Full wwPDB X-ray Structure Validation Report (i)

Sep 20, 2022 – 12:22 PM JST

PDB ID	:	7Y0C
Title	:	Crystal structure of BD55-1403 and SARS-CoV-2 Omicron RBD
Authors	:	Zhang, Z.; Xiao, J.
Deposited on	:	2022-06-04
Resolution	:	2.94 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 (1)) were used in the production of this report:

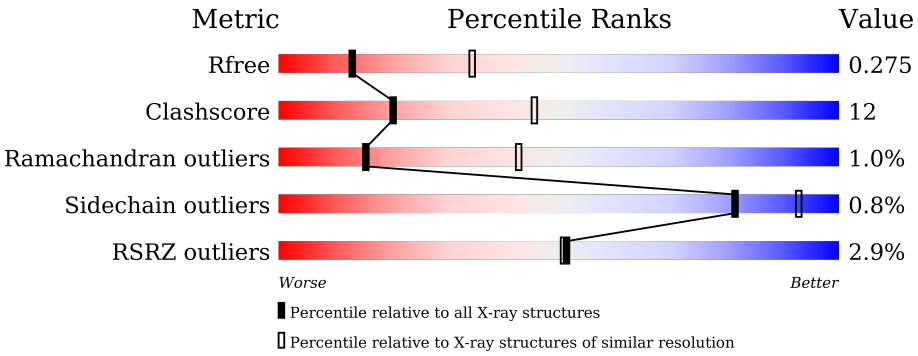
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.30
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.94 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	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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	B	214	6% 72% 27%
1	N	214	73% 23%
2	A	218	3% 78% 21%
2	M	218	69% 29%
3	E	199	71% 26%
3	R	199	4% 62% 35%

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Mol	Chain	Length	Quality of chain
4	C	4	100%
5	D	3	33% 67%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9795 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 BD55-1403 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	214	Total	C	N	O	S	0	0	0
			1652	1034	283	331	4			
1	N	214	Total	C	N	O	S	0	0	0
			1652	1034	283	331	4			

- Molecule 2 is a protein called BD55-1403 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	218	Total	C	N	O	S	0	0	0
			1620	1026	266	321	7			
2	M	218	Total	C	N	O	S	0	0	0
			1620	1026	266	321	7			

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	197	Total	C	N	O	S	0	0	0
			1582	1021	267	286	8			
3	R	197	Total	C	N	O	S	0	0	0
			1582	1021	267	286	8			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	331	LYS	ASN	variant	UNP P0DTC2
E	339	ASP	GLY	variant	UNP P0DTC2
E	371	LEU	SER	variant	UNP P0DTC2
E	373	PRO	SER	variant	UNP P0DTC2
E	375	PHE	SER	variant	UNP P0DTC2
E	417	ASN	LYS	variant	UNP P0DTC2
E	440	LYS	ASN	variant	UNP P0DTC2
E	446	SER	GLY	variant	UNP P0DTC2

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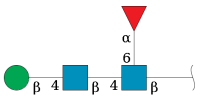
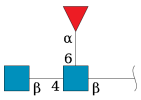
Chain	Residue	Modelled	Actual	Comment	Reference
E	477	ASN	SER	variant	UNP P0DTC2
E	478	LYS	THR	variant	UNP P0DTC2
E	484	ALA	GLU	variant	UNP P0DTC2
E	493	ARG	GLN	variant	UNP P0DTC2
E	496	SER	GLY	variant	UNP P0DTC2
E	498	ARG	GLN	variant	UNP P0DTC2
E	501	TYR	ASN	variant	UNP P0DTC2
E	505	HIS	TYR	variant	UNP P0DTC2
R	331	LYS	ASN	variant	UNP P0DTC2
R	339	ASP	GLY	variant	UNP P0DTC2
R	371	LEU	SER	variant	UNP P0DTC2
R	373	PRO	SER	variant	UNP P0DTC2
R	375	PHE	SER	variant	UNP P0DTC2
R	417	ASN	LYS	variant	UNP P0DTC2
R	440	LYS	ASN	variant	UNP P0DTC2
R	446	SER	GLY	variant	UNP P0DTC2
R	477	ASN	SER	variant	UNP P0DTC2
R	478	LYS	THR	variant	UNP P0DTC2
R	484	ALA	GLU	variant	UNP P0DTC2
R	493	ARG	GLN	variant	UNP P0DTC2
R	496	SER	GLY	variant	UNP P0DTC2
R	498	ARG	GLN	variant	UNP P0DTC2
R	501	TYR	ASN	variant	UNP P0DTC2
R	505	HIS	TYR	variant	UNP P0DTC2

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

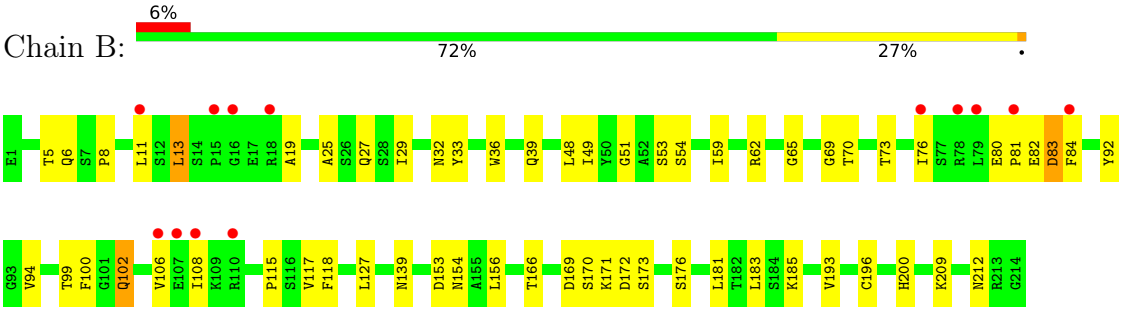


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	D	3	38	22	2	14	0	0	0

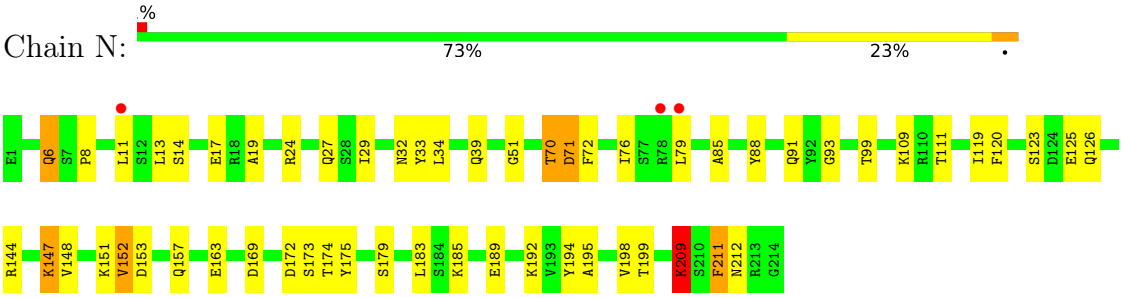
3 Residue-property plots (i)

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.

