Full wwPDB X-ray Structure Validation Report (i)

Apr 30, 2024 – 11:41 pm BST

PDB ID	:	2XBO
Title	:	Equine Rhinitis A Virus in Complex with its Sialic Acid Receptor
Authors	:	Fry, E.E.; Tuthill, T.J.; Harlos, K.; Walter, T.S.; Rowlands, D.J.; Stuart, D.I.
Deposited on	:	2010-04-14
Resolution	:	4.00 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:

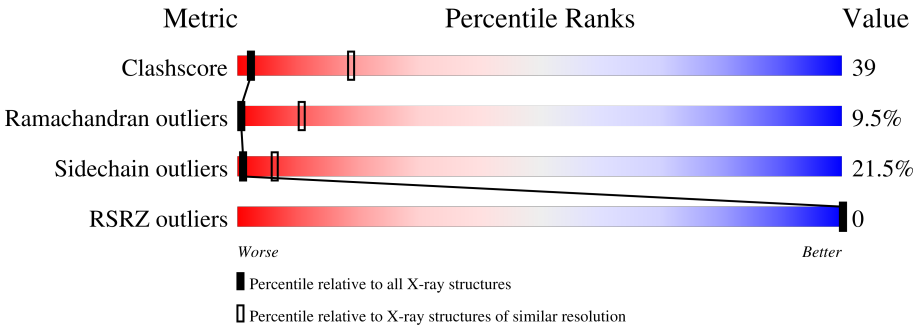
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 4.00 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))
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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	1	248	29% 46% 19% 6%
2	2	230	29% 43% 12% • 13%
3	3	226	35% 50% 14% •
4	4	80	18% 6% • • 72%
5	A	3	33% 33% 33%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5415 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 P1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	247	Total	C	N	O	S	0	0	1
			1929	1240	330	351	8			

- Molecule 2 is a protein called P1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	200	Total	C	N	O	S	0	0	0
			1554	997	266	284	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	85	SER	GLY	conflict	UNP B9VV85

- Molecule 3 is a protein called P1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	226	Total	C	N	O	S	0	0	0
			1723	1112	279	326	6			

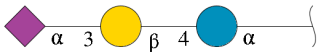
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	59	LYS	ARG	conflict	UNP B9VV85
3	107	TYR	ARG	conflict	UNP B9VV85

- Molecule 4 is a protein called P1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	22	Total	C	N	O	S	0	0	1
			166	101	29	35	1			

- Molecule 5 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galacto pyranose-(1-4)-alpha-D-glucopyranose.



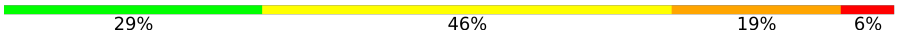
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	A	3	Total	C	N	O	0	0	0
			43	23	1	19			

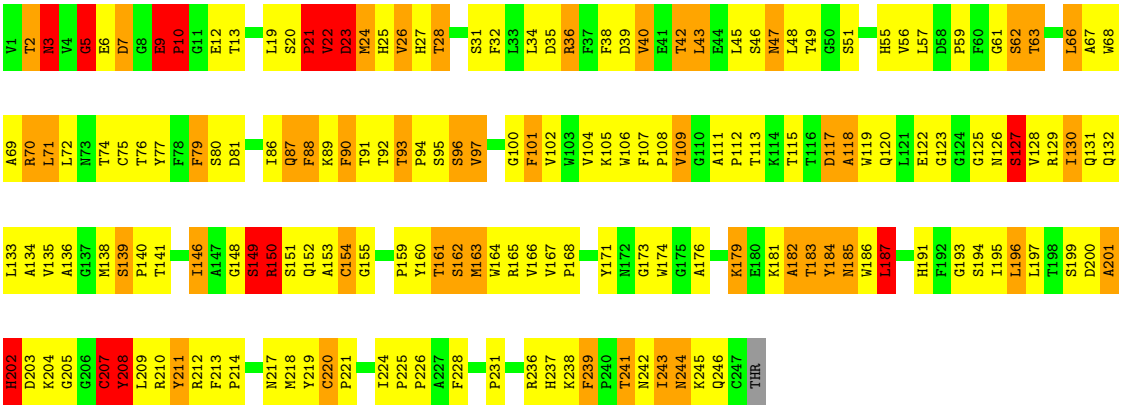
3 Residue-property plots (i)

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: P1

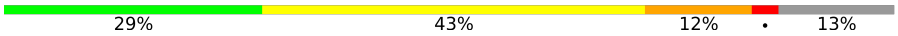
Chain 1:

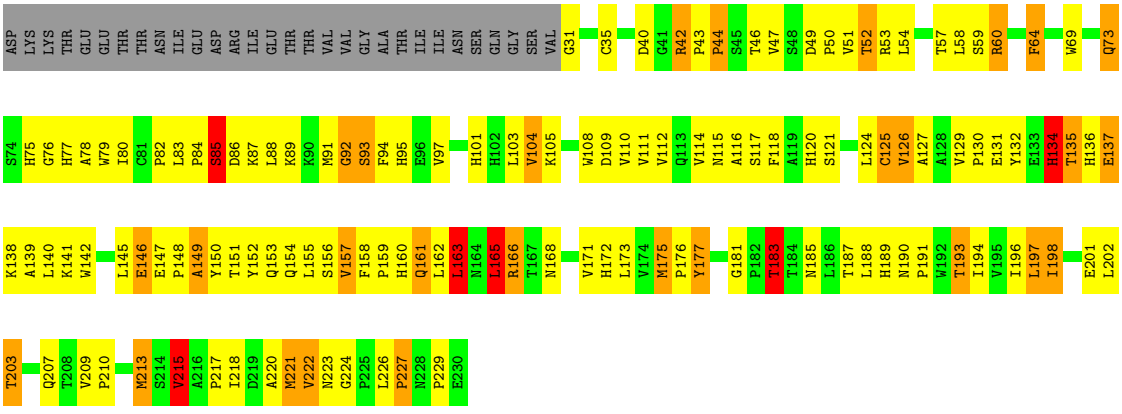




- Molecule 2: P1

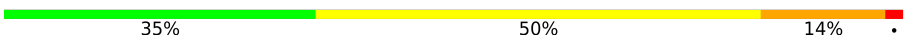
Chain 2:

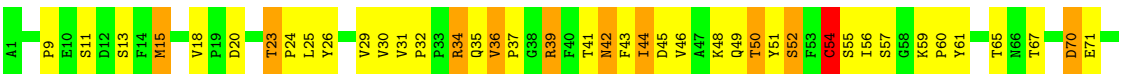


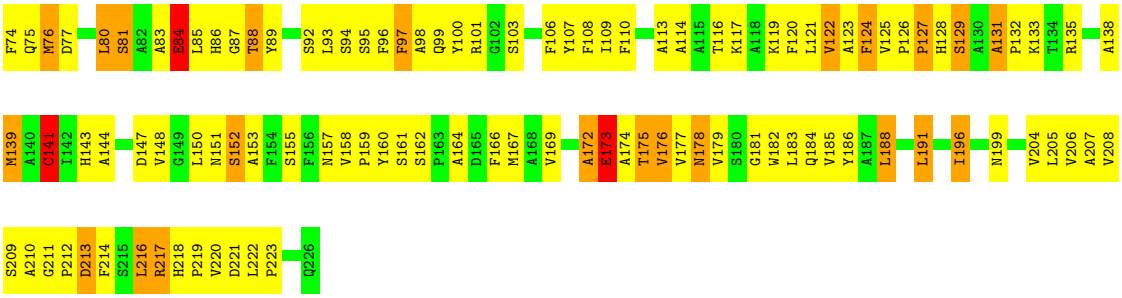


- Molecule 3: P1

Chain 3:

