Full wwPDB X-ray Structure Validation Report ⓘ

Dec 19, 2023 – 04:24 PM JST

PDB ID	:	7Y3N
Title	:	Crystal structure of SARS-CoV receptor binding domain in complex with human antibody BIOLS56
Authors	:	Rao, X.; Chai, Y.; Wu, Y.; Gao, F.
Deposited on	:	2022-06-11
Resolution	:	2.97 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:

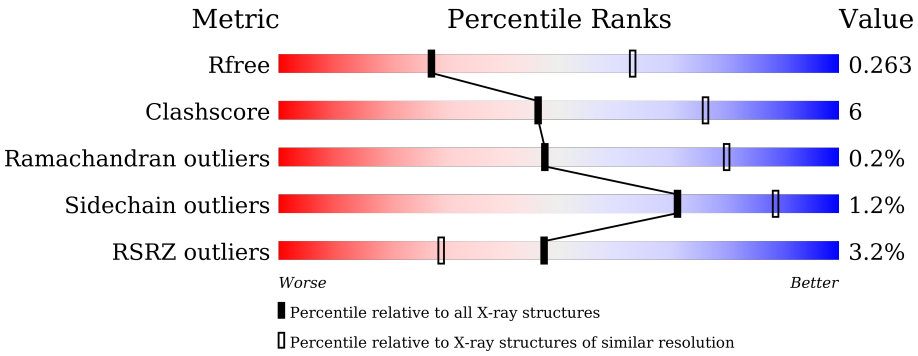
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.97 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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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	228	3% 65% 20% • 14%
1	B	228	3% 67% 18% 14%
1	E	228	5% 64% 18% • 17%
2	C	237	2% 82% 12% 6%
2	F	237	3% 81% 13% 7%
2	H	237	% 85% 9% 6%

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Mol	Chain	Length	Quality of chain
3	D	215	2% 88% 11%
3	G	215	8% 80% 18%
3	L	215	% 91% 9%
4	I	3	33% 33% 33%

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
4	NAG	I	2	-	-	-	X
5	NAG	B	301	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14620 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	0	0	0
			1560	1008	254	289	9			
1	B	195	Total	C	N	O	S	0	0	0
			1553	1004	253	287	9			
1	E	190	Total	C	N	O	S	0	0	0
			1516	983	246	278	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	223	HIS	-	expression tag	UNP P59594
A	224	HIS	-	expression tag	UNP P59594
A	225	HIS	-	expression tag	UNP P59594
A	226	HIS	-	expression tag	UNP P59594
A	227	HIS	-	expression tag	UNP P59594
A	228	HIS	-	expression tag	UNP P59594
B	223	HIS	-	expression tag	UNP P59594
B	224	HIS	-	expression tag	UNP P59594
B	225	HIS	-	expression tag	UNP P59594
B	226	HIS	-	expression tag	UNP P59594
B	227	HIS	-	expression tag	UNP P59594
B	228	HIS	-	expression tag	UNP P59594
E	223	HIS	-	expression tag	UNP P59594
E	224	HIS	-	expression tag	UNP P59594
E	225	HIS	-	expression tag	UNP P59594
E	226	HIS	-	expression tag	UNP P59594
E	227	HIS	-	expression tag	UNP P59594
E	228	HIS	-	expression tag	UNP P59594

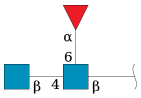
- Molecule 2 is a protein called Heavy chain of BIOLS56.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	223	Total	C	N	O	S	0	0	0
			1677	1061	278	330	8			
2	C	223	Total	C	N	O	S	0	0	0
			1677	1061	278	330	8			
2	F	221	Total	C	N	O	S	0	0	0
			1665	1055	276	327	7			

- Molecule 3 is a protein called Light chain of BIOLS56.

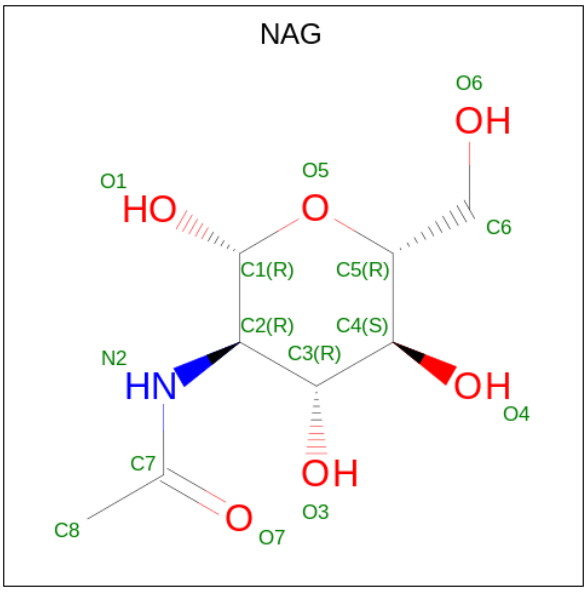
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	215	Total	C	N	O	S	0	0	0
			1646	1029	274	337	6			
3	D	214	Total	C	N	O	S	0	0	0
			1640	1026	273	335	6			
3	G	213	Total	C	N	O	S	0	0	0
			1634	1023	272	334	5			

- Molecule 4 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
4	I	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



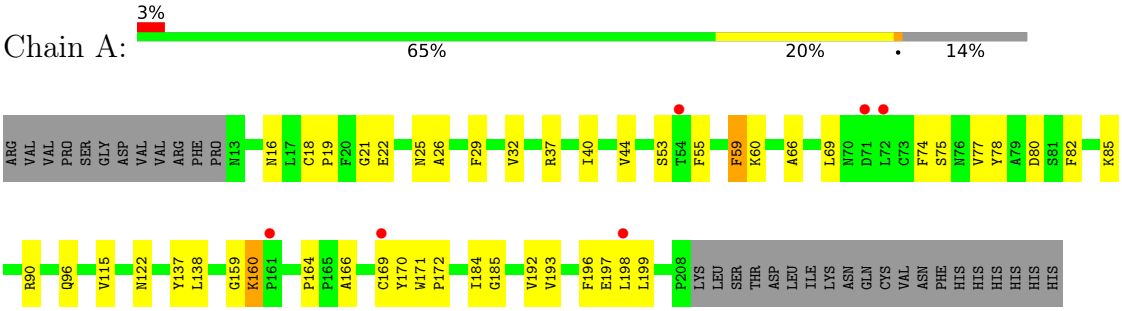
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	B	1	14	8	1	5	0	0

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.