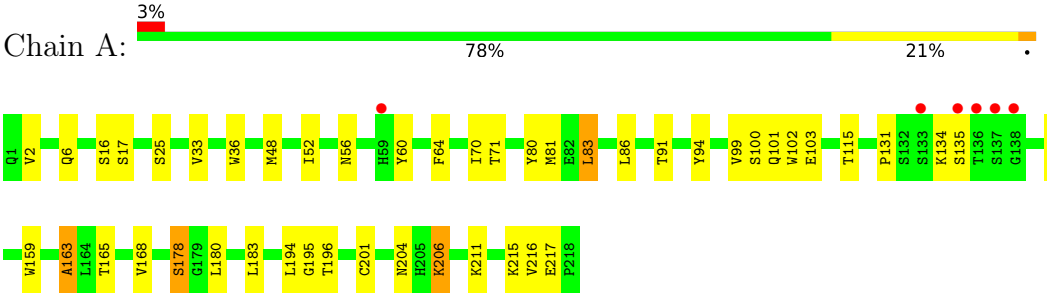
• Molecule 1: BD55-1403 Fab light chain



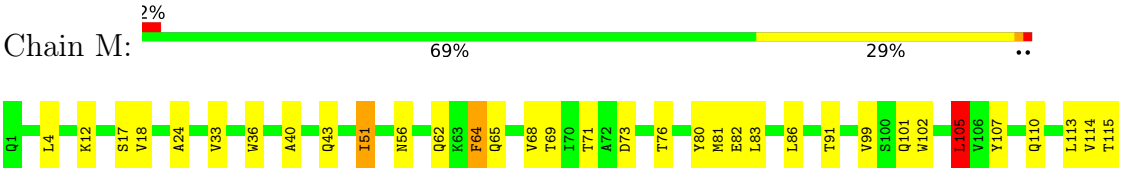
• Molecule 1: BD55-1403 Fab light chain



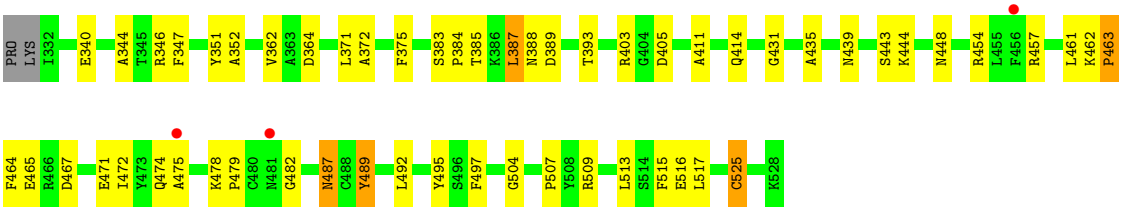
• Molecule 2: BD55-1403 Fab heavy chain



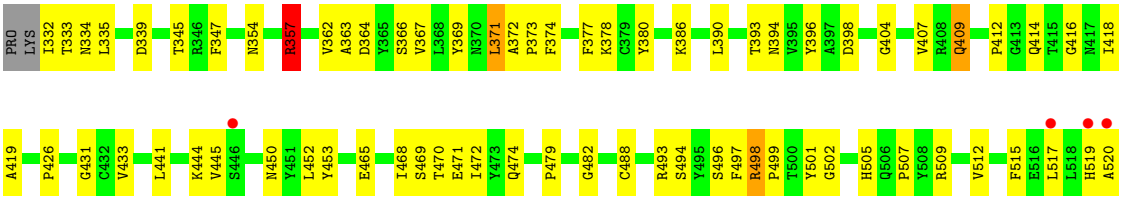
• Molecule 2: BD55-1403 Fab heavy chain



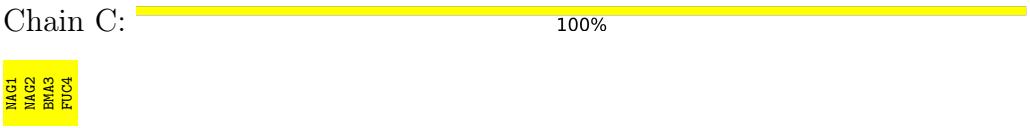
• Molecule 3: Spike protein S1



• Molecule 3: Spike protein S1



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



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	79.63Å 148.83Å 157.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.37 – 2.94 54.37 – 2.94	Depositor EDS
% Data completeness (in resolution range)	99.6 (54.37-2.94) 99.6 (54.37-2.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.202 , 0.278 0.203 , 0.275	Depositor DCC
R_{free} test set	1995 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	60.6	Xtriage
Anisotropy	0.849	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 43.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9795	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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

5.1 Standard geometry

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

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	B	0.71	1/1689 (0.1%)	0.91	4/2293 (0.2%)
1	N	0.72	3/1689 (0.2%)	0.91	3/2293 (0.1%)
2	A	0.72	2/1660 (0.1%)	0.91	4/2266 (0.2%)
2	M	0.71	0/1660	0.94	5/2266 (0.2%)
3	E	0.70	1/1629 (0.1%)	0.93	6/2217 (0.3%)
3	R	0.75	1/1629 (0.1%)	0.97	9/2217 (0.4%)
All	All	0.72	8/9956 (0.1%)	0.93	31/13552 (0.2%)

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	N	0	3
2	M	0	3
3	E	0	1
3	R	0	4
All	All	0	11

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	206	LYS	CD-CE	9.49	1.75	1.51
1	N	209	LYS	CE-NZ	8.82	1.71	1.49
1	B	196	CYS	CB-SG	-6.52	1.71	1.82
2	A	206	LYS	CE-NZ	6.46	1.65	1.49
1	N	147	LYS	CD-CE	5.83	1.65	1.51
3	R	465	GLU	CG-CD	5.72	1.60	1.51
3	E	471	GLU	CG-CD	5.64	1.60	1.51
1	N	24	ARG	CB-CG	-5.19	1.38	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	206	LYS	CA-CB-CG	-10.41	90.50	113.40
2	M	105	LEU	CA-CB-CG	8.94	135.87	115.30
2	M	153	GLU	OE1-CD-OE2	-8.31	113.33	123.30
3	E	347	PHE	CB-CG-CD2	-7.75	115.38	120.80
2	A	206	LYS	CD-CE-NZ	-7.17	95.21	111.70
1	N	209	LYS	CD-CE-NZ	-7.12	95.32	111.70
3	R	409	GLN	CA-CB-CG	6.92	128.61	113.40
1	N	24	ARG	CG-CD-NE	-6.86	97.39	111.80
3	R	357	ARG	CB-CG-CD	6.29	127.95	111.60
1	B	39	GLN	C-N-CA	-6.20	106.20	121.70
1	B	13	LEU	CB-CG-CD2	5.98	121.17	111.00
1	B	83	ASP	CB-CA-C	5.93	122.26	110.40
3	R	517	LEU	CA-CB-CG	5.86	128.78	115.30
2	M	105	LEU	CB-CG-CD2	-5.83	101.08	111.00
3	E	387	LEU	CB-CG-CD2	-5.74	101.25	111.00
3	R	488	CYS	CA-CB-SG	-5.65	103.82	114.00
1	B	156	LEU	CB-CG-CD2	5.57	120.47	111.00
3	E	517	LEU	CB-CG-CD2	5.55	120.43	111.00
3	R	498	ARG	CB-CG-CD	5.52	125.96	111.60
3	E	487	ASN	CB-CA-C	5.46	121.33	110.40
3	R	441	LEU	CB-CG-CD2	-5.43	101.78	111.00
3	R	357	ARG	NE-CZ-NH2	-5.35	117.63	120.30
3	R	369	TYR	CB-CG-CD2	-5.34	117.80	121.00
3	E	346	ARG	NE-CZ-NH1	5.32	122.96	120.30
2	A	183	LEU	CB-CG-CD1	-5.29	102.00	111.00
1	N	6	GLN	C-N-CA	5.21	134.74	121.70
2	M	153	GLU	CG-CD-OE2	-5.19	107.92	118.30
3	R	371	LEU	C-N-CA	5.12	134.49	121.70
2	M	126	VAL	C-N-CA	5.07	134.38	121.70
3	E	489	TYR	CB-CA-C	-5.05	100.30	110.40
2	A	83	LEU	CB-CG-CD2	5.01	119.51	111.00

