710	NAG	O7-C7-N2-C2
4	B	810	NAG	C8-C7-N2-C2
4	B	810	NAG	O7-C7-N2-C2
4	B	810	NAG	C4-C5-C6-O6
4	A	710	NAG	C4-C5-C6-O6
4	B	810	NAG	O5-C5-C6-O6
4	A	710	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	556/580 (95%)	0.27	24 (4%) 35 34	37, 122, 137, 148	0
1	B	546/580 (94%)	0.66	55 (10%) 7 6	33, 127, 137, 145	0
1	C	545/580 (93%)	0.53	44 (8%) 12 11	33, 123, 134, 139	0
1	D	541/580 (93%)	1.12	126 (23%) 0 1	34, 130, 138, 152	0
All	All	2188/2320 (94%)	0.64	249 (11%) 5 4	33, 126, 137, 152	0

All (249) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	557	PHE	8.2
1	C	92	SER	7.1
1	C	91	ALA	6.9
1	D	57	GLU	6.8
1	D	437	ASP	6.4
1	D	493	PRO	6.0
1	B	558	ILE	5.9
1	D	421	PRO	5.9
1	D	343	GLN	5.8
1	D	54	VAL	5.8
1	D	263	GLY	5.5
1	D	317	CYS	5.4
1	C	560	THR	5.4
1	D	318	ASP	5.0
1	D	264	SER	4.9
1	D	423	GLY	4.8
1	D	473	ASP	4.7
1	D	132	THR	4.7
1	C	59	ASN	4.6
1	B	555	THR	4.6
1	D	528	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	408	PHE	4.5
1	D	292	GLY	4.5
1	D	424	LYS	4.4
1	D	596	ASN	4.3
1	A	420	TYR	4.3
1	D	111	HIS	4.3
1	D	53	GLY	4.2
1	D	446	MET	4.2
1	D	223	SER	4.2
1	D	416	ASN	4.2
1	B	517	ASP	4.1
1	D	488	GLN	4.0
1	B	290	GLN	4.0
1	B	268	ALA	4.0
1	C	291	SER	4.0
1	C	264	SER	4.0
1	D	372	GLU	3.9
1	D	303	GLN	3.9
1	D	182	PHE	3.9
1	A	92	SER	3.8
1	D	489	ALA	3.8
1	A	156	THR	3.8
1	B	395	ALA	3.7
1	D	370	GLN	3.7
1	D	389	LYS	3.7
1	C	362	ASP	3.7
1	C	96	VAL	3.7
1	B	264	SER	3.6
1	D	276	LEU	3.6
1	D	228	ALA	3.6
1	D	65	PRO	3.6
1	D	342	VAL	3.6
1	B	492	ARG	3.6
1	A	424	LYS	3.6
1	D	214	TYR	3.6
1	B	408	PHE	3.6
1	B	175	GLY	3.5
1	D	127	LEU	3.4
1	B	518	LEU	3.4
1	D	445	GLU	3.4
1	D	135	GLN	3.4
1	A	185	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	476	SER	3.3
1	D	265	GLY	3.3
1	C	55	ARG	3.3
1	D	129	ALA	3.3
1	B	420	TYR	3.3
1	D	291	SER	3.3
1	C	576	LYS	3.3
1	C	610	ASN	3.2
1	D	495	TRP	3.2
1	B	561	LYS	3.2
1	D	439	ALA	3.2
1	B	292	GLY	3.2
1	D	575	SER	3.2
1	D	470	LEU	3.2
1	A	423	GLY	3.1
1	B	493	PRO	3.1
1	D	224	THR	3.1
1	A	40	GLN	3.1
1	D	425	ASP	3.1
1	C	53	GLY	3.1
1	B	490	GLU	3.1
1	B	554	ASP	3.1
1	D	412	ASN	3.1
1	B	405	ALA	3.1
1	D	548	ASN	3.0
1	B	396	GLU	3.0
1	A	557	PHE	3.0
1	D	467	THR	3.0
1	B	596	ASN	3.0
1	D	591	ASP	3.0
1	B	223	SER	3.0
1	B	217	GLY	2.9
1	D	226	ASP	2.9
1	B	550	PRO	2.9
1	D	211	THR	2.9
1	D	253	GLY	2.9
1	C	565	PHE	2.9
1	C	370	GLN	2.9
1	D	492	ARG	2.9
1	D	267	GLY	2.9
1	B	291	SER	2.8
1	B	110	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	392	GLU	2.8
1	A	556	LYS	2.8
1	C	128	GLU	2.8
1	D	131	ALA	2.8
