Full wwPDB X-ray Structure Validation Report (i)

Aug 17, 2022 – 08:24 PM EDT

PDB ID	:	4MYW
Title	:	Structure of HSV-2 gD bound to nectin-1
Authors	:	Lu, G.; Zhang, N.; Qi, J.; Li, Y.; Chen, Z.; Zheng, C.; Yan, J.; Gao, G.F.
Deposited on	:	2013-09-28
Resolution	:	3.19 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 (i)) were used in the production of this report:

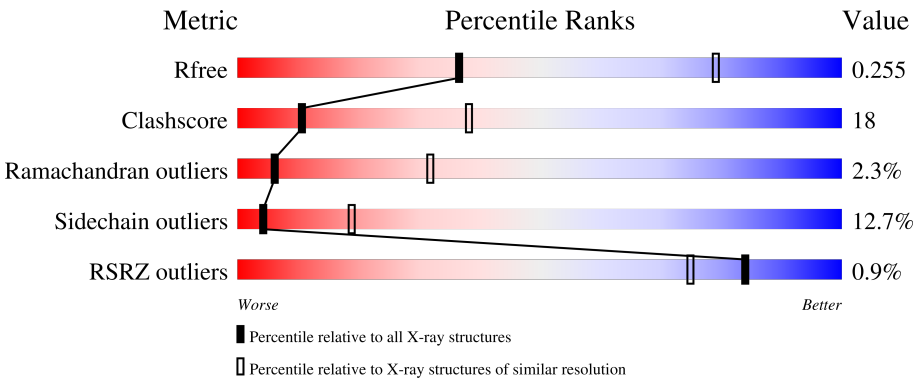
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

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	294	% 46% 28% • 21%
1	C	294	49% 25% 5% • 21%
2	B	331	% 53% 31% 7% 8%
2	D	331	% 54% 30% 7% • 8%
3	E	2	100%

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Mol	Chain	Length	Quality of chain
3	F	2	100%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8573 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 Envelope glycoprotein D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	232	1839	1184	313	332	10	0	0	0
1	C	232	1839	1184	313	332	10	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ALA	-	expression tag	UNP P03172
A	-1	ASP	-	expression tag	UNP P03172
A	0	LEU	-	expression tag	UNP P03172
A	27	GLN	ARG	SEE REMARK 999	UNP P03172
A	286	HIS	-	expression tag	UNP P03172
A	287	HIS	-	expression tag	UNP P03172
A	288	HIS	-	expression tag	UNP P03172
A	289	HIS	-	expression tag	UNP P03172
A	290	HIS	-	expression tag	UNP P03172
A	291	HIS	-	expression tag	UNP P03172
C	-2	ALA	-	expression tag	UNP P03172
C	-1	ASP	-	expression tag	UNP P03172
C	0	LEU	-	expression tag	UNP P03172
C	27	GLN	ARG	SEE REMARK 999	UNP P03172
C	286	HIS	-	expression tag	UNP P03172
C	287	HIS	-	expression tag	UNP P03172
C	288	HIS	-	expression tag	UNP P03172
C	289	HIS	-	expression tag	UNP P03172
C	290	HIS	-	expression tag	UNP P03172
C	291	HIS	-	expression tag	UNP P03172

- Molecule 2 is a protein called Poliovirus receptor-related protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	303	2377	1495	411	460	11	0	0	0
2	D	303	2377	1495	411	460	11	0	0	0

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	MET	-	expression tag	UNP Q15223
B	17	ALA	-	expression tag	UNP Q15223
B	18	SER	-	expression tag	UNP Q15223
B	19	MET	-	expression tag	UNP Q15223
B	20	THR	-	expression tag	UNP Q15223
B	21	GLY	-	expression tag	UNP Q15223
B	22	GLY	-	expression tag	UNP Q15223
B	23	GLN	-	expression tag	UNP Q15223
B	24	GLN	-	expression tag	UNP Q15223
B	25	MET	-	expression tag	UNP Q15223
B	26	GLY	-	expression tag	UNP Q15223
B	27	ARG	-	expression tag	UNP Q15223
B	28	ASP	-	expression tag	UNP Q15223
B	29	PRO	-	expression tag	UNP Q15223
B	336	ALA	-	expression tag	UNP Q15223
B	337	ALA	-	expression tag	UNP Q15223
B	338	ALA	-	expression tag	UNP Q15223
B	339	LEU	-	expression tag	UNP Q15223
B	340	GLU	-	expression tag	UNP Q15223
B	341	HIS	-	expression tag	UNP Q15223
B	342	HIS	-	expression tag	UNP Q15223
B	343	HIS	-	expression tag	UNP Q15223
B	344	HIS	-	expression tag	UNP Q15223
B	345	HIS	-	expression tag	UNP Q15223
B	346	HIS	-	expression tag	UNP Q15223
D	16	MET	-	expression tag	UNP Q15223
D	17	ALA	-	expression tag	UNP Q15223
D	18	SER	-	expression tag	UNP Q15223
D	19	MET	-	expression tag	UNP Q15223
D	20	THR	-	expression tag	UNP Q15223
D	21	GLY	-	expression tag	UNP Q15223
D	22	GLY	-	expression tag	UNP Q15223
D	23	GLN	-	expression tag	UNP Q15223
D	24	GLN	-	expression tag	UNP Q15223
D	25	MET	-	expression tag	UNP Q15223

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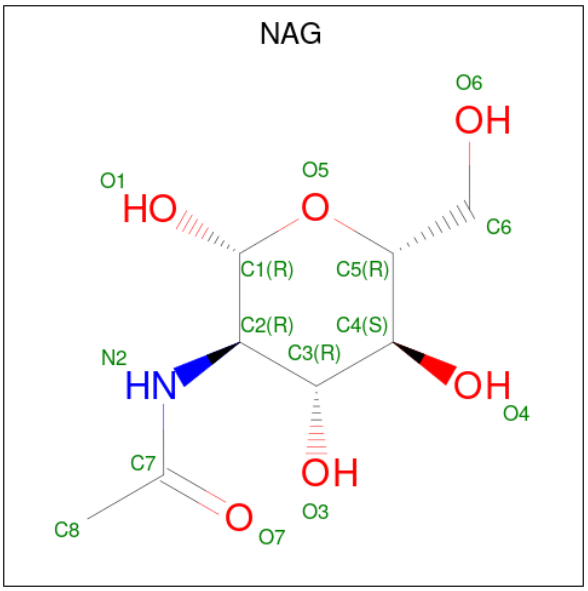
Chain	Residue	Modelled	Actual	Comment	Reference
D	26	GLY	-	expression tag	UNP Q15223
D	27	ARG	-	expression tag	UNP Q15223
D	28	ASP	-	expression tag	UNP Q15223
D	29	PRO	-	expression tag	UNP Q15223
D	336	ALA	-	expression tag	UNP Q15223
D	337	ALA	-	expression tag	UNP Q15223
D	338	ALA	-	expression tag	UNP Q15223
D	339	LEU	-	expression tag	UNP Q15223
D	340	GLU	-	expression tag	UNP Q15223
D	341	HIS	-	expression tag	UNP Q15223
D	342	HIS	-	expression tag	UNP Q15223
D	343	HIS	-	expression tag	UNP Q15223
D	344	HIS	-	expression tag	UNP Q15223
D	345	HIS	-	expression tag	UNP Q15223
D	346	HIS	-	expression tag	UNP Q15223

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	2	28	16	2	10	0	0	0
			Total	C	N	O			
3	F	2	28	16	2	10	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is water.