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	525	CYS	Mainchain
2	M	110	GLN	Sidechain
2	M	153	GLU	Sidechain
2	M	64	PHE	Peptide
1	N	211	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	N	70	THR	Peptide
1	N	71	ASP	Sidechain
3	R	357	ARG	Sidechain
3	R	469	SER	Peptide
3	R	479	PRO	Peptide
3	R	502	GLY	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	B	1652	0	1607	41	0
1	N	1652	0	1607	39	0
2	A	1620	0	1597	41	0
2	M	1620	0	1597	47	0
3	E	1582	0	1519	33	0
3	R	1582	0	1517	49	0
4	C	49	0	43	0	0
5	D	38	0	34	0	0
All	All	9795	0	9521	239	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 (239) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:206:LYS:CD	2:A:206:LYS:CE	1.75	1.64
1:N:209:LYS:CE	1:N:209:LYS:NZ	1.71	1.50
2:A:153:GLU:HG2	2:A:154:PRO:HA	1.51	0.91
2:M:91:THR:HG23	2:M:115:THR:HA	1.57	0.86
1:N:209:LYS:NZ	1:N:209:LYS:CD	2.42	0.82
2:M:153:GLU:HG2	2:M:154:PRO:HA	1.62	0.81
2:A:206:LYS:CE	2:A:206:LYS:CG	2.59	0.81
1:N:152:VAL:HG23	1:N:153:ASP:H	1.47	0.80
3:R:445:VAL:C	3:R:498:ARG:HH12	1.84	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:GLU:HB3	1:B:81:PRO:HD2	1.66	0.77
2:M:71:THR:HG23	2:M:80:TYR:HB2	1.66	0.76
2:A:71:THR:HG22	2:A:80:TYR:HB2	1.69	0.74
2:A:206:LYS:CD	2:A:206:LYS:NZ	2.51	0.73
1:B:53:SER:HB2	3:R:345:THR:HG21	1.71	0.73
2:M:131:PRO:HG3	2:M:143:LEU:HB3	1.70	0.73
1:B:139:ASN:O	1:B:176:SER:OG	2.07	0.72
2:M:17:SER:HA	2:M:86:LEU:HD11	1.72	0.71
1:B:33:TYR:HB3	1:B:92:TYR:O	1.92	0.70
3:R:498:ARG:HG2	3:R:498:ARG:HH11	1.58	0.69
2:A:33:VAL:CG1	2:A:99:VAL:HG22	2.23	0.68
2:M:40:ALA:HB3	2:M:43:GLN:HG3	1.75	0.68
1:B:118:PHE:CE1	2:A:134:LYS:HE3	2.29	0.67
3:E:461:LEU:HD22	3:E:465:GLU:HB3	1.76	0.67
1:N:172:ASP:OD1	1:N:174:THR:OG1	2.07	0.67
2:M:69:THR:HG23	2:M:82:GLU:HB3	1.77	0.67
2:A:33:VAL:HG12	2:A:99:VAL:HG22	1.78	0.66
2:M:126:VAL:O	2:M:214:LYS:HD2	1.95	0.66
3:R:519:HIS:CG	3:R:520:ALA:H	2.14	0.66
3:E:411:ALA:HB3	3:E:414:GLN:HG3	1.77	0.65
3:E:474:GLN:HB2	3:E:479:PRO:HG3	1.79	0.64
1:N:151:LYS:HG3	1:N:195:ALA:HB3	1.77	0.64
1:B:166:THR:HG22	1:B:176:SER:H	1.62	0.64
2:A:143:LEU:HD13	2:A:216:VAL:HG21	1.80	0.64
1:B:169:ASP:OD1	1:B:170:SER:N	2.31	0.63
3:R:367:VAL:O	3:R:371:LEU:HG	1.98	0.62
1:B:117:VAL:O	1:B:209:LYS:HE3	2.00	0.62
1:N:147:LYS:HB2	1:N:199:THR:HB	1.82	0.62
1:B:5:THR:HA	1:B:102:GLN:HE22	1.63	0.61
1:N:123:SER:OG	2:M:128:PRO:HD2	2.00	0.61
1:N:144:ARG:HB2	1:N:175:TYR:CE2	2.36	0.60
3:R:378:LYS:HD3	3:R:380:TYR:OH	1.99	0.60
2:A:100:SER:HB3	2:A:103:GLU:OE2	2.01	0.60
1:B:118:PHE:HE1	2:A:134:LYS:HE3	1.66	0.59
1:N:19:ALA:HB3	1:N:76:ILE:HB	1.84	0.59
2:M:36:TRP:CE2	2:M:81:MET:HB2	2.38	0.59
1:B:6:GLN:H	1:B:102:GLN:NE2	1.99	0.59
2:A:194:LEU:O	2:A:196:THR:N	2.31	0.59
2:A:101:GLN:HG3	2:A:101:GLN:O	2.02	0.59
3:R:357:ARG:HG3	3:R:396:TYR:CE1	2.38	0.58
3:R:409:GLN:HA	3:R:414:GLN:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:64:PHE:HB3	2:M:68:VAL:HG23	1.86	0.58
3:R:431:GLY:HA2	3:R:515:PHE:HD2	1.68	0.58
3:E:489:TYR:HE1	3:R:450:ASN:HB3	1.68	0.57
2:M:40:ALA:O	2:M:43:GLN:HB2	2.04	0.57
1:B:48:LEU:HA	1:B:59:ILE:HG13	1.87	0.57
1:N:76:ILE:HG21	1:N:79:LEU:HD23	1.87	0.57
1:N:39:GLN:O	1:N:85:ALA:HB1	2.05	0.56
1:N:125:GLU:OE2	1:N:125:GLU:N	2.26	0.56
1:B:62:ARG:NH2	1:B:83:ASP:OD2	2.24	0.56
3:E:431:GLY:HA2	3:E:515:PHE:HD2	1.71	0.56
3:R:433:VAL:HG22	3:R:512:VAL:HG22	1.87	0.56
3:R:496:SER:O	3:R:501:TYR:HE2	1.89	0.56
2:A:165:THR:O	2:A:168:VAL:HG12	2.06	0.56
2:M:17:SER:HA	2:M:86:LEU:CD1	2.36	0.55
2:M:62:GLN:O	2:M:65:GLN:HB2	2.07	0.55
1:N:8:PRO:HG2	1:N:11:LEU:HD21	1.88	0.55
2:M:68:VAL:HG22	2:M:83:LEU:HD13	1.89	0.54
3:R:445:VAL:O	3:R:498:ARG:NH2	2.41	0.54
3:E:454:ARG:HA	3:E:492:LEU:HD23	1.90	0.54
3:E:457:ARG:NE	3:E:467:ASP:OD2	2.31	0.54
1:B:36:TRP:HB2	1:B:49:ILE:HB	1.90	0.54
3:R:431:GLY:HA2	3:R:515:PHE:CD2	2.41	0.54
1:B:84:PHE:HB2	1:B:106:VAL:O	2.08	0.54