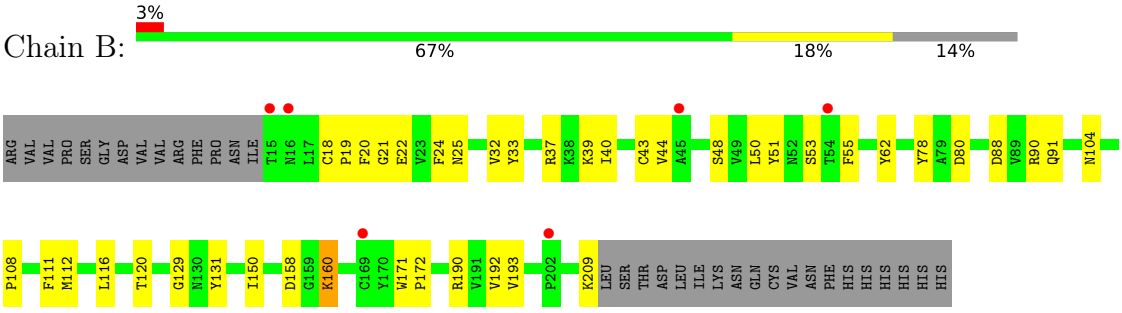
• Molecule 1: Spike protein S1

Chain A:



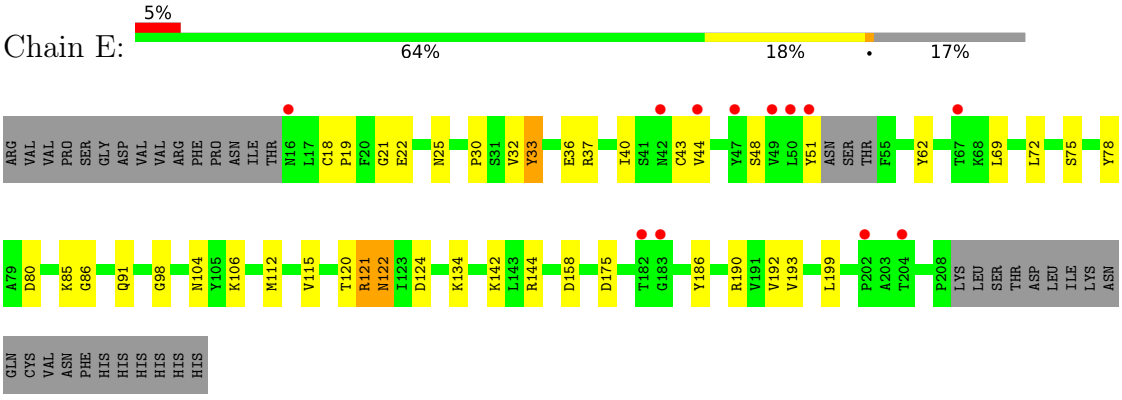
• Molecule 1: Spike protein S1

Chain B:



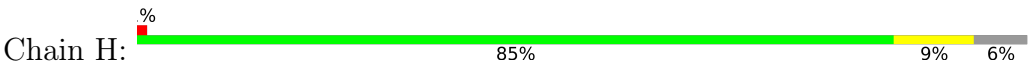
• Molecule 1: Spike protein S1

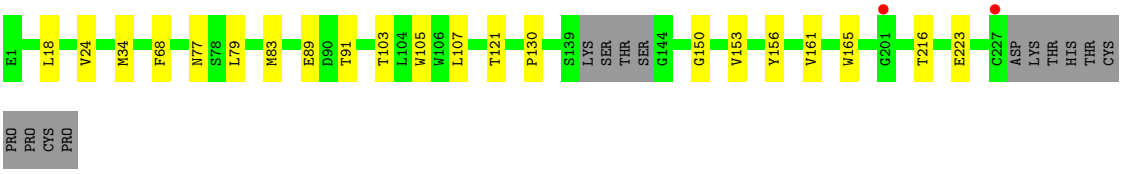
Chain E:



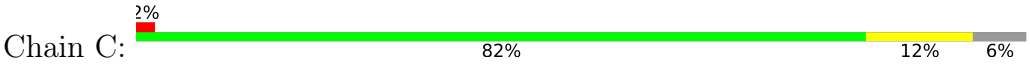
• Molecule 2: Heavy chain of BIOLS56

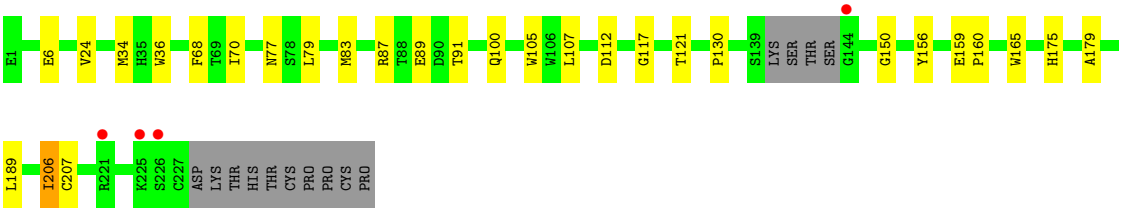
Chain H:



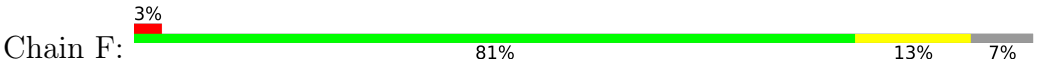


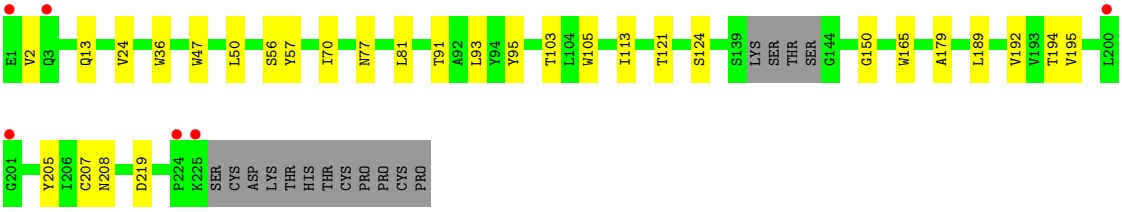
• Molecule 2: Heavy chain of BIOLS56



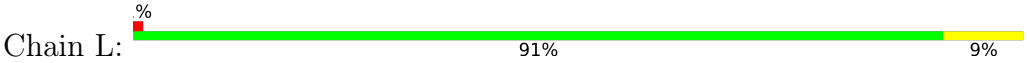


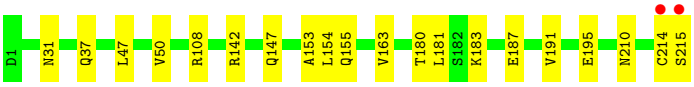
• Molecule 2: Heavy chain of BIOLS56



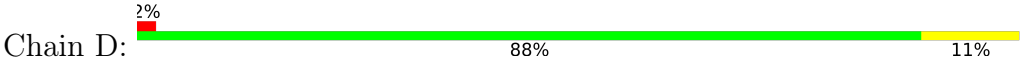


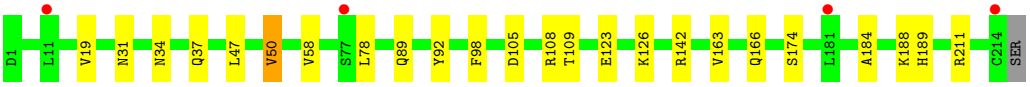
• Molecule 3: Light chain of BIOLS56



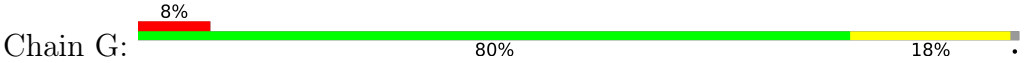


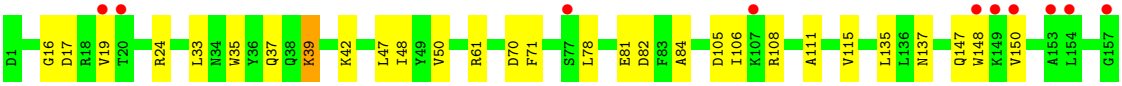
• Molecule 3: Light chain of BIOLS56





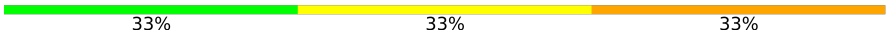
• Molecule 3: Light chain of BIOLS56





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

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	112.48Å 159.02Å 175.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.39 – 2.97 47.39 – 2.97	Depositor EDS
% Data completeness (in resolution range)	97.3 (47.39-2.97) 97.4 (47.39-2.97)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.13-2998	Depositor
R, R_{free}	0.220 , 0.263 0.220 , 0.263	Depositor DCC
R_{free} test set	3179 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	55.0	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 24.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	14620	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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

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	0.32	0/1609	0.59	0/2198
1	B	0.33	0/1602	0.59	0/2187
1	E	0.33	0/1564	0.59	0/2134
2	C	0.31	0/1719	0.57	0/2344
2	F	0.28	0/1707	0.55	0/2328
2	H	0.29	0/1719	0.53	0/2344
3	D	0.43	0/1676	0.59	0/2277
3	G	0.35	0/1670	0.62	0/2269
3	L	0.33	0/1682	0.53	0/2285
All	All	0.33	0/14948	0.57	0/20366

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1560	0	1482	28	0
1	B	1553	0	1478	27	0
1	E	1516	0	1440	35	0
2	C	1677	0	1626	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1665	0	1617	21	0
2	H	1677	0	1626	12	0
3	D	1640	0	1591	12	0
3	G	1634	0	1587	25	0
3	L	1646	0	1596	10	0
4	I	38	0	34	2	0
5	B	14	0	13	0	0
All	All	14620	0	14090	181	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 6.

