Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 03:55 AM EDT

PDB ID	:	7MZJ
Title	:	SARS-CoV-2 receptor binding domain bound to Fab WCSL 129 and Fab PDI 93
Authors	:	Pymm, P.; Dietrich, M.H.; Tan, L.L.; Chan, L.J.; Tham, W.H.
Deposited on	:	2021-05-24
Resolution	:	2.40 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:

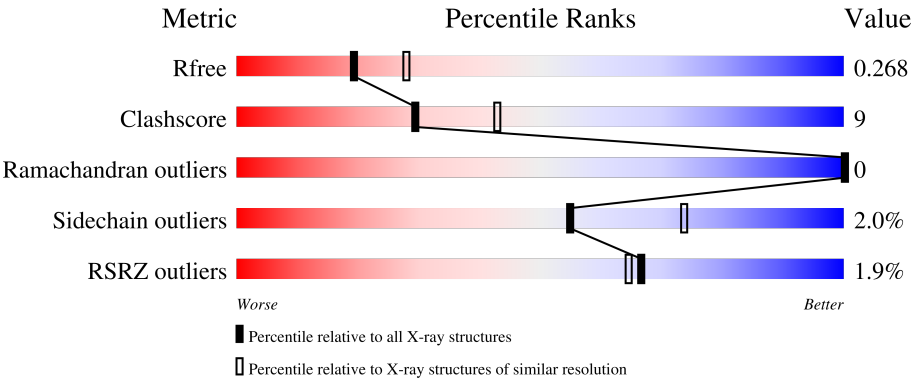
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	% 78% 20% ·
1	E	216	81% 17% ·
2	C	224	4% 65% 29% 5%
2	F	224	7% 72% 23% ·
3	A	205	77% 19% ·

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Mol	Chain	Length	Quality of chain
3	B	205	79% 17%
4	L	215	87% 12%
4	M	215	4% 79% 20%
5	H	233	79% 16% 5%
5	N	233	3% 75% 19% 6%
6	G	3	100%
6	I	3	67% 33%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 15969 atoms, of which 8 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 WCSL 129 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	212	Total	C	N	O	S	0	0	0
			1550	972	256	318	4			
1	E	212	Total	C	N	O	S	0	0	0
			1538	963	252	319	4			

- Molecule 2 is a protein called WCSL 129 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	213	Total	C	N	O	S	0	0	0
			1534	972	258	297	7			
2	F	214	Total	C	N	O	S	0	1	0
			1511	951	254	299	7			

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	198	Total	C	N	O	S	0	1	0
			1548	992	255	293	8			
3	A	196	Total	C	N	O	S	0	0	0
			1533	981	255	289	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	528	GLY	-	expression tag	UNP P0DTC2
B	529	SER	-	expression tag	UNP P0DTC2
B	530	HIS	-	expression tag	UNP P0DTC2
B	531	HIS	-	expression tag	UNP P0DTC2
B	532	HIS	-	expression tag	UNP P0DTC2
B	533	HIS	-	expression tag	UNP P0DTC2
B	534	HIS	-	expression tag	UNP P0DTC2
B	535	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	528	GLY	-	expression tag	UNP P0DTC2
A	529	SER	-	expression tag	UNP P0DTC2
A	530	HIS	-	expression tag	UNP P0DTC2
A	531	HIS	-	expression tag	UNP P0DTC2
A	532	HIS	-	expression tag	UNP P0DTC2
A	533	HIS	-	expression tag	UNP P0DTC2
A	534	HIS	-	expression tag	UNP P0DTC2
A	535	HIS	-	expression tag	UNP P0DTC2

- Molecule 4 is a protein called PDI 93 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	213	Total	C	N	O	S	0	0	0
			1603	1002	268	328	5			
4	M	212	Total	C	N	O	S	0	2	0
			1586	988	269	322	7			

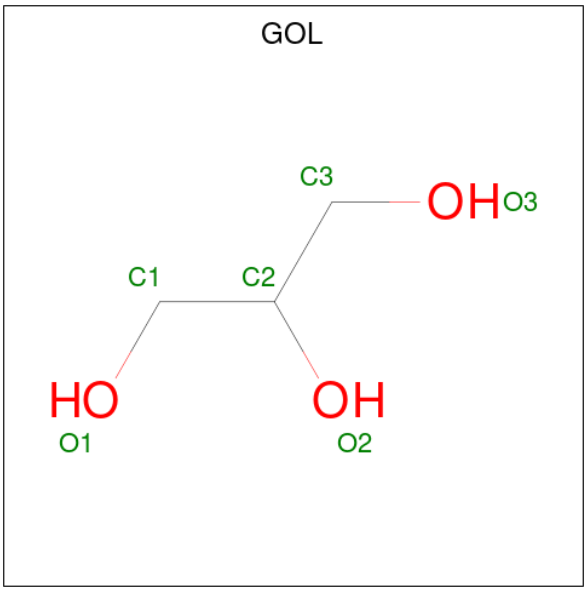
- Molecule 5 is a protein called PDI 93 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	222	Total	C	N	O	S	0	0	0
			1620	1019	271	321	9			
5	N	220	Total	C	N	O	S	0	0	0
			1596	1003	265	319	9			

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

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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C H O 14 3 8 3	0	0

- Molecule 8 is water.

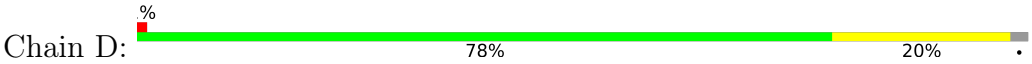
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	14	Total O 14 14	0	0
8	C	14	Total O 14 14	0	0
8	B	43	Total O 43 43	0	0
8	E	15	Total O 15 15	0	0
8	F	6	Total O 6 6	0	0
8	A	18	Total O 18 18	0	0
8	L	54	Total O 54 54	0	0
8	H	30	Total O 30 30	0	0
8	N	28	Total O 28 28	0	0
8	M	36	Total O 36 36	0	0

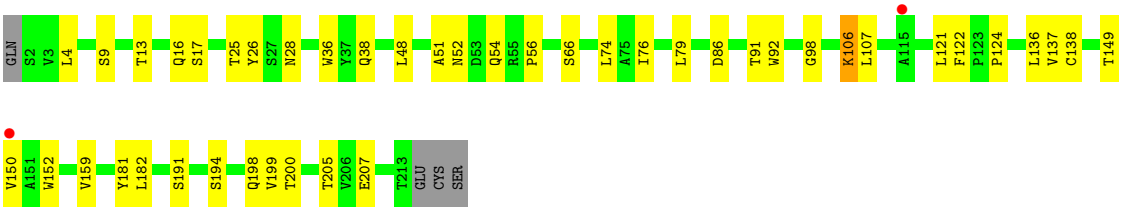
3 Residue-property plots (i)

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: WCSL 129 light chain

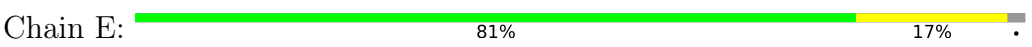
Chain D:





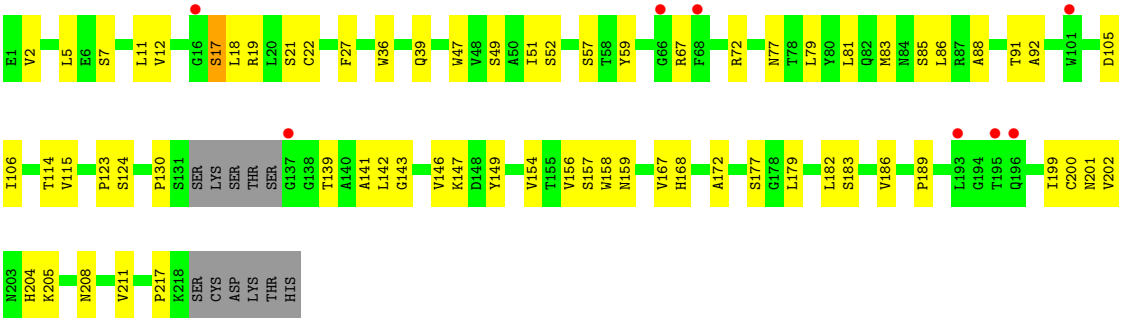
• Molecule 1: WCSL 129 light chain

Chain E:



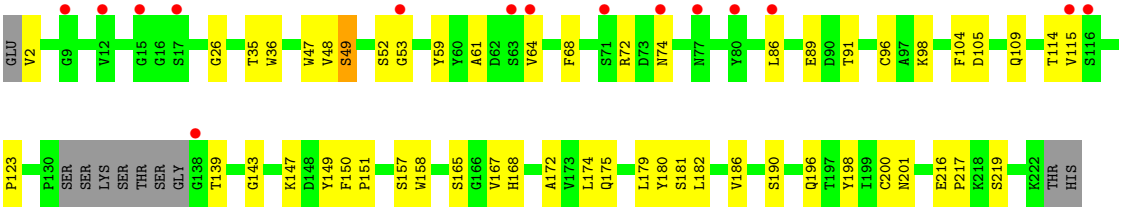
• Molecule 2: WCSL 129 heavy chain

Chain C:

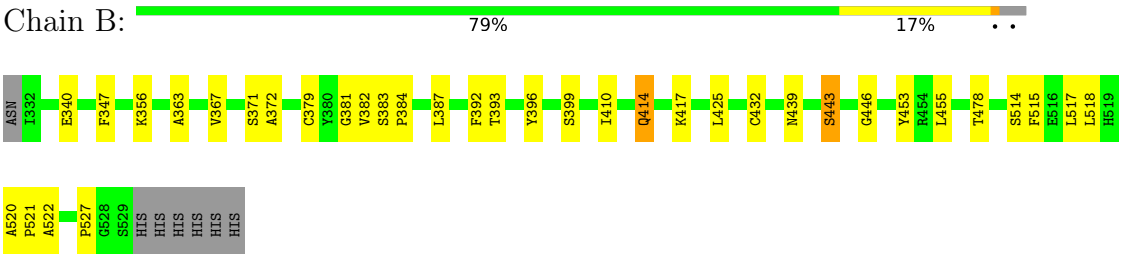


• Molecule 2: WCSL 129 heavy chain

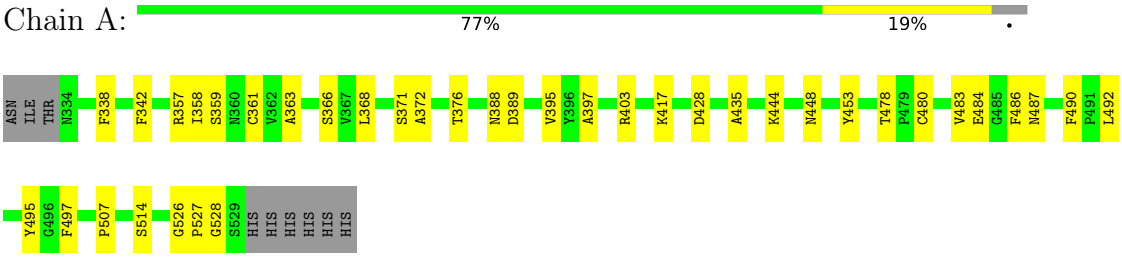
Chain F:



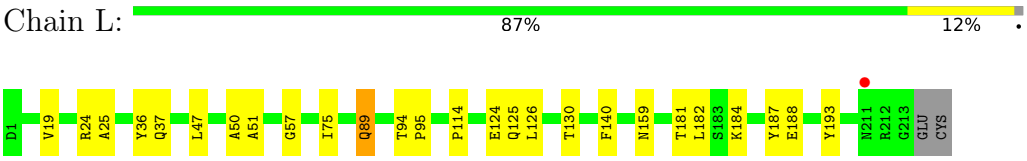
• Molecule 3: Spike protein S1



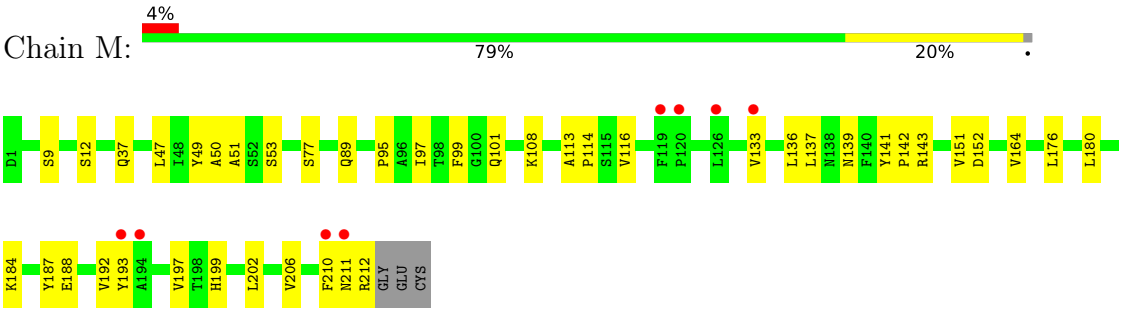
• Molecule 3: Spike protein S1



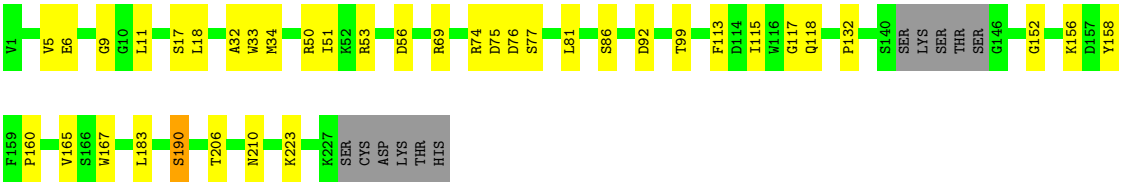
• Molecule 4: PDI 93 light chain



• Molecule 4: PDI 93 light chain

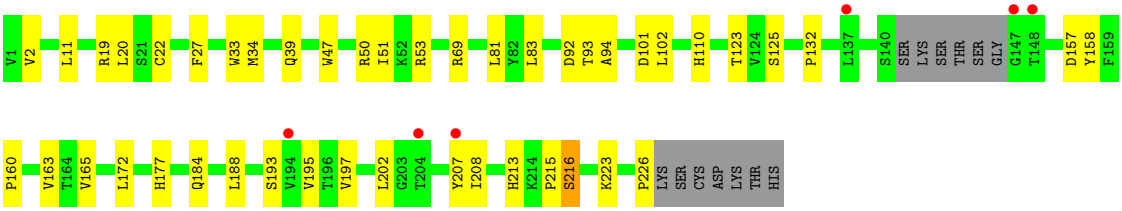


• Molecule 5: PDI 93 heavy chain



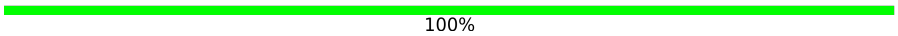
• Molecule 5: PDI 93 heavy chain

Chain N:



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

Chain G:



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

Chain I:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	39.04Å 104.72Å 127.27Å 88.72° 83.68° 82.80°	Depositor
Resolution (Å)	48.20 – 2.40 48.20 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.20-2.40) 98.5 (48.20-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.222 , 0.268 0.222 , 0.268	Depositor DCC
R_{free} test set	3828 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	46.4	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 36.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,-h+l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15969	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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: BMA, NAG, GOL

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	0.26	0/1591	0.45	0/2182
1	E	0.27	0/1580	0.44	0/2174
2	C	0.27	0/1571	0.46	0/2146
2	F	0.26	0/1548	0.48	0/2122
3	A	0.28	0/1576	0.43	0/2146
3	B	0.28	0/1592	0.43	0/2171
4	L	0.27	0/1637	0.46	0/2232
4	M	0.27	0/1620	0.46	0/2212
5	H	0.29	0/1658	0.48	0/2265
5	N	0.26	0/1634	0.47	0/2238
All	All	0.27	0/16007	0.46	0/21888

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	D	1550	0	1473	35	0
1	E	1538	0	1430	23	0
2	C	1534	0	1449	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1511	0	1366	41	0
3	A	1533	0	1432	24	0
3	B	1548	0	1437	23	0
4	L	1603	0	1523	16	0
4	M	1586	0	1477	32	0
5	H	1620	0	1537	25	0
5	N	1596	0	1481	29	0
6	G	39	0	34	0	0
6	I	39	0	34	1	0
7	B	6	8	8	0	0
8	A	18	0	0	0	0
8	B	43	0	0	2	0
8	C	14	0	0	2	0
8	D	14	0	0	0	0
8	E	15	0	0	0	0
8	F	6	0	0	1	0
8	H	30	0	0	0	0
8	L	54	0	0	1	0
8	M	36	0	0	2	0
8	N	28	0	0	2	0
All	All	15961	8	14681	288	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 (288) 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:C:199:ILE:HD12	2:C:201:ASN:HD21	1.33	0.93
5:H:9:GLY:HA2	5:H:18:LEU:HD21	1.52	0.89
4:M:37:GLN:HB2	4:M:47:LEU:HD11	1.56	0.86
1:D:74:LEU:HD22	1:D:76:ILE:HD11	1.58	0.86
1:D:86:ASP:OD1	1:D:106:LYS:HD2	1.75	0.85
2:C:167:VAL:HG22	2:C:186:VAL:HG22	1.59	0.84
5:N:34:MET:HB3	5:N:81:LEU:HD22	1.62	0.81
2:F:91:THR:HG22	2:F:115:VAL:H	1.44	0.81
2:F:91:THR:CG2	2:F:115:VAL:H	1.92	0.81
5:H:99:THR:HG21	5:H:113:PHE:HB3	1.64	0.78
2:F:89:GLU:O	8:F:301:HOH:O	2.03	0.77
5:N:208:ILE:HG22	5:N:223:LYS:HA	1.66	0.77
5:H:132:PRO:HB3	5:H:158:TYR:HB3	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:36:TRP:O	2:F:48:VAL:HG12	1.86	0.76
2:C:72:ARG:HB3	2:C:79:LEU:HD12	1.69	0.74
4:M:9:SER:OG	8:M:301:HOH:O	2.04	0.74
2:C:91:THR:HG23	2:C:114:THR:HA	1.69	0.74
2:C:51:ILE:HG21	2:C:79:LEU:HD11	1.71	0.71
2:F:167:VAL:HA	2:F:186:VAL:HG12	1.73	0.71
4:L:37:GLN:HB2	4:L:47:LEU:HD11	1.72	0.71
2:F:174:LEU:HD23	2:F:180:TYR:CE1	2.26	0.71
1:E:136:LEU:HD12	1:E:182:LEU:HD23	1.73	0.70
2:F:174:LEU:HD23	2:F:180:TYR:CD1	2.27	0.70
1:D:74:LEU:HD22	1:D:76:ILE:CD1	2.21	0.69
3:A:444:LYS:HG3	3:A:448:ASN:HB2	1.75	0.68
1:E:182:LEU:HG	1:E:184:LEU:CD2	2.22	0.68
1:E:182:LEU:HG	1:E:184:LEU:HD21	1.73	0.68
2:C:202:VAL:CG2	2:C:211:VAL:HG23	2.24	0.68
2:C:11:LEU:HD12	2:C:12:VAL:H	1.59	0.68
4:M:116:VAL:HG22	4:M:137:LEU:HD13	1.77	0.67
1:D:86:ASP:OD1	1:D:106:LYS:HA	1.95	0.66
1:D:122:PHE:HB2	1:D:137:VAL:HG22	1.78	0.66
2:C:51:ILE:HG21	2:C:79:LEU:CD1	2.25	0.66
2:C:18:LEU:HD12	2:C:19:ARG:H	1.61	0.65
3:B:410:ILE:O	3:B:425:LEU:HD12	1.96	0.65
2:F:109:GLN:HA	2:F:109:GLN:OE1	1.94	0.65
2:F:123:PRO:HB3	2:F:149:TYR:HB3	1.78	0.65
5:N:19:ARG:O	8:N:301:HOH:O	2.15	0.65
4:M:133:VAL:CG2	4:M:180:LEU:HB3	2.27	0.65
4:L:184:LYS:HE2	4:L:188:GLU:OE2	1.95	0.65
4:M:133:VAL:HG23	4:M:180:LEU:HB3	1.79	0.65
2:C:177:SER:HB3	2:C:179:LEU:HG	1.77	0.64
4:L:36:TYR:HE2	4:L:89:GLN:HG2	1.61	0.64
2:C:52:SER:HB3	2:C:57:SER:HB2	1.79	0.63
2:C:18:LEU:HD12	2:C:19:ARG:N	2.14	0.62
1:D:199:VAL:C	1:D:205:THR:HG23	2.19	0.62
2:C:156:VAL:HG23	2:C:202:VAL:HG12	1.83	0.61
1:D:152:TRP:HB2	1:D:159:VAL:HG11	1.83	0.61
2:F:147:LYS:HA	2:F:181:SER:OG	2.01	0.61
4:L:57:GLY:O	8:L:301:HOH:O	2.16	0.60
4:M:199:HIS:HB3	4:M:202:LEU:HD12	1.82	0.60
3:B:393:THR:HG22	3:B:517:LEU:HA	1.83	0.60
4:L:126:LEU:O	4:L:184:LYS:HD2	2.01	0.60
2:C:77:ASN:ND2	8:C:302:HOH:O	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:403:ARG:HG3	3:A:495:TYR:CE1	2.37	0.59
2:F:150:PHE:CE2	2:F:151:PRO:HB3	2.37	0.59
2:C:123:PRO:HB3	2:C:149:TYR:HB3	1.85	0.59
5:N:184:GLN:HG3	5:N:188:LEU:O	2.02	0.59
5:H:5:VAL:HG13	5:H:118:GLN:HE22	1.67	0.58
2:F:2:VAL:HA	2:F:26:GLY:HA3	1.85	0.58
4:L:114:PRO:HB3	4:L:140:PHE:HB3	1.85	0.58
2:F:158:TRP:CZ3	2:F:200:CYS:HB3	2.38	0.58
5:N:69:ARG:NH2	5:N:92:ASP:OD2	2.32	0.58
1:E:25:THR:HG23	1:E:27:SER:H	1.69	0.58
2:F:48:VAL:HG13	2:F:49:SER:N	2.18	0.58
4:M:151:VAL:HG22	4:M:193:TYR:CD2	2.39	0.57
1:D:150:VAL:HG12	1:D:199:VAL:HG22	1.85	0.57
2:F:59:TYR:CE1	3:A:486:PHE:HB3	2.39	0.57
3:B:367:VAL:O	8:B:701:HOH:O	2.18	0.57
4:M:101:GLN:NE2	8:M:301:HOH:O	2.15	0.57
5:N:202:LEU:HD22	5:N:226:PRO:HG3	1.86	0.56
4:M:193:TYR:HB2	4:M:210:PHE:CE1	2.40	0.56
1:E:132:ASN:HA	1:E:186:PRO:HG2	1.87	0.56
5:H:11:LEU:HB2	5:H:160:PRO:HG3	1.88	0.56
2:C:105:ASP:C	2:C:106:ILE:HD13	2.25	0.56
