Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 06:09 PM EDT

PDB ID	:	3H4Z
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 (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

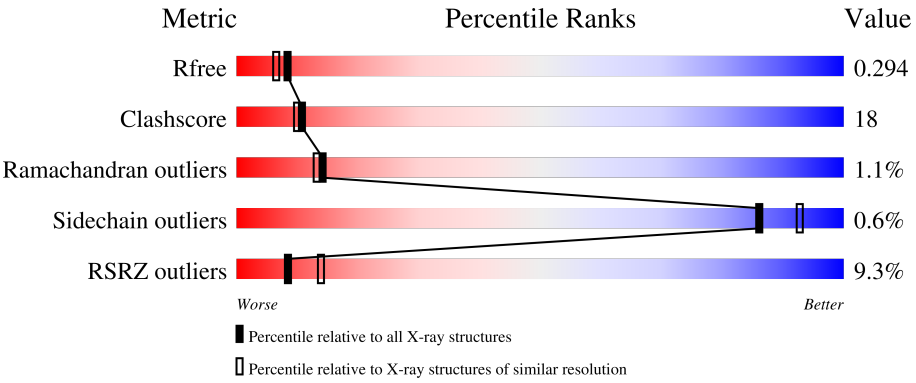
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.35 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}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (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 <=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	6% 70% 29%
1	B	568	8% 69% 29%
1	C	568	14% 54% 42%
2	D	2	100%
2	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	F	2	50% 50%

2 Entry composition (i)

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 23 12 11	0	0	0
2	E	2	Total C O 23 12 11	0	0	0
2	F	2	Total C O 23 12 11	0	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 4 is water.

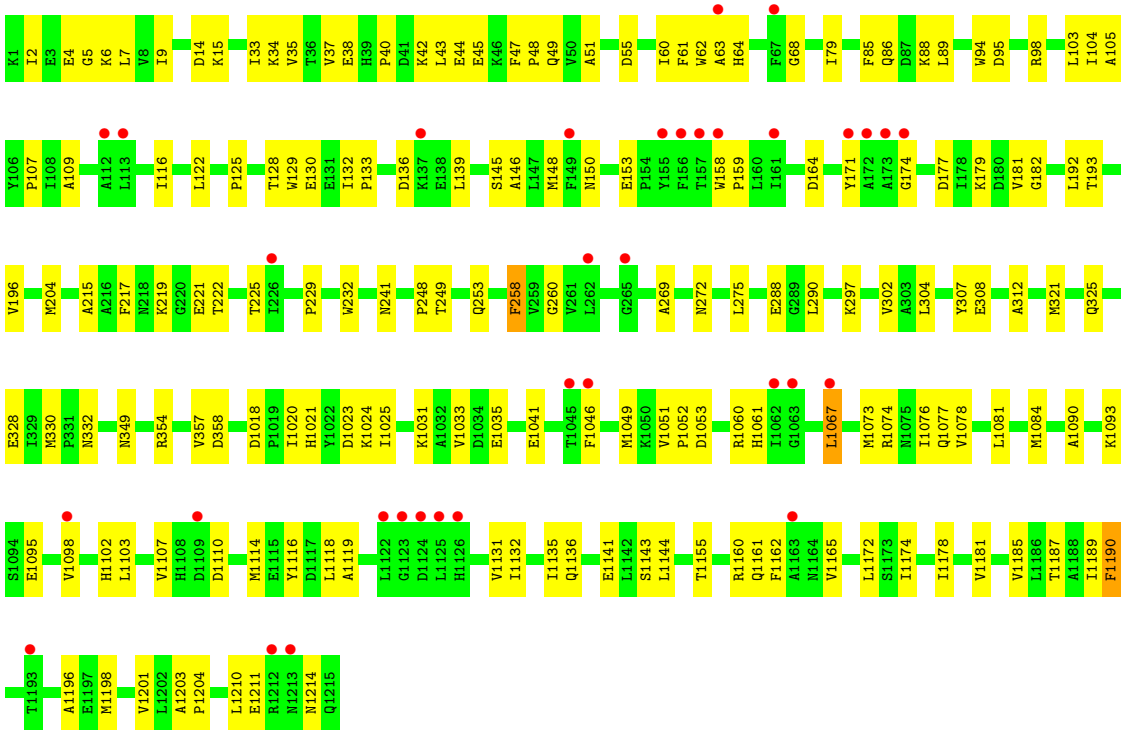
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	146	Total O 146 146	0	0
4	B	130	Total O 130 130	0	0
4	C	46	Total O 46 46	0	0

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.

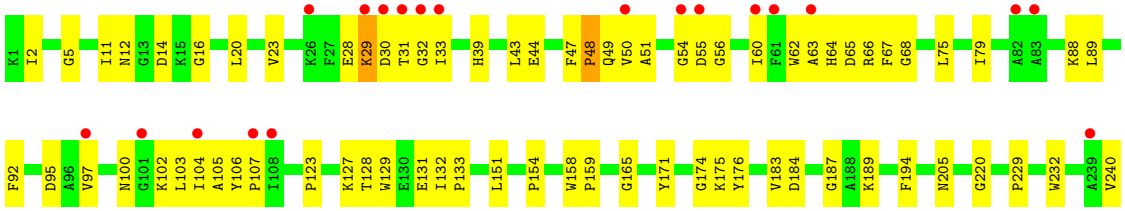
• Molecule 1: Maltose-binding periplasmic protein fused with Allergen DERP7

