



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:46 AM UTC

PDB ID : 3H4Z / pdb_00003h4z
Title : Crystal Structure of an MBP-Der p 7 fusion protein
Authors : Pedersen, L.C.; Mueller, G.A.; London, R.E.
Deposited on : 2009-04-21
Resolution : 2.35 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

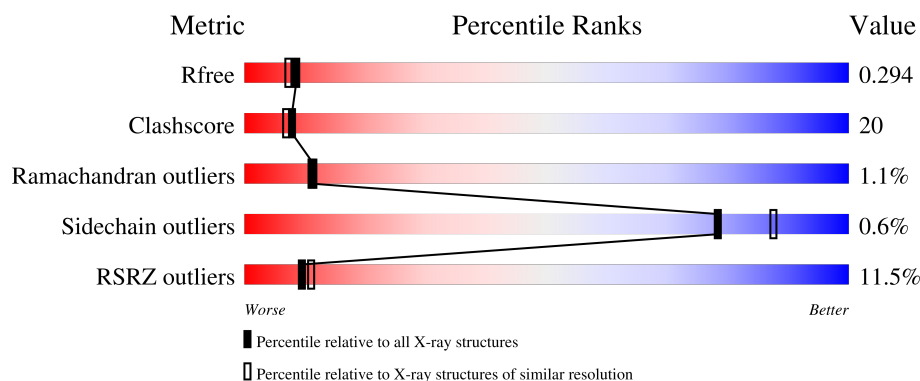
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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 $\leq 5\%$. 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	568	5% 68% 31% .
1	B	568	7% 67% 31% ..
1	C	568	21% 53% 43% ..
2	D	2	100%
2	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	F	2	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12999 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 Maltose-binding periplasmic protein fused with Allergen DERP7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	568	Total	C	N	O	S	0	0	0
			4257	2721	696	828	12			
1	B	563	Total	C	N	O	S	0	0	0
			4220	2700	691	817	12			
1	C	552	Total	C	N	O	S	0	0	0
			4130	2642	674	803	11			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	ALA	ASP	engineered mutation	UNP P0AEX9
A	83	ALA	LYS	engineered mutation	UNP P0AEX9
A	172	ALA	GLU	engineered mutation	UNP P0AEX9
A	173	ALA	ASN	engineered mutation	UNP P0AEX9
A	239	ALA	LYS	engineered mutation	UNP P0AEX9
A	359	ALA	GLU	engineered mutation	UNP P0AEX9
A	362	ALA	-	SEE REMARK 999	UNP P0AEX9
A	363	ALA	-	SEE REMARK 999	UNP P0AEX9
A	364	ALA	-	SEE REMARK 999	UNP P0AEX9
A	365	GLN	-	SEE REMARK 999	UNP P0AEX9
A	366	THR	-	SEE REMARK 999	UNP P0AEX9
A	367	ASN	-	SEE REMARK 999	UNP P0AEX9
A	368	ALA	-	SEE REMARK 999	UNP P0AEX9
A	369	ALA	-	SEE REMARK 999	UNP P0AEX9
A	370	ALA	-	SEE REMARK 999	UNP P0AEX9
B	82	ALA	ASP	engineered mutation	UNP P0AEX9
B	83	ALA	LYS	engineered mutation	UNP P0AEX9
B	172	ALA	GLU	engineered mutation	UNP P0AEX9
B	173	ALA	ASN	engineered mutation	UNP P0AEX9
B	239	ALA	LYS	engineered mutation	UNP P0AEX9
B	359	ALA	GLU	engineered mutation	UNP P0AEX9
B	362	ALA	-	SEE REMARK 999	UNP P0AEX9
B	363	ALA	-	SEE REMARK 999	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	364	ALA	-	SEE REMARK 999	UNP P0AEX9
B	365	GLN	-	SEE REMARK 999	UNP P0AEX9
B	366	THR	-	SEE REMARK 999	UNP P0AEX9
B	367	ASN	-	SEE REMARK 999	UNP P0AEX9
B	368	ALA	-	SEE REMARK 999	UNP P0AEX9
B	369	ALA	-	SEE REMARK 999	UNP P0AEX9
B	370	ALA	-	SEE REMARK 999	UNP P0AEX9
C	82	ALA	ASP	engineered mutation	UNP P0AEX9
C	83	ALA	LYS	engineered mutation	UNP P0AEX9
C	172	ALA	GLU	engineered mutation	UNP P0AEX9
C	173	ALA	ASN	engineered mutation	UNP P0AEX9
C	239	ALA	LYS	engineered mutation	UNP P0AEX9
C	359	ALA	GLU	engineered mutation	UNP P0AEX9
C	362	ALA	-	SEE REMARK 999	UNP P0AEX9
C	363	ALA	-	SEE REMARK 999	UNP P0AEX9
C	364	ALA	-	SEE REMARK 999	UNP P0AEX9
C	365	GLN	-	SEE REMARK 999	UNP P0AEX9
C	366	THR	-	SEE REMARK 999	UNP P0AEX9
C	367	ASN	-	SEE REMARK 999	UNP P0AEX9
C	368	ALA	-	SEE REMARK 999	UNP P0AEX9
C	369	ALA	-	SEE REMARK 999	UNP P0AEX9
C	370	ALA	-	SEE REMARK 999	UNP P0AEX9

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



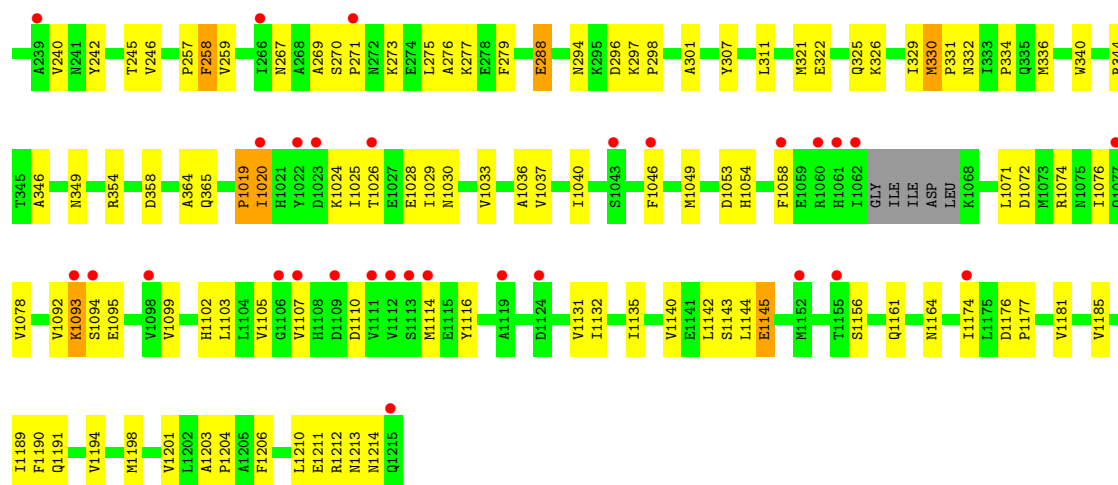
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	D	2	Total	C	O	0	0	0
			23	12	11			
2	E	2	Total	C	O	0	0	0
			23	12	11			
2	F	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

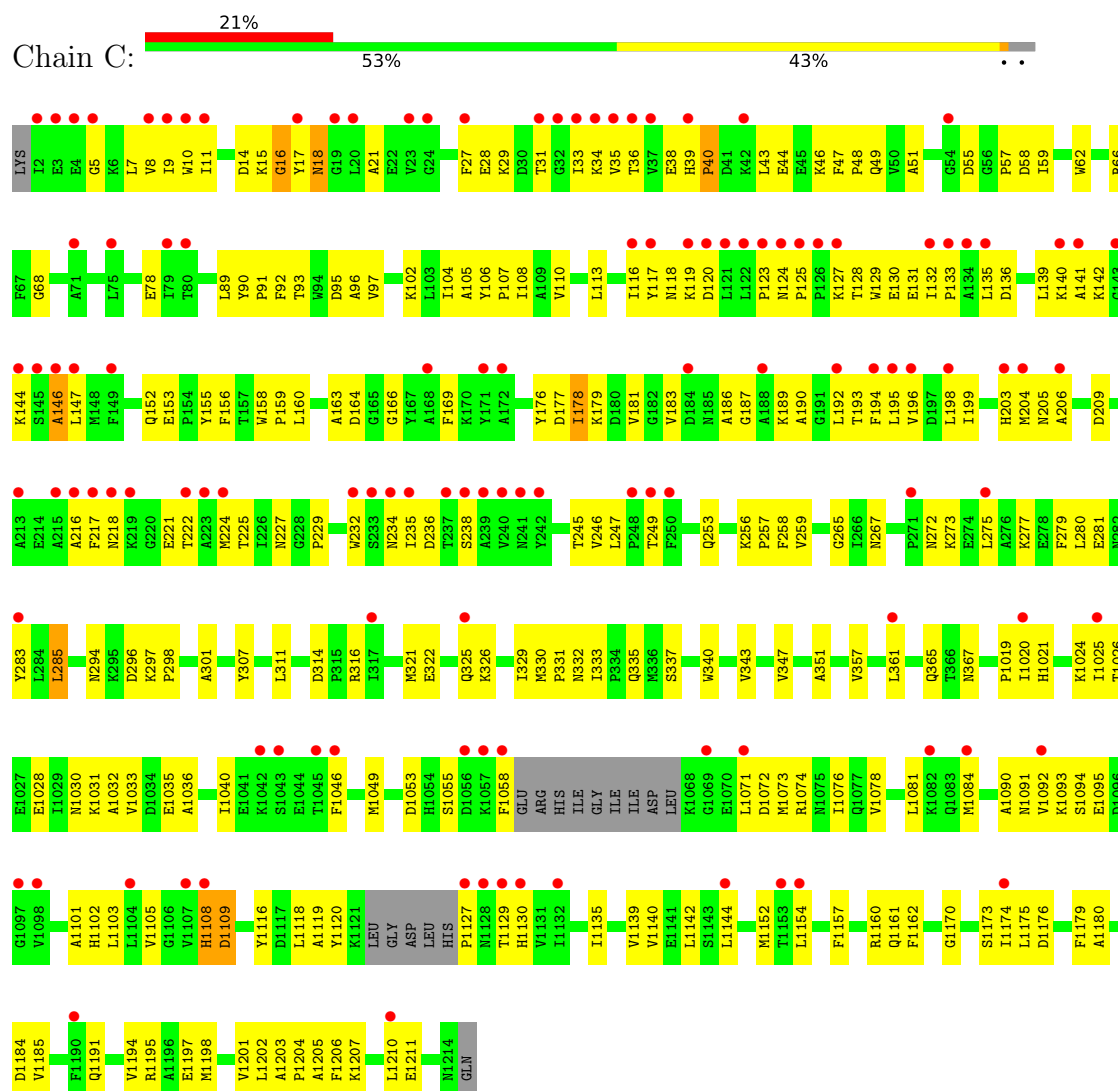
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	146	Total 146	O 146	0	0
4	B	130	Total 130	O 130	0	0
4	C	46	Total 46	O 46	0	0