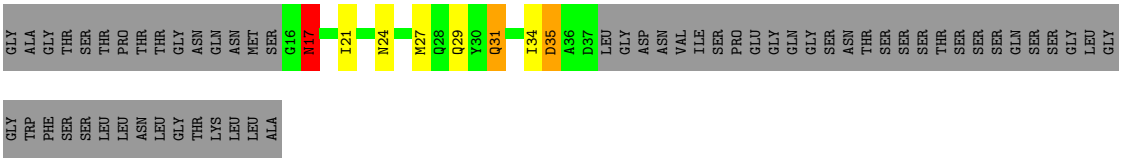






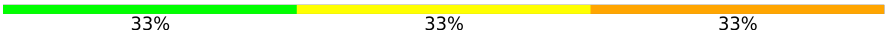
• Molecule 4: P1

Chain 4:



• Molecule 5: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	344.80Å 531.40Å 488.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.00 29.66 – 4.00	Depositor EDS
% Data completeness (in resolution range)	7.8 (20.00-4.00) 7.8 (29.66-4.00)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.247 , (Not available) 0.243 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.58 , 75.5	EDS
L-test for twinning[1]	$< \|L\| >$ = (Not available), $< L^2 >$ = (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	5415	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

[1]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: SIA, GAL, GLC

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	1	0.93	0/1993	1.23	13/2723 (0.5%)
2	2	1.00	1/1608 (0.1%)	1.19	9/2208 (0.4%)
3	3	1.02	3/1774 (0.2%)	1.12	3/2427 (0.1%)
4	4	1.16	0/168	1.13	1/226 (0.4%)
All	All	0.99	4/5543 (0.1%)	1.18	26/7584 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	1
2	2	0	1
3	3	0	2
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	54	CYS	CB-SG	-6.11	1.71	1.82
3	3	141	CYS	CB-SG	-5.83	1.72	1.81
3	3	173	GLU	CG-CD	5.78	1.60	1.51
2	2	31	GLY	N-CA	5.11	1.53	1.46

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	5	GLY	N-CA-C	9.59	137.08	113.10
1	1	7	ASP	N-CA-C	-8.08	89.19	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	207	CYS	N-CA-C	7.52	131.30	111.00
1	1	203	ASP	N-CA-C	-6.75	92.79	111.00
3	3	208	VAL	CB-CA-C	-6.45	99.15	111.40
3	3	88	THR	N-CA-C	6.22	127.80	111.00
2	2	109	ASP	N-CA-C	-6.13	94.45	111.00
1	1	201	ALA	N-CA-C	-6.09	94.54	111.00
4	4	17	ASN	N-CA-C	6.09	127.44	111.00
1	1	113	THR	N-CA-C	5.85	126.79	111.00
2	2	125	CYS	N-CA-C	-5.82	95.28	111.00
2	2	173	LEU	CA-CB-CG	5.73	128.48	115.30
2	2	138	LYS	N-CA-C	-5.65	95.75	111.00
2	2	163	LEU	CA-CB-CG	-5.56	102.50	115.30
2	2	46	THR	N-CA-C	5.42	125.64	111.00
2	2	215	VAL	CB-CA-C	-5.36	101.21	111.40
1	1	21	PRO	N-CA-C	5.34	125.99	112.10
1	1	3	ASN	N-CA-C	5.30	125.30	111.00
1	1	239	PHE	CB-CA-C	-5.28	99.84	110.40
3	3	122	VAL	N-CA-C	-5.14	97.11	111.00
2	2	92	GLY	N-CA-C	5.12	125.91	113.10
1	1	22	VAL	CB-CA-C	-5.12	101.67	111.40
1	1	23	ASP	N-CA-C	5.09	124.74	111.00
2	2	134	HIS	N-CA-C	-5.08	97.29	111.00
1	1	66	LEU	N-CA-C	5.05	124.63	111.00
1	1	127	SER	N-CA-C	5.02	124.56	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	208	TYR	Sidechain
2	2	177	TYR	Sidechain
3	3	26	TYR	Sidechain
3	3	51	TYR	Sidechain

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	1	1929	0	1864	175	0
2	2	1554	0	1523	124	0
3	3	1723	0	1680	150	0
4	4	166	0	146	8	0
5	A	43	0	37	2	0
All	All	5415	0	5250	419	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 39.

