Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 05:40 AM EDT

PDB ID	:	7SI2
Title	:	Crystal structure of neutralizing antibody 10-28 in complex with SARS-CoV-2 spike receptor binding domain (RBD)
Authors	:	Reddem, E.R.; Shapiro, L.
Deposited on	:	2021-10-12
Resolution	:	3.20 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

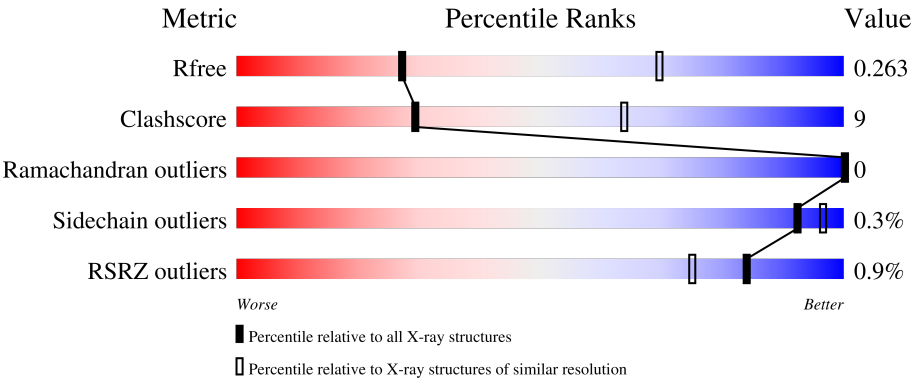
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	D	216	81% 18%
1	F	216	81% 17%
1	L	216	81% 18%
2	E	226	69% 26%
2	G	226	67% 28%

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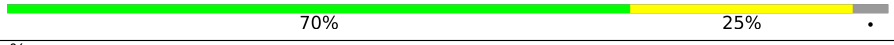
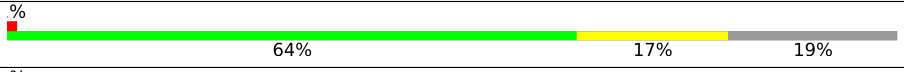
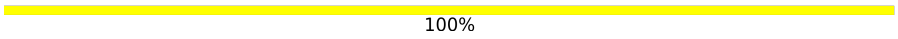
Mol	Chain	Length	Quality of chain
2	H	226	
3	A	236	
3	B	236	
3	C	236	
4	I	2	
4	J	2	
4	K	2	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14385 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 10-28 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	214	Total	C	N	O	S	0	0	0
			1630	1018	272	335	5			
1	F	214	Total	C	N	O	S	0	0	0
			1630	1018	272	335	5			
1	L	214	Total	C	N	O	S	0	0	0
			1630	1018	272	335	5			

- Molecule 2 is a protein called 10-28 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	216	Total	C	N	O	S	0	0	0
			1632	1036	272	318	6			
2	G	216	Total	C	N	O	S	0	0	0
			1632	1036	272	318	6			
2	H	216	Total	C	N	O	S	0	0	0
			1632	1036	272	318	6			

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	190	Total	C	N	O	S	0	1	0
			1505	966	249	282	8			
3	B	190	Total	C	N	O	S	0	1	0
			1505	966	249	282	8			
3	C	190	Total	C	N	O	S	0	1	0
			1505	966	249	282	8			

There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	538	GLY	-	expression tag	UNP P0DTC2
A	539	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	540	LEU	-	expression tag	UNP P0DTC2
A	541	GLU	-	expression tag	UNP P0DTC2
A	542	VAL	-	expression tag	UNP P0DTC2
A	543	LEU	-	expression tag	UNP P0DTC2
A	544	PHE	-	expression tag	UNP P0DTC2
A	545	GLN	-	expression tag	UNP P0DTC2
A	546	GLY	-	expression tag	UNP P0DTC2
A	547	PRO	-	expression tag	UNP P0DTC2
A	548	GLY	-	expression tag	UNP P0DTC2
A	549	HIS	-	expression tag	UNP P0DTC2
A	550	HIS	-	expression tag	UNP P0DTC2
A	551	HIS	-	expression tag	UNP P0DTC2
A	552	HIS	-	expression tag	UNP P0DTC2
A	553	HIS	-	expression tag	UNP P0DTC2
A	554	HIS	-	expression tag	UNP P0DTC2
B	538	GLY	-	expression tag	UNP P0DTC2
B	539	SER	-	expression tag	UNP P0DTC2
B	540	LEU	-	expression tag	UNP P0DTC2
B	541	GLU	-	expression tag	UNP P0DTC2
B	542	VAL	-	expression tag	UNP P0DTC2
B	543	LEU	-	expression tag	UNP P0DTC2
B	544	PHE	-	expression tag	UNP P0DTC2
B	545	GLN	-	expression tag	UNP P0DTC2
B	546	GLY	-	expression tag	UNP P0DTC2
B	547	PRO	-	expression tag	UNP P0DTC2
B	548	GLY	-	expression tag	UNP P0DTC2
B	549	HIS	-	expression tag	UNP P0DTC2
B	550	HIS	-	expression tag	UNP P0DTC2
B	551	HIS	-	expression tag	UNP P0DTC2
B	552	HIS	-	expression tag	UNP P0DTC2
B	553	HIS	-	expression tag	UNP P0DTC2
B	554	HIS	-	expression tag	UNP P0DTC2
C	538	GLY	-	expression tag	UNP P0DTC2
C	539	SER	-	expression tag	UNP P0DTC2
C	540	LEU	-	expression tag	UNP P0DTC2
C	541	GLU	-	expression tag	UNP P0DTC2
C	542	VAL	-	expression tag	UNP P0DTC2
C	543	LEU	-	expression tag	UNP P0DTC2
C	544	PHE	-	expression tag	UNP P0DTC2
C	545	GLN	-	expression tag	UNP P0DTC2
C	546	GLY	-	expression tag	UNP P0DTC2
C	547	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	548	GLY	-	expression tag	UNP P0DTC2
C	549	HIS	-	expression tag	UNP P0DTC2
C	550	HIS	-	expression tag	UNP P0DTC2
C	551	HIS	-	expression tag	UNP P0DTC2
C	552	HIS	-	expression tag	UNP P0DTC2
C	553	HIS	-	expression tag	UNP P0DTC2
C	554	HIS	-	expression tag	UNP P0DTC2

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

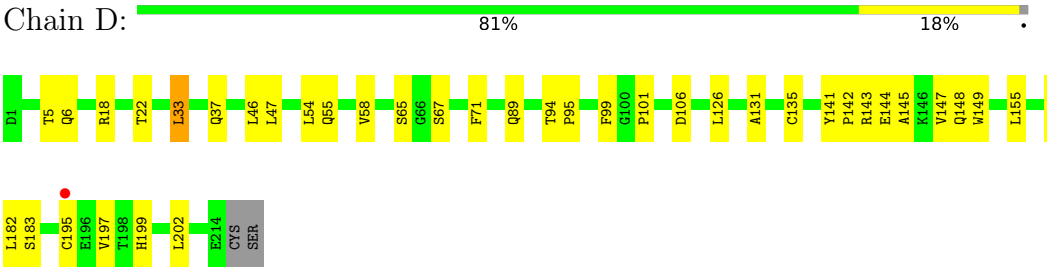
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

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.

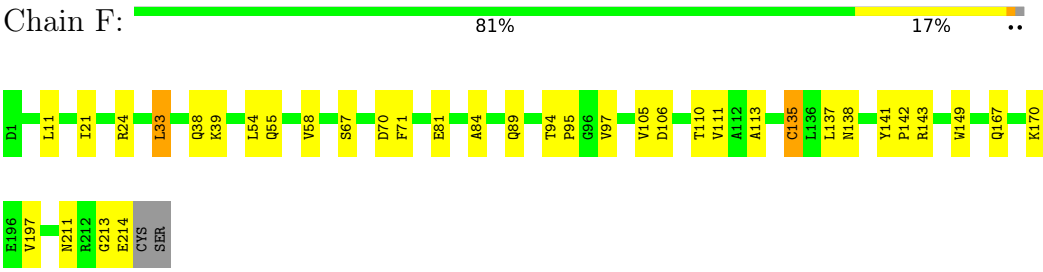
• Molecule 1: 10-28 Light Chain

Chain D:



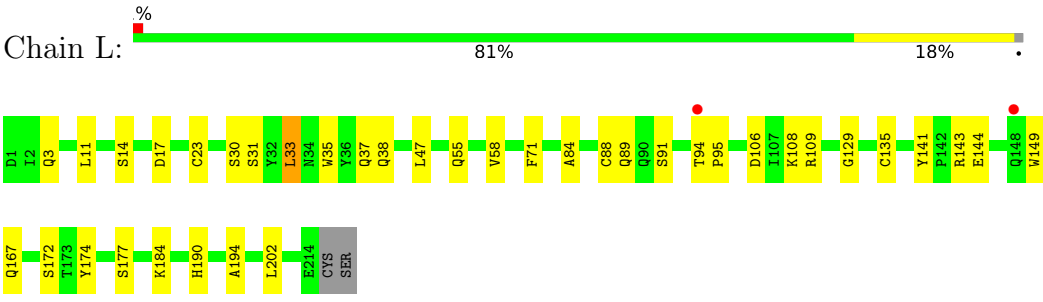
• Molecule 1: 10-28 Light Chain

Chain F:



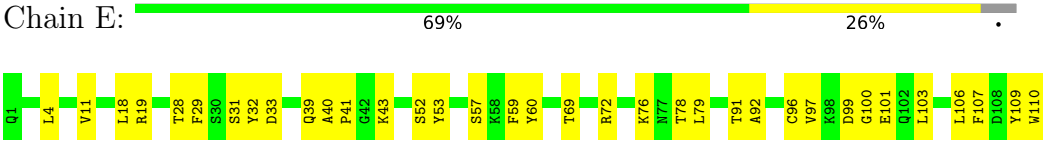
• Molecule 1: 10-28 Light Chain

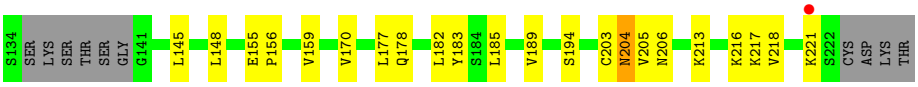
Chain L:



• Molecule 2: 10-28 Heavy Chain

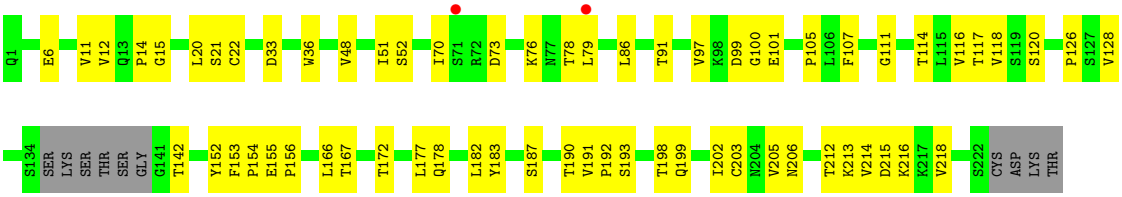
Chain E:





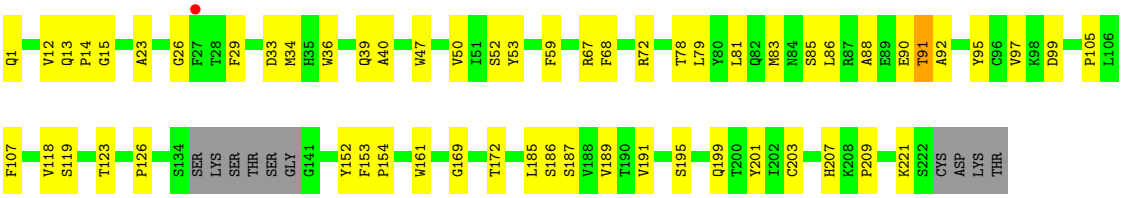
• Molecule 2: 10-28 Heavy Chain

Chain G:



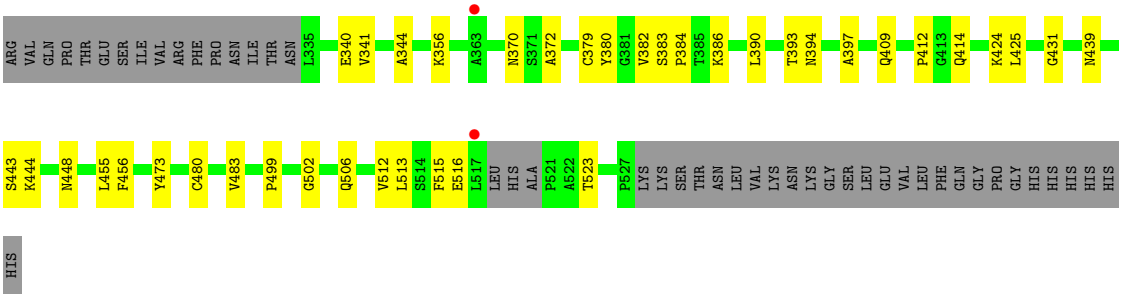
• Molecule 2: 10-28 Heavy Chain

Chain H:



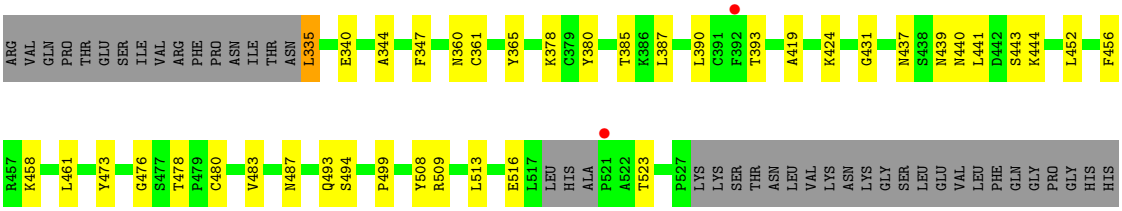
• Molecule 3: Spike protein S1

Chain A:



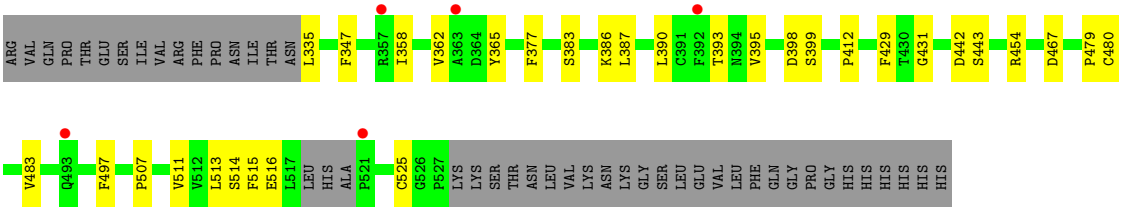
• Molecule 3: Spike protein S1

Chain B:



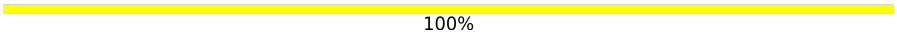
• Molecule 3: Spike protein S1

Chain C:



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

Chain I:



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

Chain J:

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

Chain K:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	123.78Å 226.68Å 186.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	108.64 – 3.20 108.64 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.7 (108.64-3.20) 97.7 (108.64-3.20)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.198 , 0.261 0.203 , 0.263	Depositor DCC
R_{free} test set	2361 reflections (5.55%)	wwPDB-VP
Wilson B-factor (Å^2)	74.9	Xtriage
Anisotropy	0.621	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.024 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.032 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14385	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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

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	D	0.61	0/1665	0.85	5/2262 (0.2%)
1	F	0.60	1/1665 (0.1%)	0.80	2/2262 (0.1%)
1	L	0.66	0/1665	0.86	2/2262 (0.1%)
2	E	0.62	0/1671	1.12	7/2274 (0.3%)
2	G	0.56	1/1671 (0.1%)	0.82	0/2274
2	H	0.64	0/1671	0.78	0/2274
3	A	0.63	1/1547 (0.1%)	0.83	1/2103 (0.0%)
3	B	0.64	0/1547	0.83	2/2103 (0.1%)
3	C	0.63	0/1547	0.83	1/2103 (0.0%)
All	All	0.62	3/14649 (0.0%)	0.86	20/19917 (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
2	E	0	1
2	G	0	1
2	H	0	1
3	C	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	424	LYS	C-N	5.52	1.46	1.34
1	F	135	CYS	CB-SG	5.08	1.90	1.82
2	G	203	CYS	CB-SG	-5.04	1.73	1.81