- Molecule 1: Maltose-binding periplasmic protein fused with Allergen DERP7



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain D:  100%



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain E:  50% 50%



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain F:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	193.35Å 117.90Å 92.44Å 90.00° 114.06° 90.00°	Depositor
Resolution (Å)	28.91 – 2.35 28.91 – 2.35	Depositor EDS
% Data completeness (in resolution range)	77.3 (28.91-2.35) 77.3 (28.91-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.36Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.249 , 0.293 0.252 , 0.294	Depositor DCC
R_{free} test set	3899 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12999	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, NA

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	0/4347	0.86	7/5925 (0.1%)
1	B	0.32	0/4311	0.82	2/5877 (0.0%)
1	C	0.31	0/4220	0.82	3/5759 (0.1%)
All	All	0.32	0/12878	0.83	12/17561 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1062	ILE	N-CA-C	9.55	116.43	106.21
1	A	1066	ASP	N-CA-C	-7.10	100.81	110.68
1	C	1109	ASP	N-CA-C	-6.42	105.74	112.93
1	C	1170	GLY	N-CA-C	6.36	118.80	111.36
1	A	1198	MET	N-CA-C	-6.34	106.08	113.88
1	B	132	ILE	CB-CA-C	-6.19	107.79	114.35
1	A	242	TYR	N-CA-C	5.75	118.61	109.81
1	A	1092	VAL	N-CA-C	5.64	117.71	108.97
1	C	18	ASN	N-CA-C	-5.33	106.29	112.89
1	A	90	TYR	CA-C-N	5.20	124.64	119.24
1	A	90	TYR	C-N-CA	5.20	124.64	119.24
1	B	330	MET	N-CA-C	5.18	116.21	109.64

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4257	0	4092	135	0
1	B	4220	0	4047	150	0
1	C	4130	0	3936	214	1
2	D	23	0	21	0	0
2	E	23	0	21	0	0
2	F	23	0	21	3	0
3	A	1	0	0	0	0
4	A	146	0	0	8	0
4	B	130	0	0	7	0
4	C	46	0	0	3	0
All	All	12999	0	12138	491	1

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 20.