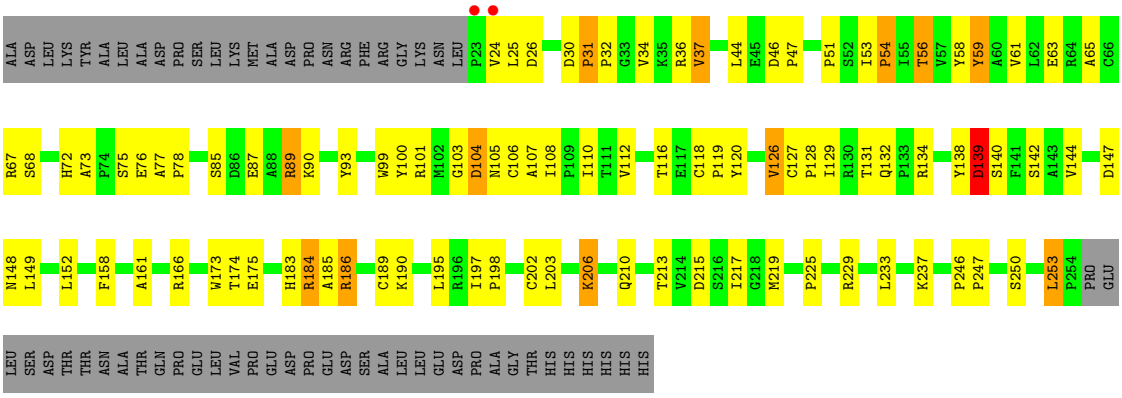
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	20	20	20	0	0
			Total	O		
5	B	13	13	13	0	0
			Total	O		
5	C	10	10	10	0	0
			Total	O		
5	D	14	14	14	0	0

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.

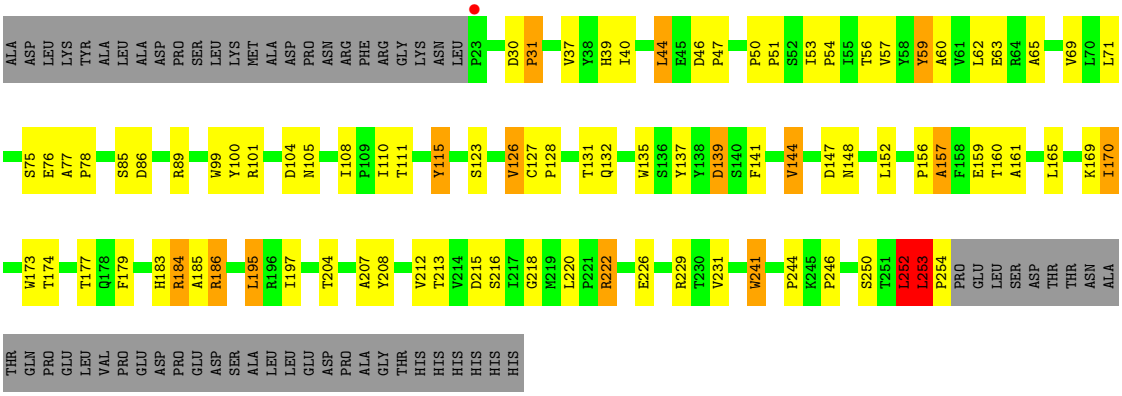
• Molecule 1: Envelope glycoprotein D

Chain A:



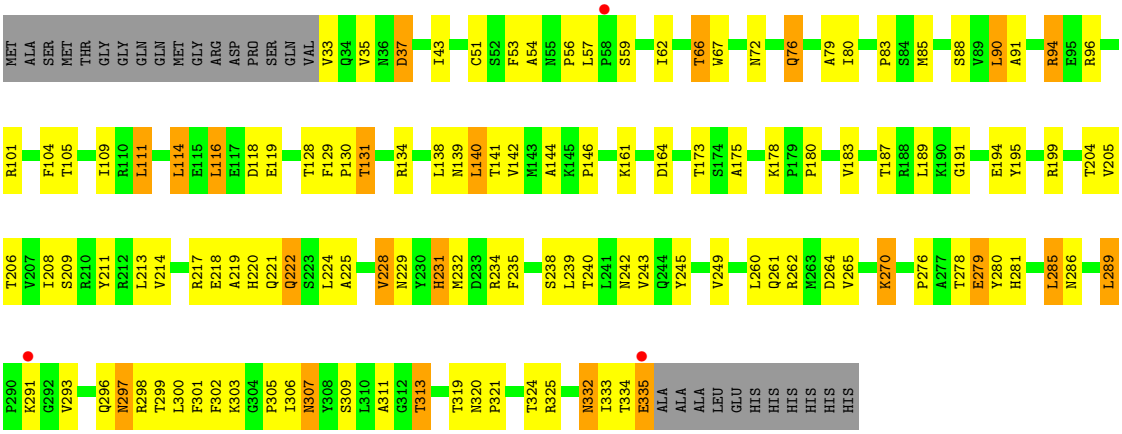
• Molecule 1: Envelope glycoprotein D

Chain C:



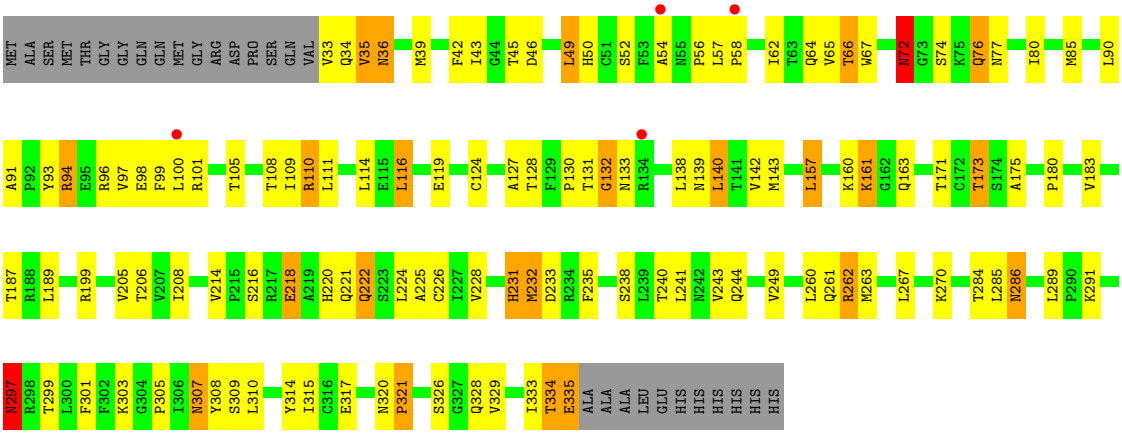
• Molecule 2: Poliovirus receptor-related protein 1

Chain B:



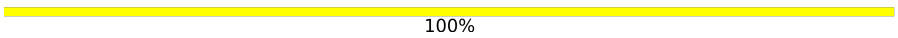
• Molecule 2: Poliovirus receptor-related protein 1

Chain D:



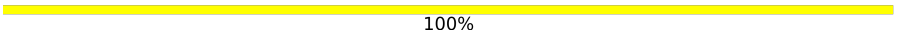
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	53.34Å 170.86Å 192.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.93 – 3.19 38.93 – 3.19	Depositor EDS
% Data completeness (in resolution range)	95.2 (38.93-3.19) 99.5 (38.93-3.19)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.85 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.196 , 0.247 0.196 , 0.255	Depositor DCC
R_{free} test set	1525 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	73.3	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 49.7	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	0.94	EDS
Total number of atoms	8573	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.11% 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 (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.36	0/1896	0.51	0/2595
1	C	0.35	0/1896	0.52	1/2595 (0.0%)
2	B	0.32	0/2429	0.50	0/3308
2	D	0.30	0/2429	0.49	0/3308
All	All	0.33	0/8650	0.50	1/11806 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	170	ILE	CB-CA-C	-5.72	100.17	111.60