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	204	ASN	CB-CG-OD1	29.14	179.88	121.60
2	E	204	ASN	CB-CG-ND2	-14.33	82.31	116.70
2	E	204	ASN	OD1-CG-ND2	-10.57	97.59	121.90
2	E	204	ASN	N-CA-CB	-8.56	95.19	110.60
1	D	54	LEU	CA-CB-CG	7.38	132.28	115.30
2	E	204	ASN	N-CA-C	6.90	129.64	111.00
1	F	135	CYS	CA-CB-SG	6.46	125.63	114.00
3	B	458	LYS	CB-CG-CD	6.32	128.02	111.60
2	E	204	ASN	CB-CA-C	6.18	122.75	110.40
1	D	144	GLU	CA-CB-CG	5.93	126.45	113.40
3	A	455	LEU	CA-CB-CG	5.63	128.25	115.30
1	F	33	LEU	CA-CB-CG	-5.61	102.40	115.30
3	B	335	LEU	CA-CB-CG	5.53	128.01	115.30
1	D	144	GLU	CB-CA-C	5.33	121.06	110.40
1	L	144	GLU	CA-CB-CG	-5.23	101.89	113.40
3	C	335	LEU	C-N-CA	5.17	134.64	121.70
1	L	33	LEU	CA-CB-CG	-5.10	103.57	115.30
1	D	46	LEU	CB-CG-CD2	-5.06	102.40	111.00
2	E	204	ASN	CA-C-N	-5.05	106.09	117.20
1	D	33	LEU	CA-CB-CG	-5.01	103.78	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	479	PRO	Peptide
2	E	203	CYS	Peptide
2	G	142	THR	Peptide
2	H	221	LYS	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	D	1630	0	1585	24	0
1	F	1630	0	1585	30	0
1	L	1630	0	1585	30	0
2	E	1632	0	1604	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	1632	0	1604	43	0
2	H	1632	0	1604	40	0
3	A	1505	0	1422	28	0
3	B	1505	0	1422	31	0
3	C	1505	0	1422	18	0
4	I	28	0	25	0	0
4	J	28	0	25	1	0
4	K	28	0	25	1	0
All	All	14385	0	13908	268	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 9.