All (419) 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)
1:1:24:MET:SD	1:1:24:MET:CE	2.03	1.44
2:2:80:ILE:HG22	2:2:82:PRO:HD3	1.29	1.11
2:2:163:LEU:HD12	2:2:171:VAL:HG23	1.37	1.04
3:3:116:THR:HG23	3:3:191:LEU:HD11	1.42	1.00
2:2:213:MET:CE	2:2:215:VAL:HG22	1.96	0.95
1:1:115:THR:HG22	1:1:131:GLN:OE1	1.67	0.94
2:2:112:VAL:HG22	2:2:213:MET:HG3	1.51	0.93
2:2:126:VAL:HG22	2:2:171:VAL:HG11	1.51	0.93
2:2:213:MET:HE1	2:2:215:VAL:HG22	1.50	0.90
1:1:88:PHE:CE1	1:1:205:GLY:HA3	2.06	0.90
1:1:109:VAL:HG11	1:1:162:SER:HA	1.55	0.88
5:A:2:GAL:H4	5:A:3:SIA:O1B	1.74	0.88
1:1:120:GLN:HG3	1:1:129:ARG:HD3	1.54	0.86
2:2:115:ASN:O	2:2:209:VAL:HG13	1.75	0.86
1:1:146:ILE:HG22	1:1:152:GLN:HG2	1.58	0.85
3:3:103:SER:O	3:3:211:GLY:HA3	1.77	0.85
2:2:114:VAL:HG22	2:2:209:VAL:HG12	1.59	0.84
1:1:87:GLN:HE21	1:1:210:ARG:HH12	1.28	0.82
2:2:69:TRP:NE1	2:2:202:LEU:HB2	1.94	0.82
1:1:243:ILE:HG22	1:1:244:ASN:H	1.44	0.82
1:1:117:ASP:HB2	1:1:129:ARG:NH1	1.96	0.80
1:1:207:CYS:O	1:1:208:TYR:HB2	1.82	0.79
2:2:75:HIS:HA	2:2:198:ILE:HG22	1.65	0.79
1:1:88:PHE:HE1	1:1:205:GLY:HA3	1.49	0.78
1:1:92:THR:HG22	1:1:93:THR:H	1.49	0.78
3:3:74:PHE:HB3	3:3:185:VAL:HG23	1.63	0.78
1:1:70:ARG:O	1:1:71:LEU:HB2	1.83	0.76
2:2:105:LYS:HG3	2:2:177:TYR:CG	2.20	0.76
1:1:219:TYR:OH	3:3:34:ARG:HD2	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:116:THR:CG2	3:3:191:LEU:HD11	2.16	0.74
2:2:54:LEU:HB2	2:2:220:ALA:HB3	1.69	0.74
2:2:161:GLN:HB3	2:2:171:VAL:HG13	1.69	0.74
3:3:122:VAL:O	3:3:143:HIS:HB2	1.87	0.74
1:1:159:PRO:HG3	3:3:29:VAL:HG21	1.69	0.74
1:1:195:ILE:HD13	1:1:197:LEU:HD21	1.70	0.73
3:3:217:ARG:HD3	3:3:218:HIS:CD2	2.24	0.73
2:2:35:CYS:HB2	2:2:175:MET:HA	1.71	0.72
2:2:121:SER:HB2	2:2:203:THR:HG23	1.71	0.72
3:3:175:THR:HG22	3:3:177:VAL:H	1.52	0.72
1:1:77:TYR:HD1	1:1:168:PRO:HA	1.53	0.72
3:3:101:ARG:O	3:3:214:PHE:HA	1.90	0.72
3:3:100:TYR:HA	3:3:216:LEU:HD12	1.73	0.71
2:2:213:MET:HE2	2:2:215:VAL:HG22	1.72	0.71
2:2:153:GLN:OE1	3:3:87:GLY:HA3	1.90	0.71
3:3:94:SER:O	3:3:169:VAL:HG11	1.90	0.71
3:3:119:LYS:HG2	3:3:147:ASP:HA	1.72	0.70
1:1:2:THR:HG21	1:1:9:GLU:OE1	1.92	0.69
3:3:55:SER:O	3:3:84:GLU:HA	1.92	0.69
2:2:116:ALA:HB2	2:2:209:VAL:HG13	1.75	0.69
3:3:217:ARG:HD3	3:3:218:HIS:NE2	2.07	0.69
1:1:22:VAL:HG12	1:1:23:ASP:N	2.08	0.69
1:1:40:VAL:HB	1:1:68:TRP:CZ2	2.27	0.69
2:2:47:VAL:HG11	2:2:223:ASN:OD1	1.92	0.69
1:1:2:THR:HB	1:1:12:GLU:HB2	1.75	0.68
2:2:86:ASP:HB2	2:2:141:LYS:HA	1.75	0.68
1:1:136:ALA:HA	1:1:141:THR:OG1	1.93	0.68
1:1:22:VAL:HG12	1:1:23:ASP:H	1.58	0.68
1:1:191:HIS:HD2	1:1:193:GLY:H	1.41	0.67
3:3:116:THR:HG23	3:3:191:LEU:CD1	2.21	0.67
2:2:114:VAL:HG22	2:2:209:VAL:CG1	2.25	0.67
3:3:160:TYR:OH	3:3:167:MET:HG2	1.95	0.67
1:1:184:TYR:O	1:1:186:TRP:N	2.28	0.66
2:2:116:ALA:HB2	2:2:209:VAL:CG1	2.26	0.66
3:3:107:TYR:CE2	3:3:155:SER:HB2	2.31	0.66
1:1:75:CYS:SG	1:1:218:MET:HG2	2.35	0.66
1:1:241:THR:H	1:1:244:ASN:ND2	1.94	0.66
1:1:45:LEU:HD12	1:1:45:LEU:H	1.60	0.66
2:2:132:TYR:HB3	2:2:193:THR:HG21	1.78	0.66
1:1:87:GLN:NE2	1:1:210:ARG:HH12	1.92	0.65
2:2:79:TRP:HE3	2:2:196:ILE:HG22	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:97:VAL:O	2:2:101:HIS:HD2	1.79	0.65
1:1:120:GLN:CG	1:1:129:ARG:HD3	2.26	0.65
3:3:42:ASN:HD22	3:3:43:PHE:N	1.95	0.65
3:3:160:TYR:HE2	3:3:167:MET:HG3	1.61	0.65
1:1:117:ASP:HB2	1:1:129:ARG:HH11	1.60	0.65
3:3:131:ALA:HB2	3:3:182:TRP:CZ2	2.32	0.65
3:3:220:VAL:HG12	3:3:221:ASP:N	2.12	0.64
2:2:79:TRP:CE3	2:2:196:ILE:HG22	2.32	0.64
1:1:38:PHE:O	1:1:210:ARG:HA	1.98	0.64
1:1:90:PHE:CE1	1:1:94:PRO:HA	2.33	0.64
2:2:64:PHE:N	2:2:64:PHE:CD1	2.65	0.64
2:2:153:GLN:CD	3:3:87:GLY:HA3	2.18	0.64
2:2:161:GLN:CB	2:2:171:VAL:HG13	2.27	0.63
2:2:197:LEU:HG	2:2:198:ILE:N	2.11	0.63
3:3:34:ARG:HB2	3:3:36:VAL:HG12	1.80	0.63
1:1:19:LEU:HB2	3:3:213:ASP:HB2	1.80	0.63
1:1:131:GLN:HB2	1:1:134:ALA:HB2	1.80	0.62
3:3:61:TYR:HB3	3:3:205:LEU:HD23	1.80	0.62
1:1:77:TYR:CD1	1:1:168:PRO:HA	2.33	0.62
1:1:159:PRO:CG	3:3:29:VAL:HG21	2.29	0.62
1:1:120:GLN:HE21	1:1:129:ARG:HE	1.44	0.62
2:2:83:LEU:HD11	2:2:194:ILE:HD12	1.81	0.62
1:1:43:LEU:HD23	1:1:43:LEU:N	2.15	0.61
1:1:164:TRP:CZ2	1:1:187:LEU:HD21	2.34	0.61
1:1:176:ALA:HB3	1:1:183:THR:HG21	1.82	0.61
3:3:97:PHE:CD1	3:3:97:PHE:N	2.68	0.61
3:3:138:ALA:O	3:3:141:CYS:SG	2.51	0.61
2:2:220:ALA:O	2:2:221:MET:HG2	2.00	0.61
3:3:42:ASN:HD22	3:3:44:ILE:H	1.48	0.61
1:1:243:ILE:HG22	1:1:244:ASN:N	2.15	0.60
1:1:224:ILE:HG13	3:3:89:TYR:CE2	2.36	0.60
1:1:236:ARG:NH1	3:3:172:ALA:O	2.34	0.60
1:1:22:VAL:O	1:1:24:MET:N	2.34	0.60
1:1:80:SER:HB2	1:1:214:PRO:O	2.01	0.60
1:1:79:PHE:HE2	3:3:31:VAL:HG11	1.67	0.60
1:1:122:GLU:HG2	1:1:123:GLY:N	2.16	0.60
2:2:185:ASN:OD1	2:2:187:THR:HB	2.02	0.59
2:2:124:LEU:HD23	2:2:198:ILE:HA	1.85	0.59
2:2:127:ALA:O	2:2:194:ILE:HA	2.01	0.59
1:1:45:LEU:HB2	1:1:202:HIS:HA	1.83	0.59
2:2:104:VAL:HG13	2:2:222:VAL:HG13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:54:CYS:HB2	3:3:206:VAL:HG13	1.83	0.59
1:1:68:TRP:O	1:1:72:LEU:HG	2.03	0.58
1:1:97:VAL:HG22	1:1:204:LYS:HD2	1.84	0.58
3:3:175:THR:CG2	3:3:176:VAL:N	2.66	0.58
3:3:127:PRO:HD3	3:3:181:GLY:CA	2.33	0.58
1:1:181:LYS:O	1:1:182:ALA:HB3	2.04	0.58
2:2:134:HIS:O	2:2:136:HIS:N	2.35	0.58
2:2:153:GLN:NE2	3:3:87:GLY:HA3	2.18	0.58
2:2:59:SER:HA	2:2:94:PHE:HB2	1.85	0.58
1:1:55:HIS:O	1:1:194:SER:HB2	2.04	0.57
2:2:160:HIS:HD1	2:2:160:HIS:H	1.52	0.57
1:1:105:LYS:HE3	1:1:139:SER:HB2	1.86	0.57
3:3:110:PHE:CD2	3:3:148:VAL:HG11	2.40	0.57
1:1:28:THR:HB	3:3:42:ASN:HD21	1.69	0.57
1:1:132:GLN:HG3	1:1:133:LEU:HD23	1.85	0.57
1:1:239:PHE:HE1	3:3:81:SER:HB3	1.69	0.57
2:2:58:LEU:O	2:2:60:ARG:HG3	2.05	0.57
2:2:85:SER:HB3	2:2:140:LEU:HB3	1.85	0.57
2:2:126:VAL:CG2	2:2:171:VAL:HG11	2.31	0.57
2:2:147:GLU:HB3	2:2:148:PRO:HD2	1.86	0.57
3:3:113:ALA:O	3:3:116:THR:HB	2.04	0.57
1:1:109:VAL:CG1	1:1:162:SER:HA	2.31	0.57
1:1:120:GLN:HG3	1:1:129:ARG:CD	2.29	0.57
1:1:130:ILE:HG13	1:1:131:GLN:N	2.19	0.57
4:4:29:GLN:HA	4:4:34:ILE:HD11	1.87	0.57
1:1:77:TYR:HB3	1:1:166:VAL:HG21	1.85	0.57
3:3:46:VAL:O	3:3:50:THR:HB	2.05	0.57
2:2:97:VAL:HG12	2:2:101:HIS:CD2	2.41	0.56
3:3:184:GLN:NE2	3:3:186:TYR:HE1	2.03	0.56