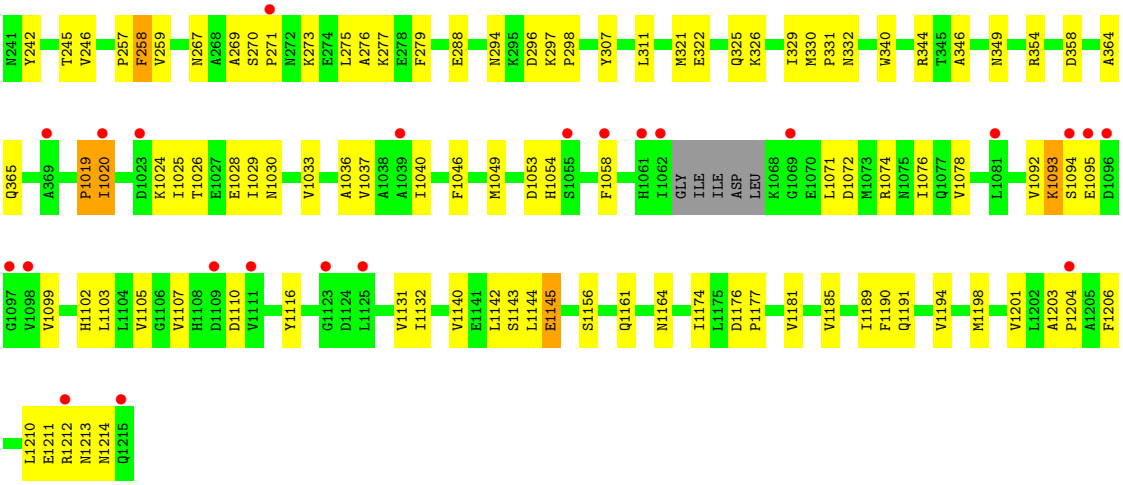
Chain A:



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

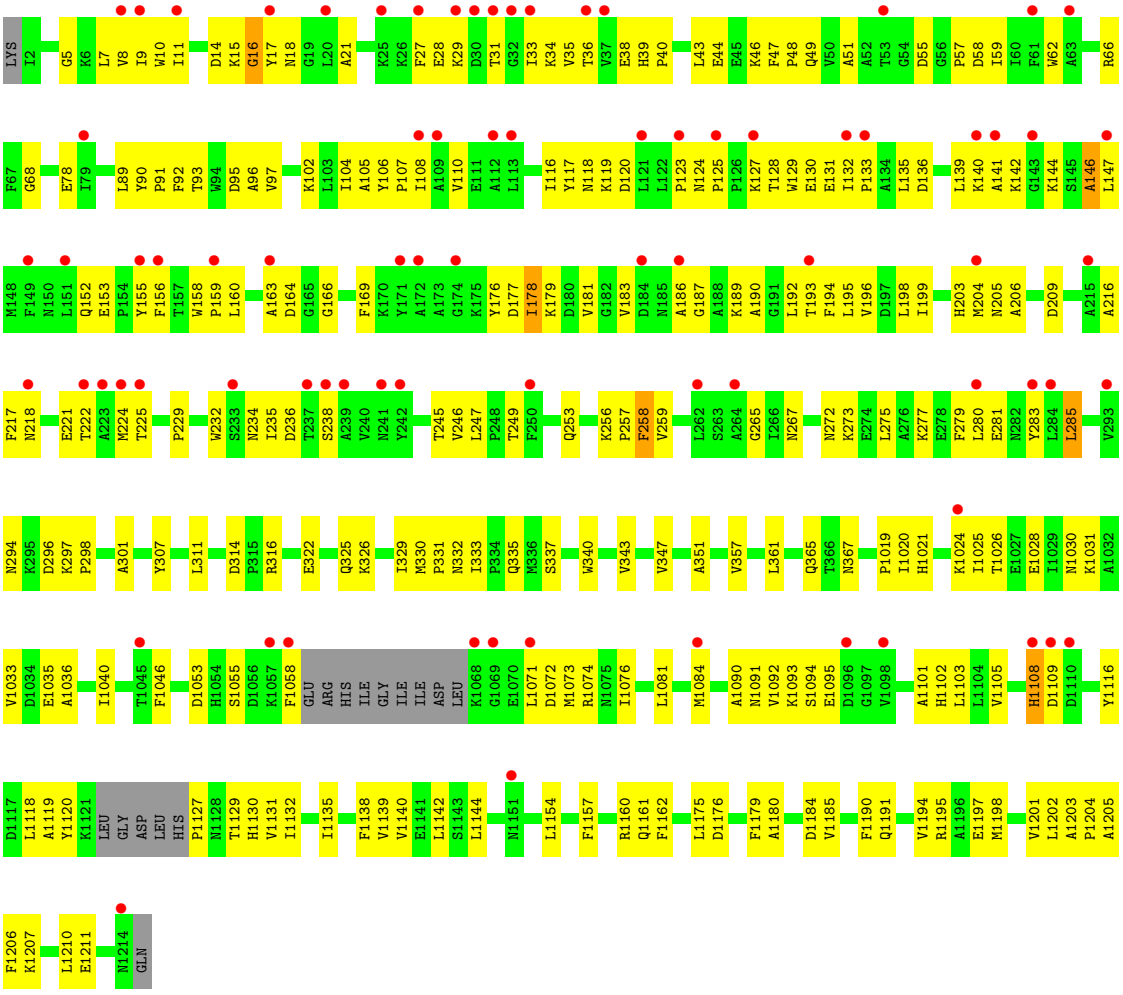
Chain B:





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

Chain C:



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

Chain D:

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

Chain E:

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

Chain F:

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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)	0.32 , 47.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	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.*

[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: 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	0.28	0/4347	0.52	0/5925
1	B	0.27	0/4311	0.49	0/5877
1	C	0.27	0/4220	0.48	0/5759
All	All	0.27	0/12878	0.50	0/17561

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	4257	0	4092	124	0
1	B	4220	0	4047	135	0
1	C	4130	0	3936	203	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	454	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 18.