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	1839	0	1819	74	0
1	C	1839	0	1819	73	0
2	B	2377	0	2324	89	0
2	D	2377	0	2324	84	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	14	0	13	0	0
4	C	14	0	13	0	0
5	A	20	0	0	0	0
5	B	13	0	0	0	0
5	C	10	0	0	0	0
5	D	14	0	0	1	0
All	All	8573	0	8362	311	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (311) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:228:VAL:HG22	2:D:235:PHE:HB3	1.51	0.93
1:A:63:GLU:HG2	1:A:184:ARG:HE	1.36	0.91
2:B:43:ILE:HD12	2:B:144:ALA:HB2	1.54	0.89
1:C:186:ARG:HG3	1:C:186:ARG:HH11	1.39	0.87
2:B:43:ILE:HD11	2:B:116:LEU:HD13	1.57	0.84
1:A:186:ARG:HH11	1:A:186:ARG:CG	1.91	0.83
1:A:85:SER:O	1:A:89:ARG:HG3	1.79	0.82
2:B:173:THR:HG23	2:B:208:ILE:HG12	1.61	0.81
1:C:253:LEU:H	1:C:254:PRO:CD	1.96	0.79
2:B:164:ASP:HA	2:B:214:VAL:HG21	1.63	0.78
2:B:297:ASN:HD22	2:B:298:ARG:H	1.33	0.76
2:D:225:ALA:HB2	2:D:238:SER:HB3	1.67	0.76
2:D:183:VAL:HG22	2:D:228:VAL:HG12	1.70	0.74
2:B:129:PHE:CD1	2:B:130:PRO:HA	2.24	0.73
2:B:228:VAL:HG13	2:B:235:PHE:HD1	1.54	0.73
1:C:253:LEU:H	1:C:254:PRO:HD2	1.52	0.72
1:C:170:ILE:HG22	1:C:170:ILE:O	1.87	0.72
2:D:66:THR:HG22	2:D:80:ILE:HG12	1.72	0.72
1:A:59:TYR:CD1	1:A:253:LEU:HD21	2.25	0.71
2:D:62:ILE:HA	2:D:128:THR:HG22	1.71	0.71
1:A:77:ALA:HB3	1:A:78:PRO:HD3	1.72	0.70
1:C:46:ASP:OD1	1:C:46:ASP:C	2.30	0.69
2:B:297:ASN:ND2	2:B:298:ARG:H	1.89	0.69
2:B:66:THR:HG23	2:B:80:ILE:HG23	1.75	0.69
2:D:100:LEU:HD21	2:D:110:ARG:HB3	1.74	0.68
2:B:91:ALA:HA	2:B:94:ARG:HG3	1.75	0.68
2:D:260:LEU:HD11	2:D:308:TYR:CE1	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:ILE:HG23	1:C:54:PRO:HD2	1.74	0.68
2:B:217:ARG:HG3	2:B:245:TYR:CD1	2.30	0.68
1:A:89:ARG:HA	1:A:120:TYR:CD1	2.30	0.67
1:C:53:ILE:HD12	1:C:173:TRP:HZ2	1.59	0.67
2:D:67:TRP:CZ3	2:D:124:CYS:HB2	2.29	0.67
1:A:53:ILE:HD12	1:A:173:TRP:HZ2	1.58	0.67
2:B:285:LEU:HD22	2:B:313:THR:HG21	1.77	0.67
2:D:43:ILE:HD11	2:D:116:LEU:HD13	1.77	0.67
1:A:186:ARG:HH11	1:A:186:ARG:HG2	1.59	0.67
2:B:119:GLU:OE2	2:B:178:LYS:HE3	1.95	0.66
2:B:54:ALA:O	2:B:56:PRO:HD3	1.95	0.66
1:A:161:ALA:HB2	1:A:183:HIS:HD2	1.61	0.66
2:D:173:THR:HG23	2:D:208:ILE:HG12	1.77	0.65
1:A:132:GLN:HG3	2:B:85:MET:SD	2.39	0.63
2:D:45:THR:HG22	2:D:46:ASP:N	2.13	0.63
1:A:63:GLU:HA	1:A:184:ARG:HB2	1.81	0.62
1:C:132:GLN:HG3	2:D:85:MET:CE	2.28	0.62
1:A:139:ASP:OD1	1:A:139:ASP:N	2.32	0.62
1:A:215:ASP:CG	2:B:90:LEU:HD22	2.20	0.62
1:A:72:HIS:HD2	1:A:73:ALA:N	1.98	0.61
1:A:186:ARG:HH11	1:A:186:ARG:HG3	1.66	0.61
2:D:54:ALA:O	2:D:56:PRO:HD3	2.01	0.61
2:B:220:HIS:HA	2:B:243:VAL:HG23	1.83	0.61
2:D:286:ASN:H	2:D:286:ASN:HD22	1.49	0.61
2:B:83:PRO:HG2	2:B:104:PHE:CZ	2.36	0.61
2:B:262:ARG:HB3	2:B:306:ILE:HD12	1.83	0.60
2:B:175:ALA:HA	2:B:206:THR:HG23	1.84	0.60
2:D:119:GLU:HG2	2:D:142:VAL:HG23	1.84	0.60
1:A:51:PRO:HA	1:A:174:THR:HG23	1.83	0.60
1:A:186:ARG:HD3	1:A:186:ARG:N	2.17	0.60
1:C:126:VAL:HG22	1:C:126:VAL:O	2.02	0.60
1:C:220:LEU:HD22	2:D:66:THR:HG21	1.84	0.60
2:B:119:GLU:HG2	2:B:142:VAL:H	1.67	0.60
2:B:183:VAL:O	2:B:195:TYR:HE1	1.85	0.60
1:A:56:THR:HB	1:A:58:TYR:HE1	1.66	0.59
1:A:186:ARG:HD3	1:A:186:ARG:H	1.65	0.59
2:B:35:VAL:CG1	2:B:138:LEU:HB3	2.33	0.59
1:C:215:ASP:HB3	2:D:77:ASN:HB2	1.83	0.59
2:D:36:ASN:OD1	2:D:50:HIS:HB2	2.03	0.59
1:C:60:ALA:HB2	1:C:250:SER:HB3	1.85	0.59
1:A:101:ARG:HB2	1:A:110:ILE:HD11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:270:LYS:HE2	2:B:298:ARG:HH12	1.69	0.58
1:A:127:CYS:HB3	1:A:128:PRO:HD2	1.86	0.58
1:C:241:TRP:CH2	1:C:244:PRO:HA	2.38	0.58
2:B:119:GLU:HG2	2:B:142:VAL:HG23	1.84	0.58
1:C:252:LEU:HD13	1:C:254:PRO:HD3	1.86	0.58
1:A:72:HIS:CD2	1:A:73:ALA:N	2.71	0.58
2:D:49:LEU:HD13	2:D:138:LEU:HD21	1.85	0.58
2:B:279:GLU:CB	2:B:319:THR:HB	2.34	0.57
1:A:59:TYR:HD1	1:A:253:LEU:HD21	1.69	0.57
2:B:289:LEU:HD22	2:B:289:LEU:H	1.70	0.57
1:A:161:ALA:HB2	1:A:183:HIS:CD2	2.39	0.56
2:D:160:LYS:HB2	2:D:163:GLN:HE21	1.70	0.56
1:C:137:TYR:CD1	1:C:197:ILE:HG12	2.40	0.56
2:B:66:THR:HG22	2:B:80:ILE:HG12	1.88	0.56
1:C:46:ASP:HB2	1:C:208:TYR:HB3	1.87	0.56
1:C:186:ARG:HH11	1:C:186:ARG:CG	2.14	0.56
2:B:307:ASN:HD22	2:B:309:SER:H	1.52	0.56
2:B:189:LEU:HG	2:B:222:GLN:HG2	1.86	0.56
2:B:325:ARG:HG3	2:B:325:ARG:HH11	1.71	0.56
1:C:132:GLN:HG3	2:D:85:MET:SD	2.46	0.56
2:D:317:GLU:HG2	2:D:326:SER:OG	2.05	0.56
2:D:220:HIS:CD2	2:D:221:GLN:HG3	2.41	0.56
2:D:334:THR:HG23	2:D:335:GLU:HB2	1.88	0.55
2:B:293:VAL:HG12	2:B:300:LEU:HD11	1.88	0.55
1:C:226:GLU:O	1:C:229:ARG:HB2	2.06	0.55
2:D:161:LYS:CD	2:D:161:LYS:H	2.19	0.55
2:D:161:LYS:H	2:D:161:LYS:HD2	1.70	0.55
1:C:186:ARG:HG3	1:C:186:ARG:NH1	2.16	0.55
2:D:138:LEU:C	2:D:138:LEU:HD12	2.28	0.55
2:D:315:ILE:HG12	2:D:328:GLN:HG2	1.89	0.55