2:2:110:VAL:HG12	2:2:215:VAL:HG13	1.88	0.56
3:3:15:MET:O	3:3:18:VAL:HG23	2.06	0.56
2:2:110:VAL:HG23	2:2:110:VAL:O	2.05	0.56
1:1:174:TRP:CE2	1:1:179:LYS:HB3	2.41	0.56
1:1:28:THR:HB	3:3:42:ASN:ND2	2.20	0.55
1:1:45:LEU:HD12	1:1:45:LEU:N	2.21	0.55
3:3:44:ILE:HG23	3:3:48:LYS:HE3	1.88	0.55
2:2:140:LEU:HD22	2:2:190:ASN:ND2	2.22	0.55
2:2:97:VAL:O	2:2:101:HIS:CD2	2.59	0.55
3:3:42:ASN:ND2	3:3:44:ILE:H	2.03	0.55
1:1:43:LEU:HD23	1:1:43:LEU:H	1.73	0.54
1:1:70:ARG:O	1:1:71:LEU:CB	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:115:ASN:HB3	2:2:210:PRO:HG2	1.88	0.54
2:2:166:ARG:HD2	3:3:110:PHE:HD2	1.73	0.54
1:1:19:LEU:HB2	3:3:213:ASP:CB	2.37	0.54
1:1:209:LEU:HD13	1:1:211:TYR:HE1	1.71	0.54
1:1:219:TYR:CE1	3:3:36:VAL:HG13	2.42	0.54
1:1:125:GLY:O	1:1:127:SER:N	2.41	0.54
1:1:207:CYS:O	1:1:208:TYR:CB	2.55	0.54
3:3:120:PHE:HB3	3:3:186:TYR:O	2.08	0.54
1:1:28:THR:CB	3:3:42:ASN:HD21	2.21	0.54
1:1:77:TYR:HB3	1:1:166:VAL:CG2	2.38	0.54
2:2:42:ARG:HG3	2:2:43:PRO:HD2	1.90	0.54
2:2:118:PHE:HB2	3:3:114:ALA:HB3	1.90	0.54
1:1:79:PHE:CD1	1:1:79:PHE:C	2.82	0.53
1:1:105:LYS:HE3	1:1:139:SER:CB	2.38	0.53
1:1:74:THR:HG21	3:3:43:PHE:CZ	2.43	0.53
1:1:163:MET:H	1:1:163:MET:HE2	1.74	0.53
2:2:75:HIS:HA	2:2:198:ILE:CG2	2.37	0.53
1:1:61:GLY:O	1:1:62:SER:HB3	2.08	0.53
1:1:35:ASP:OD2	1:1:212:ARG:HD3	2.08	0.53
3:3:106:PHE:O	3:3:155:SER:HA	2.09	0.53
1:1:13:THR:HA	3:3:144:ALA:HB2	1.90	0.53
2:2:134:HIS:HD2	2:2:145:LEU:HD13	1.75	0.52
2:2:149:ALA:HA	2:2:152:TYR:CD2	2.45	0.52
3:3:127:PRO:HD3	3:3:181:GLY:HA2	1.90	0.52
3:3:18:VAL:HG12	3:3:20:ASP:H	1.74	0.52
2:2:202:LEU:HD21	2:2:209:VAL:HG23	1.92	0.52
3:3:96:PHE:C	3:3:97:PHE:CD1	2.82	0.52
3:3:96:PHE:HB2	3:3:97:PHE:CE1	2.45	0.52
1:1:191:HIS:CD2	1:1:193:GLY:H	2.26	0.52
2:2:148:PRO:O	2:2:149:ALA:HB3	2.10	0.52
2:2:149:ALA:O	2:2:153:GLN:HG3	2.10	0.52
3:3:94:SER:OG	3:3:216:LEU:HD21	2.10	0.52
5:A:2:GAL:C4	5:A:3:SIA:O1B	2.54	0.52
1:1:7:ASP:HB2	1:1:12:GLU:OE1	2.09	0.52
1:1:219:TYR:HA	3:3:39:ARG:HA	1.90	0.52
2:2:108:TRP:HB2	2:2:175:MET:CG	2.40	0.52
4:4:17:ASN:CG	4:4:17:ASN:O	2.49	0.52
3:3:160:TYR:HE2	3:3:167:MET:CG	2.23	0.51
1:1:59:PRO:O	1:1:72:LEU:HD12	2.10	0.51
1:1:122:GLU:HG3	1:1:127:SER:HB3	1.92	0.51
1:1:76:THR:HB	1:1:220:CYS:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:43:PRO:HA	2:2:221:MET:HE1	1.92	0.51
2:2:69:TRP:CZ3	2:2:124:LEU:HG	2.46	0.51
3:3:110:PHE:CG	3:3:148:VAL:HG11	2.46	0.51
1:1:19:LEU:HD11	3:3:160:TYR:HB3	1.92	0.51
1:1:238:LYS:HA	3:3:172:ALA:HA	1.92	0.51
2:2:160:HIS:ND1	2:2:160:HIS:N	2.59	0.51
3:3:46:VAL:O	3:3:50:THR:CG2	2.58	0.51
3:3:196:ILE:HD12	3:3:199:ASN:O	2.10	0.51
2:2:132:TYR:HB3	2:2:193:THR:CG2	2.41	0.51
1:1:106:TRP:O	1:1:139:SER:HB3	2.11	0.51
1:1:109:VAL:HB	1:1:161:THR:HB	1.91	0.51
3:3:31:VAL:HG13	3:3:32:PRO:HD2	1.93	0.51
3:3:74:PHE:O	3:3:184:GLN:HA	2.11	0.51
1:1:160:TYR:OH	1:1:167:VAL:HG23	2.11	0.50
2:2:149:ALA:HA	2:2:152:TYR:CE2	2.46	0.50
2:2:120:HIS:O	3:3:113:ALA:HB2	2.12	0.50
3:3:74:PHE:HB3	3:3:185:VAL:CG2	2.36	0.50
2:2:160:HIS:HD1	2:2:160:HIS:N	2.10	0.50
1:1:5:GLY:HA2	1:1:13:THR:O	2.11	0.50
1:1:104:VAL:HA	1:1:196:LEU:O	2.11	0.50
3:3:109:ILE:N	3:3:109:ILE:HD12	2.27	0.50
2:2:69:TRP:CE2	2:2:202:LEU:HB2	2.45	0.50
1:1:102:VAL:HA	1:1:199:SER:HB2	1.94	0.50
2:2:117:SER:H	2:2:120:HIS:CE1	2.30	0.50
2:2:151:THR:O	2:2:155:LEU:N	2.45	0.50
2:2:149:ALA:O	2:2:150:TYR:C	2.51	0.49
2:2:64:PHE:HE1	2:2:215:VAL:HG23	1.76	0.49
1:1:115:THR:OG1	1:1:133:LEU:HG	2.11	0.49
3:3:42:ASN:HD22	3:3:42:ASN:C	2.14	0.49
1:1:36:ARG:O	1:1:212:ARG:HA	2.11	0.49
3:3:94:SER:HB3	3:3:169:VAL:HG13	1.94	0.49
2:2:87:LYS:HG3	2:2:142:TRP:CE2	2.47	0.49
2:2:108:TRP:HB2	2:2:175:MET:HG3	1.95	0.49
3:3:76:MET:HG3	3:3:76:MET:O	2.13	0.49
2:2:111:VAL:HG22	2:2:172:HIS:CD2	2.47	0.49
2:2:40:ASP:HB2	2:2:42:ARG:HH21	1.78	0.48
2:2:158:PHE:O	2:2:160:HIS:ND1	2.45	0.48
1:1:32:PHE:C	1:1:32:PHE:CD2	2.86	0.48
1:1:74:THR:HG21	3:3:43:PHE:CE2	2.48	0.48
3:3:116:THR:HG22	3:3:117:LYS:N	2.29	0.48
1:1:89:LYS:HB2	1:1:208:TYR:HE1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:58:LEU:O	2:2:60:ARG:N	2.46	0.48
2:2:59:SER:HB2	2:2:217:PRO:HB2	1.94	0.48
3:3:24:PRO:CG	4:4:31:GLN:HA	2.43	0.48
3:3:100:TYR:CE1	3:3:167:MET:HB3	2.48	0.48
3:3:173:GLU:HA	3:3:173:GLU:OE1	2.13	0.48
1:1:100:GLY:O	1:1:146:ILE:HG13	2.13	0.48
2:2:76:GLY:O	2:2:146:GLU:HA	2.12	0.48
1:1:224:ILE:N	2:2:154:GLN:OE1	2.46	0.48
2:2:126:VAL:HB	2:2:196:ILE:HG12	1.96	0.48
1:1:115:THR:CG2	1:1:131:GLN:OE1	2.53	0.48
2:2:129:VAL:HA	2:2:130:PRO:HD3	1.61	0.48
2:2:137:GLU:C	2:2:139:ALA:H	2.18	0.47
3:3:164:ALA:HB1	3:3:166:PHE:O	2.14	0.47
2:2:201:GLU:O	2:2:203:THR:HG22	2.14	0.47
1:1:181:LYS:O	1:1:182:ALA:CB	2.61	0.47
3:3:121:LEU:HG	3:3:143:HIS:CD2	2.48	0.47
1:1:107:PHE:HE1	1:1:196:LEU:HB2	1.80	0.47
2:2:83:LEU:HA	2:2:84:PRO:HA	1.41	0.47
3:3:46:VAL:O	3:3:50:THR:HG22	2.14	0.47
1:1:66:LEU:O	1:1:67:ALA:HB3	2.15	0.47
1:1:118:ALA:CB	1:1:132:GLN:HB2	2.45	0.47
3:3:157:ASN:O	3:3:159:PRO:HD3	2.15	0.47
1:1:166:VAL:HG22	1:1:167:VAL:N	2.29	0.47
2:2:149:ALA:C	2:2:151:THR:N	2.66	0.47
3:3:85:LEU:HD23	3:3:85:LEU:HA	1.58	0.47
3:3:169:VAL:HG12	3:3:169:VAL:O	2.13	0.47
1:1:9:GLU:HA	1:1:10:PRO:HD3	1.76	0.47
3:3:220:VAL:CG1	3:3:221:ASP:N	2.78	0.47
1:1:109:VAL:O	1:1:109:VAL:HG12	2.15	0.47
1:1:231:PRO:HG2	3:3:83:ALA:HA	1.96	0.47
3:3:121:LEU:HG	3:3:143:HIS:HD2	1.79	0.47
1:1:35:ASP:HB3	4:4:17:ASN:HB3	1.97	0.46
1:1:118:ALA:HB3	1:1:132:GLN:HB2	1.96	0.46
1:1:220:CYS:HA	1:1:221:PRO:HD2	1.76	0.46
3:3:24:PRO:HG3	4:4:31:GLN:HA	1.97	0.46
1:1:115:THR:HG23	1:1:132:GLN:HB3	1.97	0.46
3:3:184:GLN:NE2	3:3:186:TYR:CE1	2.82	0.46
1:1:21:PRO:O	1:1:22:VAL:O	2.33	0.46
2:2:198:ILE:HG22	2:2:198:ILE:O	2.14	0.46
3:3:48:LYS:HA	3:3:210:ALA:HB3	1.97	0.46
2:2:137:GLU:C	2:2:139:ALA:N	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:92:SER:O	3:3:95:SER:OG	2.33	0.46
1:1:106:TRP:HE3	1:1:140:PRO:HD2	1.81	0.46
3:3:45:ASP:O	3:3:49:GLN:HG2	2.15	0.46
3:3:80:LEU:HD12	3:3:80:LEU:HA	1.55	0.46
1:1:34:LEU:HA	1:1:34:LEU:HD23	1.72	0.46
1:1:96:SER:HB2	1:1:204:LYS:HD3	1.96	0.46
1:1:199:SER:OG	1:1:200:ASP:N	2.49	0.46