All (268) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:440:ASN:OD1	3:B:441:LEU:HG	1.06	1.22
3:B:440:ASN:OD1	3:B:441:LEU:CG	1.97	1.13
2:E:91:THR:HG22	2:E:118:VAL:H	1.26	0.99
1:D:6:GLN:HG3	1:D:101:PRO:HD2	1.49	0.95
2:H:105:PRO:HD3	3:A:383:SER:HB2	1.64	0.78
3:B:393:THR:HB	3:B:516:GLU:HB3	1.69	0.75
1:L:94:THR:HG22	3:A:379:CYS:O	1.87	0.75
1:L:94:THR:HG23	1:L:95:PRO:HD3	1.67	0.75
2:G:33:ASP:OD2	3:C:386:LYS:HE3	1.86	0.74
2:G:97:VAL:HG11	2:G:107:PHE:HB3	1.69	0.74
2:E:159:VAL:HG22	2:E:205:VAL:HG22	1.71	0.73
2:G:14:PRO:HD2	2:G:120:SER:HB2	1.75	0.69
2:H:97:VAL:HG11	2:H:107:PHE:HB3	1.75	0.68
3:C:393:THR:HB	3:C:516:GLU:HB3	1.76	0.67
1:D:18:ARG:NH1	1:F:113:ALA:O	2.27	0.67
2:G:126:PRO:HB3	2:G:152:TYR:HB3	1.78	0.66
2:E:170:VAL:HG22	2:E:189:VAL:HG22	1.77	0.65
2:E:155:GLU:CG	2:E:156:PRO:HA	2.24	0.65
2:E:40:ALA:HB3	2:E:43:LYS:HB2	1.78	0.64
3:C:347:PHE:CE2	3:C:399:SER:HB2	2.32	0.64
3:A:425:LEU:HD21	3:A:512:VAL:HG11	1.80	0.64
2:E:33:ASP:OD2	2:E:52:SER:HA	1.98	0.64
2:H:67:ARG:NH2	2:H:90:GLU:OE2	2.32	0.63
1:L:106:ASP:HB2	1:L:167:GLN:OE1	1.99	0.62
3:B:347:PHE:CE2	3:B:509:ARG:HD3	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:39:GLN:O	2:H:92:ALA:HB1	1.99	0.62
1:D:135:CYS:HB2	1:D:149:TRP:CH2	2.35	0.62
2:H:15:GLY:O	2:H:85:SER:HA	2.00	0.62
2:H:40:ALA:HA	2:H:92:ALA:HB2	1.81	0.62
1:D:65:SER:HB2	1:F:111:VAL:HG11	1.82	0.61
2:G:11:VAL:HG22	2:G:117:THR:HB	1.83	0.61
3:A:393:THR:O	3:A:523:THR:OG1	2.18	0.60
1:F:106:ASP:HB2	1:F:167:GLN:OE1	2.01	0.59
3:A:444:LYS:HG2	3:A:448:ASN:HB2	1.83	0.59
1:L:129:GLY:HA2	1:L:184:LYS:HD2	1.85	0.59
2:E:155:GLU:HG2	2:E:156:PRO:HA	1.82	0.59
1:F:67:SER:HA	1:F:71:PHE:CE2	2.37	0.59
2:H:126:PRO:HB3	2:H:152:TYR:HB3	1.85	0.59
2:H:23:ALA:HA	2:H:78:THR:HG22	1.85	0.58
2:G:99:ASP:OD1	2:G:100:GLY:N	2.36	0.58
2:G:191:VAL:HG23	2:G:193:SER:H	1.69	0.58
1:L:33:LEU:HD22	1:L:71:PHE:CG	2.38	0.58
2:G:206:ASN:ND2	2:G:213:LYS:HE2	2.18	0.58
2:E:31:SER:HA	2:E:53:TYR:HB2	1.85	0.57
2:H:195:SER:HB2	2:H:199:GLN:HG3	1.87	0.57
3:B:480:CYS:O	3:B:483:VAL:HG22	2.05	0.57
2:H:33:ASP:OD2	3:A:386:LYS:HE2	2.05	0.57
2:E:178:GLN:HG2	2:E:182:LEU:O	2.06	0.56
3:B:347:PHE:CE2	3:B:509:ARG:HB3	2.41	0.56
3:B:439:ASN:HD21	3:B:499:PRO:HA	1.71	0.56
2:E:216:LYS:HD3	2:E:217:LYS:H	1.71	0.55
1:D:106:ASP:HB2	1:D:167:GLN:OE1	2.06	0.55
3:B:347:PHE:HE2	3:B:509:ARG:HB3	1.71	0.55
3:A:431:GLY:HA2	3:A:515:PHE:CD2	2.41	0.55
1:D:95:PRO:HG2	3:B:378:LYS:HA	1.89	0.54
1:L:94:THR:HG21	3:A:382:VAL:O	2.06	0.54
2:G:155:GLU:HG2	2:G:156:PRO:HA	1.89	0.54
2:E:204:ASN:HD22	2:E:204:ASN:C	2.03	0.54
3:C:443:SER:OG	3:C:497:PHE:HB3	2.08	0.54
2:H:123:THR:HG22	2:H:154:PRO:HD3	1.89	0.54
2:G:20:LEU:HD12	2:G:114:THR:HG21	1.90	0.54
1:L:30:SER:OG	1:L:31:SER:N	2.40	0.53
1:F:33:LEU:HD22	1:F:71:PHE:CD1	2.43	0.53
2:H:40:ALA:HA	2:H:92:ALA:CB	2.37	0.53
2:H:39:GLN:C	2:H:92:ALA:HB1	2.29	0.53
3:A:480:CYS:O	3:A:483:VAL:HG12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:206:ASN:HD21	2:E:213:LYS:HE2	1.74	0.53
4:K:1:NAG:H61	4:K:2:NAG:C7	2.39	0.53
1:D:149:TRP:CZ3	1:D:195:CYS:HB3	2.43	0.53
2:H:83:MET:HE3	2:H:86:LEU:HD21	1.91	0.53
3:B:493:GLN:HG3	3:B:494:SER:N	2.24	0.53
1:L:167:GLN:NE2	1:L:172:SER:HB3	2.23	0.53
1:L:108:LYS:HA	1:L:141:TYR:OH	2.09	0.53
2:H:153:PHE:CD1	2:H:154:PRO:HA	2.44	0.52
2:H:185:LEU:HD23	2:H:186:SER:N	2.24	0.52
2:E:91:THR:HG22	2:E:118:VAL:N	2.09	0.52
2:G:172:THR:HG22	2:G:187:SER:OG	2.09	0.52
2:G:22:CYS:HB3	2:G:79:LEU:HB3	1.92	0.52
2:E:57:SER:HB2	2:E:59:PHE:CE2	2.45	0.52
2:H:52:SER:O	2:H:72:ARG:NH1	2.42	0.52
2:H:172:THR:HG22	2:H:187:SER:HB2	1.92	0.52
1:F:38:GLN:O	1:F:84:ALA:HB1	2.10	0.51
1:F:135:CYS:HB2	1:F:149:TRP:CH2	2.45	0.51
2:E:177:LEU:HD13	2:E:183:TYR:CZ	2.45	0.51
2:G:14:PRO:HG3	2:G:118:VAL:HG12	1.93	0.51
2:H:207:HIS:CD2	2:H:209:PRO:HD2	2.45	0.51
2:G:177:LEU:HD12	2:G:183:TYR:CZ	2.46	0.51
2:E:103:LEU:HD12	2:E:103:LEU:H	1.76	0.51
2:H:59:PHE:CZ	3:A:384:PRO:HB2	2.46	0.51
3:A:439:ASN:HD21	3:A:499:PRO:HA	1.76	0.51
2:E:106:LEU:C	2:E:106:LEU:HD12	2.31	0.51
2:H:172:THR:HG22	2:H:187:SER:CB	2.40	0.51
3:A:409:GLN:HA	3:A:414:GLN:HG3	1.93	0.51
3:A:379:CYS:HB2	3:A:384:PRO:HD3	1.93	0.50
2:E:18:LEU:HD12	2:E:19:ARG:H	1.77	0.50
2:H:169:GLY:O	2:H:189:VAL:HA	2.10	0.50
2:E:91:THR:CG2	2:E:118:VAL:H	2.12	0.50
2:E:100:GLY:O	2:E:101:GLU:HB2	2.10	0.50
2:G:105:PRO:HD3	3:C:383:SER:HB2	1.94	0.50
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.93	0.50
1:D:55:GLN:HB3	1:D:58:VAL:HG21	1.94	0.49
2:G:21:SER:HA	2:G:79:LEU:O	2.12	0.49
2:G:153:PHE:CD2	2:G:154:PRO:HA	2.47	0.49
1:F:94:THR:OG1	1:F:95:PRO:HD3	2.12	0.49
2:G:212:THR:HG22	2:G:214:VAL:HG23	1.94	0.49
3:B:440:ASN:OD1	3:B:441:LEU:CD2	2.60	0.49
2:E:97:VAL:HG11	2:E:107:PHE:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:153:PHE:CG	2:G:154:PRO:HA	2.48	0.49
2:H:1:GLN:NE2	2:H:26:GLY:HA2	2.26	0.49
1:L:143:ARG:HB2	1:L:174:TYR:CE2	2.47	0.49
1:F:89:GLN:HE21	1:F:97:VAL:CG1	2.26	0.49
3:C:454:ARG:NH2	3:C:467:ASP:O	2.34	0.49
1:L:177:SER:O	1:L:177:SER:OG	2.27	0.49
2:G:192:PRO:O	2:G:193:SER:HB3	2.12	0.48
2:H:29:PHE:O	2:H:72:ARG:NH2	2.46	0.48
1:D:33:LEU:HD12	1:D:89:GLN:O	2.13	0.48
2:E:206:ASN:ND2	2:E:213:LYS:HE2	2.28	0.48
3:B:452:LEU:HD23	3:B:494:SER:HA	1.95	0.48
3:C:480:CYS:O	3:C:483:VAL:HG22	2.13	0.48
2:E:155:GLU:HG3	2:E:156:PRO:HA	1.93	0.48
1:F:33:LEU:HD22	1:F:71:PHE:CG	2.47	0.48
1:F:95:PRO:HG2	3:C:377:PHE:O	2.13	0.48
1:L:38:GLN:O	1:L:84:ALA:HB1	2.14	0.48
3:A:340:GLU:O	3:A:344:ALA:HB2	2.13	0.48
1:L:108:LYS:HG2	1:L:109:ARG:N	2.29	0.48
2:H:191:VAL:HG11	2:H:201:TYR:CE1	2.47	0.47
1:L:94:THR:CG2	1:L:95:PRO:HD3	2.39	0.47
3:A:456:PHE:HB3	3:A:473:TYR:CD2	2.48	0.47
2:H:172:THR:HG22	2:H:187:SER:OG	2.14	0.47
3:A:502:GLY:O	3:A:506:GLN:HG3	2.14	0.47
2:G:128:VAL:HG21	2:G:205:VAL:HG21	1.96	0.47
2:E:32:TYR:HE1	2:E:101:GLU:HG3	1.78	0.47
1:D:55:GLN:HB3	1:D:58:VAL:CG2	2.44	0.47
2:E:4:LEU:HD13	2:E:109:TYR:HD1	1.79	0.47
1:F:54:LEU:HD11	1:F:58:VAL:HB	1.96	0.47
2:E:99:ASP:OD1	2:E:100:GLY:N	2.48	0.47
2:G:12:VAL:O	2:G:118:VAL:HA	2.15	0.47
3:A:439:ASN:OD1	3:A:443:SER:OG	2.33	0.47
3:C:398:ASP:O	3:C:511:VAL:HA	2.15	0.47
1:D:22:THR:HG21	1:F:110:THR:HG21	1.96	0.46
1:F:213:GLY:O	1:F:214:GLU:HG2	2.14	0.46
1:F:138:ASN:HD21	2:G:190:THR:HG21	1.81	0.46
3:B:360:ASN:H	3:B:523:THR:HB	1.80	0.46
3:C:358:ILE:O	3:C:395:VAL:HB	2.15	0.46
2:E:28:THR:O	2:E:28:THR:OG1	2.33	0.46
1:D:143:ARG:HB2	1:D:174:TYR:CE2	2.50	0.46
3:C:442:ASP:HB2	3:C:507:PRO:HG3	1.98	0.46