All (491) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1020:ILE:HG22	1:C:1021:HIS:H	1.27	0.95
1:C:139:LEU:HB3	1:C:144:LYS:HB2	1.53	0.91
1:B:1058:PHE:HB3	1:B:1185:VAL:HG21	1.56	0.87
1:A:9:ILE:HD11	1:A:61:PHE:CE1	2.10	0.87
1:A:1144:LEU:HD21	1:A:1210:LEU:HD13	1.57	0.86
1:C:9:ILE:HG13	1:C:59:ILE:HB	1.58	0.86
1:A:1020:ILE:HD12	1:A:1025:ILE:HD12	1.59	0.83
1:C:127:LYS:HE2	1:C:127:LYS:HA	1.58	0.83
1:A:68:GLY:HA3	1:A:332:ASN:O	1.78	0.83
1:C:7:LEU:HD12	1:C:35:VAL:HG22	1.63	0.81
1:C:189:LYS:HG2	1:C:361:LEU:HD12	1.61	0.81
1:B:1203:ALA:HB3	1:B:1204:PRO:HD3	1.62	0.80
1:A:1211:GLU:HA	1:A:1214:ASN:HB2	1.63	0.79
1:C:1026:THR:HG22	1:C:1030:ASN:HD21	1.48	0.78
1:C:1020:ILE:HG21	1:C:1025:ILE:HD11	1.66	0.78
1:C:1203:ALA:HB3	1:C:1204:PRO:HD3	1.66	0.77
1:C:1053:ASP:OD2	1:C:1074:ARG:HG2	1.85	0.76
1:C:164:ASP:O	1:C:187:GLY:HA3	1.85	0.76
1:C:181:VAL:HB	1:C:365:GLN:NE2	2.02	0.75
1:C:1144:LEU:HD21	1:C:1210:LEU:HD13	1.69	0.75
1:A:1033:VAL:HG21	1:A:1103:LEU:HD22	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1175:LEU:O	1:C:1175:LEU:HD23	1.86	0.74
1:C:1073:MET:HG3	1:C:1076:ILE:HD11	1.71	0.72
1:A:1165:VAL:HB	1:A:1187:THR:HG23	1.70	0.72
1:C:189:LYS:HG2	1:C:361:LEU:CD1	2.19	0.72
1:B:1212:ARG:C	1:B:1214:ASN:H	1.98	0.71
1:C:1033:VAL:HG21	1:C:1103:LEU:HD13	1.71	0.70
1:C:147:LEU:HA	1:C:224:MET:HB2	1.73	0.70
1:B:68:GLY:HA3	1:B:332:ASN:O	1.91	0.70
1:B:294:ASN:OD1	1:B:298:PRO:HA	1.90	0.70
1:C:181:VAL:HB	1:C:365:GLN:HE22	1.57	0.70
1:A:33:ILE:HD13	1:A:275:LEU:HD13	1.72	0.69
1:A:1076:ILE:HG23	1:A:1114:MET:HE3	1.72	0.69
1:B:44:GLU:HB2	1:B:66:ARG:HD2	1.74	0.69
1:B:165:GLY:HA3	1:B:187:GLY:HA3	1.74	0.69
1:C:1026:THR:HG22	1:C:1030:ASN:ND2	2.08	0.68
1:C:153:GLU:OE1	2:F:2:GLC:H62	1.93	0.68
1:A:1203:ALA:HB3	1:A:1204:PRO:HD3	1.75	0.68
1:A:321:MET:HE2	1:A:321:MET:HA	1.76	0.68
1:B:1143:SER:HB2	1:B:1156:SER:HB3	1.77	0.67
1:C:1020:ILE:HG22	1:C:1021:HIS:N	2.05	0.67
1:A:47:PHE:CG	1:A:60:ILE:HD12	2.30	0.67
1:C:1040:ILE:HD11	1:C:1206:PHE:HA	1.76	0.67
1:C:89:LEU:HD23	1:C:107:PRO:HG2	1.77	0.67
1:A:79:ILE:HD11	1:A:103:LEU:HB3	1.74	0.67
1:C:15:LYS:C	1:C:297:LYS:HD2	2.20	0.66
1:C:43:LEU:HD12	1:C:44:GLU:N	2.11	0.66
1:C:1081:LEU:O	1:C:1084:MET:HG2	1.95	0.66
1:C:159:PRO:HG3	1:C:257:PRO:HB3	1.77	0.66
1:C:1081:LEU:HB3	1:C:1084:MET:HE3	1.78	0.66
1:C:136:ASP:O	1:C:140:LYS:HB2	1.96	0.65
1:C:194:PHE:O	1:C:198:LEU:HG	1.96	0.65
1:C:296:ASP:OD1	1:C:297:LYS:HG3	1.96	0.65
1:B:1076:ILE:HA	1:B:1116:TYR:HB3	1.79	0.64
1:C:8:VAL:C	1:C:9:ILE:HD12	2.21	0.64
1:B:171:TYR:OH	1:B:174:GLY:HA2	1.97	0.64
1:C:198:LEU:HA	1:C:203:HIS:HD2	1.62	0.64
1:A:297:LYS:HE3	4:A:1327:HOH:O	1.97	0.64
1:A:321:MET:O	1:A:325:GLN:HG3	1.97	0.64
1:C:1180:ALA:O	1:C:1184:ASP:HB2	1.97	0.64
1:B:322:GLU:O	1:B:326:LYS:HG2	1.98	0.63
1:B:1029:ILE:HD12	1:B:1092:VAL:HG12	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:PHE:HB3	1:C:330:MET:HG2	1.78	0.63
1:B:307:TYR:CE2	1:B:311:LEU:HD11	2.33	0.63
1:C:128:THR:HG22	1:C:249:THR:OG1	1.98	0.63
1:A:1095:GLU:O	1:A:1098:VAL:HG12	1.98	0.63
1:B:1211:GLU:HA	1:B:1214:ASN:HB2	1.80	0.63
1:C:216:ALA:O	1:C:222:THR:HG22	1.99	0.63
1:C:78:GLU:OE1	1:C:102:LYS:HD3	1.98	0.62
1:B:258:PHE:CG	1:B:330:MET:HG2	2.34	0.62
1:B:1053:ASP:OD2	1:B:1074:ARG:HG2	2.00	0.62
1:B:128:THR:OG1	1:B:131:GLU:HG2	1.99	0.62
1:B:89:LEU:HD23	1:B:107:PRO:HG2	1.81	0.62
1:B:1049:MET:HE1	1:B:1198:MET:HG2	1.82	0.62
1:C:337:SER:OG	1:C:1019:PRO:HB3	1.99	0.61
1:C:116:ILE:HB	1:C:225:THR:HG23	1.82	0.61
1:C:152:GLN:HG2	1:C:209:ASP:HA	1.82	0.61
1:A:130:GLU:O	1:A:133:PRO:HD2	2.00	0.61
1:A:1141:GLU:OE1	1:A:1160:ARG:HD3	2.01	0.61
1:B:321:MET:HE2	1:B:321:MET:HA	1.82	0.61
1:C:68:GLY:HA3	1:C:332:ASN:O	2.01	0.60
1:B:1078:VAL:HG11	1:B:1198:MET:HE3	1.82	0.60
1:C:1090:ALA:HB2	1:C:1103:LEU:HD21	1.82	0.60
1:C:33:ILE:HD13	1:C:275:LEU:HD13	1.83	0.60
1:C:195:LEU:O	1:C:199:ILE:HG13	2.02	0.60
1:B:31:THR:HG22	1:B:33:ILE:HG12	1.84	0.60
1:A:14:ASP:OD1	1:A:15:LYS:HE3	2.02	0.59
1:A:1073:MET:SD	1:A:1189:ILE:HD11	2.42	0.59
1:C:1103:LEU:HB2	1:C:1142:LEU:HB2	1.84	0.59
1:B:154:PRO:HD3	1:B:344:ARG:HG3	1.83	0.59
1:C:155:TYR:HB2	2:F:2:GLC:O6	2.02	0.59
1:C:1020:ILE:HG21	1:C:1025:ILE:CD1	2.32	0.59
1:C:273:LYS:O	1:C:277:LYS:HG3	2.02	0.59
1:C:108:ILE:HD13	1:C:285:LEU:HD21	1.84	0.59
1:C:234:ASN:O	1:C:238:SER:HB2	2.01	0.59
1:C:1031:LYS:O	1:C:1035:GLU:HG3	2.03	0.59
1:B:31:THR:C	1:B:33:ILE:H	2.10	0.59
1:A:1046:PHE:CE1	1:A:1201:VAL:HG12	2.38	0.58
1:C:156:PHE:O	1:C:159:PRO:HD2	2.03	0.58
1:A:1107:VAL:HA	4:A:1345:HOH:O	2.03	0.58
1:C:62:TRP:NE1	1:C:66:ARG:HD2	2.18	0.58
1:B:1143:SER:CB	1:B:1156:SER:HB3	2.33	0.58
1:A:45:GLU:OE1	1:A:1023:ASP:HB3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1143:SER:HB3	1:A:1155:THR:HB	1.85	0.58
1:B:1107:VAL:CG1	1:B:1110:ASP:HB2	2.33	0.57
1:C:1046:PHE:CE2	1:C:1201:VAL:HG12	2.38	0.57
1:A:9:ILE:HG23	1:A:37:VAL:HA	1.86	0.57
1:C:147:LEU:HB2	1:C:224:MET:HE3	1.86	0.57
1:C:176:TYR:CE2	1:C:331:PRO:HB3	2.39	0.57
1:C:193:THR:HA	1:C:357:VAL:HG21	1.87	0.57
1:B:258:PHE:CD1	1:B:330:MET:HG2	2.39	0.57
1:C:199:ILE:HG23	1:C:205:ASN:HA	1.87	0.57
1:A:1138:PHE:HE1	1:A:1198:MET:HE3	1.68	0.57
1:A:1181:VAL:O	1:A:1185:VAL:HG23	2.05	0.57
1:B:1103:LEU:HB2	1:B:1142:LEU:HD11	1.87	0.57
1:C:246:VAL:HG12	1:C:247:LEU:N	2.19	0.57
1:B:1040:ILE:HD11	1:B:1206:PHE:HA	1.87	0.57
1:C:8:VAL:O	1:C:58:ASP:N	2.37	0.57
1:B:288:GLU:CD	1:B:288:GLU:H	2.13	0.56
1:A:42:LYS:HD3	1:A:1023:ASP:OD2	2.05	0.56
1:B:1033:VAL:HG21	1:B:1103:LEU:HD22	1.85	0.56
1:C:321:MET:HE2	1:C:321:MET:HA	1.86	0.56
1:C:1021:HIS:O	1:C:1024:LYS:HB3	2.04	0.56
1:C:130:GLU:OE1	1:C:130:GLU:N	2.36	0.56
1:C:218:ASN:HB3	1:C:238:SER:OG	2.06	0.56
1:B:104:ILE:HD12	1:B:105:ALA:N	2.20	0.56
1:B:1026:THR:HG22	1:B:1030:ASN:ND2	2.21	0.56
1:A:61:PHE:O	1:A:62:TRP:HB2	2.04	0.56
1:C:130:GLU:O	1:C:133:PRO:HD2	2.05	0.56
1:C:235:ILE:O	1:C:238:SER:HB3	2.05	0.56
1:A:89:LEU:HD23	1:A:107:PRO:HG2	1.86	0.55
1:C:367:ASN:OD1	1:C:1093:LYS:HD3	2.07	0.55
1:A:192:LEU:O	1:A:196:VAL:HG23	2.05	0.55
1:B:28:GLU:C	1:B:30:ASP:H	2.14	0.55
1:C:1046:PHE:HE2	1:C:1201:VAL:HG12	1.71	0.55
1:A:2:ILE:HD12	1:A:269:ALA:O	2.07	0.55
1:B:1107:VAL:HA	4:B:1334:HOH:O	2.05	0.55
1:A:1053:ASP:OD1	1:A:1074:ARG:HA	2.07	0.54
1:C:7:LEU:HA	1:C:58:ASP:OD1	2.07	0.54
1:B:1131:VAL:HG12	1:B:1132:ILE:N	2.22	0.54
1:C:193:THR:OG1	1:C:357:VAL:HG11	2.06	0.54
1:C:229:PRO:HA	1:C:232:TRP:CE2	2.41	0.54
1:C:1019:PRO:O	1:C:1020:ILE:HD13	2.07	0.54
1:C:9:ILE:HD12	1:C:9:ILE:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:VAL:HG22	1:B:365:GLN:NE2	2.22	0.54
1:B:1024:LYS:O	1:B:1028:GLU:HG3	2.07	0.54
1:C:1161:GLN:NE2	1:C:1191:GLN:HB2	2.22	0.54
1:B:1174:ILE:HD13	1:C:325:GLN:NE2	2.23	0.54
1:C:36:THR:HA	4:C:1233:HOH:O	2.07	0.54
1:C:1071:LEU:HD23	1:C:1071:LEU:C	2.32	0.54
1:A:229:PRO:HA	1:A:232:TRP:CE2	2.43	0.54
1:A:1076:ILE:HA	1:A:1116:TYR:HB3	1.89	0.54
1:A:302:VAL:HG21	1:A:307:TYR:HB3	1.90	0.54
1:C:8:VAL:HA	1:C:36:THR:OG1	2.08	0.54
1:A:1135:ILE:HD11	1:A:1190:PHE:HE2	1.73	0.53
1:B:79:ILE:HD11	1:B:103:LEU:HB3	1.90	0.53
1:A:64:HIS:HE1	1:A:260:GLY:HA2	1.73	0.53
1:C:1154:LEU:HD21	1:C:1157:PHE:HB2	1.90	0.53
1:A:164:ASP:HA	1:A:253:GLN:NE2	2.23	0.53
1:B:1144:LEU:HD21	1:B:1210:LEU:HD13	1.91	0.53
1:C:18:ASN:O	1:C:21:ALA:HB3	2.08	0.53
