Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 02:38 AM EDT

PDB ID	:	6NZ7
Title	:	Crystal structure of broadly neutralizing Influenza A antibody 429 B01 in complex with Hemagglutinin Hong Kong 1968
Authors	:	Zhou, T.; Kwong, P.D.
Deposited on	:	2019-02-13
Resolution	:	2.95 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:

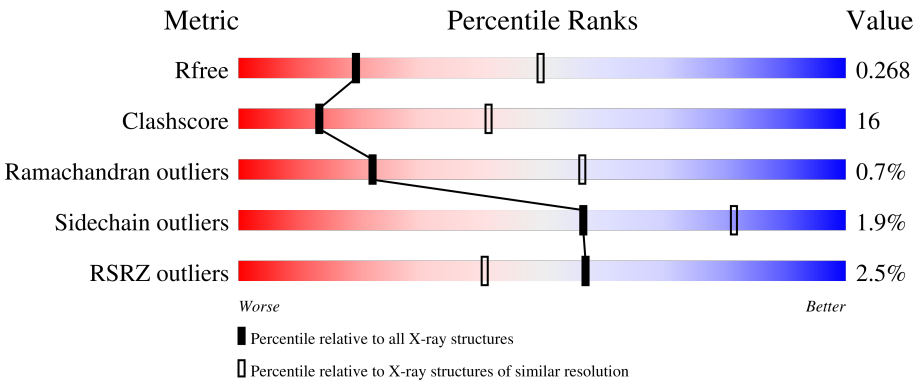
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	319	84% 15% •
1	E	319	6% 80% 18% •
2	B	173	% 72% 21% • 5%
2	F	173	4% 65% 25% • 9%
3	G	228	2% 64% 30% • •

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Mol	Chain	Length	Quality of chain
3	H	228	2% 61% 34%
4	I	214	% 66% 30%
4	L	214	2% 74% 26%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 17212 atoms, of which 2914 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	319	2467	1544	433	477	13	0	0	0
1	E	319	2467	1544	433	477	13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	218	GLU	GLY	conflict	UNP Q91MA7
E	218	GLU	GLY	conflict	UNP Q91MA7

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	165	1343	833	235	269	6	0	0	0
2	F	157	1271	788	221	256	6	0	0	0

- Molecule 3 is a protein called 429 B01 FAB heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	H	220	2307	1038	664	278	322	5	0	0	0
3	G	221	2333	1045	679	280	324	5	0	0	0

- Molecule 4 is a protein called 429 B01 FAB light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	L	214	2428	1023	788	280	331	6	0	0	0

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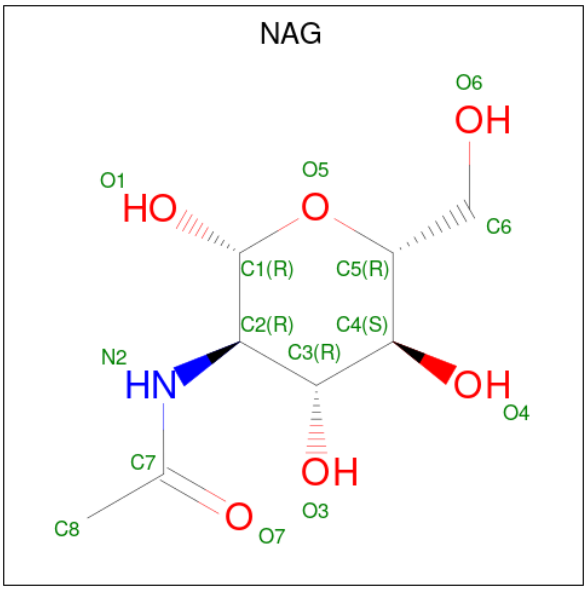
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	I	214	2423	1023	783	280	331	6	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
5	A	1	14	8	1	5	0	0
5	A	1	14	8	1	5	0	0
5	A	1	14	8	1	5	0	0
5	B	1	14	8	1	5	0	0
5	H	1	14	8	1	5	0	0
5	E	1	14	8	1	5	0	0
5	E	1	14	8	1	5	0	0
5	E	1	14	8	1	5	0	0
5	F	1	14	8	1	5	0	0