All (454) 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
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: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: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:B:1143:SER:HB2	1:B:1156:SER:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:1212:ARG:C	1:B:1214:ASN:H	1.98	0.65
1:B:1076:ILE:HA	1:B:1116:TYR:HB3	1.79	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
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: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:C:15:LYS:C	1:C:297:LYS:HD2	2.20	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:C:68:GLY:HA3	1:C:332:ASN:O	2.01	0.60
1:C:1090:ALA:HB2	1:C:1103:LEU:HD21	1.82	0.60
1:C:8:VAL:C	1:C:9:ILE:HD12	2.21	0.60
1:C:33:ILE:HD13	1:C:275:LEU:HD13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:31:THR:C	1:B:33:ILE:H	2.10	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
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: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:A:1114:MET:HE1	1:A:1190:PHE:CE1	2.43	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:1161:GLN:HG2	1:B:1191:GLN:NE2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:288:GLU:CD	1:B:288:GLU:H	2.13	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
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: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:A:1114:MET:HE1	1:A:1190:PHE:HE1	1.76	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:B:28:GLU:C	1:B:30:ASP:H	2.14	0.50
1:B:44:GLU:HB2	1:B:66:ARG:CD	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:C:340:TRP:CD1	2:F:2:GLC:H4	2.48	0.49
1:A:321:MET:HE2	1:A:321:MET:HA	1.94	0.49
1:C:1055:SER:CB	1:C:1072:ASP:HB3	2.42	0.49
1:C:1071:LEU:HD23	1:C:1071:LEU:C	2.32	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:104:ILE:HD12	1:B:104:ILE:C	2.33	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: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: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: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: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:B:12:ASN:HD22	1:B:14:ASP:CG	2.17	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: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
1:B:31:THR:HG22	1:B:31:THR:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:321:MET:HE2	1:B:321:MET:HA	1.97	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: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:B:1071:LEU:HD12	1:B:1071:LEU:C	2.36	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1084:MET:HE1	1:C:1138:PHE:HE2	1.81	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:164:ASP:CG	1:C:253:GLN:HG3	2.36	0.45
1:C:187:GLY:O	1:C:190:ALA:HB3	2.17	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:43:LEU:C	1:A:43:LEU:HD12	2.37	0.45
1:A:1174:ILE:HG12	1:A:1174:ILE:O	2.16	0.45
1:B:1102:HIS:C	1:B:1103:LEU:HD12	2.38	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:C:31:THR:O	1:C:31:THR:HG22	2.17	0.45
1:B:47:PHE:C	1:B:49:GLN:H	2.20	0.44
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:B:176:TYR:CZ	1:B:331:PRO:HG3	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:ILE:CG1	1:C:59:ILE:HB	2.38	0.44
1:B:88:LYS:C	1:B:89:LEU:HD12	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:43:LEU:HD12	1:B:43:LEU:C	2.38	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:219:LYS:HD2	1:A:221:GLU:CD	2.38	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:A:1196:ALA:C	1:A:1198:MET:H	2.20	0.43
1:B:11:ILE:O	1:B:39:HIS:HA	2.18	0.43
1:C:1046:PHE:CD2	1:C:1202:LEU:HD23	2.53	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:1102:HIS:C	1:A:1103:LEU:HD12	2.39	0.43
1:A:1131:VAL:HG12	1:A:1132:ILE:N	2.33	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:B:229:PRO:HA	1:B:232:TRP:CE2	2.53	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
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:177:ASP:C	1:C:179:LYS:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:A:288:GLU:CD	1:A:288:GLU:H	2.23	0.42
1:B:1049:MET:HB3	1:B:1078:VAL:HB	2.02	0.42
1:B:1142:LEU:HD12	1:B:1142:LEU:C	2.40	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: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: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: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:104:ILE:HD12	1:A:104:ILE:C	2.41	0.41
1:A:241:ASN:ND2	1:C:123:PRO:HD3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:55:ASP:CG	1:B:56:GLY:H	2.23	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:C:1161:GLN:HE21	1:C:1191:GLN:CD	2.23	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: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:236:ASP:C	1:C:238:SER:H	2.23	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:A:215:ALA:O	1:A:219:LYS:HB2	2.21	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
1:B:23:VAL:O	1:B:23:VAL:HG22	2.22	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:38:GLU:C	1:A:40:PRO:HD3	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1131:VAL:HG12	1:C:1132:ILE:N	2.37	0.40
1:A:1161:GLN:O	1:A:1161:GLN:HG3	2.21	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%)	34 38
1	B	559/568 (98%)	504 (90%)	48 (9%)	7 (1%)	12 10
1	C	546/568 (96%)	489 (90%)	48 (9%)	9 (2%)	9 8
All	All	1671/1704 (98%)	1517 (91%)	136 (8%)	18 (1%)	14 13