1:D:122:PHE:HB2	1:D:137:VAL:CG2	2.35	0.56
3:B:393:THR:HA	3:B:522:ALA:HA	1.88	0.56
5:H:99:THR:CG2	5:H:113:PHE:HB3	2.34	0.56
4:M:137:LEU:HD11	4:M:197:VAL:HG11	1.87	0.55
2:C:146:VAL:CG1	2:C:202:VAL:HG11	2.36	0.55
1:D:136:LEU:HD12	1:D:182:LEU:HD23	1.87	0.55
3:B:393:THR:HG21	3:B:518:LEU:H	1.70	0.55
2:C:146:VAL:HG11	2:C:202:VAL:HG11	1.88	0.55
5:N:132:PRO:HB3	5:N:158:TYR:HB3	1.88	0.55
2:C:105:ASP:O	2:C:106:ILE:HD13	2.07	0.54
1:D:36:TRP:CE3	1:D:74:LEU:HD12	2.42	0.54
2:C:36:TRP:CD2	2:C:81:LEU:HD12	2.42	0.54
1:E:90:SER:OG	1:E:100:LEU:O	2.17	0.54
5:H:69:ARG:NH2	5:H:92:ASP:OD2	2.39	0.54
1:D:16:GLN:HG2	1:D:17:SER:N	2.23	0.54
3:A:483:VAL:HG22	3:A:484:GLU:O	2.08	0.54
2:C:130:PRO:HB3	2:C:141:ALA:O	2.09	0.53
5:H:206:THR:HG23	5:H:223:LYS:HD2	1.91	0.53
5:N:101:ASP:OD1	5:N:110:HIS:HA	2.09	0.53
2:C:59:TYR:HE2	3:B:478:THR:HG21	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:428:ASP:OD1	3:A:428:ASP:N	2.42	0.53
1:D:13:THR:HG22	1:D:16:GLN:HE21	1.72	0.52
2:C:159:ASN:HA	2:C:199:ILE:HD11	1.91	0.52
3:A:363:ALA:O	3:A:527:PRO:HD3	2.10	0.52
2:C:199:ILE:HG13	2:C:199:ILE:O	2.08	0.52
2:C:36:TRP:CE2	2:C:81:LEU:HB2	2.44	0.52
2:C:130:PRO:HD2	2:C:217:PRO:HA	1.91	0.52
5:H:34:MET:HB3	5:H:81:LEU:HD22	1.91	0.52
5:N:2:VAL:HG12	5:N:27:PHE:HB3	1.90	0.52
2:C:172:ALA:HA	2:C:182:LEU:HB3	1.90	0.51
4:M:143:ARG:HE	4:M:164:VAL:HG11	1.76	0.51
1:D:13:THR:H	1:D:16:GLN:NE2	2.07	0.51
2:F:143:GLY:HA2	2:F:158:TRP:CH2	2.46	0.51
1:E:165:THR:HG23	1:E:180:SER:HB2	1.92	0.51
5:N:213:HIS:ND1	5:N:216:SER:HB3	2.26	0.51
2:C:88:ALA:HA	2:C:115:VAL:HB	1.93	0.51
2:F:91:THR:HG22	2:F:114:THR:HA	1.91	0.51
3:A:376:THR:HB	3:A:435:ALA:HB3	1.93	0.51
5:N:132:PRO:HA	5:N:157:ASP:O	2.10	0.50
4:L:89:GLN:O	4:L:89:GLN:HG3	2.11	0.50
5:H:33:TRP:HE1	5:H:53:ARG:HG2	1.75	0.50
3:B:520:ALA:HB1	3:B:521:PRO:HD2	1.93	0.50
1:E:93:ASP:HB3	1:E:96:LEU:HG	1.92	0.50
1:D:54:GLN:HG3	3:B:455:LEU:HD11	1.94	0.50
2:C:157:SER:OG	8:C:301:HOH:O	2.19	0.50
4:L:187:TYR:HA	4:L:193:TYR:OH	2.12	0.49
5:N:172:LEU:HD22	5:N:207:TYR:CD1	2.47	0.49
2:C:67:ARG:HD2	2:C:85:SER:HB2	1.94	0.49
2:F:91:THR:HG22	2:F:115:VAL:N	2.21	0.49
5:H:33:TRP:NE1	5:H:53:ARG:HG2	2.28	0.49
1:D:25:THR:HG22	1:D:26:TYR:H	1.78	0.49
1:D:38:GLN:HB2	1:D:48:LEU:HD11	1.95	0.49
1:E:196:SER:CA	1:E:209:THR:HG23	2.43	0.49
4:L:50:ALA:O	4:L:51:ALA:HB3	2.13	0.49
4:M:211:ASN:O	4:M:212:ARG:HB2	2.13	0.49
1:D:181:TYR:HH	2:C:183:SER:HG	1.59	0.48
1:E:36:TRP:CD2	1:E:74:LEU:HB2	2.48	0.48
5:N:177:HIS:HE1	4:M:139:ASN:HD21	1.59	0.48
2:C:172:ALA:HB2	2:C:182:LEU:HD23	1.94	0.48
3:A:371:SER:O	3:A:372:ALA:HB3	2.12	0.48
1:D:13:THR:HG22	1:D:16:GLN:NE2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:480:CYS:O	3:A:483:VAL:HG12	2.13	0.48
1:D:28:ASN:HA	1:D:92:TRP:O	2.13	0.48
2:C:52:SER:O	2:C:72:ARG:NH1	2.45	0.48
1:E:28:ASN:OD1	1:E:29:ILE:N	2.39	0.48
2:F:48:VAL:HG13	2:F:49:SER:H	1.78	0.48
3:A:342:PHE:HB2	6:I:1:NAG:H82	1.95	0.48
5:H:152:GLY:HA2	5:H:167:TRP:CZ2	2.49	0.48
4:M:116:VAL:HA	4:M:136:LEU:O	2.14	0.48
3:A:478:THR:HB	3:A:487:ASN:HD21	1.79	0.48
2:C:2:VAL:HG13	2:C:27:PHE:CD1	2.48	0.48
1:E:51:ALA:O	1:E:52:ASN:HB2	2.14	0.48
4:M:199:HIS:CB	4:M:202:LEU:HD12	2.44	0.48
1:D:181:TYR:OH	2:C:183:SER:OG	2.31	0.47
3:B:340:GLU:OE2	3:B:356:LYS:NZ	2.41	0.47
5:H:152:GLY:HA2	5:H:167:TRP:CH2	2.49	0.47
2:F:47:TRP:CZ3	2:F:61:ALA:HB2	2.50	0.47
4:L:19:VAL:HG22	4:L:75:ILE:HB	1.97	0.47
1:D:4:LEU:HD11	1:D:91:THR:HG22	1.95	0.47
2:F:35:THR:HG21	2:F:104:PHE:CE1	2.50	0.47
4:L:24:ARG:NH1	4:L:25:ALA:O	2.42	0.47
5:N:20:LEU:HD12	5:N:83:LEU:HD23	1.96	0.47
2:F:36:TRP:CZ3	2:F:96:CYS:HB2	2.49	0.47
2:F:219:SER:O	2:F:219:SER:OG	2.27	0.47
5:N:165:VAL:HG21	5:N:193:SER:OG	2.14	0.47
4:M:141:TYR:CG	4:M:142:PRO:HA	2.50	0.47
3:B:381:GLY:O	3:B:382:VAL:HG13	2.15	0.47
5:N:172:LEU:HD21	5:N:195:VAL:HG21	1.97	0.47
3:B:371:SER:O	3:B:372:ALA:HB3	2.15	0.46
4:M:49:TYR:O	4:M:53:SER:HB2	2.15	0.46
1:D:51:ALA:O	1:D:52:ASN:HB2	2.15	0.46
1:E:38:GLN:HB2	1:E:48:LEU:HD11	1.95	0.46
5:N:53:ARG:HD2	8:N:306:HOH:O	2.15	0.46
3:A:368:LEU:O	3:A:371:SER:OG	2.30	0.46
2:C:139:THR:HA	2:C:189:PRO:HA	1.97	0.46
1:D:121:LEU:HD13	1:D:138:CYS:HB2	1.98	0.46
2:C:11:LEU:HD12	2:C:12:VAL:N	2.27	0.46
2:F:86:LEU:HB3	2:F:115:VAL:HG21	1.96	0.46
3:A:358:ILE:HD11	3:A:397:ALA:HB2	1.98	0.46
2:C:17:SER:HA	2:C:86:LEU:HD23	1.98	0.46
3:B:384:PRO:HA	3:B:387:LEU:HD12	1.97	0.46
1:E:95:SER:C	1:E:96:LEU:HD23	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:GLY:HA3	2:F:47:TRP:CE3	2.50	0.46
5:H:33:TRP:CD1	5:H:53:ARG:HG2	2.50	0.46
2:C:202:VAL:HG22	2:C:211:VAL:HG23	1.97	0.46
3:B:417:LYS:HD2	3:B:453:TYR:CD1	2.51	0.46
2:F:53:GLY:HA2	2:F:72:ARG:NH1	2.30	0.46
1:E:196:SER:HB2	1:E:209:THR:HG23	1.98	0.46
3:A:358:ILE:HG22	3:A:361:CYS:SG	2.56	0.45
3:B:417:LYS:HG3	8:B:723:HOH:O	2.16	0.45
4:M:187:TYR:HA	4:M:193:TYR:OH	2.16	0.45
4:M:12:SER:OG	4:M:108:LYS:HG3	2.16	0.45
2:C:143:GLY:HA2	2:C:158:TRP:CH2	2.51	0.45
3:A:417:LYS:HD2	3:A:453:TYR:CD1	2.51	0.45
3:B:439:ASN:O	3:B:443:SER:HB2	2.17	0.45
4:M:152:ASP:HA	4:M:192:VAL:CG2	2.47	0.45
1:E:98:GLY:HA3	2:F:47:TRP:CZ3	2.52	0.45
2:F:196:GLN:HG2	2:F:198:TYR:CZ	2.52	0.45
3:A:388:ASN:HB3	3:A:527:PRO:HD2	1.97	0.45