1:F:192:VAL:HG22	1:F:211:ASN:OD1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:83:MET:CE	2:H:86:LEU:HD21	2.46	0.46
3:B:437:ASN:HB2	3:B:508:TYR:CZ	2.50	0.46
3:B:461:LEU:HD23	3:B:461:LEU:HA	1.67	0.46
2:G:76:LYS:O	2:G:78:THR:HG23	2.15	0.46
2:H:88:ALA:O	2:H:91:THR:HG22	2.16	0.46
2:E:11:VAL:HA	2:E:117:THR:O	2.16	0.45
2:G:198:THR:HG23	2:G:199:GLN:H	1.80	0.45
3:B:419:ALA:O	3:B:424:LYS:HD3	2.16	0.45
2:E:148:LEU:HD12	2:E:185:LEU:O	2.17	0.45
1:L:135:CYS:HB2	1:L:149:TRP:CH2	2.52	0.45
1:F:143:ARG:O	1:F:143:ARG:HG2	2.15	0.45
2:G:166:LEU:HD12	2:G:167:THR:N	2.32	0.45
3:A:394:ASN:N	3:A:516:GLU:OE2	2.44	0.45
1:D:202:LEU:HD23	1:D:202:LEU:HA	1.79	0.45
2:G:100:GLY:O	2:G:101:GLU:HB2	2.17	0.45
2:H:14:PRO:HD3	2:H:119:SER:O	2.16	0.45
3:B:335:LEU:C	3:B:361:CYS:HB2	2.37	0.45
1:D:94:THR:OG1	1:D:95:PRO:HD3	2.17	0.45
2:H:161:TRP:CZ3	2:H:203:CYS:HB3	2.52	0.45
2:G:155:GLU:CG	2:G:156:PRO:HA	2.47	0.45
2:H:53:TYR:HD2	3:A:386:LYS:NZ	2.14	0.45
2:G:178:GLN:HG2	2:G:182:LEU:O	2.17	0.45
2:H:91:THR:O	2:H:92:ALA:HB2	2.17	0.45
3:B:456:PHE:HB3	3:B:473:TYR:CD2	2.52	0.45
1:F:11:LEU:O	1:F:105:VAL:HA	2.17	0.44
2:G:33:ASP:OD1	2:G:52:SER:HA	2.17	0.44
1:L:3:GLN:HE22	3:B:478:THR:HG22	1.82	0.44
3:B:440:ASN:OD1	3:B:441:LEU:N	2.49	0.44
1:D:148:GLN:HB3	1:D:155:LEU:HD21	2.00	0.44
2:E:29:PHE:CE2	2:E:72:ARG:NH2	2.86	0.44
2:E:96:CYS:O	2:E:110:TRP:O	2.36	0.44
2:E:39:GLN:O	2:E:92:ALA:HB1	2.17	0.44
2:G:51:ILE:HD12	2:G:70:ILE:HG23	1.99	0.44
2:H:13:GLN:HA	2:H:119:SER:O	2.18	0.43
1:L:152:ASP:OD2	1:L:190:HIS:HB3	2.18	0.43
2:H:36:TRP:CD1	2:H:81:LEU:HD13	2.53	0.43
2:E:145:LEU:HD12	2:E:218:VAL:CG1	2.47	0.43
2:G:11:VAL:HA	2:G:117:THR:O	2.18	0.43
2:G:206:ASN:HD21	2:G:213:LYS:HE2	1.81	0.43
1:D:95:PRO:HB2	3:B:378:LYS:HG2	2.00	0.43
3:A:340:GLU:OE2	3:A:356:LYS:NZ	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:SER:HA	1:D:71:PHE:CE2	2.53	0.43
2:G:15:GLY:N	2:G:86:LEU:O	2.50	0.43
1:D:141:TYR:CD1	1:D:142:PRO:HA	2.53	0.43
1:F:54:LEU:HD11	1:F:58:VAL:CG1	2.49	0.43
3:A:390:LEU:HA	3:A:390:LEU:HD23	1.79	0.43
1:F:55:GLN:HB3	1:F:58:VAL:CG2	2.49	0.43
1:L:202:LEU:HD23	1:L:202:LEU:HA	1.79	0.43
3:B:444:LYS:O	3:B:499:PRO:HD3	2.19	0.43
1:D:126:LEU:HD21	1:D:131:ALA:HB2	2.00	0.42
2:E:103:LEU:HD12	2:E:103:LEU:N	2.34	0.42
1:F:137:LEU:HD21	1:F:197:VAL:HG13	2.01	0.42
1:L:143:ARG:HD3	1:L:174:TYR:CE1	2.54	0.42
1:L:14:SER:HB2	1:L:17:ASP:OD2	2.18	0.42
1:L:95:PRO:HG3	3:A:384:PRO:HG3	2.00	0.42
3:B:344:ALA:HB3	3:B:347:PHE:HE1	1.84	0.42
3:B:380:TYR:CD1	3:B:380:TYR:N	2.87	0.42
1:F:39:LYS:NZ	1:F:81:GLU:HB2	2.33	0.42
2:H:12:VAL:O	2:H:118:VAL:HA	2.19	0.42
1:F:33:LEU:HD12	1:F:89:GLN:O	2.20	0.42
1:F:55:GLN:HB3	1:F:58:VAL:HG21	2.01	0.42
2:H:34:MET:HE2	2:H:79:LEU:HD22	2.01	0.42
3:B:390:LEU:HA	3:B:390:LEU:HD23	1.59	0.42
3:B:476:GLY:HA3	3:B:487:ASN:HB3	2.00	0.42
1:D:145:ALA:HB2	1:D:199:HIS:HD2	1.84	0.42
3:A:439:ASN:ND2	3:A:499:PRO:HA	2.34	0.42
1:D:182:LEU:HB3	1:D:183:SER:H	1.58	0.42
2:E:216:LYS:HD3	2:E:217:LYS:N	2.34	0.42
2:G:218:VAL:HG23	2:G:218:VAL:O	2.20	0.42
1:L:11:LEU:HD12	1:L:11:LEU:HA	1.82	0.42
3:A:380:TYR:CE2	3:A:412:PRO:HD2	2.55	0.42
1:L:55:GLN:HB3	1:L:58:VAL:HG21	2.02	0.41
3:C:431:GLY:HA2	3:C:515:PHE:CE2	2.55	0.41
1:D:37:GLN:HB2	1:D:47:LEU:HD11	2.02	0.41
2:G:172:THR:HG22	2:G:187:SER:CB	2.49	0.41
1:L:150:LYS:HB2	1:L:194:ALA:HB3	2.02	0.41
4:J:1:NAG:H61	4:J:2:NAG:C7	2.50	0.41
3:A:370:ASN:O	3:A:372:ALA:N	2.53	0.41
3:B:365:TYR:CD2	3:B:387:LEU:HB3	2.55	0.41
3:B:431:GLY:HA3	3:B:513:LEU:O	2.21	0.41
3:B:439:ASN:O	3:B:443:SER:HB3	2.20	0.41
1:D:89:GLN:HG3	1:D:99:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:36:TRP:O	2:G:48:VAL:HB	2.20	0.41
1:L:94:THR:HG21	3:A:383:SER:HA	2.01	0.41
2:E:52:SER:HB3	3:B:385:THR:HB	2.01	0.41
1:D:147:VAL:HG22	1:D:197:VAL:HG22	2.02	0.41
1:F:89:GLN:HE21	1:F:97:VAL:HG11	1.84	0.41
2:G:73:ASP:OD2	2:G:76:LYS:NZ	2.25	0.41
3:B:340:GLU:O	3:B:344:ALA:HB2	2.20	0.41
2:E:60:TYR:OH	2:E:69:THR:HA	2.20	0.41
1:F:141:TYR:CD1	1:F:142:PRO:HA	2.56	0.41
1:L:23:CYS:HB2	1:L:35:TRP:CH2	2.55	0.41
1:F:21:ILE:HG21	1:F:21:ILE:HD13	1.83	0.41
1:L:89:GLN:HE22	1:L:91:SER:HB3	1.86	0.41
2:G:6:GLU:OE2	2:G:111:GLY:HA3	2.21	0.41
2:G:91:THR:HG23	2:G:116:VAL:O	2.20	0.41
2:H:36:TRP:HA	2:H:95:TYR:O	2.21	0.41
1:L:109:ARG:HG3	1:L:141:TYR:CD2	2.55	0.41
1:F:24:ARG:HG3	1:F:70:ASP:OD1	2.21	0.41
2:G:202:ILE:HD11	2:G:215:ASP:HB3	2.03	0.41
2:G:216:LYS:HE3	2:G:216:LYS:HB3	1.90	0.41
2:H:33:ASP:HB2	2:H:99:ASP:CB	2.51	0.41
3:A:341:VAL:HG11	3:A:397:ALA:HB1	2.02	0.41
2:G:91:THR:HG23	2:G:117:THR:HA	2.03	0.40
3:A:513:LEU:HD23	3:A:513:LEU:HA	1.80	0.40
3:C:362:VAL:HG13	3:C:525:CYS:O	2.21	0.40
2:E:72:ARG:HB3	2:E:79:LEU:HD12	2.03	0.40
2:H:47:TRP:HZ2	2:H:50:VAL:HG12	1.87	0.40
3:C:395:VAL:HA	3:C:514:SER:O	2.21	0.40
2:E:76:LYS:O	2:E:78:THR:HG23	2.22	0.40
1:F:39:LYS:HZ1	1:F:81:GLU:HB2	1.85	0.40
2:H:68:PHE:N	2:H:68:PHE:CD1	2.89	0.40
3:C:412:PRO:HG3	3:C:429:PHE:HB3	2.03	0.40
3:C:431:GLY:HA3	3:C:513:LEU:O	2.21	0.40
2:E:40:ALA:HA	2:E:92:ALA:HB2	2.02	0.40
2:E:41:PRO:HD3	2:E:91:THR:O	2.21	0.40
1:F:170:LYS:HA	1:F:170:LYS:HD3	1.79	0.40
1:L:33:LEU:HD11	1:L:88:CYS:HB2	2.04	0.40
3:C:365:TYR:CD2	3:C:387:LEU:HB3	2.57	0.40
3:C:386:LYS:O	3:C:390:LEU:HG	2.22	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	D	212/216 (98%)	202 (95%)	10 (5%)	0	100	100
1	F	212/216 (98%)	202 (95%)	10 (5%)	0	100	100
1	L	212/216 (98%)	197 (93%)	15 (7%)	0	100	100
2	E	212/226 (94%)	200 (94%)	12 (6%)	0	100	100
2	G	212/226 (94%)	199 (94%)	13 (6%)	0	100	100
2	H	212/226 (94%)	200 (94%)	12 (6%)	0	100	100
3	A	186/236 (79%)	170 (91%)	16 (9%)	0	100	100
3	B	186/236 (79%)	173 (93%)	13 (7%)	0	100	100
3	C	186/236 (79%)	173 (93%)	13 (7%)	0	100	100
All	All	1830/2034 (90%)	1716 (94%)	114 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	D	188/190 (99%)	187 (100%)	1 (0%)	88	95
1	F	188/190 (99%)	187 (100%)	1 (0%)	88	95
1	L	188/190 (99%)	188 (100%)	0	100	100
2	E	184/193 (95%)	182 (99%)	2 (1%)	73	88
2	G	184/193 (95%)	184 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	H	184/193 (95%)	183 (100%)	1 (0%)	88 95
3	A	164/206 (80%)	164 (100%)	0	100 100
3	B	164/206 (80%)	164 (100%)	0	100 100
3	C	164/206 (80%)	164 (100%)	0	100 100
All	All	1608/1767 (91%)	1603 (100%)	5 (0%)	92 96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	5	THR
2	E	194	SER
2	E	221	LYS
1	F	195	CYS
2	H	91	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	1	GLN
3	C	450	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)