1:C:1129:THR:HG22	1:C:1130:HIS:N	2.23	0.53
1:A:171:TYR:OH	1:A:174:GLY:HA2	2.07	0.53
1:B:79:ILE:HG12	1:B:103:LEU:O	2.09	0.53
1:B:1026:THR:HG22	1:B:1030:ASN:HD21	1.72	0.53
1:C:1207:LYS:HG3	1:C:1211:GLU:OE2	2.09	0.53
1:B:92:PHE:HA	1:B:95:ASP:OD2	2.08	0.53
1:C:1036:ALA:O	1:C:1040:ILE:HG13	2.08	0.53
1:B:273:LYS:O	1:B:277:LYS:HG3	2.07	0.53
1:C:18:ASN:HB2	1:C:296:ASP:OD2	2.09	0.53
1:B:104:ILE:HD12	1:B:104:ILE:C	2.33	0.53
1:B:1161:GLN:HG2	1:B:1191:GLN:NE2	2.24	0.53
1:B:1114:MET:HE2	1:B:1135:ILE:CG1	2.39	0.53
1:A:1046:PHE:O	1:A:1049:MET:HB2	2.09	0.52
1:B:346:ALA:HB2	1:B:364:ALA:HB2	1.90	0.52
1:A:33:ILE:HD13	1:A:275:LEU:CD1	2.39	0.52
1:B:12:ASN:HD22	1:B:14:ASP:CG	2.17	0.52
1:C:1055:SER:HB3	1:C:1072:ASP:HB3	1.90	0.52
1:C:217:PHE:HD1	1:C:222:THR:HG23	1.73	0.52
1:A:1076:ILE:CG2	1:A:1114:MET:HE3	2.39	0.52
1:B:1033:VAL:O	1:B:1037:VAL:HG23	2.10	0.52
1:C:11:ILE:CG2	1:C:17:TYR:HB3	2.39	0.52
1:A:1107:VAL:HG12	1:A:1110:ASP:HB2	1.91	0.52
1:B:47:PHE:CG	1:B:60:ILE:HD12	2.44	0.52
1:B:349:ASN:OD1	1:B:354:ARG:HD3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:VAL:HB	1:C:301:ALA:HB3	1.92	0.51
1:C:1197:GLU:O	1:C:1201:VAL:HG23	2.09	0.51
1:A:1135:ILE:HD11	1:A:1190:PHE:CE2	2.45	0.51
1:C:258:PHE:HB3	1:C:330:MET:CG	2.40	0.51
1:B:1071:LEU:HD12	1:B:1071:LEU:C	2.36	0.51
1:A:9:ILE:HD11	1:A:61:PHE:HE1	1.70	0.51
1:B:100:ASN:O	1:B:102:LYS:HG3	2.11	0.51
1:B:175:LYS:HA	4:B:1313:HOH:O	2.11	0.51
1:C:44:GLU:HB2	1:C:66:ARG:HD3	1.93	0.51
1:C:322:GLU:O	1:C:326:LYS:HG2	2.10	0.51
1:B:48:PRO:HA	1:B:75:LEU:HD13	1.93	0.51
1:B:1190:PHE:HA	1:B:1194:VAL:HB	1.93	0.51
1:B:1071:LEU:HD12	1:B:1071:LEU:O	2.11	0.50
1:B:1142:LEU:O	1:B:1142:LEU:HD12	2.12	0.50
1:C:194:PHE:CE2	1:C:198:LEU:HD11	2.45	0.50
1:C:1025:ILE:HG21	1:C:1092:VAL:HG11	1.94	0.50
1:C:1194:VAL:O	1:C:1198:MET:HG3	2.11	0.50
1:B:14:ASP:O	1:B:297:LYS:HD3	2.11	0.50
1:A:1031:LYS:O	1:A:1035:GLU:HG3	2.11	0.50
1:B:344:ARG:HG2	1:B:344:ARG:HH11	1.77	0.50
1:C:106:TYR:HE2	1:C:281:GLU:HG2	1.76	0.50
1:A:128:THR:HG22	1:A:249:THR:HG1	1.77	0.50
1:B:44:GLU:HB2	1:B:66:ARG:CD	2.40	0.50
1:C:164:ASP:CG	1:C:253:GLN:HG3	2.36	0.50
1:B:276:ALA:O	1:B:279:PHE:HB3	2.12	0.50
1:C:135:LEU:HD22	4:C:1250:HOH:O	2.11	0.50
1:A:86:GLN:HA	1:A:94:TRP:CZ2	2.47	0.50
1:A:1020:ILE:HD12	1:A:1025:ILE:CD1	2.39	0.50
1:A:1189:ILE:HG22	4:A:1343:HOH:O	2.12	0.50
1:A:6:LYS:HG2	1:A:7:LEU:N	2.26	0.50
1:A:241:ASN:HD21	1:C:123:PRO:HB3	1.76	0.50
1:B:1020:ILE:HG12	1:B:1025:ILE:CD1	2.42	0.50
1:C:5:GLY:O	1:C:33:ILE:HG23	2.11	0.50
1:B:198:LEU:HD13	1:B:204:MET:HE2	1.94	0.50
1:B:1212:ARG:C	1:B:1214:ASN:N	2.67	0.50
1:C:128:THR:OG1	1:C:131:GLU:HG3	2.12	0.50
1:C:1020:ILE:CG2	1:C:1021:HIS:H	2.10	0.50
1:C:1049:MET:HE1	1:C:1198:MET:HG2	1.94	0.50
1:A:43:LEU:C	1:A:43:LEU:HD12	2.37	0.49
1:A:181:VAL:HG12	1:A:182:GLY:N	2.27	0.49
1:C:11:ILE:HG21	1:C:17:TYR:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:ASP:HA	1:C:146:ALA:HB2	1.94	0.49
1:A:241:ASN:HD21	1:C:123:PRO:CG	2.26	0.49
1:B:127:LYS:HE2	1:B:127:LYS:HA	1.93	0.49
1:B:267:ASN:HB3	1:B:270:SER:HB2	1.94	0.49
1:B:1036:ALA:O	1:B:1040:ILE:HG13	2.12	0.49
1:B:1102:HIS:C	1:B:1103:LEU:HD12	2.38	0.49
1:C:340:TRP:CD1	2:F:2:GLC:H4	2.48	0.49
1:B:47:PHE:C	1:B:49:GLN:H	2.20	0.49
1:C:1055:SER:CB	1:C:1072:ASP:HB3	2.42	0.49
1:C:199:ILE:HA	1:C:204:MET:O	2.12	0.49
1:C:1120:TYR:O	1:C:1127:PRO:HD2	2.13	0.49
1:B:29:LYS:HG2	1:B:29:LYS:O	2.12	0.49
1:B:1164:ASN:HB2	4:B:1239:HOH:O	2.12	0.49
1:A:1143:SER:CB	1:A:1155:THR:HB	2.43	0.49
1:B:88:LYS:C	1:B:89:LEU:HD12	2.38	0.49
1:C:39:HIS:ND1	1:C:39:HIS:O	2.46	0.49
1:C:1026:THR:CG2	1:C:1030:ASN:HD21	2.21	0.49
1:A:1196:ALA:C	1:A:1198:MET:H	2.20	0.48
1:B:43:LEU:HD12	1:B:43:LEU:C	2.38	0.48
1:A:150:ASN:ND2	1:A:153:GLU:HB2	2.29	0.48
1:C:7:LEU:HD12	1:C:35:VAL:CG2	2.39	0.48
1:C:16:GLY:N	1:C:297:LYS:HD2	2.29	0.48
1:C:51:ALA:HA	1:C:55:ASP:O	2.13	0.48
1:A:1073:MET:HE3	1:A:1116:TYR:CZ	2.48	0.48
1:B:1020:ILE:HG12	1:B:1025:ILE:HD12	1.94	0.48
1:C:1161:GLN:HE21	1:C:1191:GLN:NE2	2.11	0.48
1:A:219:LYS:HD2	1:A:221:GLU:CD	2.38	0.48
1:B:123:PRO:HD2	4:B:1263:HOH:O	2.14	0.48
1:C:178:ILE:HG13	1:C:179:LYS:NZ	2.29	0.48
1:A:290:LEU:HD13	1:A:302:VAL:HB	1.96	0.48
1:B:51:ALA:HA	1:B:55:ASP:O	2.14	0.48
1:C:158:TRP:N	1:C:159:PRO:CD	2.77	0.48
1:A:116:ILE:HG22	1:A:217:PHE:CZ	2.49	0.48
1:A:1102:HIS:C	1:A:1103:LEU:HD12	2.39	0.48
1:B:198:LEU:CD1	1:B:204:MET:HE2	2.44	0.47
1:C:183:VAL:O	1:C:361:LEU:HD22	2.13	0.47
1:C:314:ASP:OD2	1:C:316:ARG:HB2	2.14	0.47
1:A:1073:MET:HE3	1:A:1116:TYR:CE1	2.49	0.47
1:C:177:ASP:C	1:C:179:LYS:H	2.22	0.47
1:A:95:ASP:HA	1:A:98:ARG:NH1	2.29	0.47
1:A:258:PHE:CG	1:A:330:MET:HG2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:THR:HG22	1:B:31:THR:O	2.13	0.47
1:B:151:LEU:HD12	1:B:205:ASN:O	2.15	0.47
1:A:258:PHE:CD1	1:A:330:MET:HG2	2.49	0.47
1:C:1090:ALA:HB2	1:C:1103:LEU:CD2	2.44	0.47
1:A:85:PHE:O	1:A:88:LYS:HG2	2.14	0.47
1:B:65:ASP:HA	1:B:332:ASN:HA	1.96	0.47
1:B:245:THR:OG1	1:B:246:VAL:N	2.47	0.47
1:B:1046:PHE:CE1	1:B:1201:VAL:HG12	2.50	0.47
1:C:29:LYS:O	1:C:29:LYS:HG2	2.14	0.47
1:C:1176:ASP:O	1:C:1179:PHE:HB3	2.15	0.47
1:A:4:GLU:HA	1:A:272:ASN:HD21	1.80	0.47
1:A:51:ALA:HA	1:A:55:ASP:O	2.14	0.47
1:A:288:GLU:CD	1:A:288:GLU:H	2.23	0.47
1:A:1136:GLN:HA	4:A:1347:HOH:O	2.15	0.47
1:B:20:LEU:HD12	1:B:23:VAL:CG1	2.45	0.47
1:B:1142:LEU:HD12	1:B:1142:LEU:C	2.40	0.47
1:C:47:PHE:N	1:C:48:PRO:HD2	2.30	0.47
1:A:193:THR:HA	1:A:357:VAL:HG21	1.96	0.46
1:C:10:TRP:CH2	1:C:57:PRO:HD3	2.50	0.46
1:C:57:PRO:O	1:C:267:ASN:HB2	2.16	0.46
1:C:1161:GLN:HE21	1:C:1191:GLN:CD	2.23	0.46
1:A:64:HIS:CE1	1:A:260:GLY:HA2	2.50	0.46
1:A:136:ASP:HA	1:A:146:ALA:HB2	1.98	0.46
1:A:1051:VAL:HB	1:A:1076:ILE:CG2	2.45	0.46
1:A:328:GLU:HG2	4:A:1285:HOH:O	2.15	0.46
1:A:1077:GLN:O	1:A:1114:MET:HA	2.15	0.46
1:B:50:VAL:O	1:B:55:ASP:HB3	2.15	0.46
1:B:158:TRP:N	1:B:159:PRO:CD	2.78	0.46
1:C:28:GLU:OE2	1:C:34:LYS:HA	2.16	0.46
1:C:59:ILE:HD13	1:C:280:LEU:HD21	1.98	0.46
1:C:1139:VAL:HG11	1:C:1160:ARG:NH2	2.31	0.46
1:C:8:VAL:HB	1:C:57:PRO:HA	1.97	0.46
1:C:1058:PHE:CB	1:C:1185:VAL:HG21	2.46	0.46
1:C:1105:VAL:HB	1:C:1140:VAL:HB	1.97	0.46
1:A:104:ILE:HD12	1:A:104:ILE:C	2.41	0.46
1:B:132:ILE:HB	1:B:133:PRO:HD3	1.97	0.46
1:B:1078:VAL:HG11	1:B:1198:MET:CE	2.46	0.46
1:C:245:THR:OG1	1:C:246:VAL:N	2.48	0.46
1:B:55:ASP:CG	1:B:56:GLY:H	2.23	0.46
1:C:178:ILE:HG13	1:C:179:LYS:HZ2	1.80	0.46
1:C:1139:VAL:HG21	1:C:1160:ARG:HH21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LYS:HD2	1:A:35:VAL:H	1.81	0.46
1:A:349:ASN:OD1	1:A:354:ARG:HD3	2.15	0.46
1:A:104:ILE:O	1:A:105:ALA:HB2	2.16	0.46
1:A:1081:LEU:O	1:A:1084:MET:HG2	2.15	0.46
1:B:31:THR:C	1:B:33:ILE:N	2.74	0.46
1:A:128:THR:HG22	1:A:249:THR:OG1	2.16	0.46
1:B:159:PRO:HG3	1:B:257:PRO:HB3	1.97	0.46
1:C:1076:ILE:HA	1:C:1116:TYR:HB3	1.98	0.46
1:B:1026:THR:O	1:B:1030:ASN:ND2	2.49	0.45
1:C:187:GLY:O	1:C:190:ALA:HB3	2.17	0.45
1:C:236:ASP:C	1:C:238:SER:H	2.23	0.45
1:A:45:GLU:O	1:A:48:PRO:HG2	2.16	0.45
1:B:64:HIS:NE2	1:B:330:MET:O	2.49	0.45
1:C:129:TRP:HD1	1:C:249:THR:O	1.99	0.45
1:C:279:PHE:O	1:C:283:TYR:HB2	2.16	0.45
1:A:272:ASN:HA	4:A:1233:HOH:O	2.16	0.45
1:C:27:PHE:HA	1:C:283:TYR:CE2	2.52	0.45
1:C:49:GLN:HG2	1:C:1021:HIS:CE1	2.52	0.45
1:C:206:ALA:CB	1:C:351:ALA:HB1	2.47	0.45