1:N:148:VAL:HG11	1:N:179:SER:HB2	1.89	0.54
3:E:340:GLU:O	3:E:344:ALA:HB2	2.08	0.53
1:B:27:GLN:O	1:B:70:THR:HG22	2.08	0.53
1:B:82:GLU:O	1:B:82:GLU:HG3	2.08	0.53
2:M:146:LEU:HD21	2:M:148:LYS:HD3	1.91	0.53
3:E:387:LEU:O	3:E:389:ASP:N	2.41	0.53
1:N:8:PRO:HG2	1:N:11:LEU:CD2	2.38	0.53
2:A:134:LYS:HG3	2:A:135:SER:H	1.74	0.53
3:R:386:LYS:O	3:R:390:LEU:HD12	2.08	0.53
3:E:431:GLY:HA3	3:E:513:LEU:O	2.09	0.53
1:N:33:TYR:CD1	1:N:93:GLY:HA2	2.44	0.53
2:M:132:SER:H	2:M:134:LYS:HE2	1.72	0.53
2:A:153:GLU:CG	2:A:154:PRO:HA	2.31	0.52
1:B:32:ASN:O	1:B:51:GLY:HA2	2.10	0.52
2:A:102:TRP:CD1	3:R:367:VAL:HG21	2.44	0.52
2:M:33:VAL:CG1	2:M:99:VAL:HG22	2.38	0.52
3:E:387:LEU:C	3:E:389:ASP:H	2.12	0.52
1:B:8:PRO:HG3	1:B:11:LEU:HG	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:445:VAL:O	3:R:498:ARG:NH1	2.38	0.52
1:N:169:ASP:O	1:N:173:SER:HA	2.10	0.51
2:A:6:GLN:NE2	2:A:94:TYR:O	2.37	0.51
2:M:164:LEU:HD21	2:M:187:VAL:HG21	1.93	0.51
3:R:354:ASN:O	3:R:398:ASP:HA	2.11	0.51
3:E:463:PRO:HG2	3:E:464:PHE:H	1.76	0.51
1:N:91:GLN:HG3	1:N:99:THR:HG22	1.93	0.51
1:N:14:SER:N	1:N:17:GLU:OE2	2.39	0.51
2:A:178:SER:HB2	2:A:180:LEU:H	1.75	0.51
2:M:205:HIS:ND1	2:M:208:SER:HB3	2.25	0.51
2:A:159:TRP:CH2	2:A:201:CYS:HB3	2.45	0.50
2:A:91:THR:HG23	2:A:115:THR:HA	1.93	0.50
2:A:131:PRO:HD3	2:A:143:LEU:CB	2.41	0.50
1:N:8:PRO:HG2	1:N:11:LEU:HG	1.93	0.50
2:M:135:SER:OG	2:M:139:GLY:HA2	2.11	0.50
2:A:131:PRO:HD3	2:A:143:LEU:HB3	1.94	0.50
1:N:148:VAL:HG12	1:N:163:GLU:OE2	2.12	0.50
3:R:474:GLN:HG3	3:R:474:GLN:O	2.11	0.50
3:R:519:HIS:CG	3:R:520:ALA:N	2.80	0.50
1:B:153:ASP:C	1:B:154:ASN:HD22	2.15	0.50
1:N:27:GLN:O	1:N:70:THR:HG22	2.11	0.50
1:B:169:ASP:OD1	1:B:171:LYS:HG2	2.12	0.49
3:R:332:ILE:O	3:R:333:THR:HB	2.12	0.49
3:R:409:GLN:HG2	3:R:418:ILE:HB	1.93	0.49
2:M:73:ASP:CG	2:M:76:THR:HG22	2.31	0.49
2:M:113:LEU:HD12	2:M:114:VAL:H	1.78	0.49
3:R:444:LYS:HG2	3:R:445:VAL:H	1.78	0.49
3:R:377:PHE:CG	3:R:377:PHE:O	2.65	0.49
2:A:36:TRP:CE2	2:A:81:MET:HB2	2.48	0.49
2:A:83:LEU:HD22	2:A:86:LEU:HD23	1.95	0.49
2:M:153:GLU:CG	2:M:154:PRO:HA	2.37	0.49
2:A:48:MET:HG2	2:A:64:PHE:CE2	2.48	0.48
2:A:134:LYS:HG3	2:A:135:SER:N	2.27	0.48
1:B:118:PHE:CD1	2:A:134:LYS:HE3	2.48	0.48
1:B:171:LYS:HG3	1:B:172:ASP:H	1.79	0.48
3:R:453:TYR:OH	3:R:493:ARG:HD3	2.14	0.48
3:R:471:GLU:HG2	3:R:472:ILE:H	1.78	0.48
1:B:181:LEU:HG	1:B:183:LEU:HD11	1.96	0.48
2:M:73:ASP:OD2	2:M:76:THR:HG22	2.14	0.48
3:R:404:GLY:O	3:R:407:VAL:HG23	2.14	0.47
3:E:364:ASP:H	2:M:101:GLN:HE22	1.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:185:LYS:O	1:N:189:GLU:HG2	2.14	0.47
3:E:444:LYS:HG3	3:E:448:ASN:HB2	1.96	0.47
2:M:51:ILE:HD11	2:M:56:ASN:HD22	1.80	0.47
2:A:60:TYR:HE1	2:A:70:ILE:HG13	1.80	0.47
3:R:334:ASN:O	3:R:362:VAL:HG12	2.14	0.47
3:R:347:PHE:CE2	3:R:509:ARG:HB3	2.49	0.47
3:R:364:ASP:OD1	3:R:366:SER:HB2	2.14	0.47
2:M:12:LYS:HG3	2:M:18:VAL:HB	1.97	0.47
3:E:405:ASP:OD1	3:E:504:GLY:O	2.33	0.47
3:E:393:THR:HG22	3:E:516:GLU:O	2.15	0.47
2:A:2:VAL:HG13	2:A:25:SER:O	2.16	0.46
2:A:204:ASN:ND2	2:A:211:LYS:HD2	2.31	0.46
3:E:383:SER:OG	3:E:385:THR:HG22	2.16	0.46
1:B:11:LEU:HD22	1:B:13:LEU:HD11	1.97	0.46
1:B:181:LEU:HG	1:B:183:LEU:CD1	2.45	0.46
2:M:159:TRP:CH2	2:M:201:CYS:HB3	2.51	0.46
1:N:34:LEU:HD22	1:N:72:PHE:CD1	2.51	0.46
2:M:134:LYS:HD2	2:M:142:ALA:H	1.80	0.46
3:E:405:ASP:OD1	3:E:405:ASP:N	2.48	0.46
3:R:363:ALA:O	3:R:527:PRO:HD3	2.16	0.46
3:R:357:ARG:HD2	3:R:394:ASN:OD1	2.16	0.46
1:B:19:ALA:HB3	1:B:76:ILE:HB	1.98	0.46
1:B:54:SER:OG	3:R:345:THR:HB	2.16	0.46
2:A:215:LYS:HD2	2:A:217:GLU:OE1	2.16	0.46
1:N:209:LYS:NZ	1:N:209:LYS:HD3	2.30	0.45
3:E:431:GLY:HA2	3:E:515:PHE:CD2	2.49	0.45
3:E:475:ALA:HB3	3:E:487:ASN:HB3	1.97	0.45
3:R:367:VAL:HG12	3:R:371:LEU:HD11	1.99	0.45
3:E:497:PHE:CG	3:E:507:PRO:HG3	2.50	0.45
1:N:32:ASN:O	1:N:51:GLY:HA2	2.16	0.45