6 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	I	1	4,3	14,14,15	0.67	1 (7%)	17,19,21	0.98	1 (5%)
4	NAG	I	2	4	14,14,15	0.68	1 (7%)	17,19,21	1.21	2 (11%)
4	NAG	J	1	4,3	14,14,15	0.43	0	17,19,21	0.86	1 (5%)
4	NAG	J	2	4	14,14,15	0.42	0	17,19,21	0.97	1 (5%)
4	NAG	K	1	4,3	14,14,15	0.45	0	17,19,21	0.70	1 (5%)
4	NAG	K	2	4	14,14,15	0.62	0	17,19,21	1.01	1 (5%)

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	I	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	NAG	J	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	1	NAG	O5-C1	-2.23	1.40	1.43
4	I	2	NAG	O5-C1	-2.10	1.40	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	2	NAG	C1-O5-C5	3.96	117.56	112.19
4	K	2	NAG	C1-O5-C5	3.62	117.10	112.19
4	J	2	NAG	C1-O5-C5	3.26	116.61	112.19
4	I	1	NAG	O4-C4-C5	-2.94	101.99	109.30
4	J	1	NAG	C1-O5-C5	2.91	116.13	112.19
4	K	1	NAG	C1-O5-C5	2.15	115.10	112.19
4	I	2	NAG	C2-N2-C7	2.06	125.83	122.90

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	1	NAG	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6

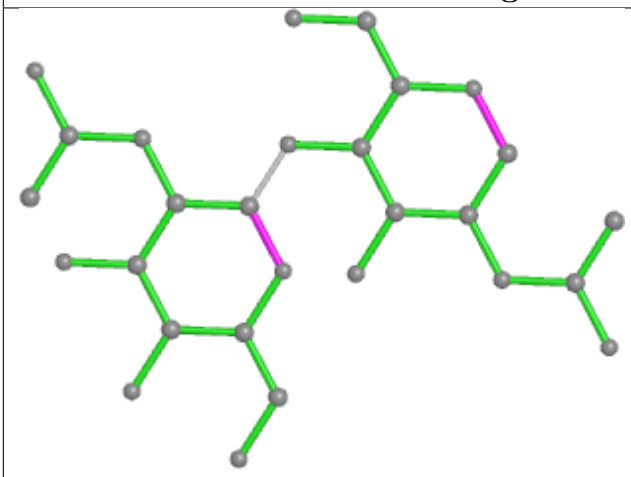
There are no ring outliers.

4 monomers are involved in 2 short contacts:

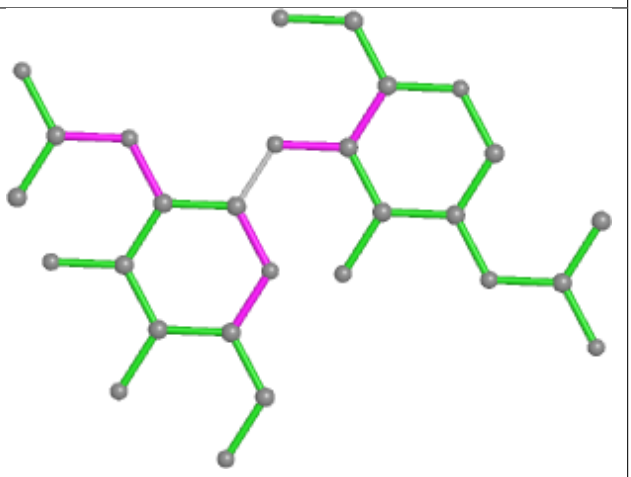
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	1	NAG	1	0
4	K	2	NAG	1	0
4	J	2	NAG	1	0
4	J	1	NAG	1	0