1:1:80:SER:OG	1:1:213:PHE:HB3	2.16	0.46
3:3:120:PHE:HA	3:3:188:LEU:H	1.81	0.46
1:1:43:LEU:N	1:1:43:LEU:CD2	2.79	0.46
1:1:171:TYR:HA	2:2:131:GLU:OE1	2.15	0.46
2:2:157:VAL:HG13	2:2:157:VAL:O	2.15	0.46
3:3:83:ALA:C	3:3:85:LEU:H	2.19	0.46
2:2:52:THR:HB	2:2:222:VAL:HG23	1.98	0.46
3:3:125:VAL:HG21	3:3:132:PRO:HG3	1.97	0.45
1:1:89:LYS:HD2	1:1:90:PHE:H	1.81	0.45
1:1:120:GLN:CB	1:1:129:ARG:HD3	2.46	0.45
1:1:149:SER:O	1:1:151:SER:N	2.49	0.45
1:1:173:GLY:CA	2:2:188:LEU:O	2.63	0.45
2:2:77:HIS:O	2:2:78:ALA:HB2	2.17	0.45
2:2:85:SER:HA	2:2:88:LEU:HB2	1.97	0.45
1:1:154:CYS:SG	1:1:155:GLY:N	2.88	0.45
1:1:173:GLY:HA2	2:2:188:LEU:O	2.17	0.45
3:3:44:ILE:CG2	3:3:48:LYS:HE3	2.46	0.45
3:3:206:VAL:HG13	3:3:206:VAL:O	2.16	0.45
2:2:85:SER:O	2:2:86:ASP:HB3	2.17	0.45
2:2:148:PRO:O	2:2:149:ALA:CB	2.65	0.45
1:1:128:VAL:CG1	1:1:129:ARG:N	2.80	0.45
3:3:121:LEU:HD21	3:3:123:ALA:HB2	1.99	0.45
3:3:35:GLN:O	3:3:36:VAL:C	2.56	0.45
3:3:220:VAL:HG12	3:3:221:ASP:H	1.78	0.45
1:1:79:PHE:CE2	3:3:34:ARG:NH2	2.85	0.45
2:2:134:HIS:C	2:2:136:HIS:H	2.21	0.45
3:3:106:PHE:CE1	3:3:158:VAL:HG21	2.52	0.45
1:1:87:GLN:O	1:1:87:GLN:HG3	2.17	0.44
1:1:228:PHE:CE2	1:1:239:PHE:HE2	2.36	0.44
3:3:83:ALA:O	3:3:85:LEU:N	2.50	0.44
3:3:106:PHE:HE1	3:3:158:VAL:HG21	1.81	0.44
2:2:124:LEU:HA	2:2:197:LEU:O	2.16	0.44
3:3:48:LYS:HD3	3:3:212:PRO:HA	1.99	0.44
3:3:166:PHE:CE2	3:3:217:ARG:HG2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:35:ASP:OD1	4:4:35:ASP:N	2.50	0.44
1:1:88:PHE:N	1:1:207:CYS:O	2.49	0.44
2:2:91:MET:O	2:2:93:SER:N	2.50	0.44
1:1:146:ILE:HG22	1:1:152:GLN:CG	2.40	0.44
3:3:65:THR:C	3:3:67:THR:H	2.21	0.44
3:3:108:PHE:HB3	3:3:204:VAL:CG1	2.48	0.44
1:1:140:PRO:HG3	3:3:25:LEU:O	2.18	0.44
2:2:165:LEU:N	2:2:165:LEU:HD23	2.33	0.44
3:3:128:HIS:HB3	3:3:129:SER:H	1.56	0.44
1:1:241:THR:HG22	1:1:242:ASN:H	1.82	0.44
1:1:62:SER:O	1:1:63:THR:HB	2.18	0.44
1:1:119:TRP:HB3	1:1:130:ILE:HG12	2.00	0.44
3:3:70:ASP:HB3	3:3:135:ARG:H	1.82	0.44
3:3:222:LEU:HA	3:3:223:PRO:HD2	1.87	0.44
1:1:79:PHE:CE2	3:3:31:VAL:HG11	2.51	0.43
2:2:177:TYR:CZ	2:2:183:THR:HA	2.54	0.43
1:1:68:TRP:O	1:1:68:TRP:HE3	2.01	0.43
2:2:220:ALA:C	2:2:221:MET:HG2	2.38	0.43
3:3:175:THR:HB	3:3:178:ASN:ND2	2.33	0.43
3:3:160:TYR:CE2	3:3:167:MET:CG	3.02	0.43
1:1:47:ASN:HD22	1:1:48:LEU:H	1.67	0.43
1:1:69:ALA:C	1:1:70:ARG:O	2.57	0.43
1:1:199:SER:C	1:1:201:ALA:H	2.22	0.43
3:3:125:VAL:HA	3:3:126:PRO:HD2	1.80	0.43
1:1:86:ILE:N	1:1:86:ILE:HD12	2.33	0.43
2:2:175:MET:H	2:2:175:MET:HG2	1.67	0.43
3:3:60:PRO:HD2	3:3:61:TYR:CD2	2.53	0.43
3:3:132:PRO:O	3:3:133:LYS:HG3	2.19	0.43
3:3:175:THR:HG22	3:3:176:VAL:N	2.33	0.43
2:2:181:GLY:C	2:2:183:THR:H	2.21	0.42
3:3:34:ARG:HB2	3:3:36:VAL:CG1	2.45	0.42
1:1:42:THR:O	1:1:42:THR:HG22	2.19	0.42
3:3:196:ILE:HD12	3:3:196:ILE:HA	1.84	0.42
1:1:148:GLY:O	1:1:150:ARG:N	2.52	0.42
3:3:172:ALA:O	3:3:173:GLU:C	2.58	0.42
1:1:89:LYS:HB2	1:1:208:TYR:CE1	2.55	0.42
1:1:212:ARG:NH2	3:3:18:VAL:O	2.45	0.42
1:1:40:VAL:HB	1:1:68:TRP:CE2	2.54	0.42
1:1:57:LEU:H	1:1:57:LEU:HG	1.65	0.42
1:1:71:LEU:O	1:1:218:MET:CE	2.68	0.42
1:1:101:PHE:HD1	1:1:101:PHE:HA	1.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:161:GLN:OE1	2:2:171:VAL:HA	2.19	0.42
3:3:23:THR:HA	3:3:24:PRO:HD3	1.69	0.42
3:3:44:ILE:HA	3:3:44:ILE:HD12	1.59	0.42
2:2:155:LEU:HD12	2:2:155:LEU:HA	1.50	0.42
2:2:226:LEU:HA	2:2:227:PRO:HD3	1.80	0.42
3:3:76:MET:HB3	3:3:84:GLU:HG3	2.02	0.42
1:1:81:ASP:HB2	1:1:214:PRO:HG2	2.02	0.42
2:2:131:GLU:CD	2:2:189:HIS:HE2	2.23	0.42
3:3:30:VAL:HG22	4:4:34:ILE:HB	2.02	0.42
3:3:84:GLU:CD	3:3:84:GLU:H	2.22	0.42
3:3:98:ALA:HB3	3:3:218:HIS:HB2	2.02	0.42
2:2:84:PRO:O	2:2:85:SER:O	2.37	0.41
3:3:175:THR:HG23	3:3:176:VAL:H	1.85	0.41
3:3:85:LEU:O	3:3:86:HIS:C	2.58	0.41
3:3:108:PHE:O	3:3:153:ALA:HA	2.21	0.41
1:1:25:HIS:O	1:1:27:HIS:N	2.53	0.41
1:1:106:TRP:HA	1:1:195:ILE:HG22	2.02	0.41
2:2:35:CYS:O	2:2:176:PRO:HD3	2.20	0.41
2:2:175:MET:HA	2:2:176:PRO:HD3	1.86	0.41
3:3:75:GLN:HG3	3:3:184:GLN:HG2	2.02	0.41
1:1:71:LEU:O	1:1:218:MET:HE1	2.21	0.41
2:2:49:ASP:HA	2:2:50:PRO:HD2	1.93	0.41
2:2:129:VAL:HG22	2:2:158:PHE:CD1	2.56	0.41
3:3:52:SER:O	3:3:207:ALA:HB1	2.20	0.41
1:1:164:TRP:CH2	1:1:187:LEU:HD21	2.56	0.41
3:3:162:SER:C	3:3:164:ALA:N	2.74	0.41
1:1:241:THR:N	1:1:244:ASN:ND2	2.65	0.41
2:2:220:ALA:C	2:2:221:MET:CG	2.88	0.41
3:3:36:VAL:HA	3:3:37:PRO:HD3	1.85	0.41
3:3:127:PRO:CD	3:3:181:GLY:HA2	2.50	0.41
1:1:74:THR:O	1:1:74:THR:HG22	2.21	0.41
1:1:88:PHE:CD2	1:1:88:PHE:O	2.74	0.41
1:1:111:ALA:HB1	1:1:112:PRO:HD2	2.03	0.41
1:1:168:PRO:O	1:1:168:PRO:HG2	2.20	0.41
1:1:191:HIS:HD2	1:1:193:GLY:N	2.13	0.41
2:2:80:ILE:HG22	2:2:82:PRO:CD	2.22	0.41
2:2:140:LEU:HD22	2:2:190:ASN:CG	2.41	0.41
3:3:99:GLN:HB3	3:3:166:PHE:HB3	2.03	0.41
3:3:120:PHE:CD1	3:3:120:PHE:N	2.89	0.41
4:4:17:ASN:O	4:4:17:ASN:ND2	2.54	0.41
1:1:26:VAL:HG12	1:1:26:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:87:GLN:HA	1:1:153:ALA:HB2	2.03	0.41
1:1:241:THR:N	1:1:244:ASN:HD21	2.19	0.41
1:1:241:THR:HB	1:1:243:ILE:H	1.85	0.41
2:2:94:PHE:O	2:2:95:HIS:C	2.59	0.41
3:3:93:LEU:O	3:3:93:LEU:HD23	2.21	0.41
3:3:124:PHE:CD1	3:3:124:PHE:C	2.93	0.41
1:1:151:SER:C	1:1:153:ALA:H	2.25	0.40
1:1:186:TRP:O	1:1:187:LEU:O	2.39	0.40
1:1:211:TYR:N	1:1:211:TYR:CD1	2.89	0.40
2:2:73:GLN:HA	2:2:73:GLN:NE2	2.37	0.40
2:2:166:ARG:HD3	3:3:152:SER:HB3	2.03	0.40
1:1:108:PRO:CB	1:1:161:THR:HG21	2.52	0.40
1:1:211:TYR:N	1:1:211:TYR:HD1	2.19	0.40
3:3:218:HIS:HA	3:3:219:PRO:HD2	1.91	0.40
1:1:219:TYR:CD2	1:1:219:TYR:N	2.90	0.40
1:1:225:PRO:HA	1:1:226:PRO:HD3	1.71	0.40
2:2:69:TRP:CG	2:2:202:LEU:HD22	2.56	0.40
2:2:114:VAL:CG2	2:2:209:VAL:HG12	2.41	0.40
1:1:217:ASN:OD1	3:3:39:ARG:NH1	2.55	0.40
2:2:58:LEU:HD23	2:2:58:LEU:HA	1.82	0.40
3:3:46:VAL:O	3:3:50:THR:CB	2.68	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	1	245/248 (99%)	173 (71%)	41 (17%)	31 (13%)	0 5
2	2	198/230 (86%)	154 (78%)	27 (14%)	17 (9%)	1 12
3	3	224/226 (99%)	181 (81%)	28 (12%)	15 (7%)	1 17
4	4	20/80 (25%)	12 (60%)	6 (30%)	2 (10%)	0 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	687/784 (88%)	520 (76%)	102 (15%)	65 (10%)	0 10