1:C:53:ILE:HD12	1:C:173:TRP:CZ2	2.40	0.54
2:B:228:VAL:HG13	2:B:235:PHE:CD1	2.39	0.54
1:C:44:LEU:HB2	1:C:212:VAL:O	2.07	0.54
1:C:85:SER:O	1:C:89:ARG:HG3	2.08	0.54
2:D:36:ASN:OD1	2:D:36:ASN:N	2.39	0.54
1:C:253:LEU:O	1:C:254:PRO:C	2.46	0.54
1:C:47:PRO:HG3	1:C:100:TYR:CZ	2.42	0.54
1:C:108:ILE:HD13	1:C:197:ILE:HG21	1.90	0.54
1:C:139:ASP:OD1	1:C:139:ASP:N	2.38	0.54
1:C:144:VAL:O	1:C:229:ARG:NH1	2.41	0.54
1:A:75:SER:HB3	1:A:149:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ALA:HB2	1:A:185:ALA:HB3	1.89	0.53
1:A:225:PRO:O	1:A:229:ARG:HG3	2.09	0.53
2:B:138:LEU:C	2:B:138:LEU:HD12	2.29	0.53
2:D:260:LEU:O	2:D:261:GLN:HB2	2.07	0.53
1:A:99:TRP:CZ3	1:A:166:ARG:HB2	2.44	0.53
1:C:147:ASP:O	1:C:148:ASN:HB2	2.08	0.53
1:A:108:ILE:HD13	1:A:197:ILE:HG21	1.89	0.53
2:B:33:VAL:CG1	2:B:134:ARG:HB3	2.39	0.53
2:B:307:ASN:ND2	2:B:309:SER:OG	2.42	0.53
2:D:66:THR:HG23	2:D:80:ILE:HG23	1.91	0.53
1:C:47:PRO:HG3	1:C:100:TYR:CE1	2.43	0.52
1:A:61:VAL:HG12	1:A:63:GLU:HG3	1.91	0.52
1:A:72:HIS:HD2	1:A:73:ALA:H	1.55	0.52
2:B:35:VAL:HG11	2:B:138:LEU:HB3	1.92	0.52
1:C:75:SER:O	1:C:78:PRO:HD2	2.09	0.52
2:B:279:GLU:HB2	2:B:319:THR:HB	1.90	0.52
2:B:62:ILE:HG13	2:B:128:THR:HG22	1.90	0.52
1:C:135:TRP:HB2	1:C:222:ARG:HG3	1.92	0.52
1:C:137:TYR:N	1:C:137:TYR:CD2	2.78	0.52
2:D:180:PRO:HG3	2:D:205:VAL:HG21	1.92	0.52
1:A:53:ILE:HD13	1:A:76:GLU:HG3	1.92	0.51
2:B:180:PRO:HG3	2:B:205:VAL:HG21	1.92	0.51
1:C:213:THR:O	1:C:216:SER:HB3	2.11	0.51
1:C:218:GLY:HA2	2:D:77:ASN:OD1	2.10	0.51
1:A:53:ILE:HD12	1:A:173:TRP:CZ2	2.43	0.51
2:D:72:ASN:N	2:D:72:ASN:HD22	2.07	0.51
2:B:320:ASN:HB2	2:B:321:PRO:CD	2.41	0.51
1:C:99:TRP:HB2	1:C:111:THR:HG22	1.93	0.51
1:C:253:LEU:N	1:C:254:PRO:HD2	2.23	0.51
2:D:261:GLN:HA	2:D:305:PRO:HB2	1.92	0.51
2:D:286:ASN:H	2:D:286:ASN:ND2	2.08	0.50
2:D:45:THR:CG2	2:D:46:ASP:N	2.74	0.50
2:D:67:TRP:CD1	2:D:109:ILE:HD13	2.47	0.50
1:A:30:ASP:HB3	1:A:34:VAL:HB	1.94	0.49
1:C:139:ASP:OD2	1:C:222:ARG:NE	2.45	0.49
1:A:47:PRO:HG3	1:A:100:TYR:CE1	2.46	0.49
1:A:108:ILE:HG12	1:A:202:CYS:HA	1.95	0.49
2:B:220:HIS:O	2:B:221:GLN:HB2	2.12	0.49
2:D:97:VAL:HG12	2:D:98:GLU:N	2.27	0.49
1:C:63:GLU:HG2	1:C:184:ARG:HE	1.78	0.49
2:B:178:LYS:HB2	2:B:204:THR:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:PRO:HG3	1:A:100:TYR:CZ	2.48	0.48
2:B:54:ALA:C	2:B:56:PRO:HD3	2.33	0.48
2:B:299:THR:HG21	2:B:301:PHE:CZ	2.49	0.48
1:C:37:VAL:O	1:C:131:THR:HA	2.12	0.48
2:D:286:ASN:HD22	2:D:286:ASN:N	2.09	0.48
1:A:126:VAL:HG22	1:A:126:VAL:O	2.13	0.48
2:B:191:GLY:HA3	2:B:211:TYR:CE1	2.48	0.48
2:B:224:LEU:HD12	2:B:225:ALA:N	2.29	0.48
2:B:164:ASP:HA	2:B:214:VAL:CG2	2.38	0.48
1:C:231:VAL:HG12	2:D:130:PRO:HB3	1.96	0.48
2:D:138:LEU:HD12	2:D:138:LEU:O	2.14	0.48
1:C:46:ASP:OD1	1:C:47:PRO:N	2.47	0.47
1:C:253:LEU:N	1:C:254:PRO:CD	2.69	0.47
2:D:34:GLN:HG3	2:D:35:VAL:N	2.29	0.47
1:A:233:LEU:HB3	1:A:237:LYS:HD2	1.97	0.47
2:D:160:LYS:CB	2:D:163:GLN:HE21	2.26	0.47
1:C:46:ASP:HA	1:C:47:PRO:HD3	1.62	0.47
2:D:267:LEU:HD13	2:D:329:VAL:HG11	1.97	0.47
1:A:53:ILE:CD1	1:A:173:TRP:HZ2	2.28	0.47
1:A:87:GLU:O	1:A:90:LYS:CG	2.63	0.47
1:C:101:ARG:HB2	1:C:110:ILE:HD11	1.95	0.47
2:D:173:THR:CG2	2:D:208:ILE:HG12	2.43	0.47
1:A:65:ALA:HB2	1:A:185:ALA:CB	2.45	0.47
2:D:310:LEU:HB2	2:D:333:ILE:HD11	1.96	0.47
2:B:265:VAL:O	2:B:302:PHE:HB2	2.15	0.47
1:C:186:ARG:CG	1:C:186:ARG:NH1	2.76	0.47
1:A:87:GLU:O	1:A:90:LYS:HG3	2.14	0.46
2:D:33:VAL:HA	5:D:401:HOH:O	2.15	0.46
2:D:43:ILE:HD11	2:D:116:LEU:CD1	2.44	0.46
2:D:260:LEU:HD11	2:D:308:TYR:CZ	2.50	0.46
1:A:158:PHE:CE1	1:A:186:ARG:HA	2.51	0.46
2:D:62:ILE:HD12	2:D:62:ILE:N	2.29	0.46
2:B:94:ARG:HG3	2:B:94:ARG:H	1.48	0.46
2:B:279:GLU:HB3	2:B:319:THR:HB	1.96	0.46
1:C:169:LYS:HG3	1:C:174:THR:OG1	2.16	0.46
2:D:157:LEU:HB2	2:D:243:VAL:HG12	1.98	0.46
1:C:69:VAL:O	1:C:152:LEU:HD12	2.16	0.46
2:D:93:TYR:HB3	2:D:97:VAL:CG2	2.46	0.46
2:D:93:TYR:HB3	2:D:97:VAL:HG23	1.98	0.46
2:D:225:ALA:CB	2:D:238:SER:HB3	2.43	0.46
1:A:106:CYS:HB2	1:A:203:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ARG:HG3	1:A:186:ARG:NH1	2.29	0.46
1:C:30:ASP:O	1:C:31:PRO:C	2.54	0.46
1:C:39:HIS:HE1	1:C:215:ASP:OD2	1.99	0.46
2:D:91:ALA:HA	2:D:94:ARG:HG3	1.98	0.46
2:D:127:ALA:HA	2:D:133:ASN:OD1	2.16	0.46
2:D:76:GLN:HE21	2:D:76:GLN:HB3	1.56	0.46
1:C:59:TYR:HD1	1:C:60:ALA:N	2.14	0.45
2:D:220:HIS:HB2	2:D:243:VAL:HG23	1.97	0.45
1:A:103:GLY:O	1:A:104:ASP:C	2.54	0.45
1:C:71:LEU:HD22	1:C:179:PHE:HB3	1.98	0.45
2:B:194:GLU:O	2:B:209:SER:HA	2.17	0.45
2:B:130:PRO:O	2:B:131:THR:O	2.34	0.45
2:D:54:ALA:C	2:D:56:PRO:HD3	2.37	0.45
2:D:232:MET:HA	2:D:232:MET:CE	2.46	0.45
1:C:127:CYS:HB3	1:C:128:PRO:HD2	1.99	0.45
1:C:195:LEU:HD23	1:C:195:LEU:HA	1.79	0.45
1:C:139:ASP:HB2	1:C:222:ARG:HD2	1.99	0.45