1:B:193:VAL:HG22	1:B:212:ASN:OD1	2.16	0.45
1:B:25:ALA:HB2	1:B:29:ILE:HD12	1.98	0.45
3:E:362:VAL:HA	3:E:525:CYS:O	2.17	0.45
3:R:452:LEU:HD23	3:R:494:SER:HA	1.99	0.45
2:A:163:ALA:O	2:A:165:THR:HG23	2.17	0.45
3:E:371:LEU:HB2	3:E:375:PHE:CZ	2.52	0.45
3:R:409:GLN:NE2	3:R:416:GLY:HA3	2.32	0.45
3:R:501:TYR:HB3	3:R:505:HIS:HB2	1.99	0.44
2:M:86:LEU:HD23	2:M:116:VAL:HG21	1.98	0.44
3:R:380:TYR:CE1	3:R:412:PRO:HD2	2.52	0.44
3:E:351:TYR:CE1	3:E:352:ALA:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:153:GLU:HG2	2:A:154:PRO:CA	2.34	0.44
1:N:192:LYS:O	1:N:212:ASN:O	2.35	0.44
1:N:194:TYR:HB2	1:N:211:PHE:CE1	2.52	0.44
2:M:193:SER:HA	2:M:196:THR:HG22	2.00	0.44
2:M:215:LYS:HB2	2:M:215:LYS:HE3	1.78	0.44
1:N:11:LEU:HB3	1:N:13:LEU:CD2	2.48	0.44
1:N:152:VAL:HG13	1:N:157:GLN:HG3	2.00	0.44
2:M:151:PHE:CD1	2:M:152:PRO:HA	2.53	0.44
2:A:16:SER:OG	2:A:17:SER:N	2.51	0.44
1:N:29:ILE:HD11	1:N:72:PHE:CE2	2.53	0.43
3:R:468:ILE:HD12	3:R:468:ILE:HA	1.86	0.43
3:R:470:THR:OG1	3:R:471:GLU:N	2.52	0.43
3:E:462:LYS:HB3	3:E:463:PRO:HD2	2.00	0.43
3:R:444:LYS:O	3:R:499:PRO:HD3	2.19	0.43
1:B:166:THR:HG21	1:B:176:SER:HB2	2.01	0.43
2:A:103:GLU:H	3:R:339:ASP:HB3	1.84	0.43
3:E:462:LYS:HB2	3:E:465:GLU:OE2	2.18	0.43
2:M:159:TRP:CZ3	2:M:201:CYS:HB3	2.54	0.43
1:N:211:PHE:CD2	1:N:212:ASN:N	2.87	0.43
1:B:127:LEU:HD22	1:B:185:LYS:HG3	2.01	0.43
2:A:33:VAL:HB	2:A:52:ILE:HD13	2.01	0.43
1:N:152:VAL:HG23	1:N:153:ASP:N	2.25	0.43
2:M:153:GLU:HG2	2:M:154:PRO:CA	2.41	0.43
3:E:462:LYS:HB3	3:E:463:PRO:CD	2.49	0.42
2:M:194:LEU:HD23	2:M:194:LEU:HA	1.87	0.42
1:N:8:PRO:HG2	1:N:11:LEU:CG	2.50	0.42
1:N:119:ILE:HG12	1:N:120:PHE:H	1.85	0.42
3:R:372:ALA:HB1	3:R:373:PRO:CD	2.49	0.42
2:A:194:LEU:C	2:A:196:THR:H	2.19	0.42
2:M:4:LEU:HD23	2:M:24:ALA:HB2	2.02	0.42
3:E:403:ARG:HG3	3:E:495:TYR:CE1	2.55	0.42
1:N:148:VAL:HG23	1:N:198:VAL:HG22	2.01	0.42
2:A:71:THR:CG2	2:A:80:TYR:HB2	2.45	0.42
3:E:384:PRO:HA	3:E:387:LEU:HD12	2.01	0.42
3:E:472:ILE:HG13	3:E:482:GLY:HA2	2.01	0.42
2:M:183:LEU:HD23	2:M:184:SER:N	2.34	0.42
3:R:393:THR:HG23	3:R:521:PRO:O	2.19	0.42
1:B:127:LEU:HD23	1:B:127:LEU:HA	1.81	0.42
1:B:183:LEU:HD12	1:B:183:LEU:N	2.35	0.42
2:M:151:PHE:HB2	2:M:180:LEU:HD23	2.01	0.42
1:N:123:SER:HB3	1:N:126:GLN:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:409:GLN:HG2	3:R:419:ALA:H	1.84	0.42
1:B:115:PRO:HD3	1:B:200:HIS:ND1	2.34	0.41
2:M:64:PHE:HB3	2:M:68:VAL:CG2	2.50	0.41
3:R:373:PRO:HB2	3:R:374:PHE:CD2	2.55	0.41
2:M:105:LEU:HD23	2:M:107:TYR:CZ	2.56	0.41
1:N:6:GLN:HE22	1:N:88:TYR:HA	1.85	0.41
1:B:94:VAL:O	3:R:335:LEU:HD21	2.20	0.41
1:B:169:ASP:OD1	1:B:171:LYS:N	2.43	0.41
3:E:372:ALA:O	3:E:375:PHE:HB2	2.20	0.41
3:E:439:ASN:O	3:E:443:SER:HB3	2.21	0.41
3:R:497:PHE:CE2	3:R:507:PRO:HB3	2.56	0.41
3:E:435:ALA:HA	3:E:509:ARG:O	2.21	0.41
1:B:65:GLY:HA2	1:B:73:THR:O	2.20	0.41
1:B:80:GLU:HB3	1:B:81:PRO:CD	2.44	0.41
1:B:169:ASP:O	1:B:173:SER:HA	2.20	0.41
1:N:183:LEU:HD23	1:N:183:LEU:HA	1.94	0.41
2:M:113:LEU:HD12	2:M:114:VAL:N	2.35	0.41
2:M:126:VAL:HG22	2:M:147:VAL:HG22	2.03	0.40
1:B:99:THR:HG22	1:B:100:PHE:N	2.36	0.40
2:A:33:VAL:HB	2:A:52:ILE:CD1	2.49	0.40
2:A:159:TRP:HD1	2:A:168:VAL:HG21	1.87	0.40
2:M:101:GLN:HG2	2:M:102:TRP:CD1	2.56	0.40
2:M:150:TYR:HE1	2:M:153:GLU:HG3	1.87	0.40
2:M:153:GLU:OE2	2:M:173:ALA:HB3	2.22	0.40
3:R:471:GLU:HG2	3:R:472:ILE:N	2.37	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	B	212/214 (99%)	193 (91%)	17 (8%)	2 (1%)	17 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	N	212/214 (99%)	179 (84%)	32 (15%)	1 (0%)	29 60
2	A	216/218 (99%)	197 (91%)	15 (7%)	4 (2%)	8 26
2	M	216/218 (99%)	206 (95%)	9 (4%)	1 (0%)	29 60
3	E	195/199 (98%)	170 (87%)	23 (12%)	2 (1%)	15 43
3	R	195/199 (98%)	161 (83%)	32 (16%)	2 (1%)	15 43
All	All	1246/1262 (99%)	1106 (89%)	128 (10%)	12 (1%)	15 43