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	5	GLY
1	1	9	GLU
1	1	10	PRO
1	1	21	PRO
1	1	22	VAL
1	1	23	ASP
1	1	26	VAL
1	1	88	PHE
1	1	126	ASN
1	1	127	SER
1	1	150	ARG
1	1	184	TYR
2	2	85	SER
2	2	92	GLY
2	2	134	HIS
2	2	135	THR
2	2	137	GLU
2	2	149	ALA
3	3	11	SER
3	3	36	VAL
3	3	129	SER
4	4	17	ASN
1	1	6	GLU
1	1	109	VAL
1	1	149	SER
1	1	162	SER
1	1	185	ASN
1	1	208	TYR
1	1	243	ILE
2	2	60	ARG
2	2	73	GLN
2	2	93	SER
2	2	165	LEU
2	2	183	THR
2	2	224	GLY
2	2	229	PRO
3	3	9	PRO

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Mol	Chain	Res	Type
3	3	15	MET
3	3	57	SER
3	3	84	GLU
1	1	62	SER
1	1	179	LYS
1	1	182	ALA
3	3	54	CYS
3	3	88	THR
3	3	127	PRO
4	4	31	GLN
1	1	3	ASN
1	1	202	HIS
1	1	244	ASN
2	2	227	PRO
3	3	131	ALA
3	3	172	ALA
3	3	174	ALA
1	1	63	THR
1	1	118	ALA
1	1	135	VAL
1	1	187	LEU
2	2	44	PRO
2	2	156	SER
3	3	139	MET
3	3	196	ILE
1	1	220	CYS
1	1	20	SER
2	2	191	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	1	208/210 (99%)	158 (76%)	50 (24%)	0 4
2	2	176/203 (87%)	141 (80%)	35 (20%)	1 8
3	3	190/190 (100%)	152 (80%)	38 (20%)	1 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	4	18/65 (28%)	14 (78%)	4 (22%)	1 6
All	All	592/668 (89%)	465 (78%)	127 (22%)	1 6