1	C	567	GLU	2.8
1	D	234	GLY	2.8
1	C	182	PHE	2.7
1	D	409	THR	2.7
1	B	562	PRO	2.7
1	D	184	HIS	2.7
1	B	588	ARG	2.7
1	D	381	GLY	2.7
1	C	290	GLN	2.7
1	C	265	GLY	2.7
1	C	588	ARG	2.7
1	D	270	CYS	2.7
1	D	130	ALA	2.7
1	D	319	ARG	2.7
1	B	496	ALA	2.6
1	D	42	PRO	2.6
1	D	511	PRO	2.6
1	A	291	SER	2.6
1	C	97	ARG	2.6
1	D	396	GLU	2.6
1	D	288	ILE	2.6
1	D	499	ALA	2.6
1	A	398	GLU	2.6
1	C	234	GLY	2.6
1	D	344	PRO	2.6
1	B	560	THR	2.6
1	D	231	GLY	2.6
1	B	571	SER	2.6
1	C	210	VAL	2.6
1	B	557	PHE	2.6
1	B	397	SER	2.6
1	D	576	LYS	2.5
1	C	372	GLU	2.5
1	D	438	TRP	2.5
1	B	112	GLY	2.5
1	A	421	PRO	2.5
1	C	531	SER	2.5
1	B	265	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	562	PRO	2.5
1	D	474	TYR	2.5
1	D	45	ASN	2.5
1	B	407	ASP	2.5
1	D	268	ALA	2.5
1	A	265	GLY	2.5
1	B	269	SER	2.5
1	C	562	PRO	2.5
1	B	495	TRP	2.5
1	D	610	ASN	2.5
1	D	484	TYR	2.5
1	C	329	LEU	2.5
1	D	66	VAL	2.5
1	B	303	GLN	2.5
1	D	422	GLU	2.4
1	D	79	LEU	2.4
1	D	128	GLU	2.4
1	D	361	PRO	2.4
1	D	77	PRO	2.4
1	D	420	TYR	2.4
1	B	62	ILE	2.4
1	C	213	ASN	2.4
1	D	60	ASN	2.4
1	D	331	ARG	2.4
1	D	400	GLY	2.4
1	D	501	GLY	2.4
1	D	550	PRO	2.4
1	D	490	GLU	2.4
1	D	549	GLN	2.4
1	A	490	GLU	2.3
1	C	292	GLY	2.3
1	B	263	GLY	2.3
1	C	268	ALA	2.3
1	D	569	VAL	2.3
1	C	421	PRO	2.3
1	D	518	LEU	2.3
1	D	313	ALA	2.3
1	D	517	ASP	2.3
1	C	361	PRO	2.3
1	A	264	SER	2.3
1	A	263	GLY	2.3
1	C	269	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	61	GLU	2.3
1	A	135	GLN	2.3
1	D	573	PHE	2.3
1	D	269	SER	2.2
1	B	185	GLY	2.2
1	C	184	HIS	2.2
1	D	500	HIS	2.2
1	D	368	MET	2.2
1	C	134	VAL	2.2
1	C	381	GLY	2.2
1	C	558	ILE	2.2
1	B	267	GLY	2.2
1	C	110	LEU	2.2
1	D	123	PHE	2.2
1	C	226	ASP	2.2
1	D	58	LEU	2.2
1	C	371	GLY	2.2
1	A	585	LEU	2.2
1	D	362	ASP	2.2
1	D	502	ASP	2.2
1	D	220	GLY	2.2
1	D	181	LEU	2.2
1	C	369	GLN	2.2
1	D	252	PHE	2.2
1	B	216	LEU	2.2
1	B	515	ALA	2.2
1	D	204	TYR	2.2
1	A	134	VAL	2.2
1	C	186	GLY	2.2
1	D	334	SER	2.1
1	D	87	PRO	2.1
1	C	373	PHE	2.1
1	A	320	GLU	2.1
1	D	197	ASP	2.1
1	D	136	ASN	2.1
1	B	73	PRO	2.1
1	B	174	SER	2.1
1	B	373	PHE	2.1
1	B	113	ALA	2.1
1	D	62	ILE	2.1
1	D	609	HIS	2.1
1	B	564	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	215	ARG	2.1
1	B	494	GLU	2.1
1	D	307	TYR	2.1
1	A	155	LEU	2.1
1	D	316	GLY	2.1
1	D	436	THR	2.1
1	B	355	VAL	2.1
1	D	391	VAL	2.1
1	C	225	GLY	2.1
1	D	262	PHE	2.0
1	A	471	HIS	2.0
1	B	591	ASP	2.0
1	D	251	HIS	2.0
1	D	110	LEU	2.0
1	B	182	PHE	2.0
1	A	495	TRP	2.0
1	D	287	ALA	2.0
1	D	366	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)