5:N:197:VAL:HG11	5:N:207:TYR:CZ	2.52	0.45
3:A:338:PHE:CE1	3:A:358:ILE:HD13	2.52	0.45
3:A:395:VAL:HA	3:A:514:SER:O	2.16	0.45
5:H:53:ARG:HG3	5:H:56:ASP:HB2	1.99	0.45
1:E:18:VAL:HG22	1:E:19:SER:N	2.31	0.44
2:F:157:SER:OG	2:F:201:ASN:HB2	2.18	0.44
2:F:158:TRP:CH2	2:F:200:CYS:HB3	2.52	0.44
5:H:75:ASP:OD1	5:H:77:SER:OG	2.29	0.44
2:C:154:VAL:CG2	2:C:182:LEU:HD21	2.47	0.44
3:A:338:PHE:HE1	3:A:358:ILE:HD13	1.83	0.44
4:L:124:GLU:OE1	4:L:124:GLU:N	2.47	0.44
2:C:149:TYR:CE2	2:C:154:VAL:HG13	2.53	0.44
1:E:121:LEU:HD13	1:E:138:CYS:HB2	1.99	0.44
5:H:156:LYS:HA	5:H:190:SER:HB2	2.00	0.44
1:D:200:THR:HG23	1:D:205:THR:OG1	2.17	0.44
5:H:17:SER:OG	5:H:86:SER:HA	2.18	0.44
3:B:379:CYS:HA	3:B:432:CYS:HA	1.98	0.44
2:F:174:LEU:HD13	2:F:175:GLN:O	2.18	0.44
3:A:357:ARG:HG2	3:A:359:SER:OG	2.18	0.44
3:B:363:ALA:O	3:B:527:PRO:HD3	2.18	0.43
2:F:216:GLU:HB3	2:F:217:PRO:HD2	2.00	0.43
3:A:497:PHE:CD2	3:A:507:PRO:HB3	2.52	0.43
5:N:172:LEU:HD22	5:N:207:TYR:HD1	1.81	0.43
1:D:98:GLY:HA3	2:C:47:TRP:CE3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:39:GLN:C	5:N:94:ALA:HB1	2.38	0.43
5:N:93:THR:HG23	5:N:123:THR:HA	2.00	0.43
3:A:363:ALA:O	3:A:526:GLY:HA2	2.18	0.43
2:C:130:PRO:HG3	2:C:142:LEU:HB3	2.00	0.43
5:N:33:TRP:CE3	5:N:50:ARG:HD2	2.53	0.43
1:D:48:LEU:O	1:D:56:PRO:HD2	2.18	0.43
1:D:137:VAL:HG12	1:D:181:TYR:CD2	2.54	0.43
3:B:446:GLY:HA3	4:M:95:PRO:HD3	2.00	0.43
2:F:98:LYS:HE2	2:F:105:ASP:OD1	2.17	0.43
1:D:198:GLN:HG2	1:D:207:GLU:HG3	2.00	0.43
4:L:94:THR:N	4:L:95:PRO:HD2	2.34	0.43
4:L:125:GLN:HG2	4:L:130:THR:O	2.18	0.43
2:C:159:ASN:HA	2:C:199:ILE:CG1	2.49	0.43
5:H:6:GLU:OE2	5:H:117:GLY:HA3	2.19	0.43
5:N:50:ARG:HG2	5:N:51:ILE:N	2.34	0.43
5:H:50:ARG:HG2	5:H:51:ILE:N	2.33	0.43
4:L:181:THR:O	4:L:182:LEU:HD23	2.19	0.43
5:N:177:HIS:CE1	4:M:139:ASN:HD21	2.37	0.42
1:D:16:GLN:CG	1:D:17:SER:N	2.82	0.42
2:C:81:LEU:HD22	2:C:83:MET:HG2	2.00	0.42
3:B:414:GLN:HE21	3:B:414:GLN:HB3	1.58	0.42
5:H:99:THR:HG23	5:H:115:ILE:O	2.19	0.42
2:F:172:ALA:HA	2:F:182:LEU:HB3	2.02	0.42
5:H:165:VAL:HA	5:H:210:ASN:O	2.19	0.42
4:M:184:LYS:O	4:M:188:GLU:HG3	2.19	0.42
4:M:151:VAL:HG22	4:M:193:TYR:HD2	1.84	0.42
1:D:149:THR:OG1	1:D:200:THR:HB	2.19	0.42
4:M:89:GLN:HB2	4:M:99:PHE:CD2	2.55	0.42
4:M:137:LEU:HD11	4:M:197:VAL:HG21	2.01	0.42
2:C:146:VAL:HG23	2:C:146:VAL:O	2.19	0.42
2:F:174:LEU:HD23	2:F:180:TYR:CZ	2.54	0.42
5:N:197:VAL:HG11	5:N:207:TYR:CE1	2.55	0.42
4:M:137:LEU:HB2	4:M:176:LEU:HB3	2.01	0.42
1:E:49:ILE:HD13	1:E:55:ARG:HG3	2.01	0.42
2:F:174:LEU:HD22	2:F:179:LEU:O	2.20	0.42
5:H:32:ALA:O	5:H:74:ARG:NH2	2.44	0.42
5:H:74:ARG:HD3	5:H:76:ASP:OD1	2.20	0.42
5:N:11:LEU:HB2	5:N:160:PRO:HG3	2.02	0.41
4:M:50:ALA:O	4:M:51:ALA:HB3	2.19	0.41
2:F:172:ALA:HB2	2:F:182:LEU:HD23	2.02	0.41
2:C:204:HIS:O	2:C:208:ASN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:139:THR:N	2:F:190:SER:OG	2.53	0.41
1:E:64:SER:OG	1:E:75:ALA:HB3	2.21	0.41
2:F:64:VAL:HG21	2:F:68:PHE:CD2	2.56	0.41
3:A:389:ASP:HA	3:A:528:GLY:O	2.20	0.41
5:N:163:VAL:HG12	5:N:213:HIS:CD2	2.55	0.41
3:B:392:PHE:CD1	3:B:515:PHE:HB3	2.56	0.41
3:B:347:PHE:CE2	3:B:399:SER:HB2	2.56	0.41
4:L:159:ASN:OD1	4:L:159:ASN:N	2.54	0.41
2:C:81:LEU:HD22	2:C:83:MET:CG	2.50	0.41
3:A:490:PHE:CE2	3:A:492:LEU:HB2	2.55	0.41
4:M:152:ASP:HA	4:M:192:VAL:HG22	2.03	0.41
3:B:393:THR:CG2	3:B:518:LEU:H	2.33	0.41
3:B:396:TYR:HB2	3:B:514:SER:OG	2.21	0.41
2:F:143:GLY:HA2	2:F:158:TRP:HH2	1.86	0.41
1:D:98:GLY:HA3	2:C:47:TRP:CZ3	2.55	0.41
1:D:124:PRO:HD3	1:D:136:LEU:CD2	2.51	0.41
1:D:136:LEU:HB2	1:D:182:LEU:HB3	2.03	0.41
2:C:205:LYS:C	2:C:208:ASN:H	2.24	0.41
5:N:47:TRP:CD2	4:M:97:ILE:HB	2.55	0.41
4:M:113:ALA:HA	4:M:114:PRO:HD3	1.96	0.40
4:M:202:LEU:HD22	4:M:206:VAL:CG2	2.51	0.40
2:C:5:LEU:O	2:C:22:CYS:HA	2.21	0.40
2:F:48:VAL:CG1	2:F:49:SER:N	2.82	0.40
5:N:213:HIS:CD2	5:N:215:PRO:HD2	2.57	0.40
1:D:79:LEU:HD21	1:D:107:LEU:HD21	2.03	0.40
5:H:183:LEU:HD12	5:H:183:LEU:HA	1.92	0.40
2:C:39:GLN:C	2:C:92:ALA:HB1	2.41	0.40
1:E:82:GLU:CD	1:E:82:GLU:H	2.25	0.40
1:E:124:PRO:HD3	1:E:136:LEU:HD23	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	D	210/216 (97%)	200 (95%)	10 (5%)	0	100	100
1	E	210/216 (97%)	199 (95%)	11 (5%)	0	100	100
2	C	209/224 (93%)	197 (94%)	12 (6%)	0	100	100
2	F	211/224 (94%)	204 (97%)	7 (3%)	0	100	100
3	A	194/205 (95%)	185 (95%)	9 (5%)	0	100	100
3	B	197/205 (96%)	187 (95%)	10 (5%)	0	100	100
4	L	211/215 (98%)	202 (96%)	9 (4%)	0	100	100
4	M	212/215 (99%)	202 (95%)	10 (5%)	0	100	100
5	H	218/233 (94%)	211 (97%)	7 (3%)	0	100	100
5	N	216/233 (93%)	204 (94%)	12 (6%)	0	100	100
All	All	2088/2186 (96%)	1991 (95%)	97 (5%)	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	171/181 (94%)	166 (97%)	5 (3%)	42	62
1	E	168/181 (93%)	164 (98%)	4 (2%)	49	68
2	C	158/184 (86%)	150 (95%)	8 (5%)	24	39
2	F	151/184 (82%)	146 (97%)	5 (3%)	38	57
3	A	164/177 (93%)	163 (99%)	1 (1%)	86	94
3	B	165/177 (93%)	162 (98%)	3 (2%)	59	76
4	L	178/189 (94%)	177 (99%)	1 (1%)	86	94
4	M	173/189 (92%)	172 (99%)	1 (1%)	86	94
5	H	175/197 (89%)	174 (99%)	1 (1%)	86	94
5	N	169/197 (86%)	165 (98%)	4 (2%)	49	68
All	All	1672/1856 (90%)	1639 (98%)	33 (2%)	55	74