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	2	THR
1	1	3	ASN
1	1	9	GLU
1	1	10	PRO
1	1	24	MET
1	1	28	THR
1	1	31	SER
1	1	36	ARG
1	1	39	ASP
1	1	40	VAL
1	1	42	THR
1	1	43	LEU
1	1	46	SER
1	1	47	ASN
1	1	49	THR
1	1	51	SER
1	1	56	VAL
1	1	70	ARG
1	1	71	LEU
1	1	79	PHE
1	1	87	GLN
1	1	90	PHE
1	1	91	THR
1	1	93	THR
1	1	95	SER
1	1	96	SER
1	1	97	VAL
1	1	101	PHE
1	1	117	ASP
1	1	130	ILE
1	1	138	MET
1	1	139	SER
1	1	146	ILE
1	1	149	SER
1	1	150	ARG
1	1	154	CYS

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Mol	Chain	Res	Type
1	1	161	THR
1	1	163	MET
1	1	165	ARG
1	1	183	THR
1	1	185	ASN
1	1	187	LEU
1	1	196	LEU
1	1	202	HIS
1	1	207	CYS
1	1	211	TYR
1	1	237	HIS
1	1	241	THR
1	1	245	LYS
1	1	246	GLN
2	2	42	ARG
2	2	44	PRO
2	2	51	VAL
2	2	52	THR
2	2	53	ARG
2	2	57	THR
2	2	64	PHE
2	2	85	SER
2	2	89	LYS
2	2	103	LEU
2	2	104	VAL
2	2	125	CYS
2	2	126	VAL
2	2	135	THR
2	2	146	GLU
2	2	157	VAL
2	2	159	PRO
2	2	161	GLN
2	2	162	LEU
2	2	163	LEU
2	2	165	LEU
2	2	166	ARG
2	2	168	ASN
2	2	175	MET
2	2	183	THR
2	2	193	THR
2	2	197	LEU
2	2	198	ILE

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Mol	Chain	Res	Type
2	2	203	THR
2	2	207	GLN
2	2	213	MET
2	2	215	VAL
2	2	218	ILE
2	2	221	MET
2	2	222	VAL
3	3	13	SER
3	3	23	THR
3	3	34	ARG
3	3	39	ARG
3	3	41	THR
3	3	42	ASN
3	3	44	ILE
3	3	50	THR
3	3	52	SER
3	3	56	ILE
3	3	59	LYS
3	3	70	ASP
3	3	71	GLU
3	3	76	MET
3	3	77	ASP
3	3	80	LEU
3	3	81	SER
3	3	84	GLU
3	3	97	PHE
3	3	124	PHE
3	3	139	MET
3	3	141	CYS
3	3	150	LEU
3	3	151	ASN
3	3	152	SER
3	3	161	SER
3	3	173	GLU
3	3	175	THR
3	3	176	VAL
3	3	178	ASN
3	3	179	VAL
3	3	183	LEU
3	3	188	LEU
3	3	191	LEU
3	3	209	SER

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Mol	Chain	Res	Type
3	3	213	ASP
3	3	216	LEU
3	3	217	ARG
4	4	21	ILE
4	4	24	ASN
4	4	27	MET
4	4	35	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	3	ASN
1	1	47	ASN
1	1	87	GLN
1	1	120	GLN
1	1	191	HIS
1	1	244	ASN
2	2	73	GLN
2	2	95	HIS
2	2	101	HIS
2	2	134	HIS
2	2	172	HIS
3	3	42	ASN
3	3	49	GLN
3	3	75	GLN
3	3	184	GLN
4	4	17	ASN
4	4	24	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

3 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GLC	A	1	5	12,12,12	0.70	0	17,17,17	0.68	0
5	GAL	A	2	5	11,11,12	0.65	0	15,15,17	0.73	0
5	SIA	A	3	5	20,20,21	1.11	2 (10%)	24,28,31	1.67	4 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GLC	A	1	5	-	2/2/22/22	0/1/1/1
5	GAL	A	2	5	-	2/2/19/22	0/1/1/1
5	SIA	A	3	5	-	2/18/34/38	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	3	SIA	C7-C6	-2.27	1.50	1.53
5	A	3	SIA	C4-C5	-2.26	1.51	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	3	SIA	C3-C4-C5	-5.14	105.25	111.46
5	A	3	SIA	C8-C7-C6	-3.18	107.00	113.03
5	A	3	SIA	C6-O6-C2	2.39	116.45	111.34
5	A	3	SIA	O1B-C1-C2	2.05	118.89	113.03