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

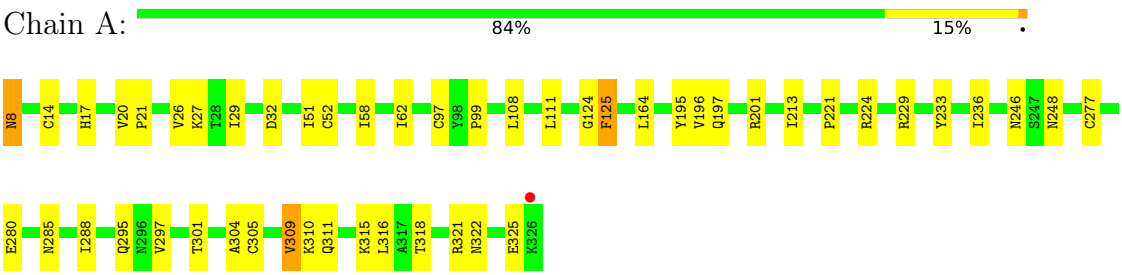
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	8	8	8	0	0
6	B	1	1	1	0	0
6	H	3	3	3	0	0
6	L	4	4	4	0	0
6	E	1	1	1	0	0
6	F	1	1	1	0	0
6	G	1	1	1	0	0

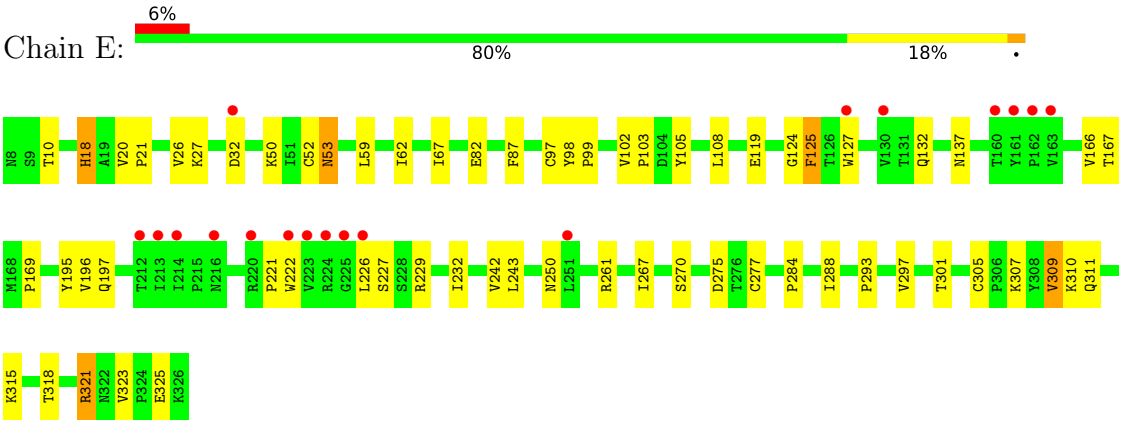
3 Residue-property plots (i)

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.