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

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Mol	Chain	Res	Type
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 (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	426/461 (92%)	422 (99%)	4 (1%)	78	87
1	B	421/461 (91%)	419 (100%)	2 (0%)	88	94
1	C	412/461 (89%)	410 (100%)	2 (0%)	88	94
All	All	1259/1383 (91%)	1251 (99%)	8 (1%)	86	93

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

Mol	Chain	Res	Type
1	A	44	GLU
1	A	258	PHE
1	A	358	ASP
1	A	1190	PHE
1	B	258	PHE
1	B	1176	ASP
1	C	258	PHE
1	C	1190	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	100	ASN
1	A	241	ASN
1	A	253	GLN
1	B	12	ASN
1	B	18	ASN
1	B	241	ASN
1	B	365	GLN
1	B	1054	HIS
1	C	100	ASN
1	C	203	HIS
1	C	241	ASN
1	C	282	ASN
1	C	1030	ASN
1	C	1161	GLN
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GLC	D	2	2	11,11,12	0.47	0	15,15,17	0.62	0
2	GLC	E	1	2	12,12,12	0.42	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	0.36	0	17,17,17	0.31	0
2	GLC	F	2	2	11,11,12	0.42	0	15,15,17	0.60	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(^{o})	Ideal(^{o})
2	E	2	GLC	C1-O5-C5	2.03	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

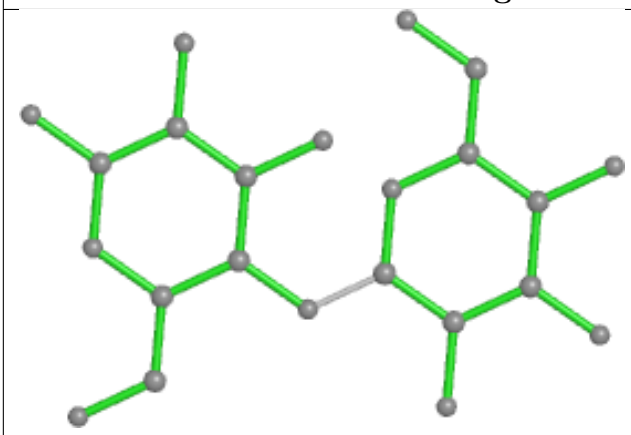
There are no ring outliers.

1 monomer is involved in 3 short contacts:

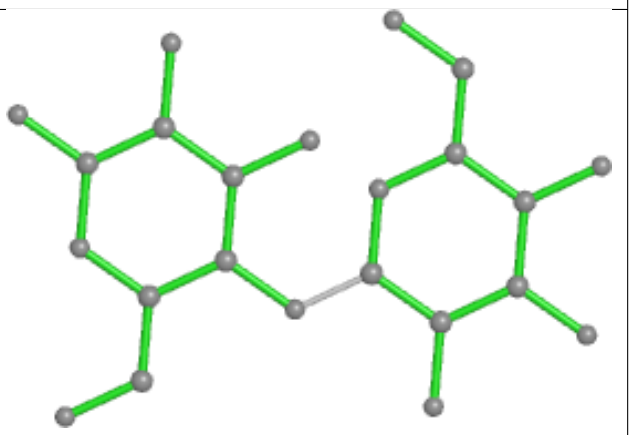
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2	GLC	3	0