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2	GAL	O5-C5-C6-O6

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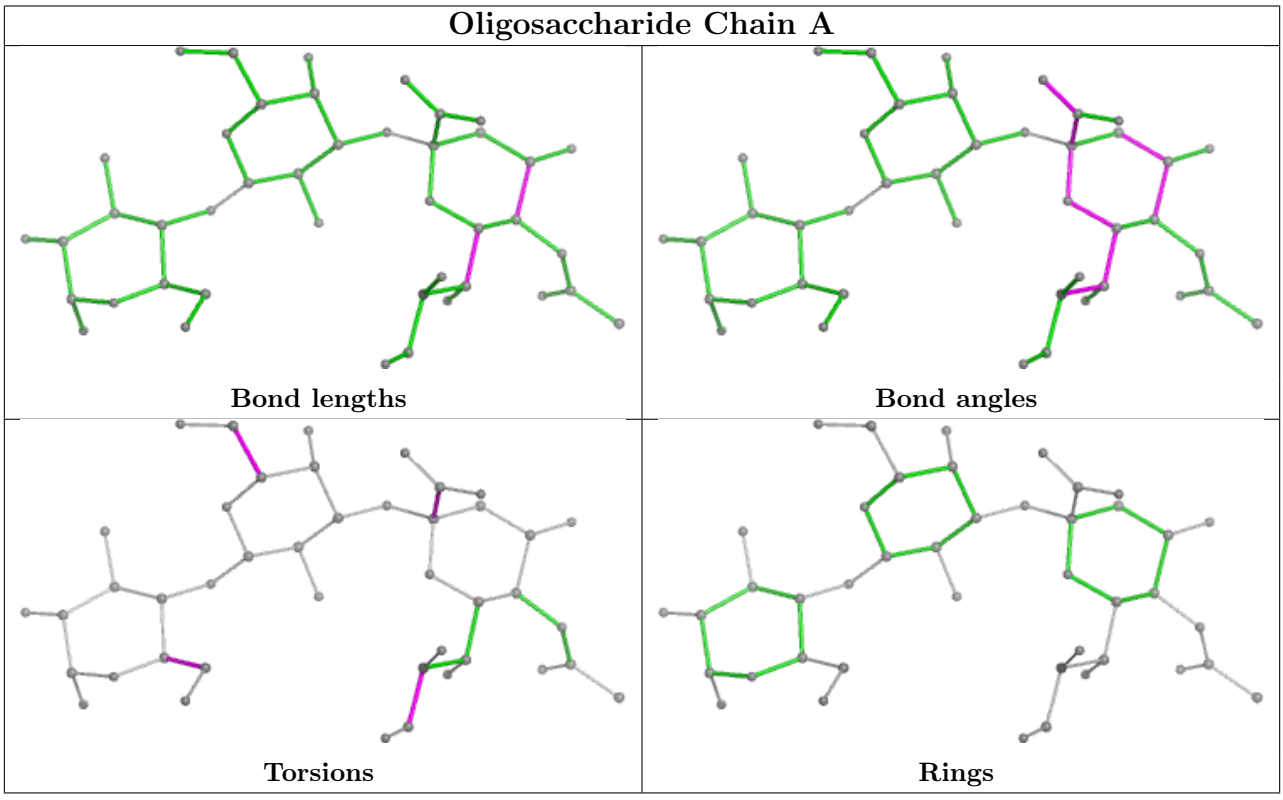
Mol	Chain	Res	Type	Atoms
5	A	1	GLC	O5-C5-C6-O6
5	A	2	GAL	C4-C5-C6-O6
5	A	1	GLC	C4-C5-C6-O6
5	A	3	SIA	O8-C8-C9-O9
5	A	3	SIA	O1A-C1-C2-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2	GAL	2	0
5	A	3	SIA	2	0

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



5.6 Ligand geometry (i)

There are no ligands in this entry.

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	1	247/248 (99%)	-1.12	0	100	100	2, 10, 44, 101	0
2	2	200/230 (86%)	-1.19	0	100	100	2, 6, 43, 88	0
3	3	226/226 (100%)	-1.25	0	100	100	2, 4, 26, 61	0
4	4	22/80 (27%)	-0.75	0	100	100	15, 37, 55, 71	0
All	All	695/784 (88%)	-1.17	0	100	100	2, 6, 44, 101	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

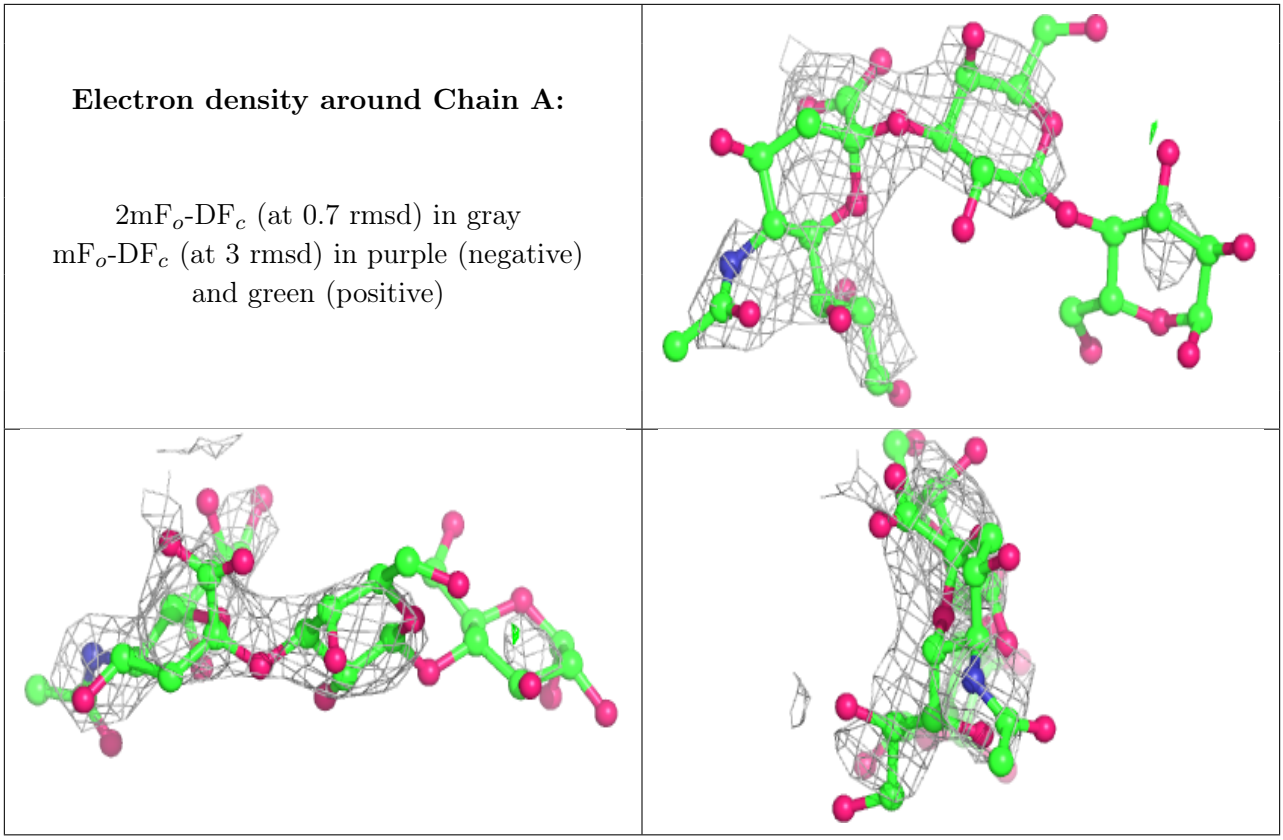
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GLC	A	1	12/12	0.86	0.94	62,73,74,75	12
5	GAL	A	2	11/12	0.94	0.54	35,47,53,55	11
5	SIA	A	3	20/21	0.96	0.32	3,18,26,27	20

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 A:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.