1:A:148:MET:HB2	1:A:222:THR:HG21	1.97	0.45
1:B:259:VAL:HB	1:B:329:ILE:HA	1.98	0.45
1:C:272:ASN:HB3	1:C:275:LEU:HD12	1.99	0.45
1:B:1072:ASP:HB3	1:B:1074:ARG:NH1	2.31	0.45
1:C:89:LEU:N	1:C:89:LEU:HD12	2.31	0.45
1:C:116:ILE:O	1:C:225:THR:HG22	2.16	0.45
1:C:1024:LYS:HE3	1:C:1028:GLU:OE1	2.16	0.45
1:A:38:GLU:C	1:A:40:PRO:HD3	2.41	0.45
1:A:1174:ILE:HG12	1:A:1174:ILE:O	2.16	0.45
1:C:116:ILE:HB	1:C:225:THR:CG2	2.45	0.45
1:B:28:GLU:O	1:B:32:GLY:N	2.46	0.45
1:B:129:TRP:HB3	1:B:194:PHE:CE2	2.53	0.44
1:B:1054:HIS:CD2	1:B:1189:ILE:HD13	2.52	0.44
1:C:232:TRP:CH2	1:C:316:ARG:HB3	2.52	0.44
1:A:1090:ALA:HA	1:A:1103:LEU:HG	1.99	0.44
1:C:93:THR:O	1:C:96:ALA:HB3	2.17	0.44
1:A:45:GLU:O	1:A:49:GLN:HG3	2.17	0.44
1:A:1021:HIS:O	1:A:1024:LYS:HB3	2.17	0.44
1:B:1190:PHE:HD1	1:B:1194:VAL:HG21	1.82	0.44
1:A:88:LYS:O	1:A:304:LEU:HD12	2.17	0.44
1:A:172:ALA:O	1:A:173:ALA:C	2.61	0.44
1:B:176:TYR:CZ	1:B:331:PRO:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ASN:HD22	1:A:14:ASP:CG	2.25	0.44
1:C:97:VAL:HG21	1:C:107:PRO:HD3	2.00	0.44
1:C:1191:GLN:HA	1:C:1195:ARG:HB2	1.99	0.44
1:C:9:ILE:CG1	1:C:59:ILE:HB	2.38	0.44
1:B:1054:HIS:HD2	1:B:1189:ILE:HD13	1.83	0.44
1:C:92:PHE:HA	1:C:95:ASP:OD2	2.18	0.44
1:B:47:PHE:N	1:B:48:PRO:HD2	2.33	0.44
1:B:50:VAL:HG23	1:B:51:ALA:N	2.32	0.44
1:B:54:GLY:HA2	1:B:269:ALA:CB	2.48	0.44
1:B:1019:PRO:O	1:B:1020:ILE:HB	2.18	0.44
1:C:129:TRP:CE2	1:C:160:LEU:HD13	2.53	0.44
1:A:177:ASP:OD1	1:A:179:LYS:HB2	2.18	0.43
1:A:79:ILE:HG12	1:A:103:LEU:O	2.17	0.43
1:A:1049:MET:HB3	1:A:1078:VAL:HB	1.99	0.43
1:B:79:ILE:HD12	1:B:106:TYR:CE2	2.53	0.43
1:B:321:MET:O	1:B:325:GLN:HG2	2.18	0.43
1:B:5:GLY:O	1:B:33:ILE:HD12	2.17	0.43
1:B:340:TRP:O	1:B:344:ARG:HB2	2.19	0.43
1:C:123:PRO:HG2	1:C:124:ASN:H	1.84	0.43
1:B:11:ILE:O	1:B:39:HIS:HA	2.18	0.43
1:B:334:PRO:C	1:B:336:MET:H	2.25	0.43
1:C:1046:PHE:CD2	1:C:1202:LEU:HD23	2.53	0.43
1:C:1073:MET:HE3	1:C:1116:TYR:CE1	2.54	0.43
1:C:132:ILE:HB	1:C:133:PRO:HD3	2.01	0.43
1:A:158:TRP:N	1:A:159:PRO:CD	2.81	0.43
1:A:1060:ARG:O	1:A:1067:LEU:HB3	2.19	0.43
1:A:1131:VAL:HG12	1:A:1132:ILE:N	2.33	0.43
1:C:31:THR:O	1:C:31:THR:HG22	2.17	0.43
1:C:192:LEU:O	1:C:196:VAL:HG23	2.18	0.43
1:B:16:GLY:HA2	1:B:296:ASP:OD2	2.18	0.43
1:C:178:ILE:HB	1:C:335:GLN:HG3	1.99	0.43
1:B:220:GLY:HA2	4:B:1251:HOH:O	2.18	0.43
1:B:1107:VAL:HG13	1:B:1110:ASP:HB2	1.99	0.43
1:B:1174:ILE:CD1	1:C:325:GLN:NE2	2.82	0.43
1:B:1025:ILE:HG22	1:B:1092:VAL:HG11	2.01	0.43
1:C:10:TRP:HA	1:C:38:GLU:O	2.19	0.43
1:A:1114:MET:HE2	1:A:1190:PHE:HE1	1.82	0.43
1:B:229:PRO:HA	1:B:232:TRP:CE2	2.53	0.43
1:C:1173:SER:C	1:C:1175:LEU:N	2.76	0.43
1:A:116:ILE:HB	1:A:225:THR:HG23	2.00	0.42
1:A:302:VAL:HG23	1:A:308:GLU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:GLU:C	1:B:30:ASP:N	2.76	0.42
1:B:189:LYS:HD3	1:B:358:ASP:OD2	2.19	0.42
1:B:1144:LEU:O	1:B:1145:GLU:HB2	2.18	0.42
1:C:1032:ALA:CB	1:C:1152:MET:HE1	2.48	0.42
1:A:129:TRP:CD1	1:A:248:PRO:HB2	2.54	0.42
1:B:62:TRP:HB3	1:B:67:PHE:HE1	1.84	0.42
1:B:89:LEU:CD2	1:B:107:PRO:HG2	2.49	0.42
1:B:184:ASP:HB3	1:B:365:GLN:HB2	2.00	0.42
1:A:1118:LEU:HD12	1:A:1119:ALA:H	1.85	0.42
1:C:104:ILE:O	1:C:105:ALA:HB2	2.19	0.42
1:C:118:ASN:OD1	1:C:120:ASP:HB2	2.19	0.42
1:C:307:TYR:CE2	1:C:311:LEU:HD11	2.54	0.42
1:C:1078:VAL:HG11	1:C:1198:MET:HE3	2.01	0.42
1:A:1172:LEU:HD21	1:A:1178:ILE:HG23	2.01	0.42
1:B:1093:LYS:HE2	1:B:1095:GLU:OE2	2.19	0.42
1:C:10:TRP:CD1	1:C:38:GLU:HB2	2.55	0.42
1:C:46:LYS:NZ	4:C:1219:HOH:O	2.51	0.42
1:A:1032:ALA:CB	1:A:1152:MET:HE1	2.50	0.42
1:B:1105:VAL:HB	1:B:1140:VAL:CG2	2.50	0.42
1:A:130:GLU:OE1	1:A:130:GLU:N	2.48	0.42
1:A:132:ILE:N	1:A:133:PRO:CD	2.82	0.42
1:B:240:VAL:O	1:B:242:TYR:HD1	2.03	0.42
1:B:301:ALA:HB2	1:B:321:MET:HE3	2.01	0.42
1:C:178:ILE:HG22	1:C:333:ILE:HD12	2.02	0.42
1:C:258:PHE:CG	1:C:330:MET:HG2	2.55	0.42
1:A:5:GLY:O	1:A:33:ILE:HG23	2.20	0.42
1:C:256:LYS:HG2	1:C:326:LYS:O	2.19	0.42
1:A:241:ASN:HD21	1:C:123:PRO:CB	2.33	0.42
1:B:1049:MET:HB3	1:B:1078:VAL:HB	2.02	0.42
1:A:122:LEU:HD21	1:A:125:PRO:HA	2.01	0.42
1:C:139:LEU:O	1:C:142:LYS:N	2.47	0.42
1:C:1091:ASN:O	1:C:1101:ALA:HA	2.20	0.42
1:C:1173:SER:C	1:C:1175:LEU:H	2.28	0.42
1:A:1051:VAL:HA	1:A:1052:PRO:HD3	1.93	0.41
1:B:97:VAL:HG21	1:B:105:ALA:O	2.20	0.41
1:B:209:ASP:OD1	1:B:209:ASP:C	2.63	0.41
1:C:169:PHE:CD2	1:C:333:ILE:HD11	2.55	0.41
1:C:1094:SER:O	1:C:1095:GLU:HB2	2.20	0.41
1:A:241:ASN:HD21	1:C:123:PRO:HD3	1.85	0.41
1:B:1094:SER:CB	1:B:1099:VAL:HG22	2.50	0.41
1:C:43:LEU:HD12	1:C:43:LEU:C	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:VAL:O	1:A:308:GLU:HB2	2.20	0.41
1:B:2:ILE:O	1:B:271:PRO:HG3	2.20	0.41
1:B:1074:ARG:NH2	4:B:1267:HOH:O	2.52	0.41
1:B:1107:VAL:HG13	4:B:1334:HOH:O	2.21	0.41
1:C:59:ILE:HA	1:C:265:GLY:O	2.21	0.41
1:C:259:VAL:HB	1:C:329:ILE:HA	2.01	0.41
1:A:241:ASN:ND2	1:C:123:PRO:HD3	2.36	0.41
1:A:1149:GLU:CD	1:A:1149:GLU:N	2.78	0.41
1:B:164:ASP:O	1:B:164:ASP:CG	2.64	0.41
1:B:173:ALA:O	1:B:174:GLY:C	2.62	0.41
1:B:340:TRP:HA	1:B:340:TRP:CE3	2.53	0.41
1:C:258:PHE:CB	1:C:330:MET:HG2	2.49	0.41
1:C:1108:HIS:HB3	1:C:1109:ASP:H	1.69	0.41
1:C:1135:ILE:HD13	1:C:1162:PHE:CE1	2.56	0.41
1:A:241:ASN:ND2	1:C:123:PRO:HG3	2.36	0.41
1:C:1154:LEU:C	1:C:1154:LEU:HD23	2.45	0.41
1:A:308:GLU:O	1:A:312:ALA:HB2	2.21	0.41
1:A:109:ALA:CB	1:A:302:VAL:HA	2.51	0.41
1:A:62:TRP:CD1	1:A:63:ALA:N	2.88	0.41
1:A:204:MET:HB2	4:A:1226:HOH:O	2.21	0.41
1:A:1022:TYR:O	1:A:1023:ASP:C	2.63	0.41
1:C:10:TRP:CZ3	1:C:57:PRO:HD3	2.56	0.41
1:C:16:GLY:N	1:C:297:LYS:HB2	2.35	0.41
1:C:206:ALA:HB2	1:C:351:ALA:HB1	2.00	0.41
1:C:216:ALA:HA	1:C:221:GLU:OE1	2.21	0.41
1:C:340:TRP:CE3	1:C:340:TRP:HA	2.56	0.41
1:A:1041:GLU:HB2	4:A:1283:HOH:O	2.21	0.41
1:A:1093:LYS:HE2	1:A:1095:GLU:HG2	2.03	0.41
1:B:48:PRO:HA	1:B:75:LEU:CD1	2.50	0.41
1:B:296:ASP:O	1:B:297:LYS:HG3	2.20	0.41
1:B:365:GLN:HE21	1:B:365:GLN:HA	1.86	0.41
1:C:38:GLU:C	1:C:40:PRO:HD3	2.45	0.41
1:C:279:PHE:HA	1:C:283:TYR:CD1	2.56	0.41
1:C:343:VAL:O	1:C:347:VAL:HG23	2.21	0.41
1:A:1135:ILE:HD13	1:A:1162:PHE:CE1	2.55	0.41
1:C:113:LEU:HD23	1:C:227:ASN:C	2.46	0.41
1:A:215:ALA:O	1:A:219:LYS:HB2	2.21	0.40
1:B:195:LEU:HD12	1:B:204:MET:HE1	2.04	0.40
1:C:117:TYR:CE2	1:C:125:PRO:HD3	2.57	0.40
1:C:1046:PHE:CZ	1:C:1205:ALA:HB2	2.55	0.40
1:C:1140:VAL:HG11	1:C:1157:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:VAL:O	1:B:23:VAL:HG22	2.22	0.40
1:B:1114:MET:HE2	1:B:1135:ILE:HG13	2.03	0.40
1:C:14:ASP:O	1:C:297:LYS:HD3	2.21	0.40
1:A:139:LEU:HD13	1:A:145:SER:O	2.21	0.40
1:B:62:TRP:CD1	1:B:63:ALA:N	2.90	0.40
1:C:90:TYR:HA	1:C:91:PRO:HD3	1.95	0.40
1:C:294:ASN:OD1	1:C:298:PRO:HA	2.20	0.40
1:C:1118:LEU:HD12	1:C:1119:ALA:H	1.86	0.40
1:A:1018:ASP:O	1:A:1020:ILE:HG23	2.21	0.40
1:A:1185:VAL:O	1:A:1189:ILE:HG23	2.21	0.40
1:C:164:ASP:HB2	1:C:253:GLN:HG3	2.04	0.40
1:C:1091:ASN:HB2	1:C:1102:HIS:HB2	2.04	0.40
1:A:1161:GLN:O	1:A:1161:GLN:HG3	2.21	0.40
1:A:1209:GLU:C	1:A:1211:GLU:H	2.30	0.40
1:A:1211:GLU:O	1:A:1214:ASN:HB3	2.20	0.40
1:B:33:ILE:HG13	1:B:275:LEU:HD11	2.02	0.40
1:B:1131:VAL:CG1	1:B:1132:ILE:N	2.84	0.40
1:B:1177:PRO:O	1:B:1181:VAL:HG23	2.22	0.40
1:C:160:LEU:HA	1:C:163:ALA:HB2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:ALA:O	1:C:141:ALA:O[2_555]	1.89	0.31