All (181) 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:F:103:THR:HG22	2:F:105:TRP:H	1.40	0.86
2:H:103:THR:HG22	2:H:105:TRP:H	1.46	0.81
1:E:30:PRO:HG3	1:E:36:GLU:HG3	1.67	0.75
3:G:161:GLU:HG2	3:G:175:LEU:HD21	1.73	0.71
3:D:47:LEU:HA	3:D:58:VAL:HG21	1.74	0.70
3:G:19:VAL:HG21	3:G:78:LEU:HD12	1.74	0.69
2:H:91:THR:HG23	2:H:121:THR:HA	1.77	0.66
1:A:164:PRO:HA	1:A:166:ALA:H	1.60	0.66
3:D:108:ARG:HG2	3:D:109:THR:N	2.11	0.66
1:A:37:ARG:HD2	1:A:78:TYR:CD1	2.31	0.65
2:F:13:GLN:HG2	2:F:124:SER:HA	1.78	0.64
2:C:91:THR:HG23	2:C:121:THR:HA	1.78	0.64
1:E:120:THR:HG21	1:E:190:ARG:HG3	1.78	0.64
1:A:18:CYS:SG	1:A:40:ILE:HG23	2.37	0.64
1:A:164:PRO:HD3	1:A:169:CYS:HB3	1.80	0.64
2:F:36:TRP:HD1	2:F:70:ILE:HD12	1.63	0.63
2:C:36:TRP:HD1	2:C:70:ILE:HD12	1.65	0.62
1:E:75:SER:HB3	1:E:199:LEU:HD12	1.83	0.61
3:L:147:GLN:OE1	3:L:154:LEU:HD21	2.01	0.61
3:G:24:ARG:HH21	3:G:24:ARG:HG3	1.66	0.61
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.81	0.61
1:B:37:ARG:HD2	1:B:78:TYR:CD1	2.36	0.61
1:B:18:CYS:SG	1:B:40:ILE:HG23	2.41	0.60
3:G:159:SER:HB3	3:G:179:LEU:HD12	1.84	0.60
1:E:37:ARG:HD2	1:E:78:TYR:CD1	2.36	0.60
1:E:121:ARG:O	1:E:122:ASN:C	2.40	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:ASN:OD1	1:E:122:ASN:N	2.34	0.59
1:A:184:ILE:H	1:A:184:ILE:HD12	1.66	0.58
3:G:61:ARG:NE	3:G:82:ASP:OD2	2.36	0.58
1:B:32:VAL:HG22	1:B:104:ASN:HB3	1.85	0.58
1:A:164:PRO:HA	1:A:166:ALA:N	2.20	0.57
3:G:61:ARG:NH2	3:G:81:GLU:OE2	2.30	0.56
2:H:24:VAL:HG22	2:H:77:ASN:HB3	1.86	0.56
1:A:122:ASN:OD1	1:A:122:ASN:N	2.36	0.56
1:E:144:ARG:HH12	2:F:57:TYR:HA	1.69	0.56
3:G:105:ASP:HB2	3:G:166:GLN:OE1	2.05	0.56
1:E:69:LEU:HA	1:E:72:LEU:HD12	1.88	0.56
3:D:37:GLN:HB2	3:D:47:LEU:HD11	1.88	0.55
1:B:32:VAL:O	1:B:33:TYR:HD1	1.90	0.55
1:E:19:PRO:HB2	1:E:22:GLU:HG2	1.89	0.54
1:E:43:CYS:SG	1:E:44:VAL:N	2.81	0.54
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.90	0.53
1:A:19:PRO:HB2	1:A:22:GLU:HG2	1.90	0.53
3:D:105:ASP:HB2	3:D:166:GLN:OE1	2.08	0.53
1:E:144:ARG:NH1	2:F:56:SER:O	2.42	0.53
3:L:183:LYS:O	3:L:187:GLU:HG2	2.09	0.52
2:F:91:THR:HG23	2:F:121:THR:HA	1.90	0.52
1:E:144:ARG:NH1	2:F:57:TYR:HA	2.25	0.52
1:A:53:SER:C	1:A:55:PHE:H	2.13	0.52
2:F:103:THR:HG22	2:F:105:TRP:N	2.18	0.52
1:E:80:ASP:O	1:E:192:VAL:HA	2.09	0.51
2:C:87:ARG:C	2:C:89:GLU:H	2.13	0.51
3:L:147:GLN:HB2	3:L:195:GLU:HB3	1.93	0.51
1:B:19:PRO:HB2	1:B:22:GLU:HG2	1.92	0.51
3:D:142:ARG:HE	3:D:163:VAL:HG11	1.76	0.51
1:B:129:GLY:HA3	1:B:131:TYR:CE1	2.45	0.50
1:B:48:SER:HA	1:B:51:TYR:HD2	1.76	0.50
1:A:59:PHE:C	1:A:60:LYS:HD2	2.32	0.50
1:B:80:ASP:HB2	1:B:193:VAL:HB	1.93	0.50
1:A:137:TYR:CD2	1:A:138:LEU:HD13	2.47	0.50
1:E:32:VAL:O	1:E:33:TYR:HD1	1.94	0.50
2:F:93:LEU:HD23	2:F:95:TYR:CZ	2.46	0.50
1:B:43:CYS:SG	1:B:44:VAL:N	2.85	0.49
2:H:150:GLY:HA2	2:H:165:TRP:CH2	2.47	0.49
1:B:150:ILE:HD13	3:D:92:TYR:CD2	2.47	0.49
3:L:142:ARG:HD2	3:L:163:VAL:HG11	1.95	0.49
1:E:91:GLN:CD	1:E:98:GLY:HA3	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:VAL:HG22	1:A:196:PHE:HD1	1.77	0.49