2:B:67:TRP:CD1	2:B:109:ILE:HD13	2.52	0.44
2:D:49:LEU:CD1	2:D:138:LEU:HD11	2.47	0.44
2:D:175:ALA:HA	2:D:206:THR:HG23	1.98	0.44
2:D:189:LEU:HG	2:D:222:GLN:HG2	1.98	0.44
1:A:147:ASP:O	1:A:148:ASN:HB2	2.17	0.44
1:C:104:ASP:O	1:C:105:ASN:HB2	2.18	0.44
1:A:118:CYS:HA	1:A:119:PRO:HD3	1.73	0.44
2:D:187:THR:HB	2:D:224:LEU:HD12	1.99	0.44
2:B:262:ARG:O	2:B:306:ILE:HG13	2.18	0.44
2:D:262:ARG:HG3	2:D:263:MET:N	2.32	0.44
1:A:186:ARG:N	1:A:186:ARG:CD	2.80	0.44
2:B:111:LEU:HD13	2:B:114:LEU:HD11	1.99	0.44
2:D:57:LEU:HG	2:D:58:PRO:HD2	2.00	0.44
2:D:314:TYR:O	2:D:328:GLN:HA	2.17	0.44
1:A:30:ASP:HA	1:A:31:PRO:HD2	1.66	0.44
2:B:296:GLN:HB3	2:B:297:ASN:H	1.59	0.44
1:C:77:ALA:N	1:C:78:PRO:CD	2.81	0.44
2:D:43:ILE:CD1	2:D:116:LEU:HD13	2.46	0.43
1:A:116:THR:HG22	1:A:129:ILE:HB	2.00	0.43
2:B:57:LEU:C	2:B:59:SER:H	2.21	0.43
2:B:279:GLU:HG3	2:B:281:HIS:CE1	2.53	0.43
2:B:79:ALA:HA	2:B:88:SER:O	2.18	0.43
2:B:96:ARG:NH2	2:B:118:ASP:OD2	2.52	0.43
2:D:297:ASN:ND2	2:D:297:ASN:H	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:PHE:HE1	1:A:186:ARG:HA	1.83	0.43
1:C:62:LEU:HD13	1:C:69:VAL:HB	2.00	0.43
1:C:252:LEU:HA	1:C:252:LEU:HD23	1.78	0.43
1:A:46:ASP:HA	1:A:47:PRO:HD3	1.82	0.43
2:B:228:VAL:CG1	2:B:235:PHE:HD1	2.27	0.43
2:B:324:THR:O	2:B:325:ARG:HD2	2.19	0.43
1:A:99:TRP:CH2	1:A:166:ARG:HB2	2.54	0.43
2:B:119:GLU:OE2	2:B:141:THR:HG23	2.18	0.43
1:C:161:ALA:HB2	1:C:183:HIS:CD2	2.54	0.43
2:D:160:LYS:HD3	2:D:160:LYS:HA	1.89	0.43
1:C:50:PRO:HA	1:C:51:PRO:HD3	1.74	0.43
2:B:180:PRO:HG3	2:B:205:VAL:CG2	2.49	0.43
2:B:187:THR:HB	2:B:224:LEU:HD13	2.00	0.43
1:A:100:TYR:HB3	1:A:107:ALA:HB1	2.01	0.43
2:D:42:PHE:CD1	2:D:143:MET:HB2	2.54	0.43
1:A:173:TRP:CH2	1:A:175:GLU:HB2	2.54	0.42
2:B:229:ASN:HD21	2:B:234:ARG:HG3	1.83	0.42
1:A:138:TYR:C	1:A:140:SER:H	2.23	0.42
2:B:43:ILE:HD11	2:B:116:LEU:CD1	2.40	0.42
2:B:62:ILE:N	2:B:62:ILE:HD12	2.34	0.42
2:B:219:ALA:HB3	2:B:243:VAL:HG21	2.02	0.42
2:D:116:LEU:HD12	2:D:116:LEU:HA	1.78	0.42
2:D:231:HIS:HB3	2:D:232:MET:H	1.55	0.42
2:B:116:LEU:HD21	2:B:204:THR:HG23	2.02	0.42
1:C:137:TYR:N	1:C:137:TYR:HD2	2.18	0.42
1:A:44:LEU:HD21	1:A:112:VAL:HG21	2.01	0.42
1:A:206:LYS:O	1:A:210:GLN:HG2	2.19	0.42
1:A:253:LEU:HD13	1:A:253:LEU:HA	1.88	0.42
1:C:115:TYR:N	1:C:115:TYR:CD1	2.87	0.42
1:C:252:LEU:HB3	1:C:253:LEU:H	1.66	0.42
2:D:39:MET:HB2	2:D:140:LEU:HD23	2.02	0.42
2:D:99:PHE:HA	2:D:108:THR:O	2.20	0.42
1:A:51:PRO:HB2	1:A:53:ILE:O	2.20	0.42
2:B:280:TYR:HB3	2:B:297:ASN:O	2.20	0.42
2:D:307:ASN:ND2	2:D:309:SER:OG	2.53	0.42
1:C:204:THR:O	1:C:207:ALA:HB3	2.20	0.42
1:A:217:ILE:HG13	1:A:219:MET:HG3	2.02	0.42
2:D:299:THR:HG21	2:D:301:PHE:CZ	2.55	0.42
1:A:37:VAL:O	1:A:131:THR:HA	2.20	0.41
2:D:320:ASN:HB2	2:D:321:PRO:HD2	2.02	0.41
2:B:76:GLN:HE21	2:B:76:GLN:HB3	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:VAL:HG12	1:A:131:THR:HG22	2.03	0.41
1:A:246:PRO:HA	1:A:247:PRO:HD2	1.84	0.41
1:C:157:ALA:HB1	1:C:159:GLU:OE1	2.21	0.41
2:B:53:PHE:HB3	2:B:105:THR:HG22	2.01	0.41
2:B:260:LEU:HD12	2:B:335:GLU:O	2.20	0.41
2:B:285:LEU:HD12	2:B:285:LEU:HA	1.74	0.41
2:B:319:THR:HG23	2:B:324:THR:OG1	2.20	0.41
1:C:40:ILE:HG13	1:C:131:THR:CG2	2.51	0.41
2:B:261:GLN:HA	2:B:305:PRO:HB2	2.02	0.41
2:D:67:TRP:CH2	2:D:124:CYS:HB2	2.55	0.41
1:A:189:CYS:SG	1:A:190:LYS:N	2.93	0.41
1:A:142:SER:HA	1:A:152:LEU:O	2.20	0.41
2:B:140:LEU:HD22	2:B:141:THR:N	2.35	0.41
2:B:320:ASN:CB	2:B:321:PRO:CD	2.98	0.41
1:C:56:THR:OG1	1:C:177:THR:HG23	2.20	0.41
1:A:93:TYR:CE2	1:A:118:CYS:HB2	2.55	0.41
1:A:134:ARG:HB3	1:A:219:MET:HB3	2.02	0.41
2:B:116:LEU:HD12	2:B:116:LEU:HA	1.88	0.41
2:B:262:ARG:HB3	2:B:306:ILE:CD1	2.50	0.41
2:D:52:SER:HA	2:D:105:THR:O	2.21	0.41
2:D:132:GLY:O	2:D:133:ASN:OD1	2.39	0.41
1:A:197:ILE:HA	1:A:198:PRO:HD2	1.84	0.41
1:C:141:PHE:CD2	1:C:141:PHE:N	2.89	0.41
1:C:77:ALA:HB1	1:C:170:ILE:HD11	2.03	0.40
1:C:126:VAL:O	1:C:126:VAL:CG2	2.69	0.40
2:B:33:VAL:HG11	2:B:134:ARG:HB3	2.03	0.40
2:B:231:HIS:HB3	2:B:232:MET:H	1.58	0.40
1:A:53:ILE:HG22	1:A:54:PRO:O	2.22	0.40
2:B:114:LEU:HD12	2:B:114:LEU:HA	1.83	0.40
2:B:225:ALA:HB2	2:B:238:SER:HB3	2.02	0.40
1:C:156:PRO:HB2	1:C:160:THR:OG1	2.21	0.40
1:A:36:ARG:HA	1:A:36:ARG:HD3	1.92	0.40
2:B:311:ALA:HB2	2:B:333:ILE:HD12	2.03	0.40
1:A:68:SER:O	1:A:247:PRO:HA	2.22	0.40
2:B:240:THR:HG23	1:C:86:ASP:OD2	2.22	0.40
2:B:332:ASN:O	2:B:332:ASN:ND2	2.54	0.40
2:D:216:SER:OG	2:D:218:GLU:HG2	2.21	0.40
2:D:220:HIS:HB2	2:D:243:VAL:CG2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	230/294 (78%)	205 (89%)	20 (9%)	5 (2%)	6	33
1	C	230/294 (78%)	202 (88%)	19 (8%)	9 (4%)	3	19
2	B	301/331 (91%)	268 (89%)	28 (9%)	5 (2%)	9	40
2	D	301/331 (91%)	273 (91%)	23 (8%)	5 (2%)	9	40
All	All	1062/1250 (85%)	948 (89%)	90 (8%)	24 (2%)	6	32