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	9	SER
1	D	66	SER
1	D	106	LYS
1	D	191	SER
1	D	194	SER
2	C	7	SER
2	C	17	SER
2	C	21	SER
2	C	49	SER
2	C	124	SER
2	C	147	LYS
2	C	168	HIS
2	C	200	CYS
3	B	383	SER
3	B	414	GLN
3	B	443	SER
1	E	17	SER
1	E	169	SER
1	E	194	SER
1	E	196	SER
2	F	49	SER
2	F	52	SER
2	F	74	ASN
2	F	165	SER
2	F	168	HIS
3	A	366	SER
4	L	89	GLN
5	H	190	SER
5	N	22	CYS
5	N	102	LEU
5	N	125	SER
5	N	216	SER
4	M	77	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	16	GLN
1	D	38	GLN
2	C	208	ASN
3	B	414	GLN

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Mol	Chain	Res	Type
2	F	77	ASN
2	F	204	HIS
3	A	394	ASN
5	H	118	GLN
4	M	138	ASN
4	M	139	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

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	$\#\|Z\| > 2$
6	NAG	G	1	6,3	14,14,15	0.34	0	17,19,21	0.45	0
6	NAG	G	2	6	14,14,15	0.23	0	17,19,21	0.44	0
6	BMA	G	3	6	11,11,12	0.78	0	15,15,17	0.77	0
6	NAG	I	1	6,3	14,14,15	0.33	0	17,19,21	0.42	0
6	NAG	I	2	6	14,14,15	0.35	0	17,19,21	0.39	0
6	BMA	I	3	6	11,11,12	0.72	0	15,15,17	0.69	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
6	NAG	G	1	6,3	-	1/6/23/26	0/1/1/1
6	NAG	G	2	6	-	3/6/23/26	0/1/1/1
6	BMA	G	3	6	-	0/2/19/22	0/1/1/1
6	NAG	I	1	6,3	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	4/6/23/26	0/1/1/1
6	BMA	I	3	6	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	2	NAG	C4-C5-C6-O6
6	G	2	NAG	O5-C5-C6-O6
6	I	2	NAG	C4-C5-C6-O6
6	I	3	BMA	O5-C5-C6-O6
6	G	1	NAG	O5-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
6	I	2	NAG	C1-C2-N2-C7
6	G	2	NAG	C3-C2-N2-C7
6	I	2	NAG	C3-C2-N2-C7