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

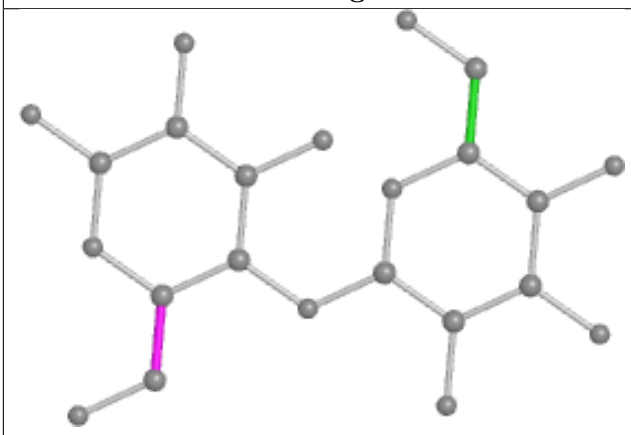
Oligosaccharide Chain D



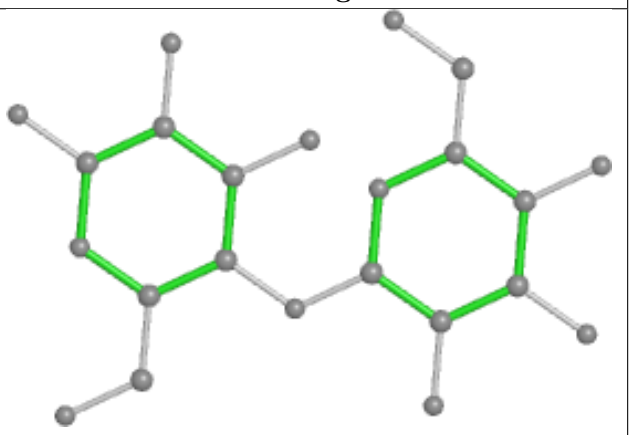
Bond lengths



Bond angles

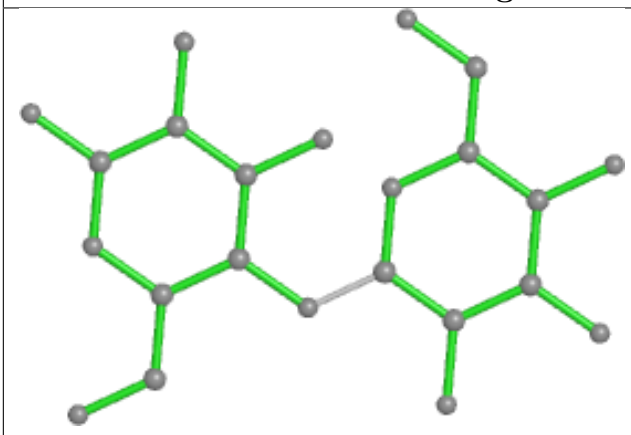


Torsions

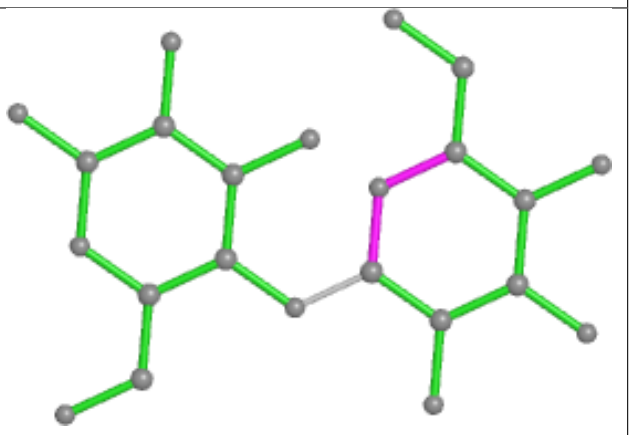


Rings

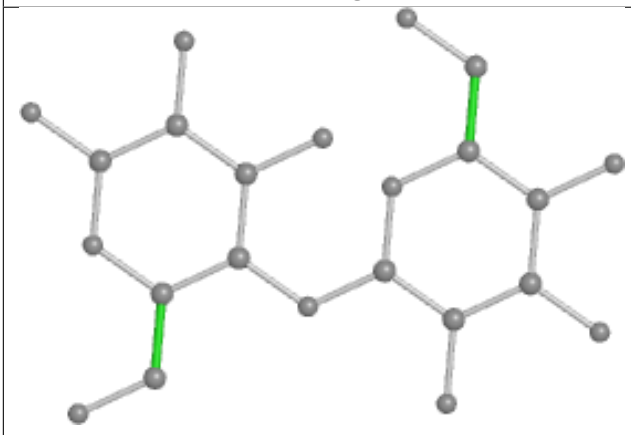
Oligosaccharide Chain E



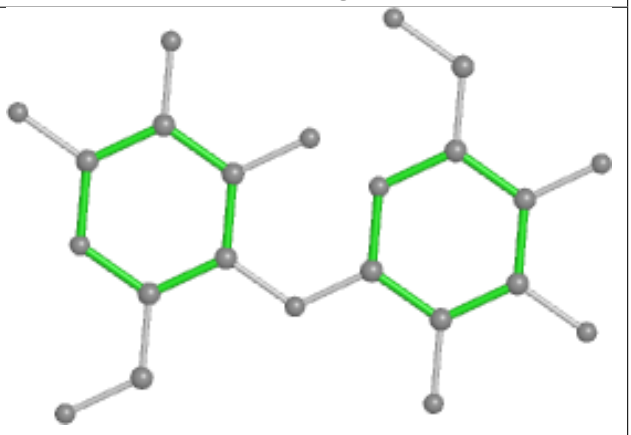
Bond lengths



Bond angles

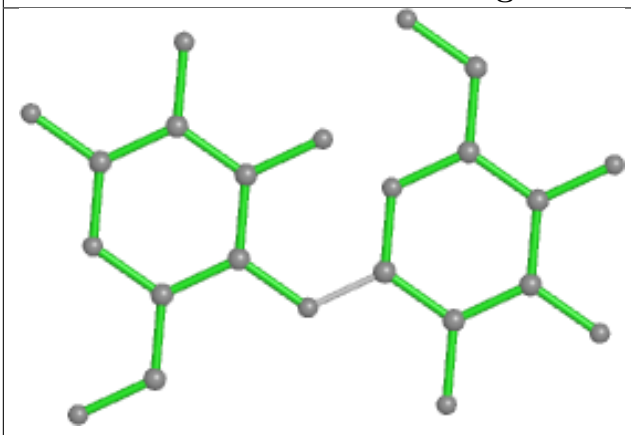


Torsions

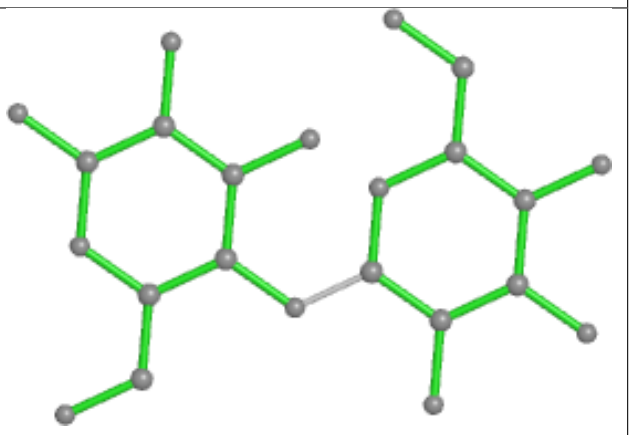


Rings

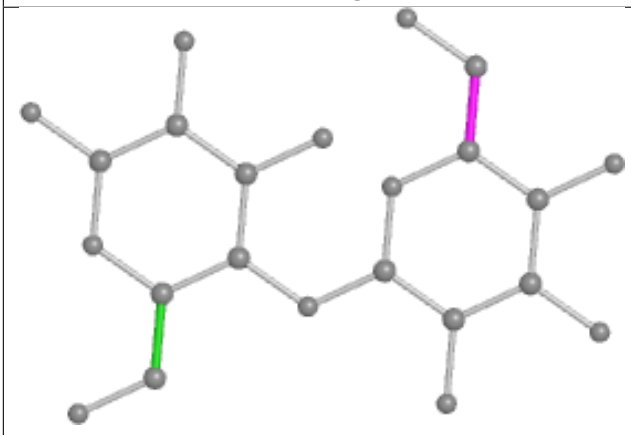
Oligosaccharide Chain F



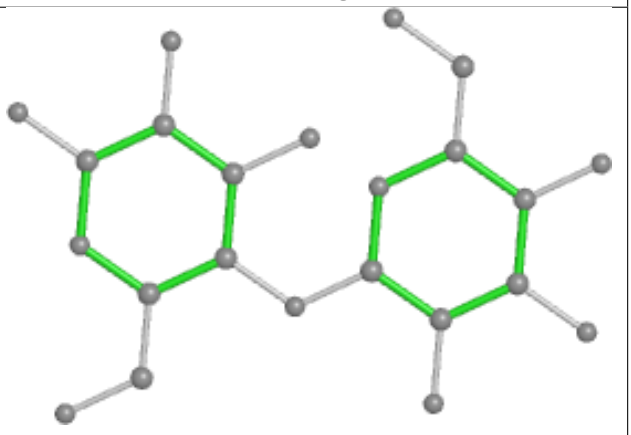
Bond lengths



Bond angles



Torsions



Rings

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 (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	568/568 (100%)	0.40	34 (5%) 21 32	19, 42, 75, 90	0
1	B	563/568 (99%)	0.55	43 (7%) 13 21	22, 47, 73, 96	0
1	C	552/568 (97%)	1.00	79 (14%) 2 4	35, 61, 81, 96	0
All	All	1683/1704 (98%)	0.65	156 (9%) 8 14	19, 50, 78, 96	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1124	ASP	7.4
1	C	31	THR	7.0
1	C	1069	GLY	7.0
1	C	33	ILE	5.9
1	A	1123	GLY	5.4
1	C	32	GLY	5.2
1	C	239	ALA	4.8
1	B	1062	ILE	4.8
1	C	1058	PHE	4.7
1	C	242	TYR	4.6
1	A	1067	LEU	4.4
1	C	141	ALA	4.3
1	C	155	TYR	4.2
1	B	1094	SER	4.1
1	C	36	THR	3.9
1	C	1057	LYS	3.9
1	A	1125	LEU	3.9
1	C	222	THR	3.9
1	B	1058	PHE	3.9
1	B	1061	HIS	3.8
1	B	1109	ASP	3.7
1	A	1109	ASP	3.6
1	C	11	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	1098	VAL	3.6
1	A	173	ALA	3.5
1	C	238	SER	3.5
1	C	250	PHE	3.4
1	A	172	ALA	3.4
1	B	101	GLY	3.3
1	C	215	ALA	3.3
1	A	1063	GLY	3.3
1	C	125	PRO	3.3
1	A	1046	PHE	3.2
1	B	54	GLY	3.2
1	C	1108	HIS	3.2
1	C	143	GLY	3.2
1	C	9	ILE	3.1
1	A	1122	LEU	3.1
1	C	113	LEU	3.1
1	C	133	PRO	3.1
1	C	109	ALA	3.1
1	C	1109	ASP	3.0
1	A	155	TYR	3.0
1	C	17	TYR	3.0
1	C	20	LEU	3.0
1	C	79	ILE	3.0
1	B	239	ALA	3.0
1	C	61	PHE	3.0
1	A	171	TYR	2.9