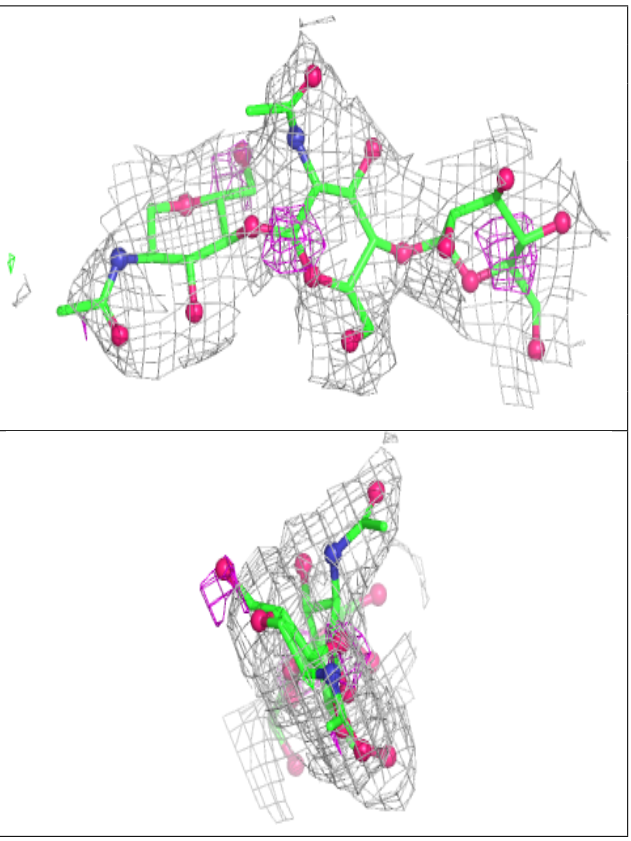
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MAN	E	3	11/12	0.56	0.40	155,157,157,157	0
3	MAN	F	5	11/12	0.74	0.46	112,113,113,114	0
2	NAG	E	2	14/15	0.81	0.46	148,149,151,153	0
3	MAN	F	6	11/12	0.81	0.37	112,113,115,115	0
2	NAG	E	1	14/15	0.82	0.34	136,138,140,144	0
3	MAN	F	4	11/12	0.84	0.38	99,105,108,110	0
3	NAG	F	1	14/15	0.90	0.25	95,99,101,103	0
3	MAN	F	7	11/12	0.92	0.36	89,91,93,95	0
3	NAG	F	2	14/15	0.93	0.30	89,90,93,93	0
3	BMA	F	3	11/12	0.93	0.20	87,88,91,94	0

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

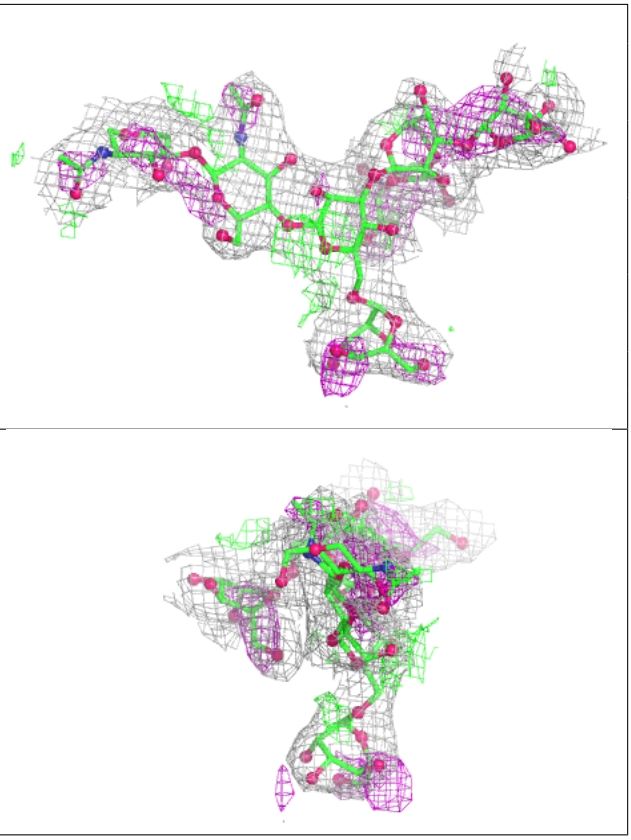
Electron density around Chain E:

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



Electron density around Chain F:

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



6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	A	710	14/15	0.44	0.69	174,176,176,176	0
4	NAG	B	810	14/15	0.65	0.57	142,144,144,144	0

6.5 Other polymers (i)

There are no such residues in this entry.