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

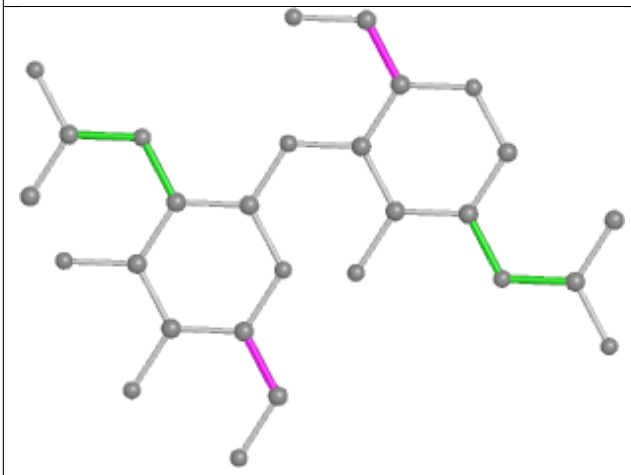
Oligosaccharide Chain I



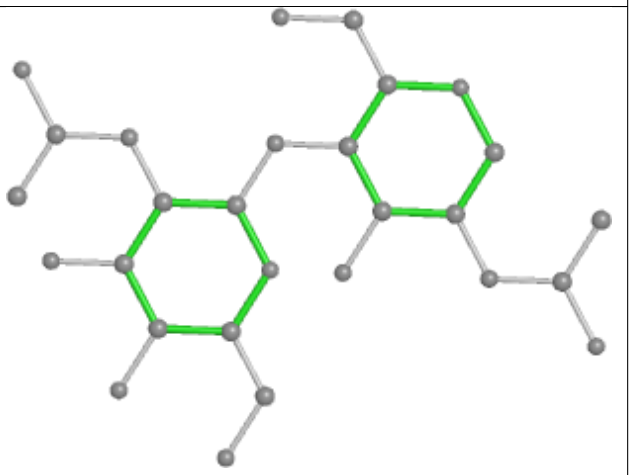
Bond lengths



Bond angles

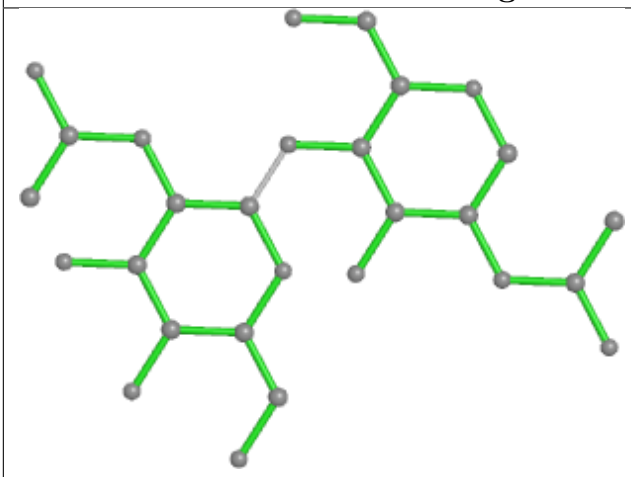


Torsions

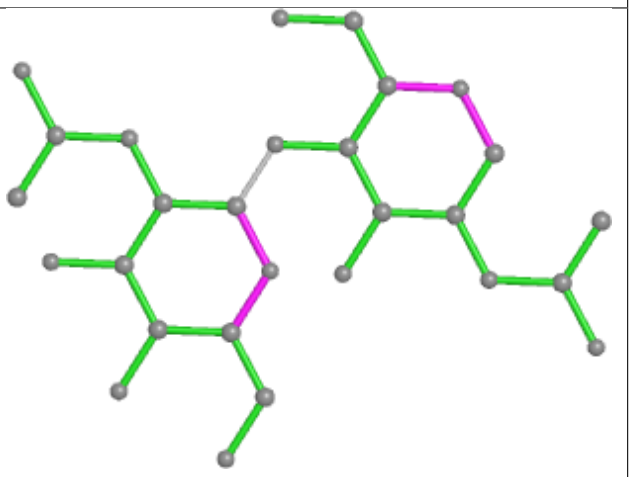


Rings

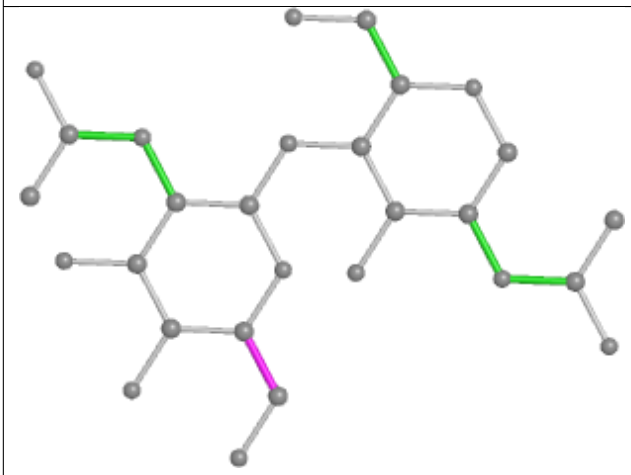
Oligosaccharide Chain J



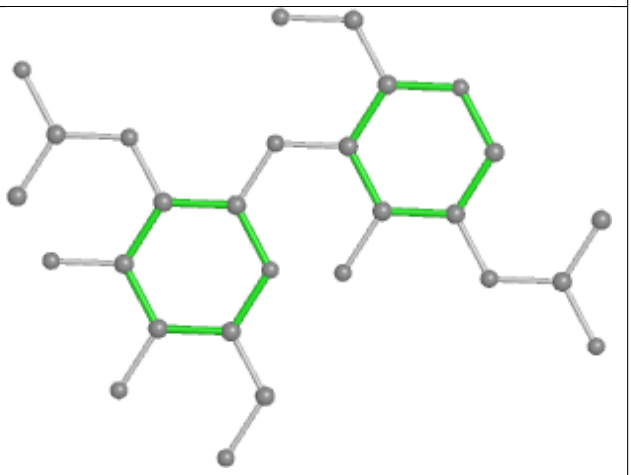
Bond lengths



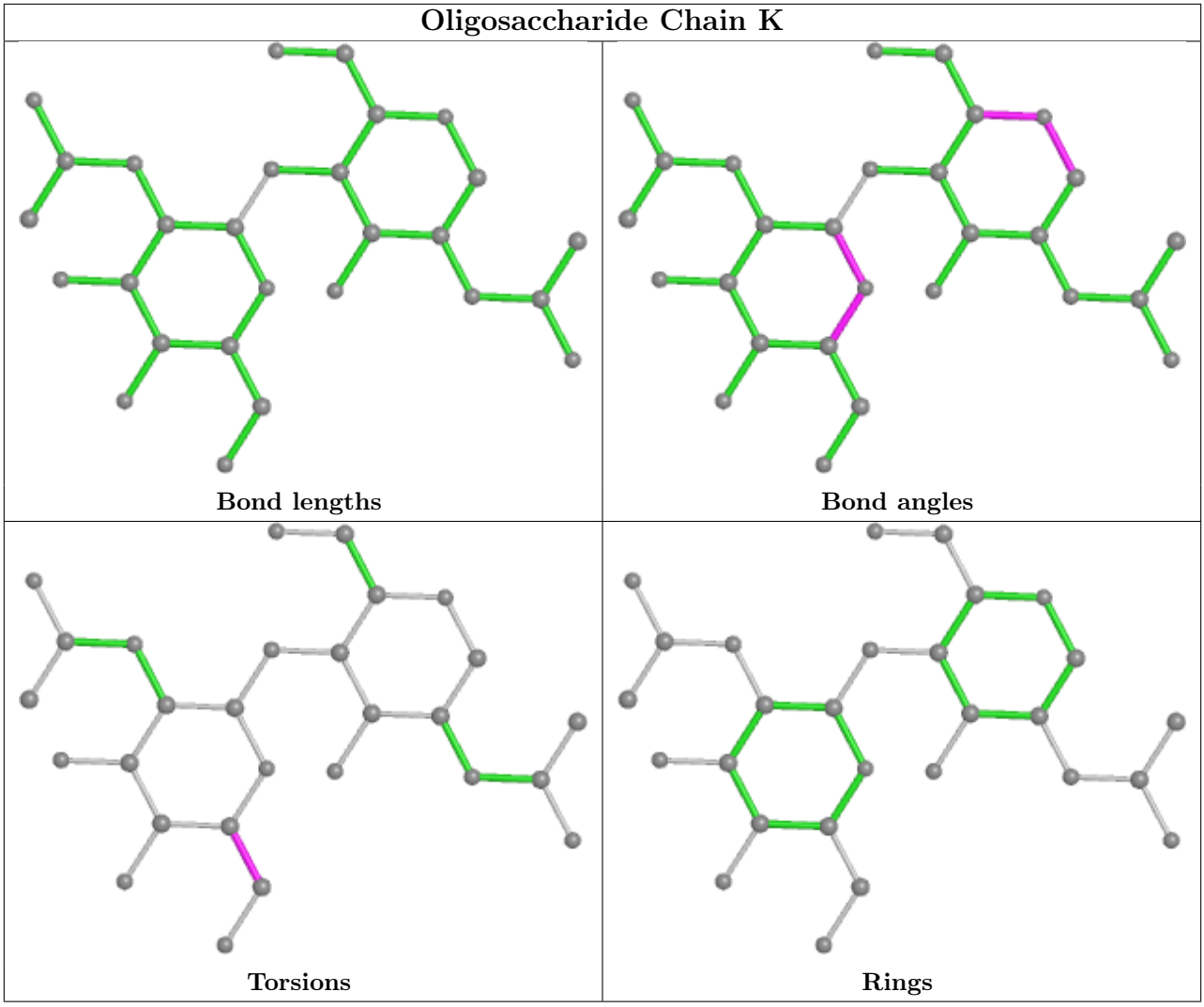
Bond angles



Torsions



Rings



5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	D	214/216 (99%)	0.19	1 (0%)	91	86	30, 72, 101, 120	0
1	F	214/216 (99%)	0.18	1 (0%)	91	86	30, 69, 96, 123	0
1	L	214/216 (99%)	0.22	2 (0%)	84	75	50, 69, 94, 102	0
2	E	216/226 (95%)	0.28	1 (0%)	91	86	57, 79, 98, 111	0
2	G	216/226 (95%)	0.24	2 (0%)	84	75	62, 82, 111, 133	0
2	H	216/226 (95%)	0.18	1 (0%)	91	86	52, 69, 89, 105	0
3	A	190/236 (80%)	0.21	2 (1%)	80	69	30, 77, 119, 142	0
3	B	190/236 (80%)	0.21	2 (1%)	80	69	30, 77, 110, 124	0
3	C	190/236 (80%)	0.40	5 (2%)	56	40	30, 89, 123, 146	0
All	All	1860/2034 (91%)	0.24	17 (0%)	84	75	30, 75, 106, 146	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	94	THR	3.8
3	C	521	PRO	3.0
1	D	195	CYS	2.8
2	H	27	PHE	2.7
3	C	363	ALA	2.5
3	C	493	GLN	2.3
2	G	71	SER	2.2
3	C	357	ARG	2.2
3	B	392	PHE	2.2
3	A	517	LEU	2.2
3	C	392	PHE	2.1
2	E	221	LYS	2.1
3	B	521	PRO	2.1
3	A	363	ALA	2.1
2	G	79	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	148	GLN	2.0
1	F	192	VAL	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)