1	B	1023	ASP	2.9
1	B	1097	GLY	2.9
1	C	123	PRO	2.9
1	C	149	PHE	2.9
1	C	8	VAL	2.9
1	C	147	LEU	2.9
1	A	113	LEU	2.9
1	A	63	ALA	2.8
1	C	172	ALA	2.8
1	C	264	ALA	2.8
1	C	1071	LEU	2.8
1	A	226	ILE	2.8
1	C	1068	LYS	2.8
1	A	174	GLY	2.8
1	B	108	ILE	2.8
1	B	63	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	265	GLY	2.8
1	A	1212	ARG	2.8
1	C	204	MET	2.7
1	A	1062	ILE	2.7
1	B	33	ILE	2.7
1	A	157	THR	2.7
1	C	218	ASN	2.7
1	A	1045	THR	2.7
1	C	283	TYR	2.7
1	C	29	LYS	2.6
1	B	1095	GLU	2.6
1	A	1098	VAL	2.6
1	B	50	VAL	2.6
1	B	369	ALA	2.6
1	C	174	GLY	2.6
1	A	1193	THR	2.6
1	A	67	PHE	2.6
1	C	1098	VAL	2.6
1	B	83	ALA	2.6
1	B	97	VAL	2.6
1	C	37	VAL	2.6
1	C	121	LEU	2.5
1	B	1096	ASP	2.5
1	C	262	LEU	2.5
1	C	223	ALA	2.5
1	C	127	LYS	2.5
1	B	104	ILE	2.5
1	C	1151	ASN	2.5
1	C	63	ALA	2.4
1	B	31	THR	2.4
1	C	224	MET	2.4
1	C	53	THR	2.4
1	C	233	SER	2.4
1	A	156	PHE	2.3
1	B	61	PHE	2.3
1	B	82	ALA	2.3
1	A	158	TRP	2.3
1	A	1213	ASN	2.3
1	B	1069	GLY	2.3
1	A	149	PHE	2.3
1	B	1111	VAL	2.3
1	B	1212	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	241	ASN	2.3
1	B	1039	ALA	2.3
1	B	1215	GLN	2.3
1	B	32	GLY	2.3
1	A	161	ILE	2.2
1	B	29	LYS	2.2
1	B	55	ASP	2.2
1	B	1204	PRO	2.2
1	A	112	ALA	2.2
1	C	1110	ASP	2.2
1	B	107	PRO	2.2
1	C	1024	LYS	2.2
1	C	30	ASP	2.2
1	C	171	TYR	2.2
1	C	108	ILE	2.2
1	A	137	LYS	2.2
1	B	1123	GLY	2.2
1	A	1163	ALA	2.2
1	C	184	ASP	2.2
1	C	151	LEU	2.1
1	C	27	PHE	2.1
1	C	156	PHE	2.1
1	C	186	ALA	2.1
1	B	60	ILE	2.1
1	A	262	LEU	2.1
1	B	1055	SER	2.1
1	C	284	LEU	2.1
1	C	132	ILE	2.1
1	B	30	ASP	2.1
1	A	1126	HIS	2.1
1	B	1020	ILE	2.1
1	C	1084	MET	2.1
1	C	1214	ASN	2.1
1	C	293	VAL	2.1
1	C	159	PRO	2.1
1	B	1081	LEU	2.0
1	B	26	LYS	2.0
1	C	140	LYS	2.0
1	C	193	THR	2.0
1	C	237	THR	2.0
1	C	1045	THR	2.0
1	C	112	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	271	PRO	2.0
1	C	1096	ASP	2.0
1	B	1125	LEU	2.0
1	C	280	LEU	2.0
1	C	25	LYS	2.0
1	C	225	THR	2.0
1	C	163	ALA	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)