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	56	ASN
2	A	195	GLY
3	E	388	ASN
3	E	463	PRO
1	N	152	VAL
2	M	133	SER
3	R	426	PRO
1	B	102	GLN
2	A	178	SER
3	R	482	GLY
2	A	163	ALA
1	B	69	GLY

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	B	185/185 (100%)	184 (100%)	1 (0%)	88 96
1	N	185/185 (100%)	181 (98%)	4 (2%)	52 78
2	A	184/184 (100%)	184 (100%)	0	100 100
2	M	184/184 (100%)	182 (99%)	2 (1%)	73 90
3	E	172/174 (99%)	171 (99%)	1 (1%)	86 95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	R	172/174 (99%)	171 (99%)	1 (1%)	86 95
All	All	1082/1086 (100%)	1073 (99%)	9 (1%)	81 93

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	108	ILE
3	E	478	LYS
1	N	71	ASP
1	N	109	LYS
1	N	111	THR
1	N	209	LYS
2	M	51	ILE
2	M	105	LEU
3	R	528	LYS

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

Mol	Chain	Res	Type
1	B	30	ASN
1	B	102	GLN
1	B	154	ASN
2	A	101	GLN
2	A	204	ASN
3	E	370	ASN
2	M	56	ASN
2	M	169	HIS
3	R	409	GLN

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)

7 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	$\#\|Z\| > 2$
4	NAG	C	1	3,4	14,14,15	0.63	0	17,19,21	0.89	1 (5%)
4	NAG	C	2	4	14,14,15	0.94	2 (14%)	17,19,21	1.02	1 (5%)
4	BMA	C	3	4	11,11,12	1.88	3 (27%)	15,15,17	1.02	1 (6%)
4	FUC	C	4	4	10,10,11	1.99	2 (20%)	14,14,16	2.09	2 (14%)
5	NAG	D	1	3,5	14,14,15	0.52	0	17,19,21	0.66	0
5	NAG	D	2	5	14,14,15	0.77	0	17,19,21	1.35	1 (5%)
5	FUC	D	3	5	10,10,11	1.69	3 (30%)	14,14,16	1.39	1 (7%)

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	C	1	3,4	-	1/6/23/26	0/1/1/1
4	NAG	C	2	4	-	2/6/23/26	0/1/1/1
4	BMA	C	3	4	-	0/2/19/22	0/1/1/1
4	FUC	C	4	4	-	-	0/1/1/1
5	NAG	D	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	D	2	5	-	2/6/23/26	0/1/1/1
5	FUC	D	3	5	-	-	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	4	FUC	C4-C5	4.36	1.62	1.52
4	C	3	BMA	C4-C5	3.72	1.60	1.53
5	D	3	FUC	C2-C3	3.28	1.57	1.52
4	C	3	BMA	C1-C2	3.18	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2	NAG	O5-C1	-2.56	1.39	1.43
5	D	3	FUC	C4-C3	2.50	1.58	1.52
4	C	3	BMA	O2-C2	2.25	1.48	1.43
4	C	4	FUC	O5-C5	2.21	1.48	1.43
4	C	2	NAG	C1-C2	-2.20	1.49	1.52
5	D	3	FUC	O5-C5	2.18	1.48	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	4	FUC	C1-C2-C3	-5.40	103.03	109.67
5	D	2	NAG	C1-O5-C5	4.33	118.06	112.19
5	D	3	FUC	C1-C2-C3	-3.67	105.15	109.67
4	C	2	NAG	C1-O5-C5	3.23	116.57	112.19
4	C	4	FUC	C6-C5-C4	2.84	118.32	113.07
4	C	1	NAG	C3-C4-C5	-2.65	105.52	110.24
4	C	3	BMA	C1-O5-C5	2.11	115.05	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

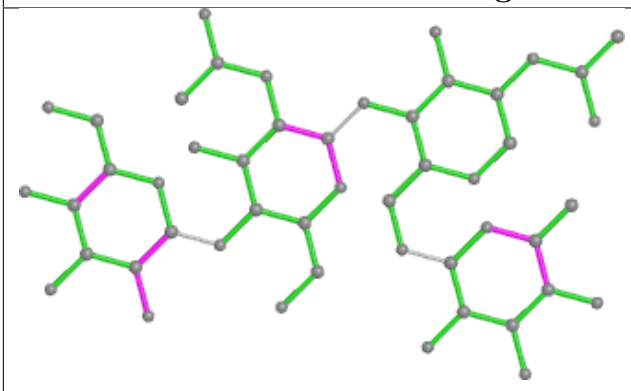
Mol	Chain	Res	Type	Atoms
4	C	2	NAG	O5-C5-C6-O6
5	D	2	NAG	O5-C5-C6-O6
4	C	2	NAG	C4-C5-C6-O6
5	D	2	NAG	C4-C5-C6-O6
4	C	1	NAG	C4-C5-C6-O6

There are no ring outliers.

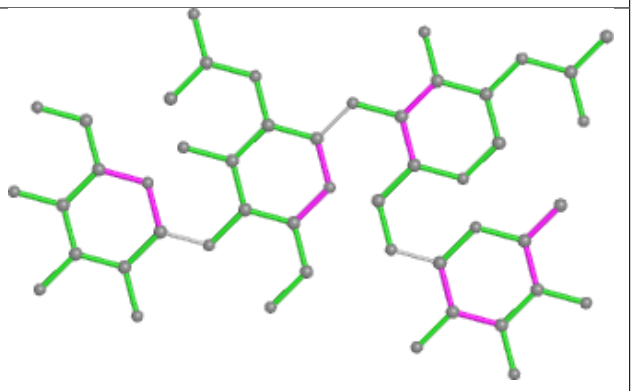
No monomer is involved in short contacts.