1:E:18:CYS:SG	1:E:40:ILE:HG23	2.53	0.48
3:G:108:ARG:NH1	3:G:111:ALA:HB2	2.28	0.48
3:G:148:TRP:CG	3:G:179:LEU:HD13	2.48	0.48
3:G:183:LYS:O	3:G:187:GLU:HG2	2.13	0.48
1:B:108:PRO:HD2	1:B:111:PHE:HB2	1.96	0.48
1:A:80:ASP:O	1:A:192:VAL:HA	2.13	0.48
1:E:85:LYS:HG2	1:E:86:GLY:N	2.29	0.48
3:G:39:LYS:HG3	3:G:84:ALA:HB2	1.94	0.48
3:G:78:LEU:HD23	3:G:82:ASP:HB2	1.95	0.48
2:C:68:PHE:CZ	2:C:83:MET:HE3	2.49	0.48
3:G:115:VAL:O	3:G:207:LYS:HE2	2.14	0.48
1:A:160:LYS:HE3	1:A:160:LYS:HB2	1.52	0.47
3:L:153:ALA:HB1	2:C:206:ILE:HD11	1.96	0.47
1:E:48:SER:HA	1:E:51:TYR:CD2	2.50	0.47
3:L:214:CYS:SG	3:L:215:SER:N	2.87	0.47
1:A:21:GLY:O	1:A:25:ASN:HB2	2.15	0.47
1:B:20:PHE:CE1	1:B:40:ILE:HD13	2.50	0.47
2:F:179:ALA:HA	2:F:189:LEU:HB3	1.97	0.46
2:C:100:GLN:HB3	2:C:112:ASP:HB3	1.98	0.46
1:A:169:CYS:C	1:A:170:TYR:HD1	2.18	0.46
2:H:216:THR:HG23	1:E:158:ASP:HA	1.96	0.46
3:D:89:GLN:HB2	3:D:98:PHE:CD2	2.50	0.46
1:A:66:ALA:HA	1:A:69:LEU:HD13	1.97	0.46
1:B:32:VAL:O	1:B:33:TYR:CD1	2.69	0.46
1:B:209:LYS:N	1:B:209:LYS:HD2	2.31	0.46
1:A:75:SER:CB	1:A:199:LEU:H	2.29	0.46
1:E:106:LYS:NZ	1:E:142:LYS:HB3	2.30	0.46
2:F:36:TRP:NE1	2:F:81:LEU:HB2	2.31	0.46
3:G:35:TRP:HB2	3:G:48:ILE:HB	1.98	0.46
1:E:62:TYR:O	1:E:112:MET:HA	2.16	0.46
4:I:1:NAG:H61	4:I:2:NAG:H82	1.98	0.46
1:B:53:SER:C	1:B:55:PHE:H	2.19	0.46
1:A:169:CYS:C	1:A:170:TYR:CD1	2.89	0.45
1:B:129:GLY:HA3	1:B:131:TYR:HE1	1.80	0.45
3:G:115:VAL:HG12	3:G:207:LYS:HG3	1.98	0.45
2:H:105:TRP:CH2	2:H:107:LEU:HB2	2.51	0.45
2:F:24:VAL:HG22	2:F:77:ASN:HB3	1.98	0.45
1:A:115:VAL:HG22	1:A:193:VAL:HG22	1.98	0.45
1:B:24:PHE:CZ	1:B:50:LEU:HD21	2.52	0.45
3:G:16:GLY:N	3:G:78:LEU:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:VAL:HG22	1:E:104:ASN:HB3	1.98	0.45
2:C:36:TRP:CD1	2:C:70:ILE:HD12	2.48	0.45
3:D:123:GLU:HA	3:D:126:LYS:HE2	1.99	0.45
2:H:68:PHE:CE1	2:H:83:MET:HB3	2.53	0.44
1:A:90:ARG:NH2	1:A:96:GLN:OE1	2.50	0.44
1:E:21:GLY:O	1:E:25:ASN:HB2	2.17	0.44
3:G:33:LEU:HD22	3:G:71:PHE:CG	2.52	0.44
1:B:62:TYR:O	1:B:112:MET:HA	2.18	0.44
3:D:19:VAL:HG21	3:D:78:LEU:HD12	2.00	0.44
1:E:120:THR:O	1:E:121:ARG:C	2.56	0.44
1:A:74:PHE:HD1	1:A:198:LEU:HG	1.82	0.44
2:C:150:GLY:HA2	2:C:165:TRP:CH2	2.52	0.44
2:F:150:GLY:HA2	2:F:165:TRP:CH2	2.53	0.44
1:E:37:ARG:HD2	1:E:78:TYR:HB3	2.00	0.44
1:E:120:THR:HG21	1:E:190:ARG:CG	2.47	0.44
2:F:47:TRP:CZ2	2:F:50:LEU:HD23	2.52	0.44
1:A:16:ASN:O	1:A:44:VAL:N	2.46	0.44
2:C:70:ILE:HD11	2:C:79:LEU:HD11	1.98	0.44
1:A:85:LYS:HG2	1:A:185:GLY:O	2.18	0.44
2:C:159:GLU:HG3	2:C:160:PRO:HA	2.00	0.44
1:E:134:LYS:HG2	1:E:175:ASP:OD1	2.18	0.44
2:F:208:ASN:ND2	2:F:219:ASP:OD1	2.46	0.44
3:G:24:ARG:NH2	3:G:70:ASP:OD1	2.51	0.43
1:E:37:ARG:HD2	1:E:78:TYR:HD1	1.83	0.43
2:H:153:VAL:HG11	2:H:161:VAL:HG11	1.99	0.43
1:A:171:TRP:HA	1:A:172:PRO:HD3	1.85	0.43
1:B:50:LEU:HD22	1:B:116:LEU:HD22	2.00	0.43
1:B:171:TRP:HA	1:B:172:PRO:HD3	1.77	0.43
1:E:121:ARG:HE	1:E:121:ARG:HB3	1.47	0.43
2:H:103:THR:HG22	2:H:105:TRP:N	2.24	0.43