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	72	ASN
2	B	131	THR
1	C	252	LEU
1	C	253	LEU
1	C	65	ALA
1	C	185	ALA
2	D	132	GLY
2	D	297	ASN
1	A	104	ASP
1	C	157	ALA
1	C	246	PRO
2	D	72	ASN
1	A	139	ASP
2	B	37	ASP
1	A	31	PRO
2	B	264	ASP
1	C	31	PRO
1	C	139	ASP
2	B	276	PRO
1	C	241	TRP
2	D	96	ARG
2	D	321	PRO

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Mol	Chain	Res	Type
1	A	32	PRO
1	A	54	PRO

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	202/255 (79%)	183 (91%)	19 (9%)	8 31
1	C	202/255 (79%)	187 (93%)	15 (7%)	13 43
2	B	264/286 (92%)	227 (86%)	37 (14%)	3 15
2	D	264/286 (92%)	217 (82%)	47 (18%)	2 8
All	All	932/1082 (86%)	814 (87%)	118 (13%)	4 19

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	25	LEU
1	A	26	ASP
1	A	37	VAL
1	A	56	THR
1	A	59	TYR
1	A	67	ARG
1	A	89	ARG
1	A	105	ASN
1	A	126	VAL
1	A	139	ASP
1	A	144	VAL
1	A	184	ARG
1	A	186	ARG
1	A	195	LEU
1	A	206	LYS
1	A	213	THR
1	A	250	SER
1	A	253	LEU

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Mol	Chain	Res	Type
2	B	37	ASP
2	B	51	CYS
2	B	66	THR
2	B	76	GLN
2	B	90	LEU
2	B	94	ARG
2	B	101	ARG
2	B	111	LEU
2	B	114	LEU
2	B	116	LEU
2	B	139	ASN
2	B	140	LEU
2	B	146	PRO
2	B	161	LYS
2	B	199	ARG
2	B	213	LEU
2	B	218	GLU
2	B	222	GLN
2	B	228	VAL
2	B	231	HIS
2	B	239	LEU
2	B	242	ASN
2	B	249	VAL
2	B	270	LYS
2	B	278	THR
2	B	279	GLU
2	B	285	LEU
2	B	286	ASN
2	B	289	LEU
2	B	291	LYS
2	B	297	ASN
2	B	303	LYS
2	B	307	ASN
2	B	313	THR
2	B	332	ASN
2	B	334	THR
2	B	335	GLU
1	C	44	LEU
1	C	57	VAL
1	C	59	TYR
1	C	76	GLU
1	C	115	TYR

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Mol	Chain	Res	Type
1	C	123	SER
1	C	126	VAL
1	C	144	VAL
1	C	165	LEU
1	C	184	ARG
1	C	186	ARG
1	C	195	LEU
1	C	222	ARG
1	C	252	LEU
1	C	253	LEU
2	D	35	VAL
2	D	36	ASN
2	D	49	LEU
2	D	64	GLN
2	D	65	VAL
2	D	66	THR
2	D	72	ASN
2	D	74	SER
2	D	76	GLN
2	D	90	LEU
2	D	94	ARG
2	D	101	ARG
2	D	110	ARG
2	D	111	LEU
2	D	114	LEU
2	D	116	LEU
2	D	131	THR
2	D	139	ASN
2	D	140	LEU
2	D	157	LEU
2	D	161	LYS
2	D	171	THR
2	D	173	THR
2	D	199	ARG
2	D	214	VAL
2	D	218	GLU
2	D	222	GLN
2	D	226	CYS
2	D	231	HIS
2	D	232	MET
2	D	233	ASP
2	D	240	THR

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Mol	Chain	Res	Type
2	D	241	LEU
2	D	244	GLN
2	D	249	VAL
2	D	262	ARG
2	D	270	LYS
2	D	284	THR
2	D	285	LEU
2	D	286	ASN
2	D	289	LEU
2	D	291	LYS
2	D	297	ASN
2	D	303	LYS
2	D	307	ASN
2	D	334	THR
2	D	335	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	72	HIS
1	A	183	HIS
1	A	210	GLN
2	B	64	GLN
2	B	76	GLN
2	B	221	GLN
2	B	229	ASN
2	B	242	ASN
2	B	274	ASN
2	B	281	HIS
2	B	297	ASN
2	B	307	ASN
2	B	332	ASN
1	C	39	HIS
1	C	183	HIS
1	C	228	GLN
2	D	34	GLN
2	D	72	ASN
2	D	76	GLN
2	D	163	GLN
2	D	244	GLN
2	D	274	ASN

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Mol	Chain	Res	Type
2	D	286	ASN
2	D	297	ASN
2	D	307	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

4 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	$\#\|Z\| > 2$
3	NAG	E	1	3,1	14,14,15	0.58	0	17,19,21	1.38	3 (17%)
3	NAG	E	2	3	14,14,15	0.40	0	17,19,21	1.22	1 (5%)
3	NAG	F	1	3,1	14,14,15	0.56	0	17,19,21	1.31	1 (5%)
3	NAG	F	2	3	14,14,15	0.45	0	17,19,21	1.05	2 (11%)

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
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	3/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	1	NAG	C1-O5-C5	3.54	116.99	112.19
3	E	2	NAG	C1-O5-C5	3.32	116.69	112.19
3	E	1	NAG	C4-C3-C2	3.12	115.59	111.02
3	F	2	NAG	C1-O5-C5	2.71	115.87	112.19
3	F	2	NAG	C2-N2-C7	-2.51	119.32	122.90
3	E	1	NAG	O4-C4-C3	-2.50	104.56	110.35
3	E	1	NAG	O5-C1-C2	-2.07	108.02	111.29

There are no chirality outliers.