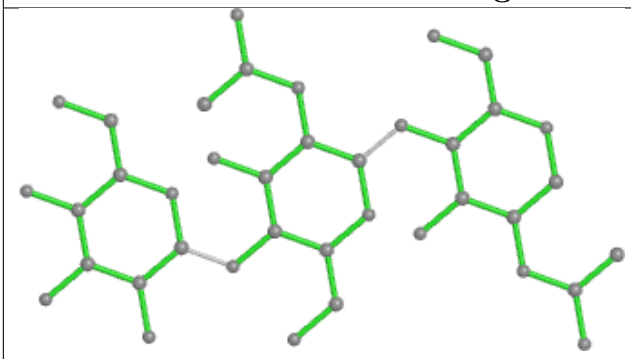
There are no ring outliers.

1 monomer is involved in 1 short contact:

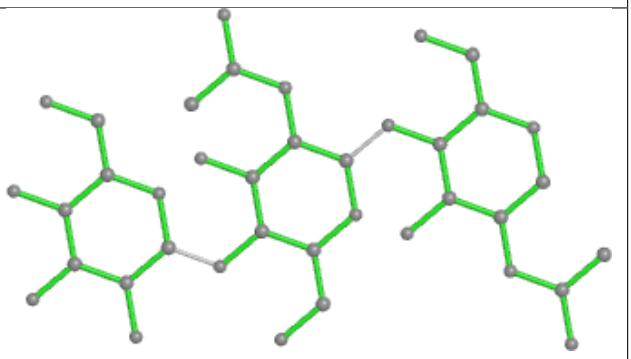
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	1	NAG	1	0

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

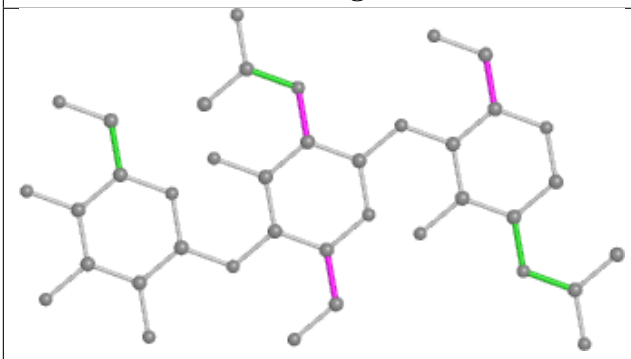
Oligosaccharide Chain G



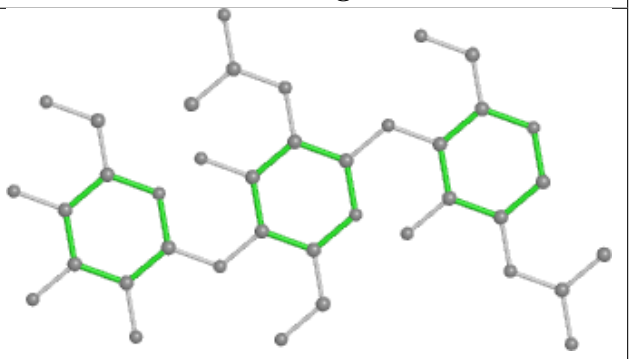
Bond lengths



Bond angles

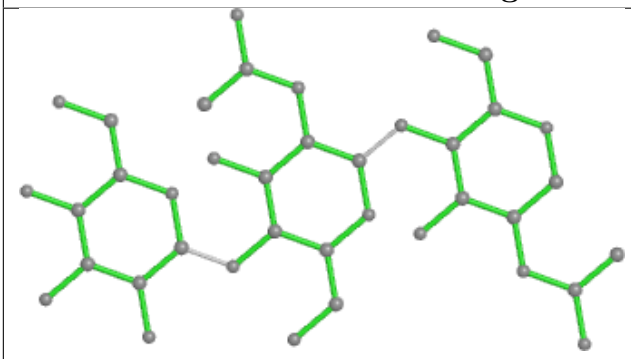


Torsions

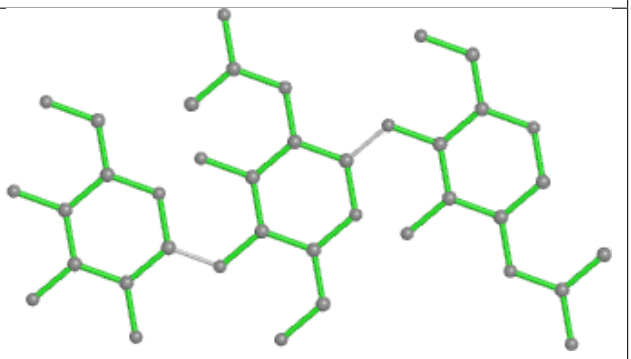


Rings

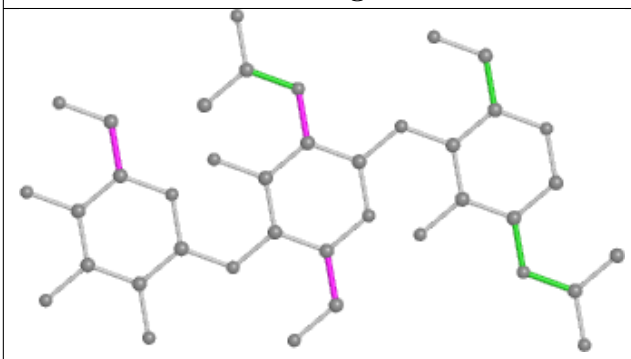
Oligosaccharide Chain I



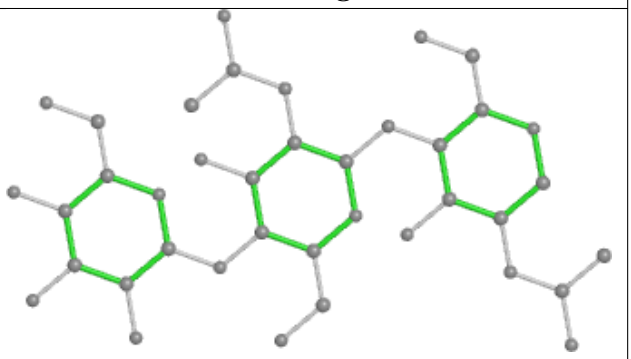
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
7	GOL	B	601	-	5,5,5	1.12	0	5,5,5	1.37	1 (20%)

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
7	GOL	B	601	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	601	GOL	C3-C2-C1	-2.71	101.18	111.70

There are no chirality outliers.

There are no torsion outliers.