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

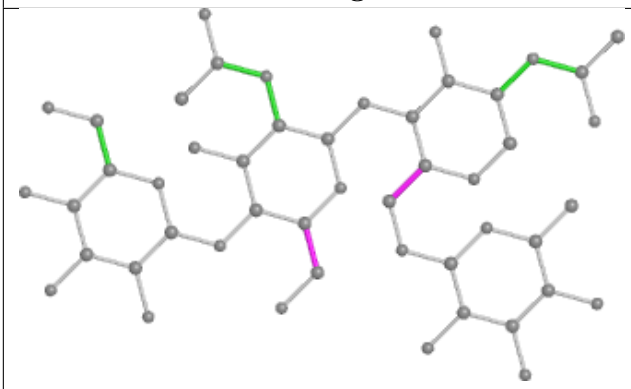
Oligosaccharide Chain C



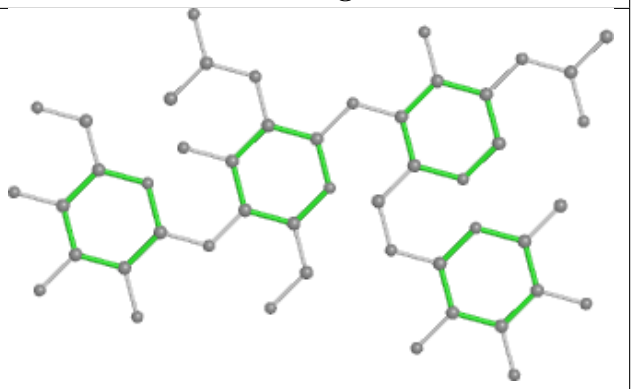
Bond lengths



Bond angles

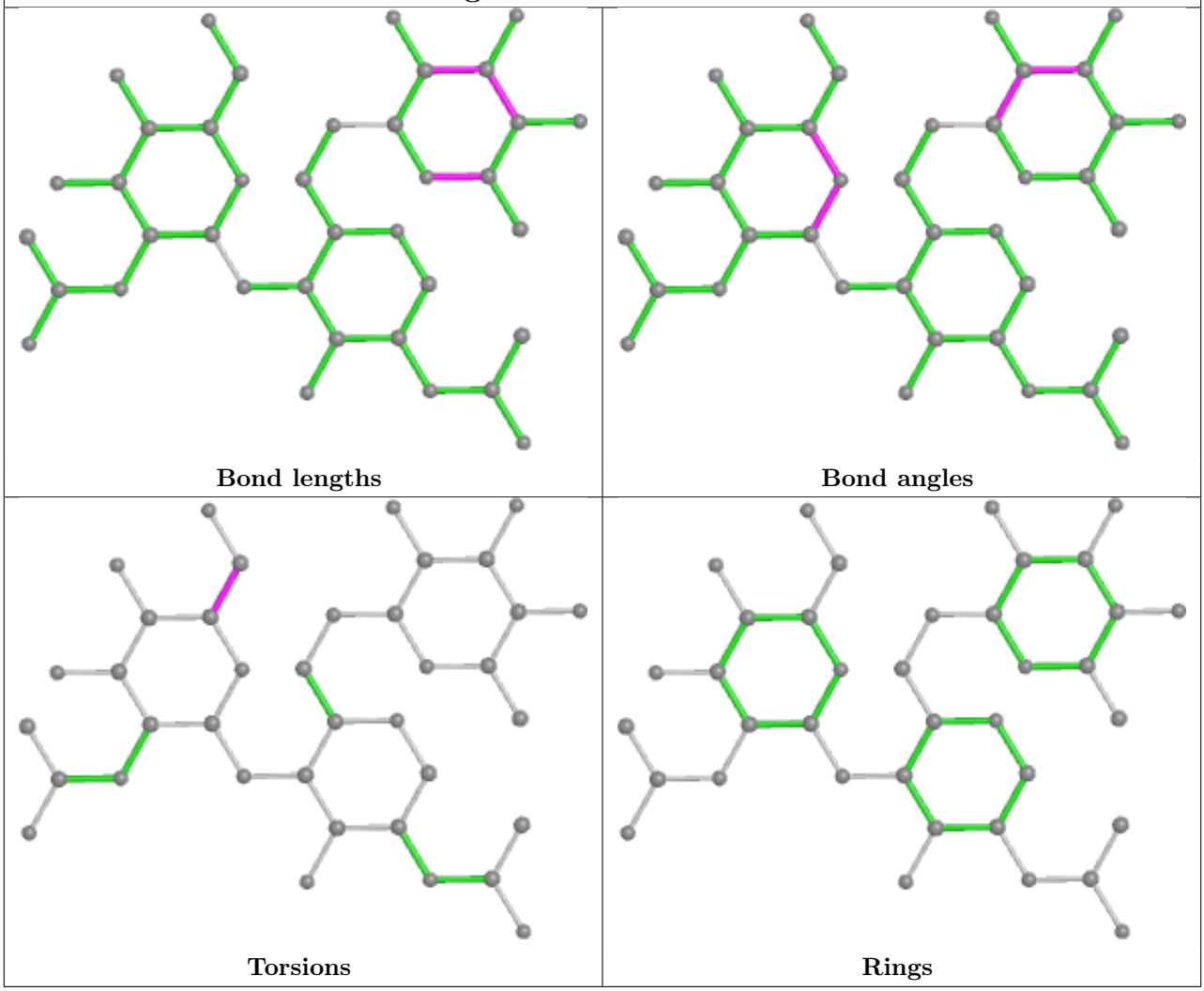


Torsions



Rings

Oligosaccharide Chain D



5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	B	214/214 (100%)	0.44	13 (6%)	21	19	44, 61, 88, 106	0
1	N	214/214 (100%)	0.34	3 (1%)	75	77	40, 62, 82, 89	0
2	A	218/218 (100%)	0.31	6 (2%)	53	53	38, 58, 104, 132	0
2	M	218/218 (100%)	0.28	5 (2%)	60	61	40, 58, 96, 126	0
3	E	197/199 (98%)	0.27	3 (1%)	73	75	39, 62, 95, 104	0
3	R	197/199 (98%)	0.29	7 (3%)	42	41	39, 63, 93, 113	0
All	All	1258/1262 (99%)	0.32	37 (2%)	51	51	38, 60, 93, 132	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	R	520	ALA	6.5
2	A	137	SER	6.4
1	B	81	PRO	5.0
2	M	135	SER	4.9
2	M	136	THR	4.8
2	A	136	THR	4.7
2	A	138	GLY	4.4
2	A	135	SER	3.9
1	B	78	ARG	3.7
3	R	522	ALA	3.5
1	B	79	LEU	3.5
1	B	11	LEU	3.3
1	B	18	ARG	3.3
3	R	446	SER	3.2
1	B	16	GLY	3.2
2	M	137	SER	3.1
1	B	107	GLU	2.9
1	B	106	VAL	2.9
1	B	84	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	N	79	LEU	2.6
1	B	76	ILE	2.6
3	E	481	ASN	2.5
2	A	59	HIS	2.5
3	E	456	PHE	2.5
3	R	525	CYS	2.4
3	E	475	ALA	2.3
1	B	15	PRO	2.3
1	N	78	ARG	2.3
2	A	133	SER	2.3
2	M	138	GLY	2.3
3	R	519	HIS	2.3
1	B	108	ILE	2.2
1	B	110	ARG	2.2
2	M	216	VAL	2.2
3	R	521	PRO	2.1
3	R	517	LEU	2.0
1	N	11	LEU	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)