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	566/568 (100%)	524 (93%)	40 (7%)	2 (0%)	30 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	559/568 (98%)	504 (90%)	48 (9%)	7 (1%)	9	8
1	C	546/568 (96%)	489 (90%)	48 (9%)	9 (2%)	7	6
All	All	1671/1704 (98%)	1517 (91%)	136 (8%)	18 (1%)	11	11

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	146	ALA
1	C	186	ALA
1	C	1108	HIS
1	B	1020	ILE
1	B	1093	LYS
1	A	1061	HIS
1	A	1067	LEU
1	B	1145	GLU
1	B	29	LYS
1	C	119	LYS
1	C	178	ILE
1	C	285	LEU
1	B	1019	PRO
1	B	1213	ASN
1	C	16	GLY
1	C	40	PRO
1	B	48	PRO
1	C	166	GLY

5.3.2 Protein sidechains ⓘ

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	426/461 (92%)	422 (99%)	4 (1%)	70	82
1	B	421/461 (91%)	418 (99%)	3 (1%)	76	86
1	C	412/461 (89%)	411 (100%)	1 (0%)	87	94
All	All	1259/1383 (91%)	1251 (99%)	8 (1%)	78	87

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	241	ASN
1	A	258	PHE
1	A	288	GLU
1	A	1174	ILE
1	B	258	PHE
1	B	288	GLU
1	B	1176	ASP
1	C	1174	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	100	ASN
1	A	152	GLN
1	A	241	ASN
1	A	253	GLN
1	A	1128	ASN
1	A	1167	ASN
1	B	12	ASN
1	B	18	ASN
1	B	152	GLN
1	B	234	ASN
1	B	241	ASN
1	B	325	GLN
1	B	355	GLN
1	B	365	GLN
1	B	1054	HIS
1	B	1167	ASN
1	C	12	ASN
1	C	72	GLN
1	C	100	ASN
1	C	203	HIS
1	C	241	ASN
1	C	1030	ASN
1	C	1054	HIS
1	C	1130	HIS
1	C	1151	ASN
1	C	1161	GLN
1	C	1167	ASN
1	C	1191	GLN

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	$\# Z > 2$
2	GLC	D	1	2	12,12,12	0.37	0	17,17,17	0.39	0
2	GLC	D	2	2	11,11,12	0.47	0	15,15,17	0.59	0
2	GLC	E	1	2	12,12,12	0.41	0	17,17,17	0.37	0
2	GLC	E	2	2	11,11,12	0.44	0	15,15,17	0.64	1 (6%)
2	GLC	F	1	2	12,12,12	0.35	0	17,17,17	0.31	0
2	GLC	F	2	2	11,11,12	0.42	0	15,15,17	0.59	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
2	GLC	D	1	2	-	2/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	GLC	E	1	2	-	0/2/22/22	0/1/1/1
2	GLC	E	2	2	-	0/2/19/22	0/1/1/1
2	GLC	F	1	2	-	0/2/22/22	0/1/1/1
2	GLC	F	2	2	-	2/2/19/22	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(°)	Ideal(°)
2	E	2	GLC	C1-O5-C5	2.06	114.95	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

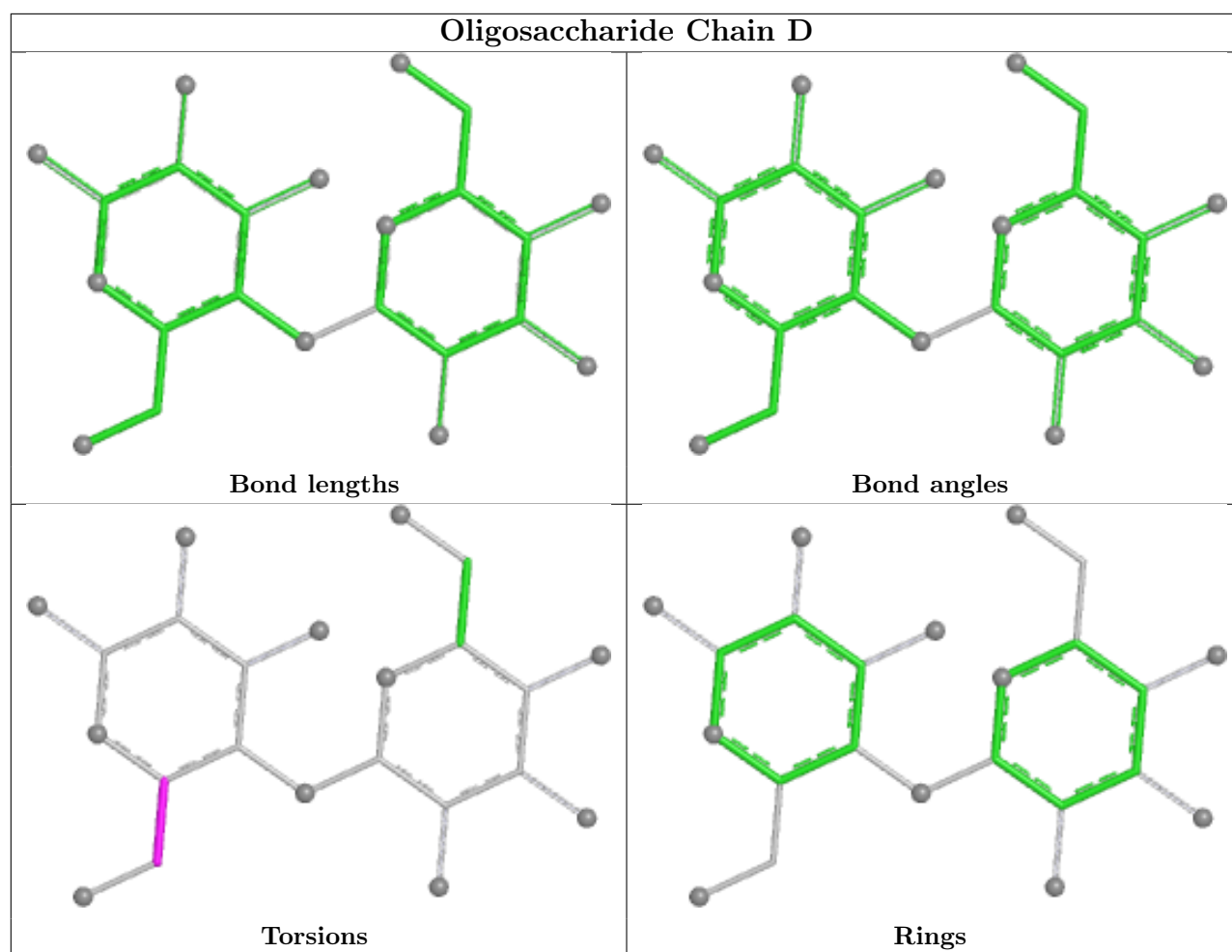
Mol	Chain	Res	Type	Atoms
2	F	2	GLC	O5-C5-C6-O6
2	F	2	GLC	C4-C5-C6-O6
2	D	1	GLC	C4-C5-C6-O6
2	D	1	GLC	O5-C5-C6-O6

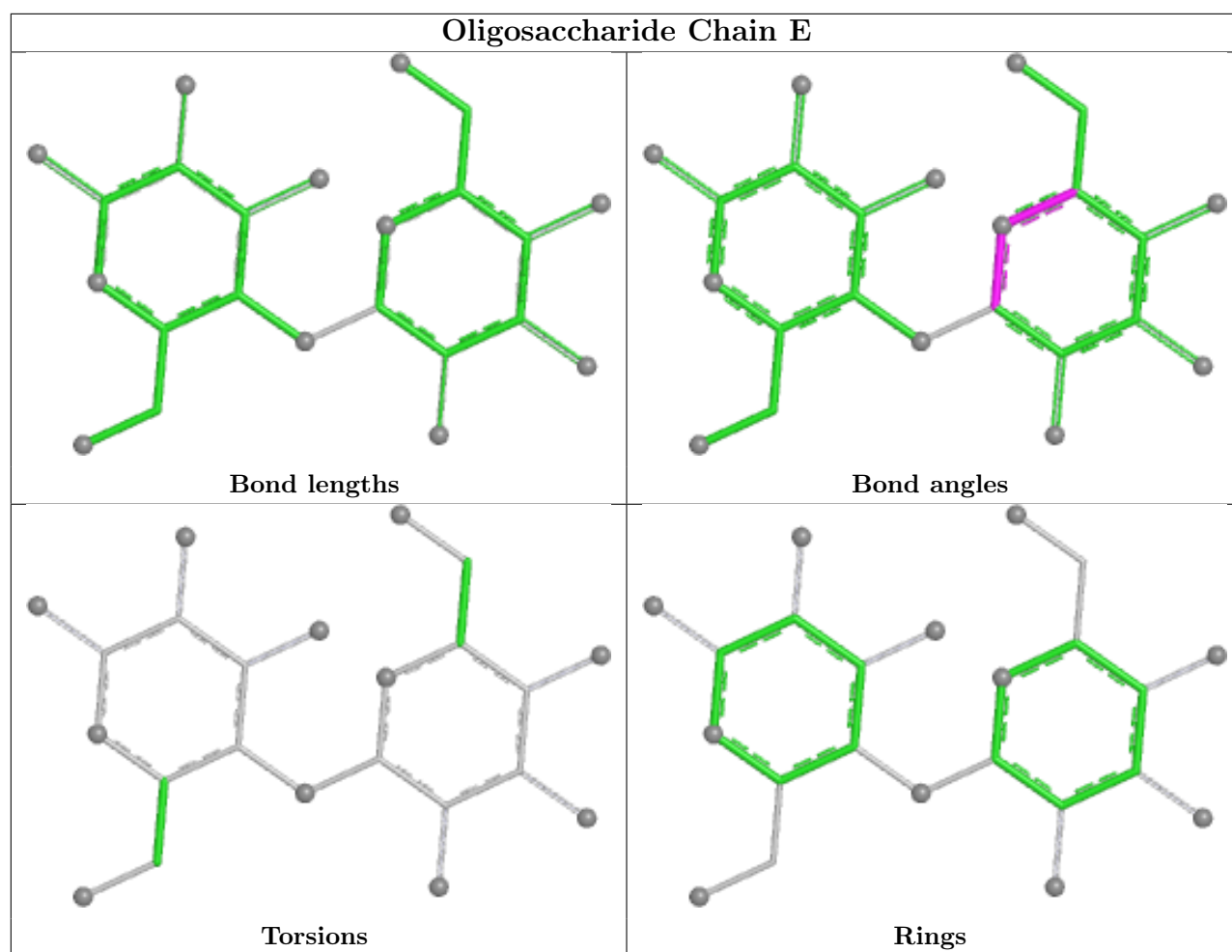
There are no ring outliers.