1:B:88:ASP:O	1:B:91:GLN:HG2	2.18	0.43
3:L:154:LEU:HD23	3:L:155:GLN:N	2.33	0.43
2:C:24:VAL:HG22	2:C:77:ASN:O	2.19	0.43
2:C:179:ALA:HA	2:C:189:LEU:HB3	2.01	0.43
2:H:89:GLU:H	2:H:89:GLU:HG3	1.61	0.43
1:B:80:ASP:O	1:B:192:VAL:HA	2.18	0.43
2:F:192:VAL:HG21	3:G:135:LEU:HD13	2.00	0.43
1:A:26:ALA:HB3	1:A:29:PHE:HE1	1.84	0.42
3:G:106:ILE:H	3:G:106:ILE:HD12	1.84	0.42
2:F:194:THR:HG21	3:G:137:ASN:ND2	2.34	0.42
1:B:37:ARG:NE	1:B:80:ASP:OD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:6:GLU:OE1	2:C:117:GLY:N	2.39	0.42
2:C:175:HIS:CE1	3:D:174:SER:HG	2.38	0.42
2:F:2:VAL:HG12	2:F:113:ILE:HG21	2.01	0.42
2:F:165:TRP:CZ3	2:F:207:CYS:HB3	2.55	0.42
2:H:130:PRO:HB3	2:H:156:TYR:HB3	2.02	0.42
1:A:197:GLU:HG2	1:A:199:LEU:HD21	2.02	0.41
1:E:36:GLU:O	1:E:80:ASP:HA	2.20	0.41
3:G:198:HIS:CD2	3:G:199:GLN:H	2.37	0.41
4:I:1:NAG:H61	4:I:2:NAG:C7	2.50	0.41
1:B:39:LYS:HE2	1:B:39:LYS:HB3	1.78	0.41
3:D:184:ALA:O	3:D:188:LYS:HG3	2.21	0.41
1:E:120:THR:OG1	1:E:124:ASP:HB2	2.20	0.41
1:B:21:GLY:O	1:B:25:ASN:HB2	2.20	0.41
1:E:37:ARG:HA	1:E:37:ARG:HD3	1.88	0.41
3:G:150:VAL:HG22	3:G:192:TYR:HD1	1.85	0.41
2:C:105:TRP:CH2	2:C:107:LEU:HB2	2.56	0.41
2:C:130:PRO:HB3	2:C:156:TYR:HB3	2.02	0.41
2:C:165:TRP:CZ3	2:C:207:CYS:HB3	2.55	0.41
2:H:34:MET:HB3	2:H:79:LEU:HD22	2.02	0.41
3:L:191:VAL:HG22	3:L:210:ASN:OD1	2.21	0.41
1:E:115:VAL:HG13	1:E:193:VAL:HG22	2.03	0.41
2:F:103:THR:CG2	2:F:105:TRP:H	2.22	0.41
2:F:195:VAL:HG11	2:F:205:TYR:CE1	2.56	0.41
3:G:37:GLN:HB2	3:G:47:LEU:HD11	2.02	0.41
1:B:90:ARG:HD2	1:B:90:ARG:C	2.41	0.40
3:D:189:HIS:O	3:D:211:ARG:NE	2.52	0.40
1:E:32:VAL:O	1:E:33:TYR:CD1	2.74	0.40
1:A:32:VAL:HA	1:A:82:PHE:HB2	2.03	0.40
3:L:180:THR:O	3:L:181:LEU:HD23	2.22	0.40
1:E:85:LYS:HG3	1:E:186:TYR:HB2	2.01	0.40
3:G:108:ARG:HH12	3:G:111:ALA:HB2	1.85	0.40
1:B:120:THR:HG21	1:B:190:ARG:HG3	2.04	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	194/228 (85%)	178 (92%)	15 (8%)	1 (0%)	29 66
1	B	193/228 (85%)	180 (93%)	12 (6%)	1 (0%)	29 66
1	E	186/228 (82%)	168 (90%)	17 (9%)	1 (0%)	29 66
2	C	219/237 (92%)	213 (97%)	6 (3%)	0	100 100
2	F	217/237 (92%)	211 (97%)	6 (3%)	0	100 100
2	H	219/237 (92%)	214 (98%)	5 (2%)	0	100 100
3	D	212/215 (99%)	203 (96%)	8 (4%)	1 (0%)	29 66
3	G	211/215 (98%)	202 (96%)	9 (4%)	0	100 100
3	L	213/215 (99%)	205 (96%)	8 (4%)	0	100 100
All	All	1864/2040 (91%)	1774 (95%)	86 (5%)	4 (0%)	47 80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	122	ASN
1	B	160	LYS
3	D	50	VAL
1	A	159	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	A	171/202 (85%)	169 (99%)	2 (1%)	71 89
1	B	170/202 (84%)	168 (99%)	2 (1%)	71 89
1	E	165/202 (82%)	163 (99%)	2 (1%)	71 89
2	C	188/202 (93%)	187 (100%)	1 (0%)	88 95
2	F	186/202 (92%)	186 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	H	188/202 (93%)	186 (99%)	2 (1%)	73 90
3	D	190/191 (100%)	187 (98%)	3 (2%)	62 85
3	G	189/191 (99%)	184 (97%)	5 (3%)	46 76
3	L	191/191 (100%)	188 (98%)	3 (2%)	62 85
All	All	1638/1785 (92%)	1618 (99%)	20 (1%)	71 89