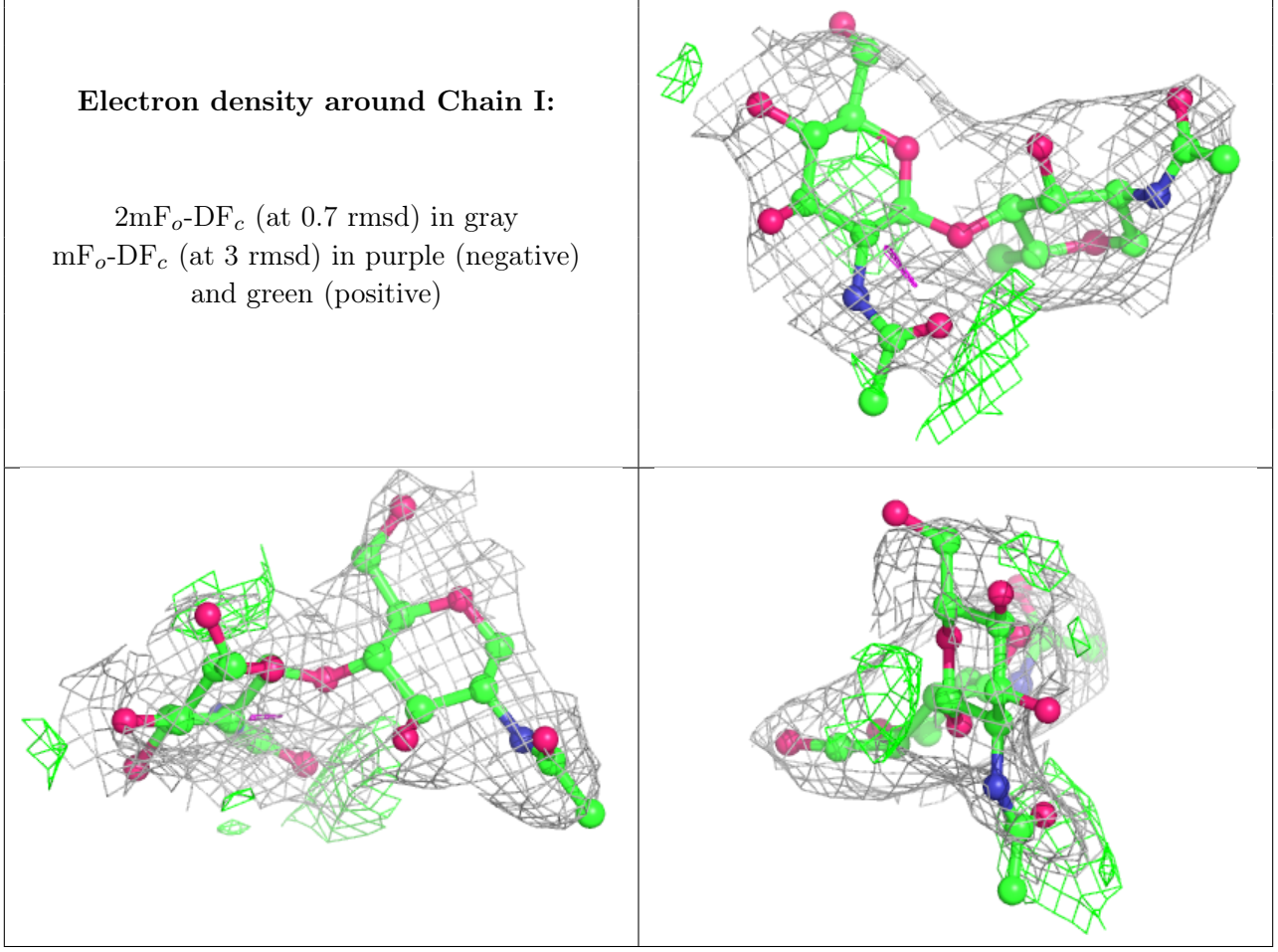
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	NAG	I	2	14/15	0.70	0.27	113,120,127,128	0
4	NAG	K	2	14/15	0.77	0.23	113,121,128,129	0
4	NAG	K	1	14/15	0.86	0.23	90,104,115,115	0
4	NAG	J	2	14/15	0.90	0.15	101,107,112,114	0
4	NAG	J	1	14/15	0.92	0.22	88,101,106,107	0
4	NAG	I	1	14/15	0.94	0.21	75,83,92,105	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.

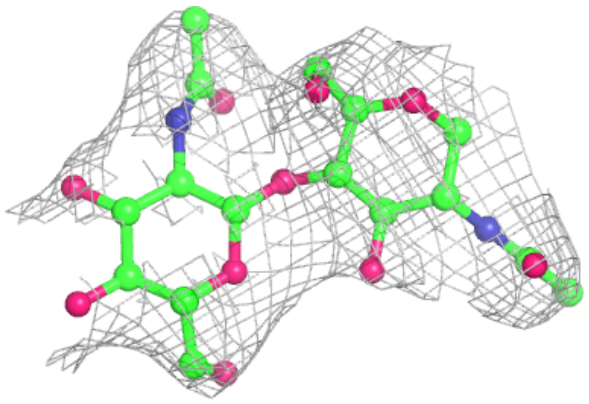
Electron density around Chain I:

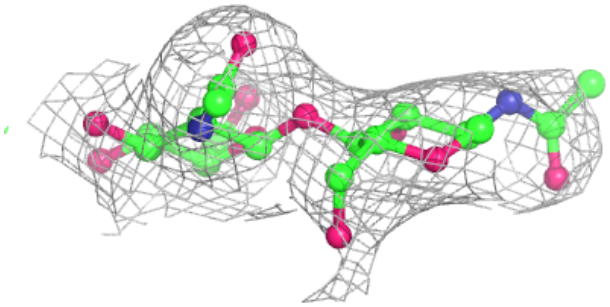
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

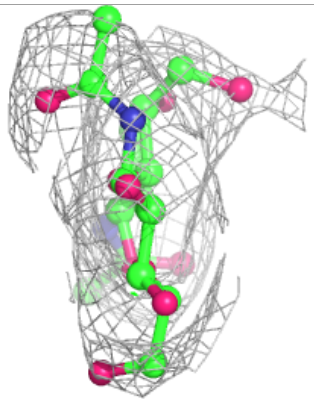


Electron density around Chain J:

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

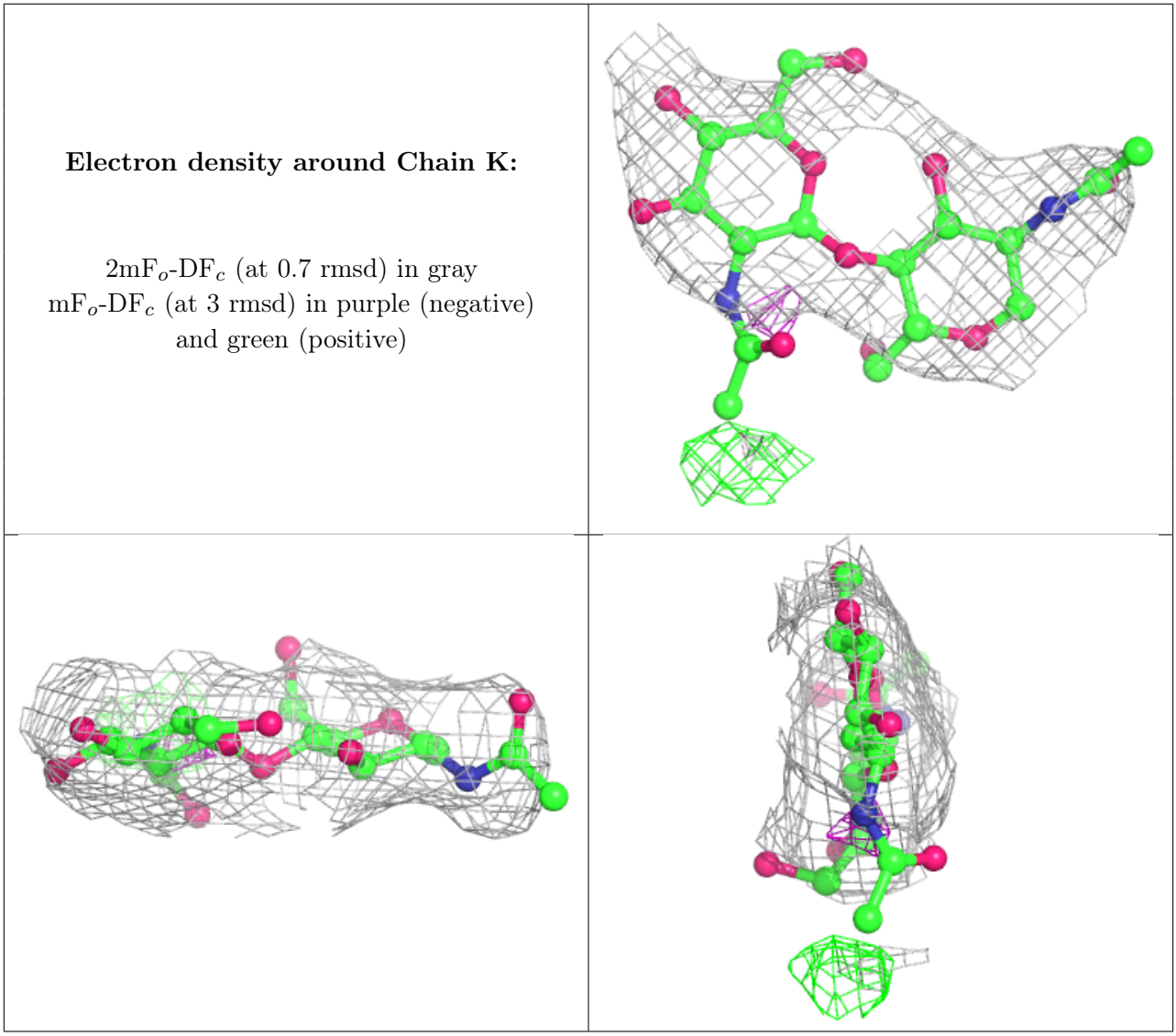






Electron density around Chain K:

$2mF_o$-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.