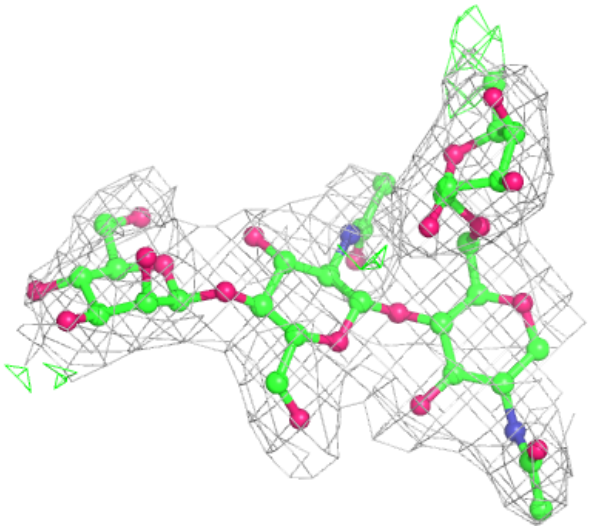
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

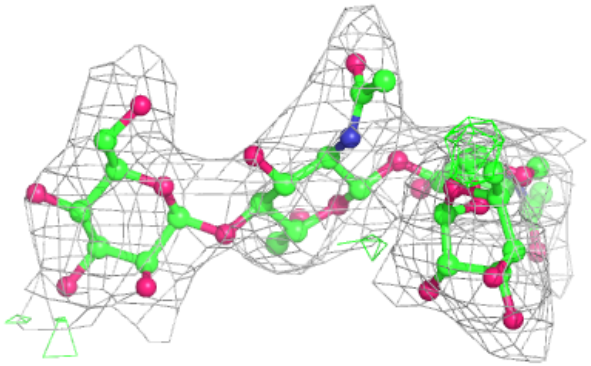
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BMA	C	3	11/12	0.86	0.15	65,73,77,79	0
4	NAG	C	2	14/15	0.92	0.18	54,60,71,81	0
5	NAG	D	2	14/15	0.93	0.16	56,69,80,82	0
4	FUC	C	4	10/11	0.94	0.19	63,69,73,76	0
5	FUC	D	3	10/11	0.95	0.16	70,76,82,88	0
5	NAG	D	1	14/15	0.96	0.19	43,53,63,74	0
4	NAG	C	1	14/15	0.97	0.17	40,49,56,58	0

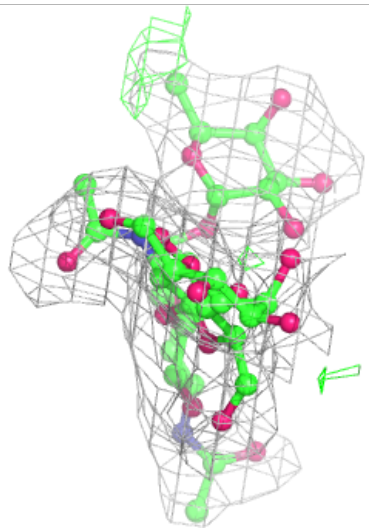
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

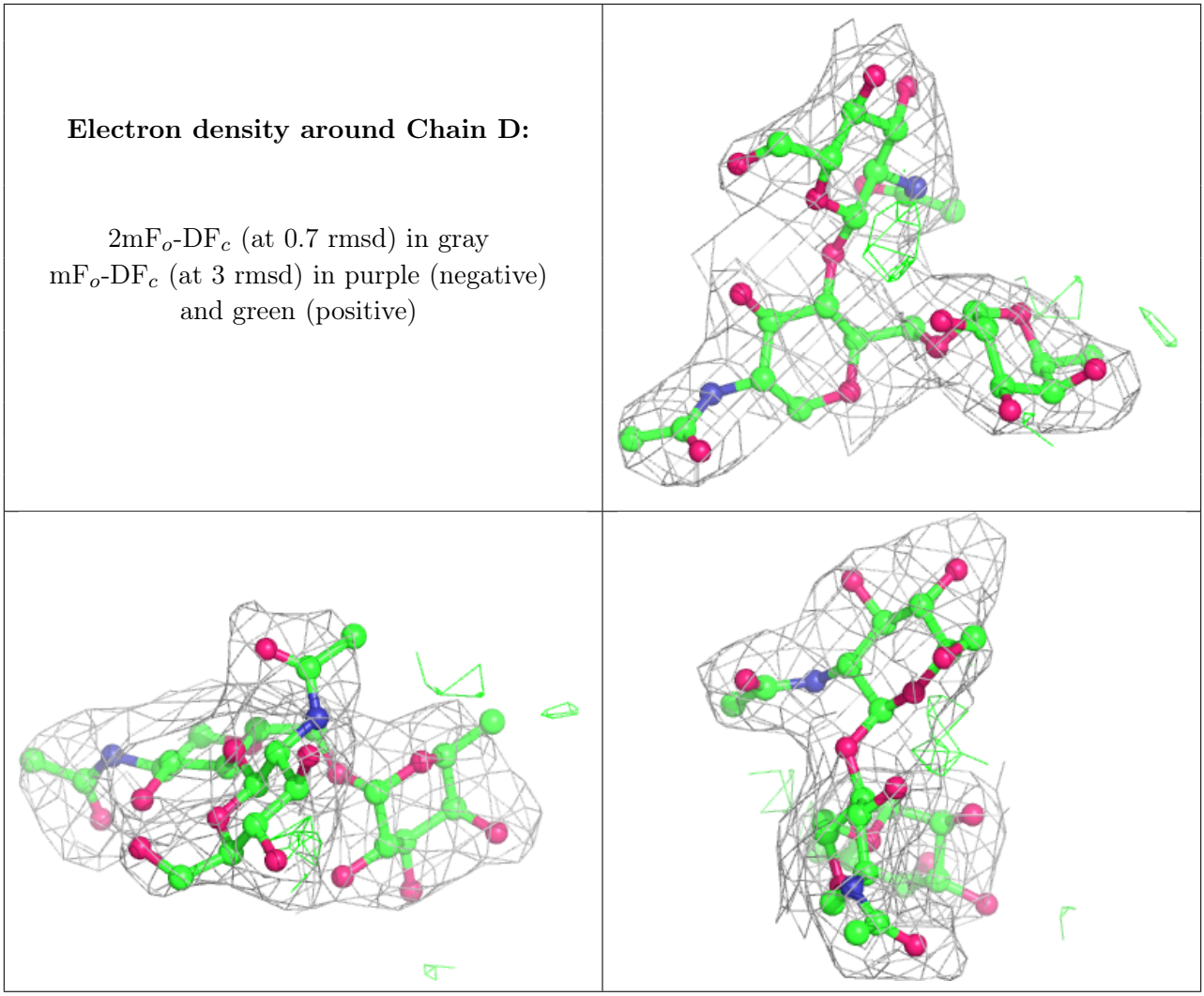






Electron density around Chain D:

$2mF_o$-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.