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	D	212/216 (98%)	-0.04	2 (0%) 84 82	39, 56, 71, 86	0
1	E	212/216 (98%)	-0.17	1 (0%) 91 89	44, 55, 69, 86	0
2	C	213/224 (95%)	0.31	8 (3%) 40 39	45, 67, 81, 91	0
2	F	214/224 (95%)	0.48	15 (7%) 16 15	49, 73, 90, 99	0
3	A	196/205 (95%)	-0.05	0 100 100	35, 52, 74, 90	0
3	B	198/205 (96%)	-0.17	0 100 100	31, 44, 66, 81	0
4	L	213/215 (99%)	-0.35	1 (0%) 91 89	34, 42, 59, 67	0
4	M	212/215 (98%)	-0.02	8 (3%) 40 39	31, 45, 77, 86	0
5	H	222/233 (95%)	-0.19	0 100 100	34, 48, 59, 74	0
5	N	220/233 (94%)	-0.01	6 (2%) 54 52	32, 54, 75, 91	0
All	All	2112/2186 (96%)	-0.02	41 (1%) 66 64	31, 54, 79, 99	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	196	GLN	4.6
4	M	126	LEU	4.4
5	N	148	THR	4.3
4	M	194	ALA	4.0
2	F	17	SER	3.8
2	C	193	LEU	3.4
2	C	137	GLY	3.4
2	C	195	THR	3.3
2	F	115	VAL	3.2
2	C	66	GLY	2.9
2	F	74	ASN	2.8
4	M	211	ASN	2.7
2	C	68	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
2	F	86	LEU	2.7
2	F	9	GLY	2.7
4	M	120	PRO	2.7
2	F	80	TYR	2.6
2	F	15	GLY	2.6
4	L	211	ASN	2.6
5	N	207	TYR	2.6
2	F	53	GLY	2.5
2	F	77	ASN	2.5
2	F	138	GLY	2.5
4	M	193	TYR	2.5
1	D	115	ALA	2.5
4	M	119	PHE	2.5
2	F	116	SER	2.4
2	F	64	VAL	2.4
5	N	204	THR	2.4
5	N	194	VAL	2.3
2	F	63	SER	2.3
5	N	137	LEU	2.3
5	N	147	GLY	2.2
4	M	133	VAL	2.2
2	C	16	GLY	2.2
4	M	210	PHE	2.2
2	F	12	VAL	2.1
2	C	101	TRP	2.1
1	D	150	VAL	2.1
2	F	71	SER	2.1
1	E	195	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)

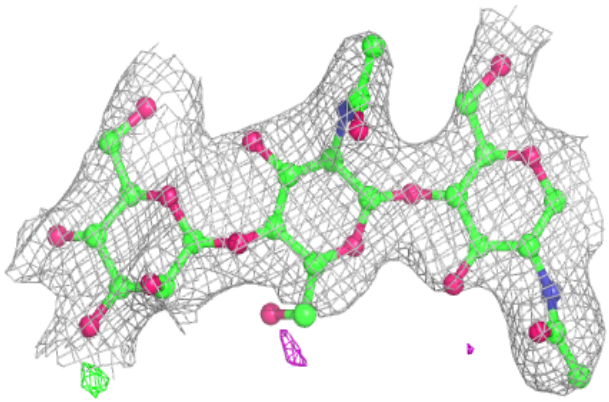
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

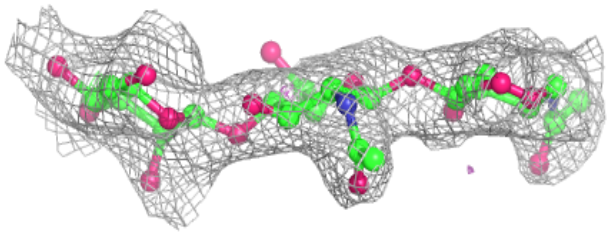
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	BMA	G	3	11/12	0.68	0.20	68,78,84,85	0
6	NAG	I	2	14/15	0.89	0.26	72,76,84,86	0
6	BMA	I	3	11/12	0.89	0.13	72,79,82,82	0
6	NAG	I	1	14/15	0.90	0.13	51,62,73,77	0
6	NAG	G	1	14/15	0.91	0.16	46,54,66,71	0
6	NAG	G	2	14/15	0.92	0.22	53,70,75,80	0

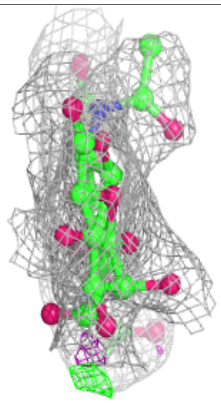
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

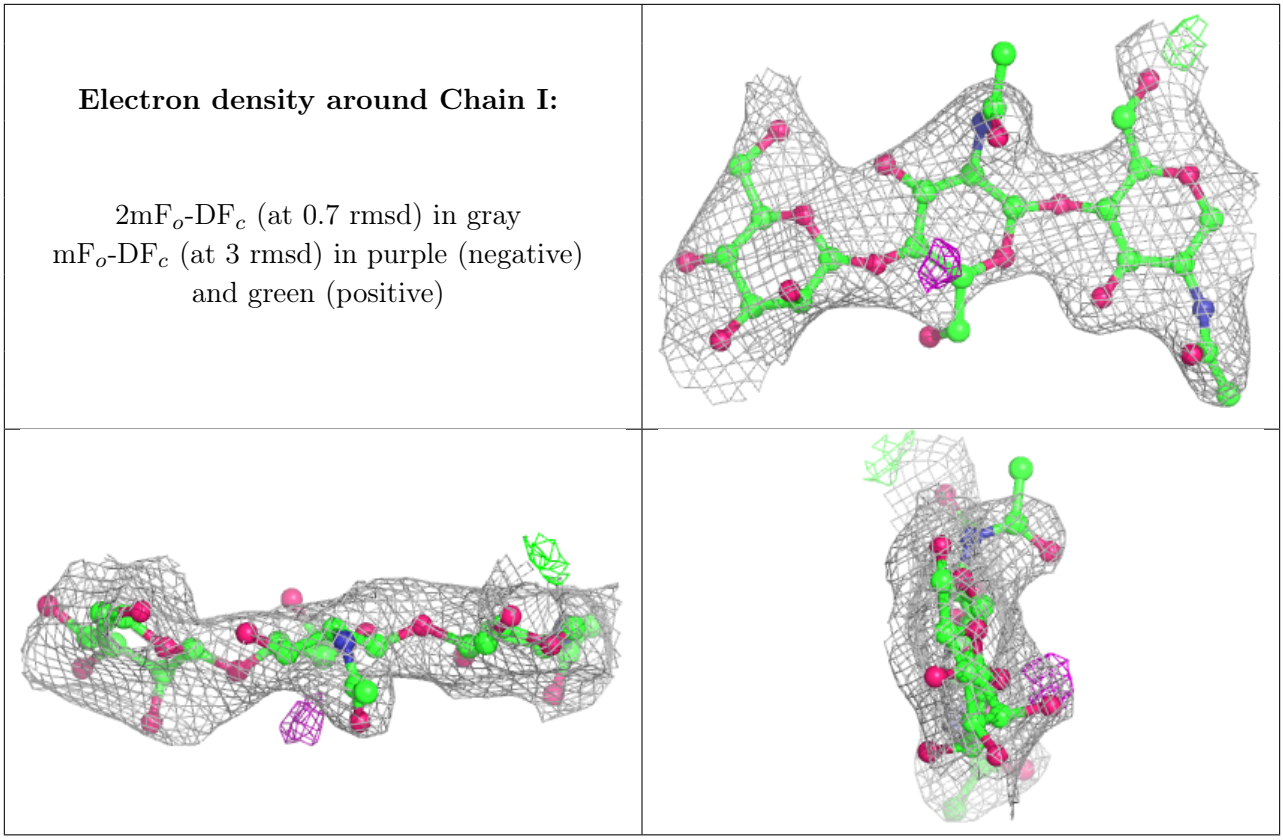






Electron density around Chain I:

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



6.4 Ligands

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
7	GOL	B	601	6/6	0.91	0.27	50,60,66,72	0

6.5 Other polymers

There are no such residues in this entry.