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	PHE
1	A	160	LYS
2	H	18	LEU
2	H	223	GLU
3	L	31	ASN
3	L	50	VAL
3	L	108	ARG
1	B	158	ASP
1	B	160	LYS
2	C	206	ILE
3	D	31	ASN
3	D	34	ASN
3	D	50	VAL
1	E	33	TYR
1	E	121	ARG
3	G	17	ASP
3	G	39	LYS
3	G	42	LYS
3	G	50	VAL
3	G	147	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
2	C	175	HIS
3	D	210	ASN
1	E	76	ASN
3	G	198	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

3 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	1,4	14,14,15	0.43	0	17,19,21	0.61	0
4	NAG	I	2	4	14,14,15	0.71	0	17,19,21	0.80	1 (5%)
4	FUC	I	3	4	10,10,11	0.94	0	14,14,16	0.63	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	I	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	FUC	I	3	4	-	-	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	2	NAG	O5-C1-C2	-2.27	107.71	111.29

There are no chirality outliers.

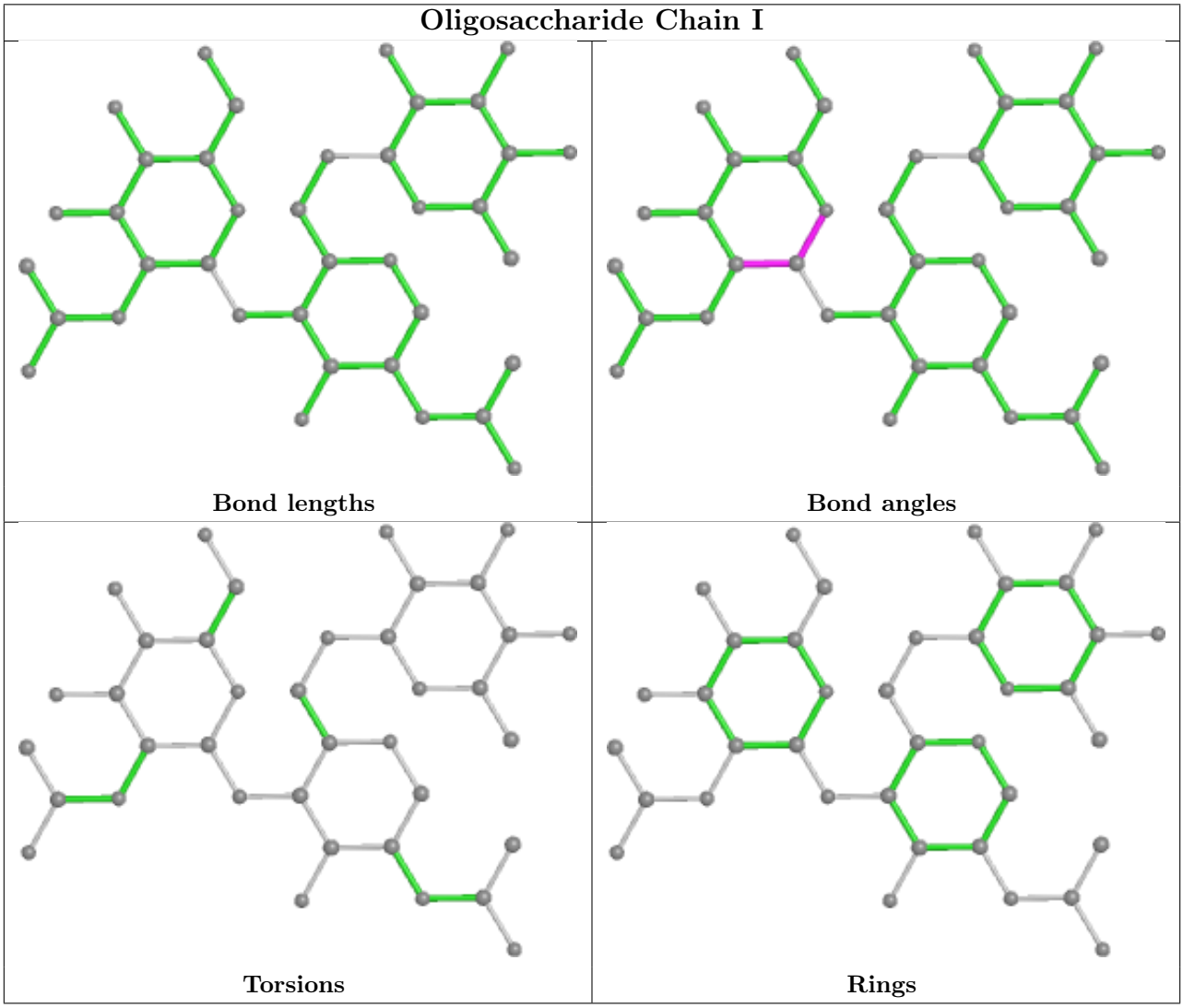
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	NAG	2	0
4	I	2	NAG	2	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.



5.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	B	301	1	14,14,15	0.38	0	17,19,21	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	301	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	301	NAG	C4-C5-C6-O6
5	B	301	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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	196/228 (85%)	0.13	6 (3%) 49 30	32, 51, 79, 96	0
1	B	195/228 (85%)	0.13	6 (3%) 49 30	30, 42, 79, 102	0
1	E	190/228 (83%)	0.38	12 (6%) 20 10	31, 50, 95, 108	0
2	C	223/237 (94%)	-0.02	4 (1%) 68 48	28, 44, 76, 118	0
2	F	221/237 (93%)	0.22	6 (2%) 54 35	38, 53, 93, 106	0
2	H	223/237 (94%)	-0.05	2 (0%) 84 69	29, 40, 71, 100	0
3	D	214/215 (99%)	0.16	4 (1%) 66 46	32, 50, 71, 102	0
3	G	213/215 (99%)	0.55	18 (8%) 10 5	42, 71, 102, 108	0
3	L	215/215 (100%)	-0.10	2 (0%) 84 69	29, 48, 62, 106	0
All	All	1890/2040 (92%)	0.15	60 (3%) 47 29	28, 48, 90, 118	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	15	THR	4.9
2	F	201	GLY	4.3
2	F	225	LYS	4.1
3	G	154	LEU	3.6
1	E	49	VAL	3.6
2	F	200	LEU	3.5
1	B	16	ASN	3.3
3	G	201	LEU	3.1
1	A	54	THR	3.1
3	G	157	GLY	3.1
3	G	199	GLN	3.0
3	G	77	SER	3.0
3	G	148	TRP	2.9
1	A	169	CYS	2.9
3	L	214	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
3	D	11	LEU	2.9
3	D	77	SER	2.9
1	E	182	THR	2.9
3	G	197	THR	2.8
2	F	1	GLU	2.8
3	G	192	TYR	2.7
2	C	144	GLY	2.7
1	E	67	THR	2.6
2	C	221	ARG	2.6
2	F	3	GLN	2.6
2	F	224	PRO	2.6
2	H	227	CYS	2.5
1	B	169	CYS	2.5
3	D	181	LEU	2.5
1	B	202	PRO	2.5
3	D	214	CYS	2.5
3	G	150	VAL	2.5
3	G	107	LYS	2.5
1	E	202	PRO	2.4
1	E	47	TYR	2.4
1	E	50	LEU	2.4
1	E	16	ASN	2.4
1	E	42	ASN	2.3
3	G	19	VAL	2.3
1	E	183	GLY	2.3
2	H	201	GLY	2.3
1	E	204	THR	2.3
1	A	161	PRO	2.2
1	B	45	ALA	2.2
1	A	71	ASP	2.2
3	G	149	LYS	2.2
1	A	198	LEU	2.2
3	G	20	THR	2.2
2	C	226	SER	2.2
3	G	193	ALA	2.2
3	G	210	ASN	2.2
2	C	225	LYS	2.1
1	E	44	VAL	2.1
3	G	194	CYS	2.1
3	G	153	ALA	2.1
3	G	212	GLY	2.1
1	A	72	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	54	THR	2.0
3	L	215	SER	2.0
1	E	51	TYR	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)