All (7) torsion outliers are listed below:

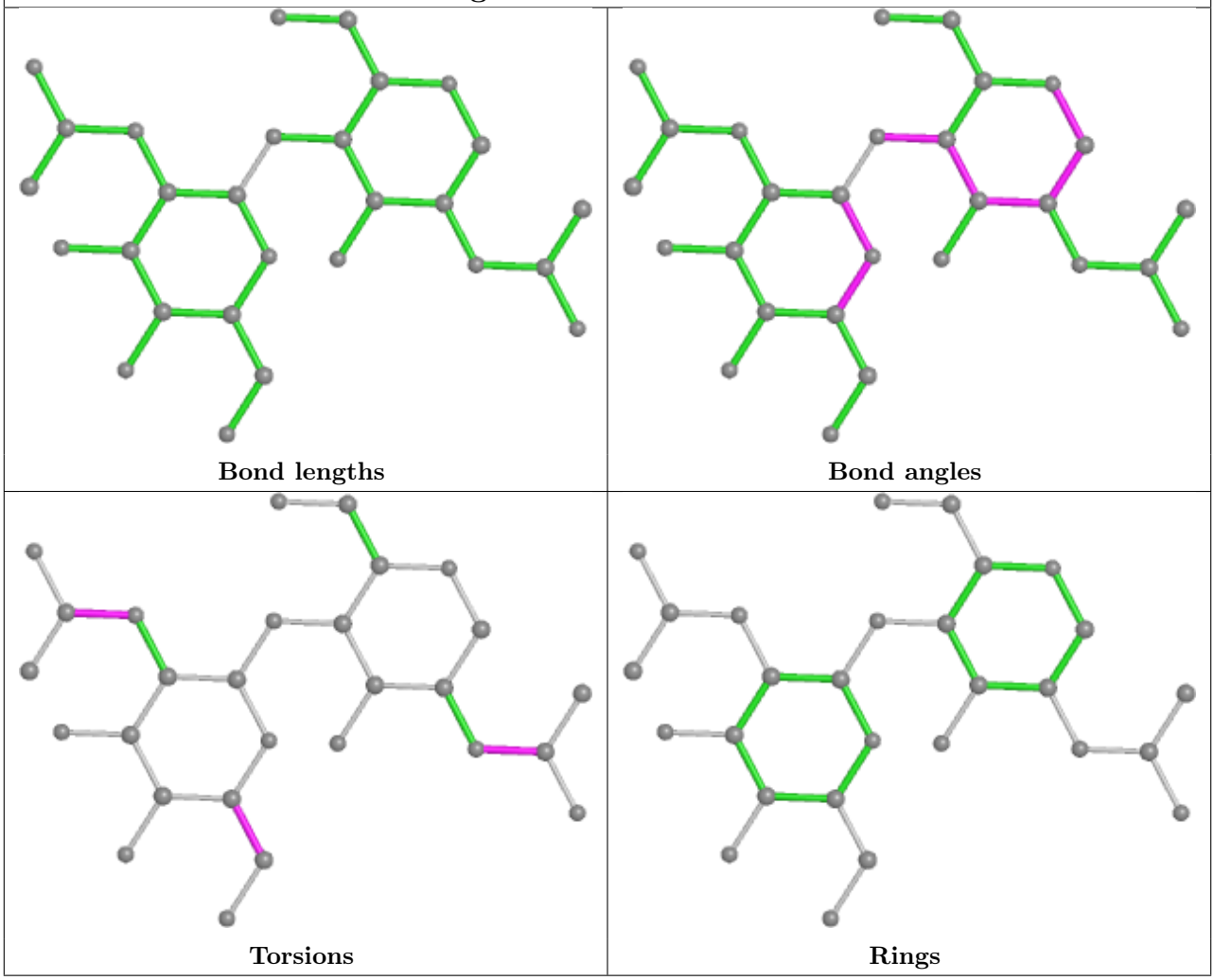
Mol	Chain	Res	Type	Atoms
3	F	2	NAG	C4-C5-C6-O6
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	F	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	E	2	NAG	O5-C5-C6-O6

There are no ring outliers.

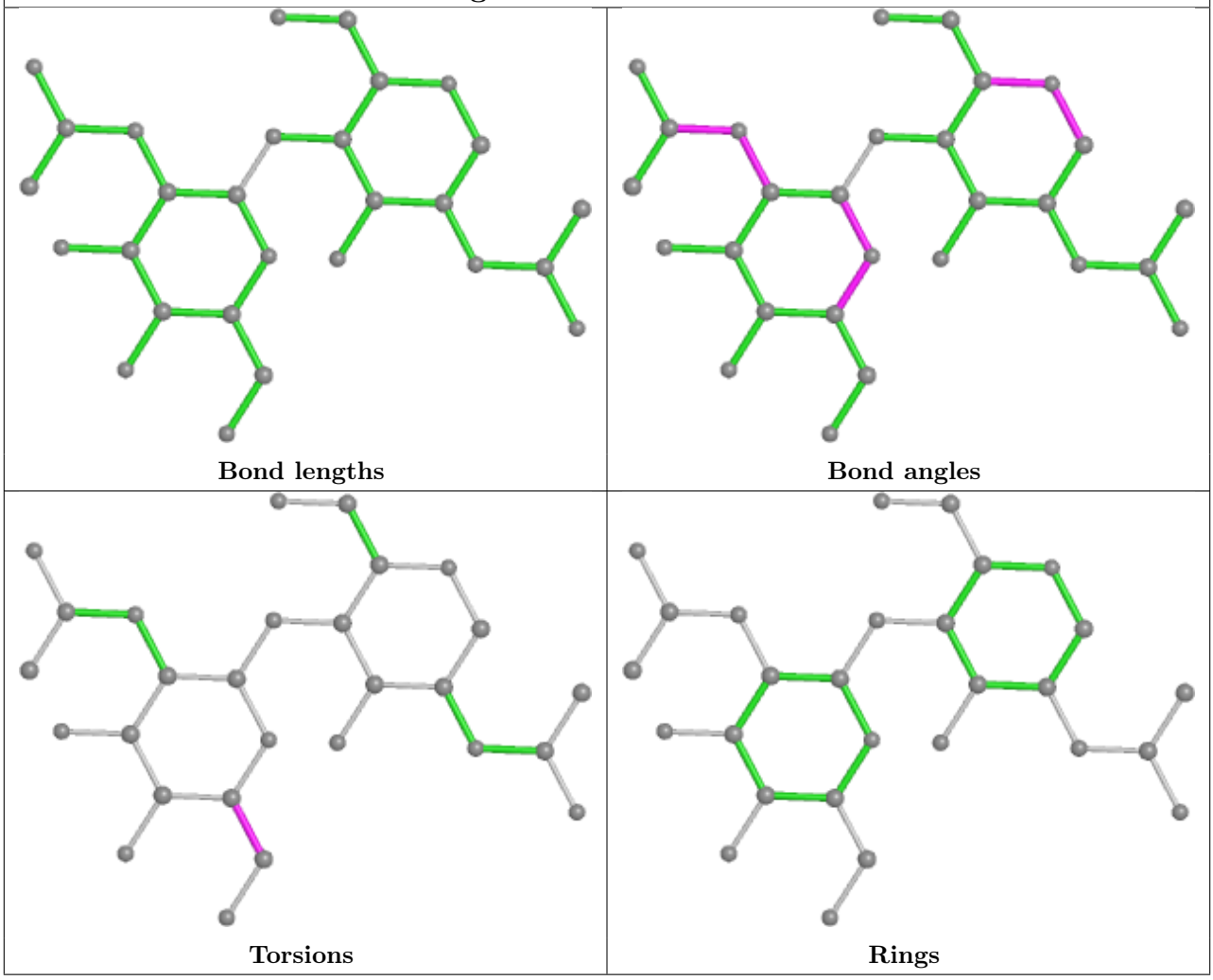
No monomer is involved in short contacts.