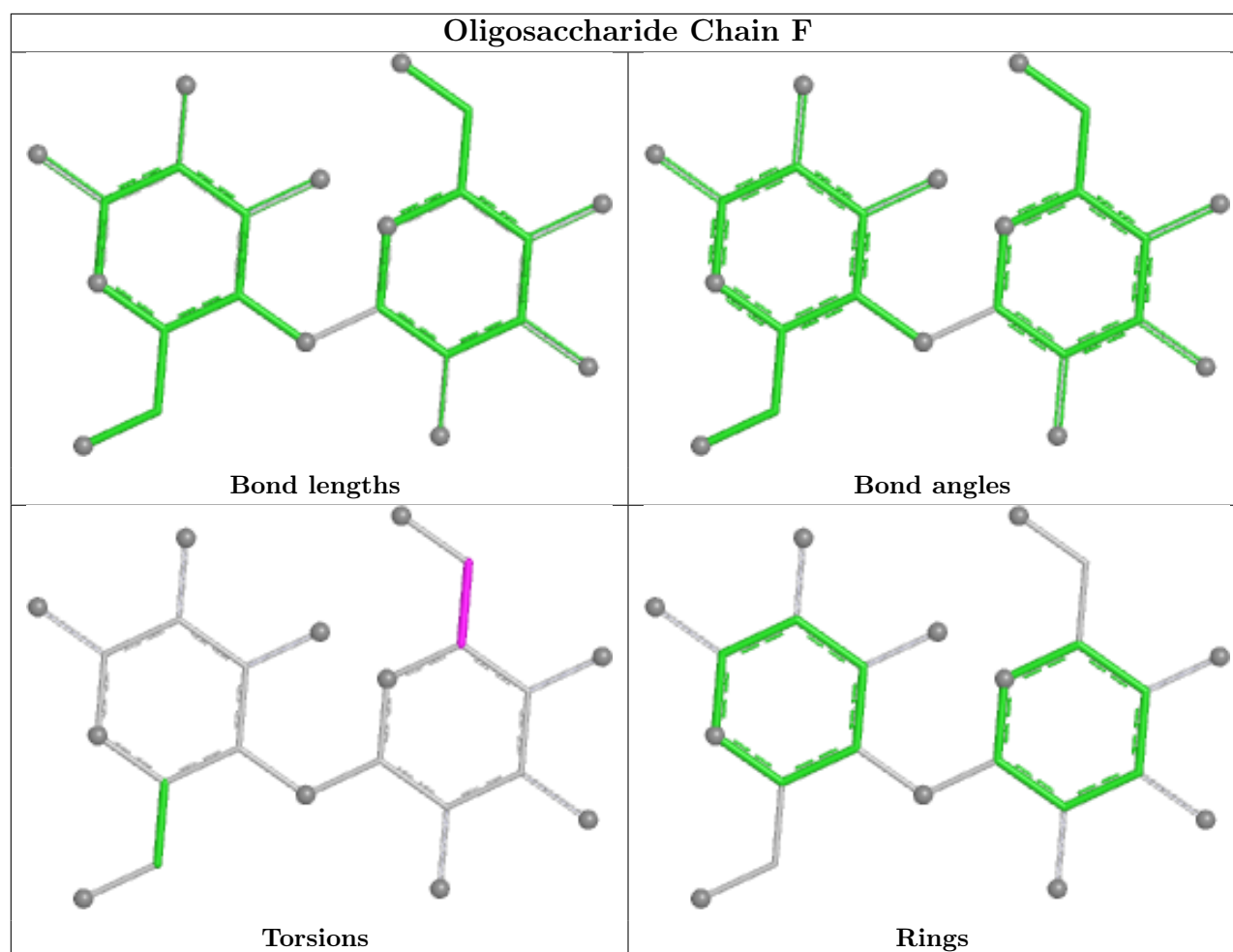
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2	GLC	3	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 [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	568/568 (100%)	0.50	29 (5%)	33 39	19, 42, 75, 90	0
1	B	563/568 (99%)	0.72	42 (7%)	20 23	22, 47, 73, 96	0
1	C	552/568 (97%)	1.39	122 (22%)	2 2	35, 61, 81, 96	0
All	All	1683/1704 (98%)	0.87	193 (11%)	9 11	19, 50, 78, 96	0

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1062	ILE	6.1
1	C	1069	GLY	5.6
1	C	222	THR	5.0
1	B	54	GLY	4.7
1	C	125	PRO	4.3
1	B	1094	SER	4.3
1	A	1213	ASN	4.2
1	C	240	VAL	4.0
1	C	121	LEU	4.0
1	C	33	ILE	3.9
1	A	1067	LEU	3.9
1	C	215	ALA	3.9
1	C	1107	VAL	3.8
1	A	1124	ASP	3.7
1	C	31	THR	3.7
1	C	133	PRO	3.7
1	C	1043	SER	3.6
1	C	9	ILE	3.6
1	C	223	ALA	3.5
1	A	1046	PHE	3.5
1	C	23	VAL	3.4
1	C	8	VAL	3.4
1	C	239	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	1061	HIS	3.3
1	C	32	GLY	3.3
1	C	3	GLU	3.3
1	C	141	ALA	3.3
1	C	27	PHE	3.3
1	C	145	SER	3.3
1	C	37	VAL	3.3
1	C	134	ALA	3.2
1	C	242	TYR	3.2
1	C	143	GLY	3.2
1	C	123	PRO	3.2
1	B	266	ILE	3.2
1	B	1020	ILE	3.2
1	C	250	PHE	3.2
1	B	1109	ASP	3.2
1	A	1125	LEU	3.2
1	C	2	ILE	3.2
1	C	79	ILE	3.1
1	C	1071	LEU	3.1
1	A	1193	THR	3.1
1	C	1129	THR	3.1
1	C	54	GLY	3.1
1	C	1127	PRO	3.1
1	C	122	LEU	3.1
1	C	147	LEU	3.1
1	B	1043	SER	3.0
1	B	1058	PHE	3.0
1	C	35	VAL	3.0
1	C	235	ILE	3.0
1	B	2	ILE	2.9
1	C	275	LEU	2.9
1	B	50	VAL	2.9
1	B	33	ILE	2.9
1	A	1122	LEU	2.8
1	C	219	LYS	2.8
1	C	241	ASN	2.8
1	C	1108	HIS	2.8
1	C	188	ALA	2.8
1	C	248	PRO	2.8
1	B	1113	SER	2.8
1	B	1114	MET	2.8
1	C	217	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	1058	PHE	2.8
1	C	126	PRO	2.7
1	B	52	ALA	2.7
1	C	117	TYR	2.7
1	C	1045	THR	2.7
1	C	1097	GLY	2.7
1	C	224	MET	2.7
1	C	238	SER	2.7
1	C	75	LEU	2.7
1	A	172	ALA	2.7
1	C	168	ALA	2.7
1	C	20	LEU	2.7
1	C	127	LYS	2.6
1	C	194	PHE	2.6
1	C	36	THR	2.6
1	A	1061	HIS	2.6
1	C	1042	LYS	2.6
1	C	216	ALA	2.6
1	C	11	ILE	2.6
1	C	1084	MET	2.6
1	C	146	ALA	2.6
1	B	32	GLY	2.6
1	C	135	LEU	2.6
1	C	10	TRP	2.6
1	C	172	ALA	2.5
1	A	1126	HIS	2.5
1	C	233	SER	2.5
1	C	1132	ILE	2.5
1	B	30	ASP	2.5
1	B	1077	GLN	2.5
1	B	1111	VAL	2.5
1	B	1174	ILE	2.5
1	C	283	TYR	2.5
1	C	361	LEU	2.5
1	C	1154	LEU	2.5
1	C	237	THR	2.4
1	B	1112	VAL	2.4
1	C	1092	VAL	2.4
1	C	234	ASN	2.4
1	C	1128	ASN	2.4
1	C	1130	HIS	2.4
1	B	173	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1112	VAL	2.4
1	C	171	TYR	2.4
1	C	184	ASP	2.4
1	C	24	GLY	2.4
1	B	1026	THR	2.4
1	B	1107	VAL	2.4
1	A	1045	THR	2.4
1	C	249	THR	2.4
1	C	1153	THR	2.4
1	A	1107	VAL	2.4
1	C	149	PHE	2.4
1	B	1124	ASP	2.3
1	C	17	TYR	2.3
1	C	218	ASN	2.3
1	B	1	LYS	2.3
1	C	19	GLY	2.3
1	C	116	ILE	2.3
1	C	1098	VAL	2.3
1	A	1066	ASP	2.3
1	A	1085	LYS	2.3
1	C	206	ALA	2.3
1	A	1114	MET	2.3
1	C	196	VAL	2.3
1	B	1152	MET	2.3
1	B	1060	ARG	2.3
1	A	1076	ILE	2.3
1	C	271	PRO	2.3
1	A	173	ALA	2.3
1	C	203	HIS	2.3
1	B	104	ILE	2.3
1	C	1046	PHE	2.2
1	C	1210	LEU	2.2
1	A	87	ASP	2.2
1	B	101	GLY	2.2
1	C	204	MET	2.2
1	B	1119	ALA	2.2
1	A	1043	SER	2.2
1	C	34	LYS	2.2
1	B	1098	VAL	2.2
1	C	198	LEU	2.2
1	C	1190	PHE	2.2
1	C	1104	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	120	ASP	2.2
1	C	5	GLY	2.2
1	C	4	GLU	2.2
1	C	213	ALA	2.2
1	B	1022	TYR	2.2
1	C	232	TRP	2.2
1	C	1025	ILE	2.2
1	C	1144	LEU	2.2
1	B	271	PRO	2.2
1	C	119	LYS	2.2
1	B	53	THR	2.2
1	B	239	ALA	2.2
1	C	80	THR	2.2
1	A	1062	ILE	2.1
1	C	132	ILE	2.1
1	C	195	LEU	2.1
1	C	1020	ILE	2.1
1	C	1174	ILE	2.1
1	A	1108	HIS	2.1
1	C	39	HIS	2.1
1	C	325	GLN	2.1
1	A	1069	GLY	2.1
1	B	1106	GLY	2.1
1	A	1060	ARG	2.1
1	B	1046	PHE	2.1
1	C	1082	LYS	2.1
1	A	1214	ASN	2.1
1	B	1215	GLN	2.1
1	C	71	ALA	2.1
1	B	1023	ASP	2.1
1	C	124	ASN	2.1
1	A	1063	GLY	2.1
1	C	144	LYS	2.0
1	A	1197	GLU	2.0
1	C	1056	ASP	2.0
1	A	1171	GLY	2.0
1	B	1093	LYS	2.0
1	C	42	LYS	2.0
1	C	140	LYS	2.0
1	B	1155	THR	2.0
1	C	192	LEU	2.0
1	A	1064	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	317	ILE	2.0
1	C	1057	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