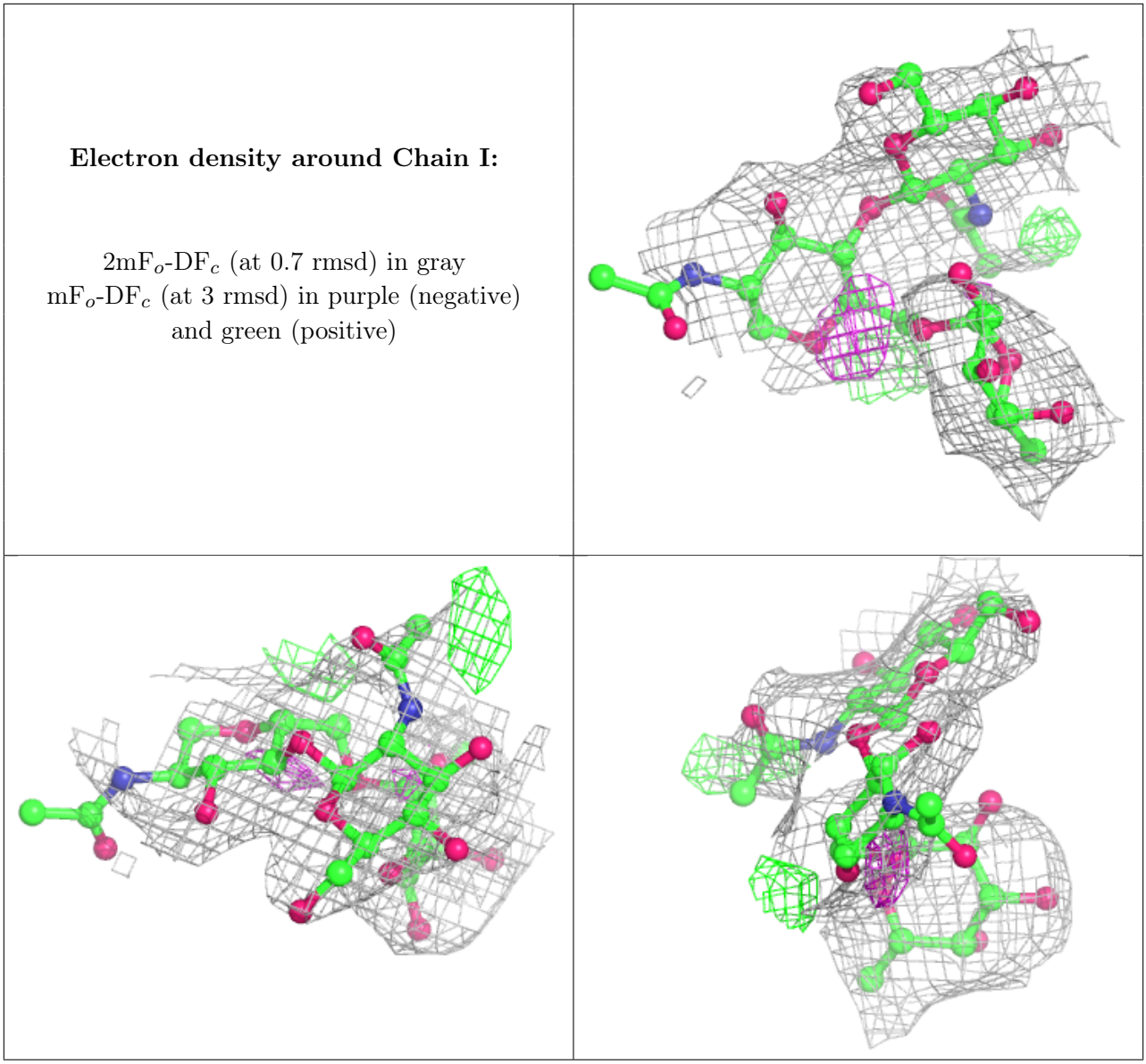
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	0.43	77,95,99,103	0
4	NAG	I	1	14/15	0.76	0.34	80,93,102,106	0
4	FUC	I	3	10/11	0.80	0.29	70,78,87,91	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)



6.4 Ligands

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
5	NAG	B	301	14/15	0.73	0.40	85,99,103,105	0

6.5 Other polymers

There are no such residues in this entry.