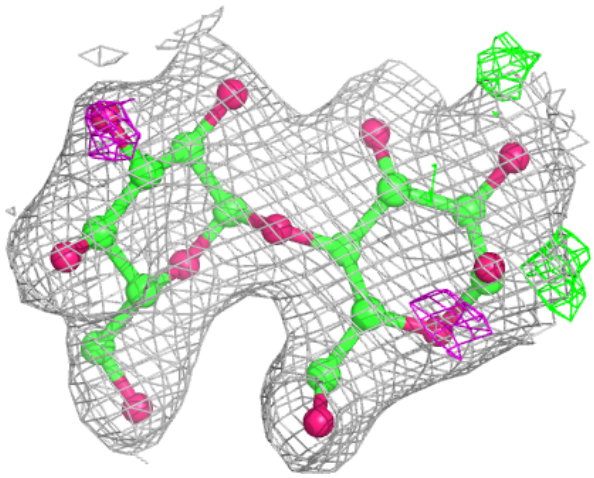
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

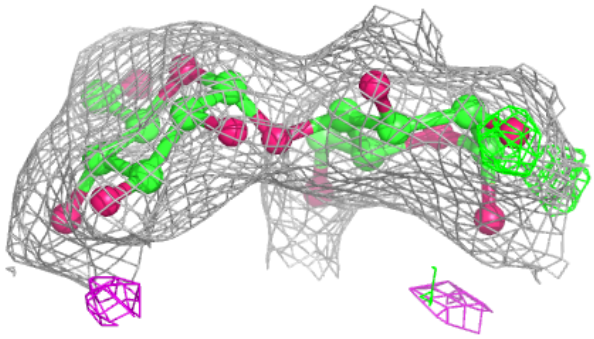
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	E	1	12/12	0.92	0.17	31,33,36,36	0
2	GLC	F	1	12/12	0.92	0.21	44,48,50,51	0
2	GLC	F	2	11/12	0.94	0.26	40,43,46,46	0
2	GLC	D	2	11/12	0.95	0.23	27,31,36,37	0
2	GLC	D	1	12/12	0.96	0.24	26,31,34,37	0
2	GLC	E	2	11/12	0.96	0.17	35,38,39,40	0

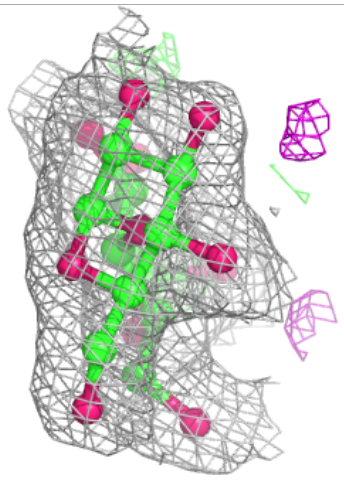
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