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 E



Oligosaccharide Chain F



5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	C	503	1	14,14,15	0.55	0	17,19,21	0.99	0
4	NAG	A	503	1	14,14,15	0.57	0	17,19,21	0.93	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	503	1	-	2/6/23/26	0/1/1/1
4	NAG	A	503	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	503	NAG	C8-C7-N2-C2
4	C	503	NAG	O7-C7-N2-C2

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	232/294 (78%)	-0.26	2 (0%)	84	75	24, 70, 113, 178	0
1	C	232/294 (78%)	-0.19	1 (0%)	92	89	24, 78, 139, 175	0
2	B	303/331 (91%)	-0.17	3 (0%)	82	72	41, 70, 124, 182	0
2	D	303/331 (91%)	-0.03	4 (1%)	77	65	45, 78, 152, 238	0
All	All	1070/1250 (85%)	-0.16	10 (0%)	84	75	24, 75, 135, 238	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	54	ALA	5.8
2	B	58	PRO	3.5
2	B	335	GLU	2.9
1	A	24	VAL	2.7
1	A	23	PRO	2.6
2	D	134	ARG	2.4
1	C	23	PRO	2.4
2	B	291	LYS	2.2
2	D	100	LEU	2.1
2	D	58	PRO	2.1

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,

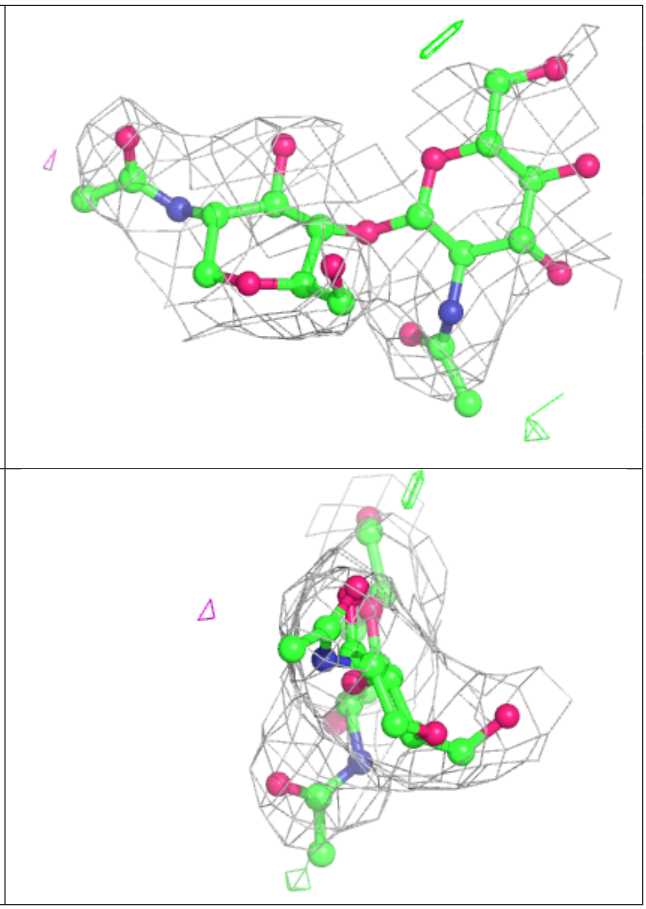
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	F	2	14/15	0.88	0.17	73,80,90,91	0
3	NAG	E	2	14/15	0.89	0.18	86,99,109,109	0
3	NAG	F	1	14/15	0.96	0.14	62,67,71,71	0
3	NAG	E	1	14/15	0.96	0.14	59,65,75,77	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.

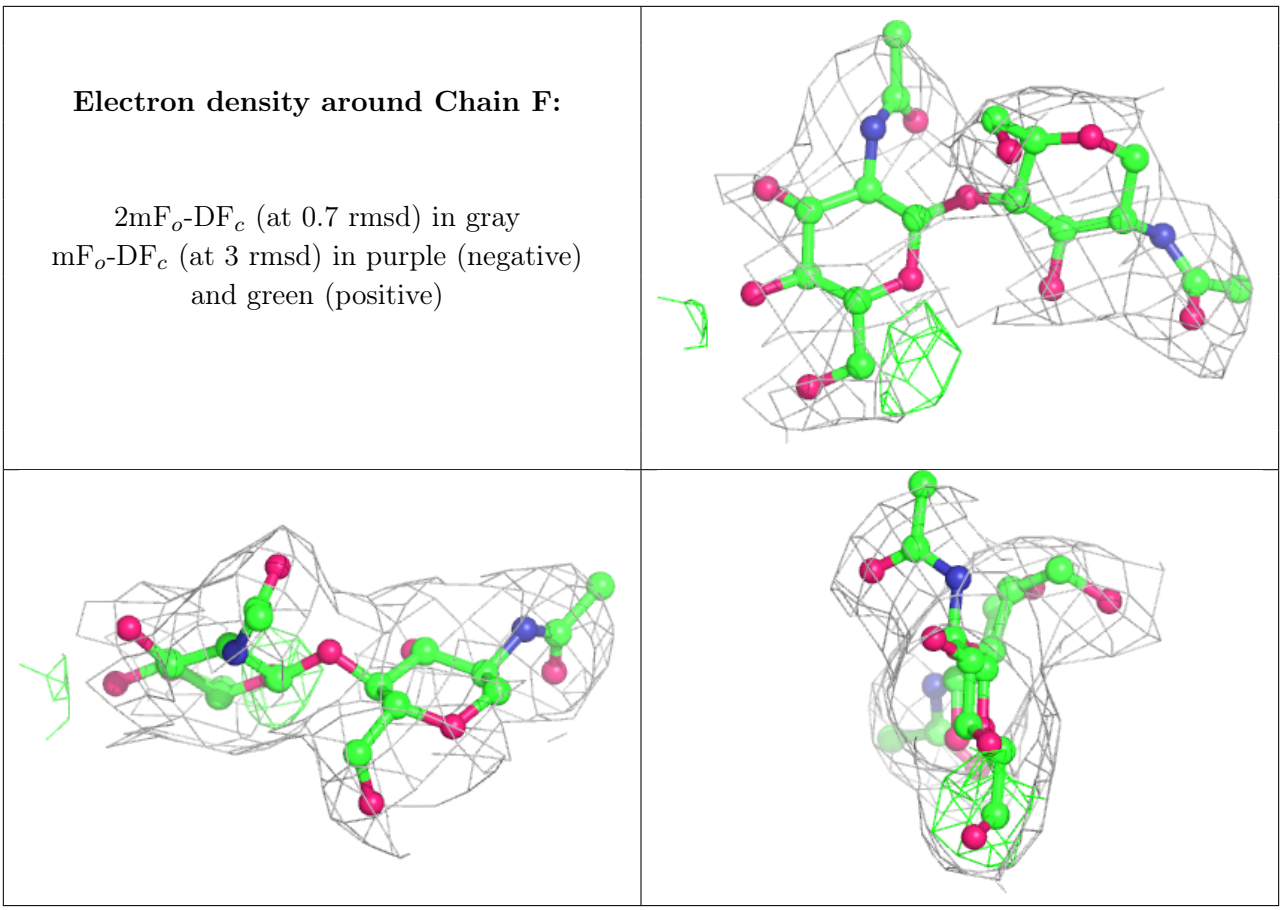
Electron density around Chain E:

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 (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
4	NAG	C	503	14/15	0.72	0.28	115,138,145,146	0
4	NAG	A	503	14/15	0.86	0.20	85,106,112,115	0

6.5 Other polymers (i)

There are no such residues in this entry.