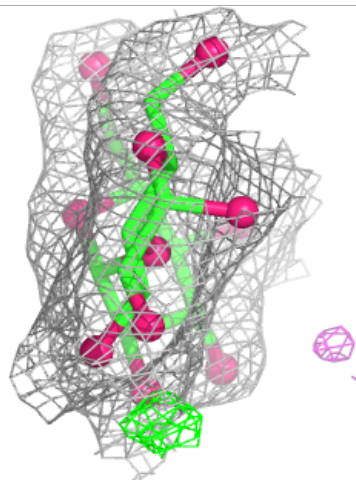
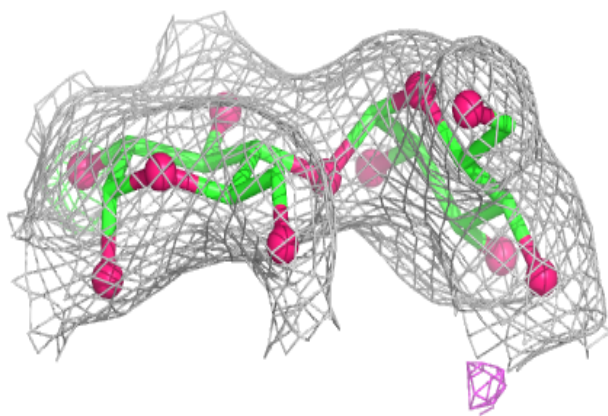
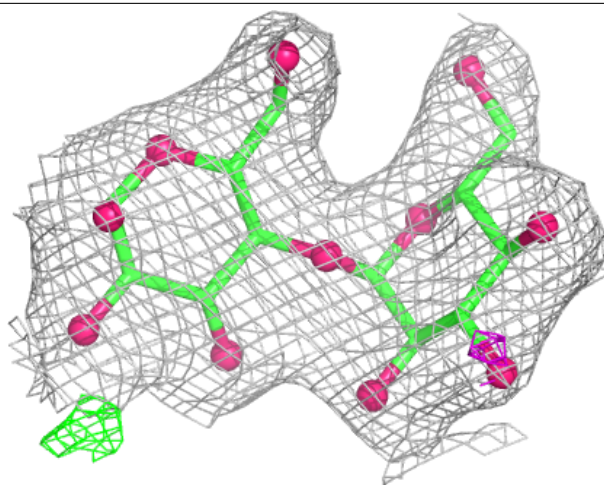
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	F	1	12/12	0.90	0.11	44,48,50,51	0
2	GLC	E	1	12/12	0.92	0.09	31,33,36,36	0
2	GLC	D	1	12/12	0.93	0.09	26,31,34,37	0
2	GLC	D	2	11/12	0.93	0.09	27,31,36,37	0
2	GLC	F	2	11/12	0.93	0.10	40,43,46,46	0
2	GLC	E	2	11/12	0.95	0.06	35,38,39,40	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.

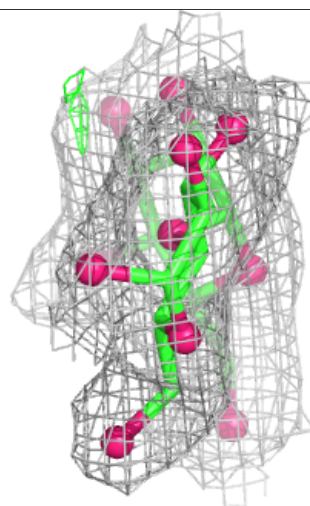
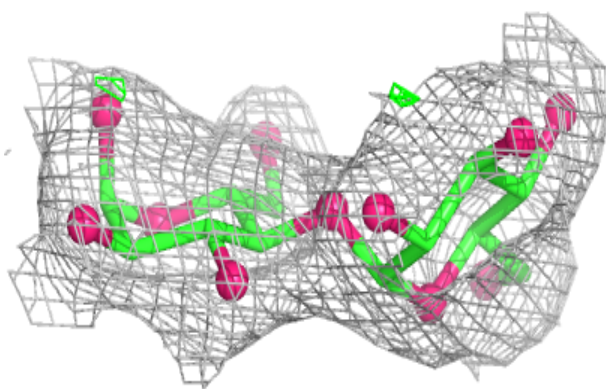
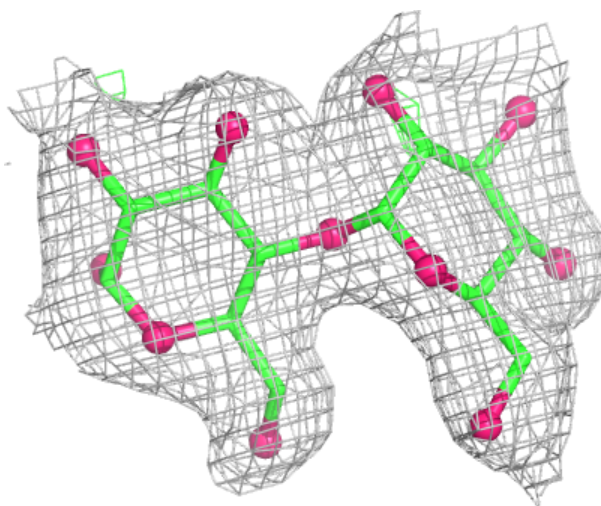
Electron density around Chain D:

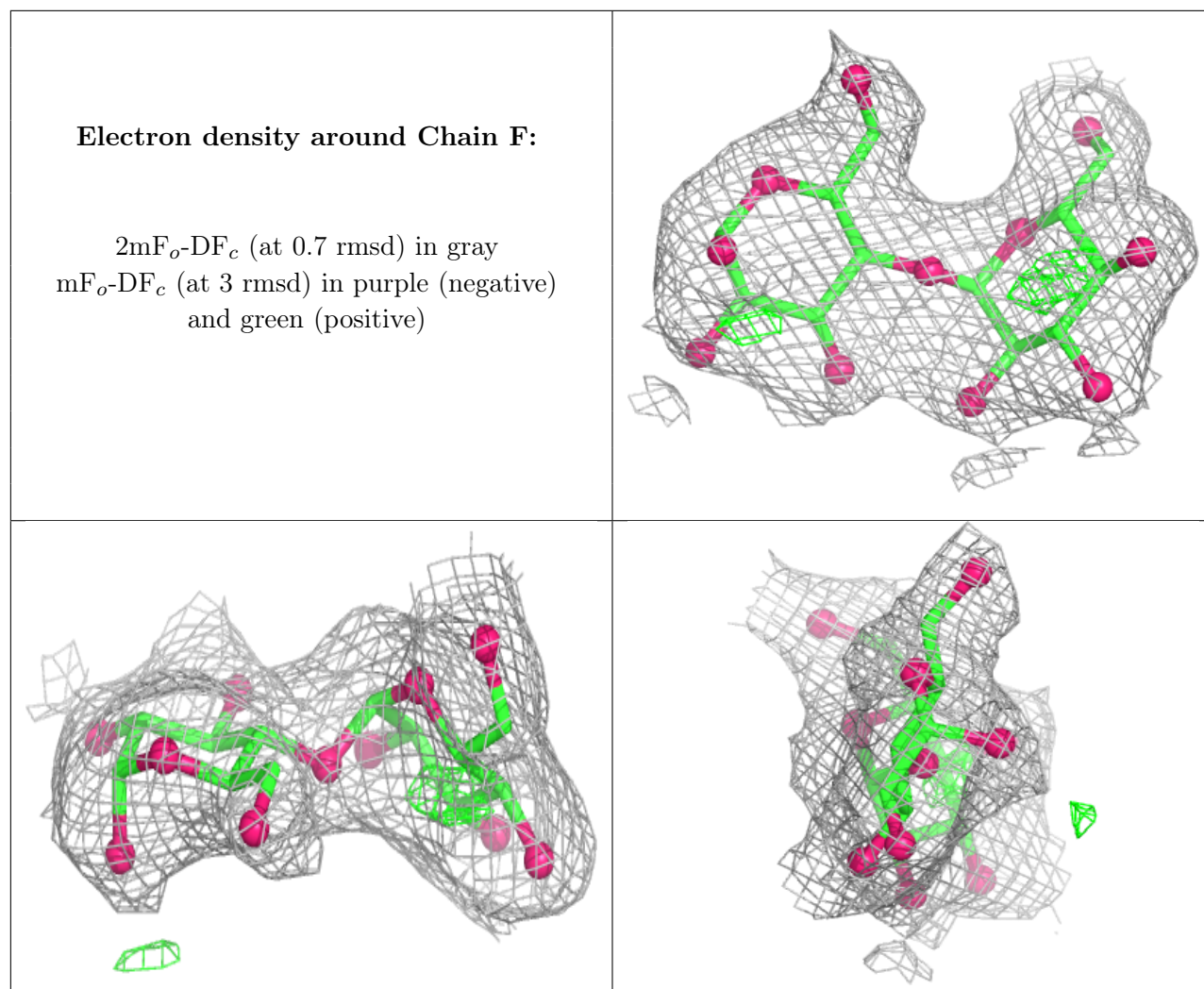
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain E:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	A	1216	1/1	0.85	0.18	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.