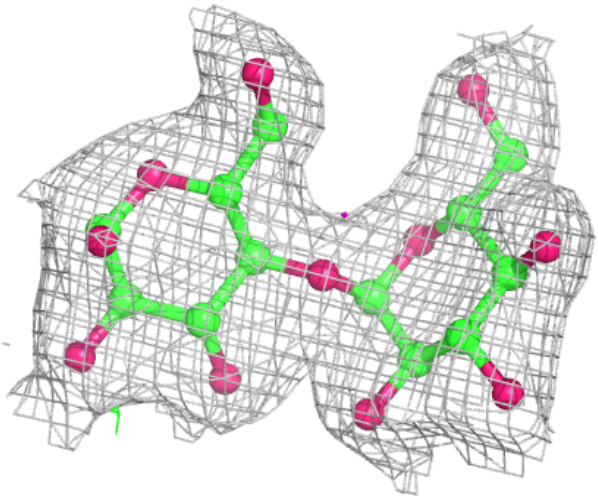


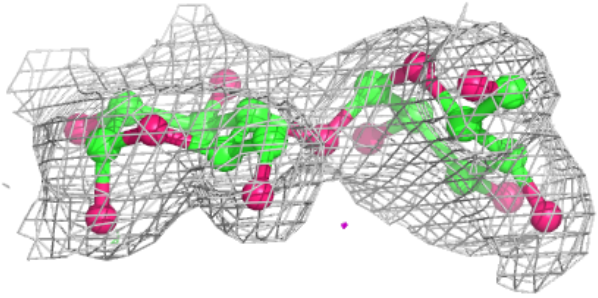


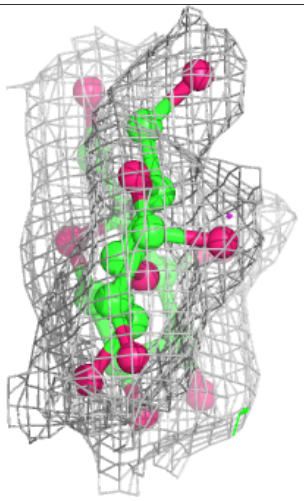


Electron density around Chain E:

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

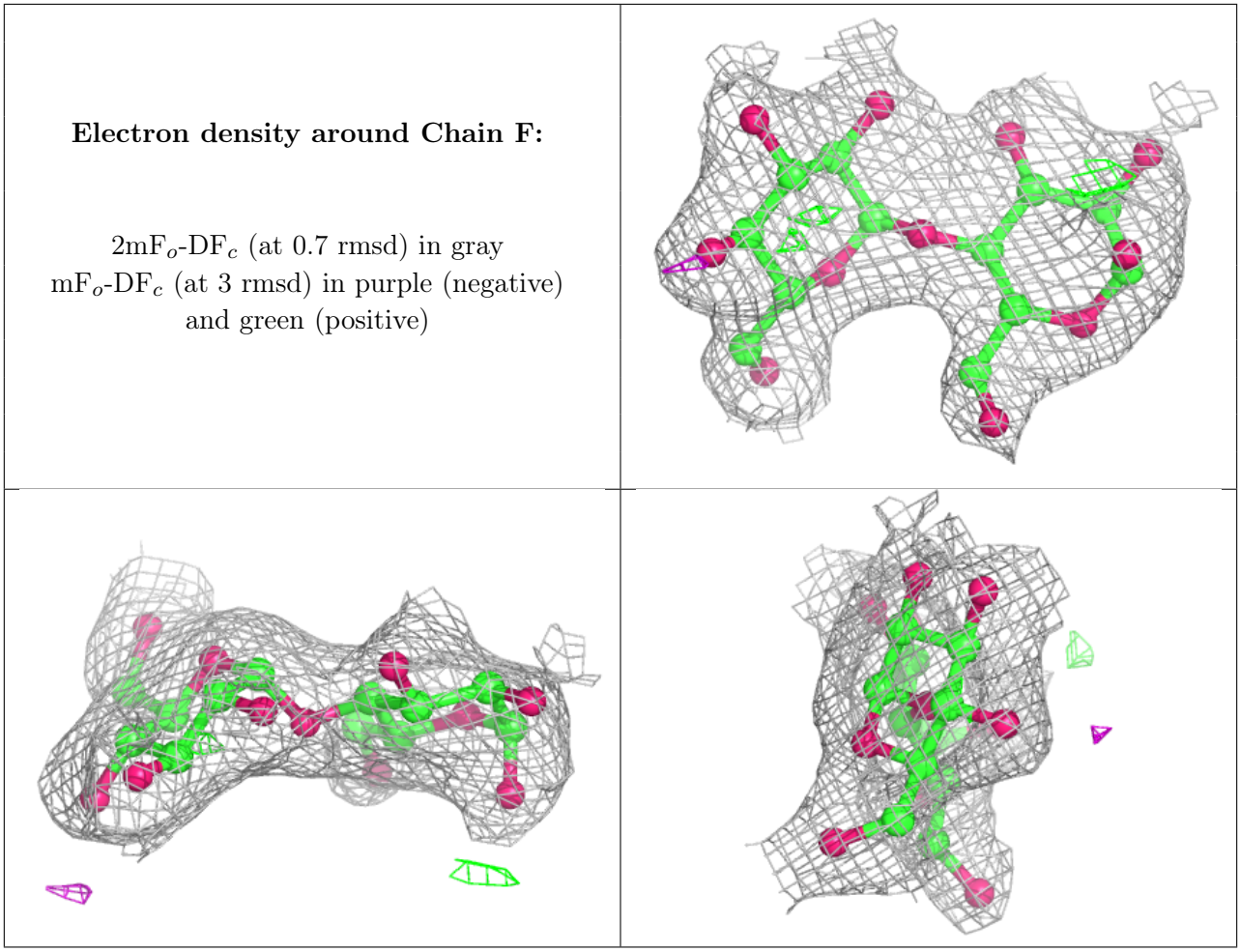






Electron density around Chain F:

$2mF_o$-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
3	NA	A	1216	1/1	0.89	0.21	46,46,46,46	0

6.5 Other polymers

There are no such residues in this entry.