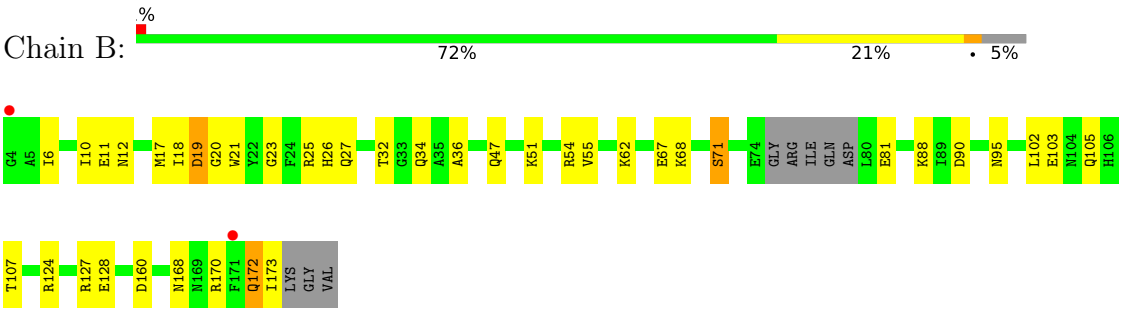
• Molecule 1: Hemagglutinin HA1 chain



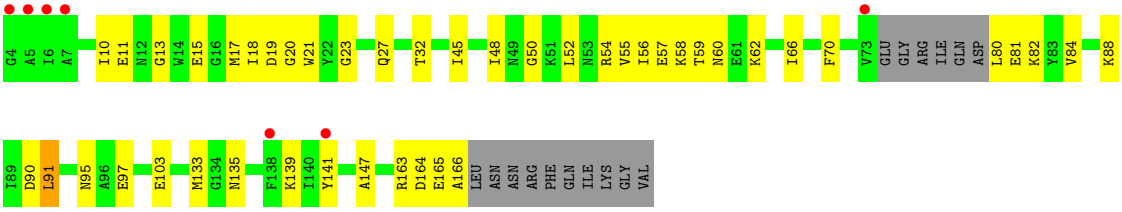
• Molecule 1: Hemagglutinin HA1 chain



• Molecule 2: Hemagglutinin HA2 chain

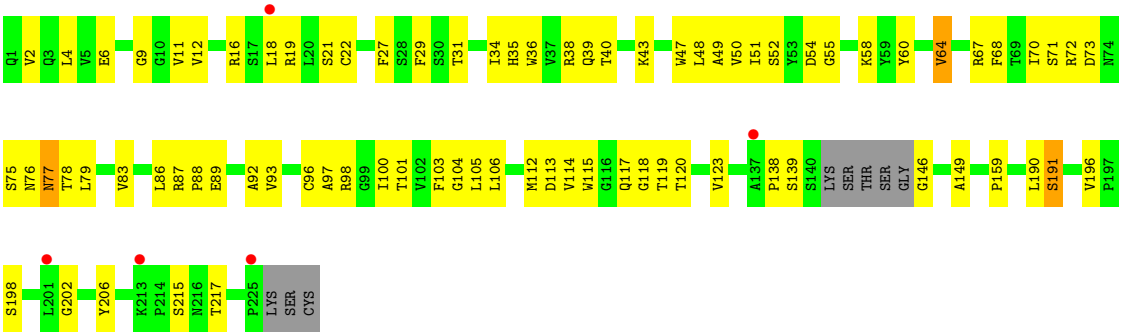


• Molecule 2: Hemagglutinin HA2 chain



- Molecule 3: 429 B01 FAB heavy chain

Chain H:

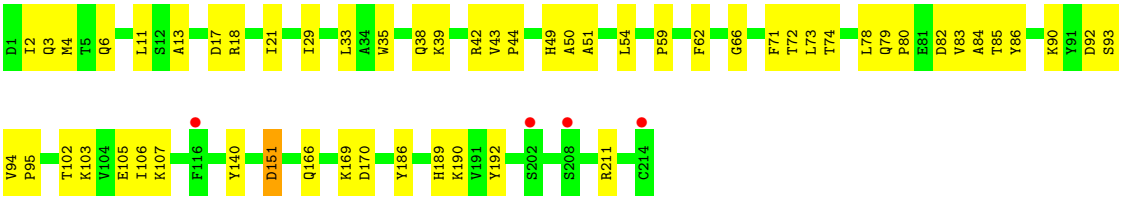


- Molecule 3: 429 B01 FAB heavy chain

Chain G:

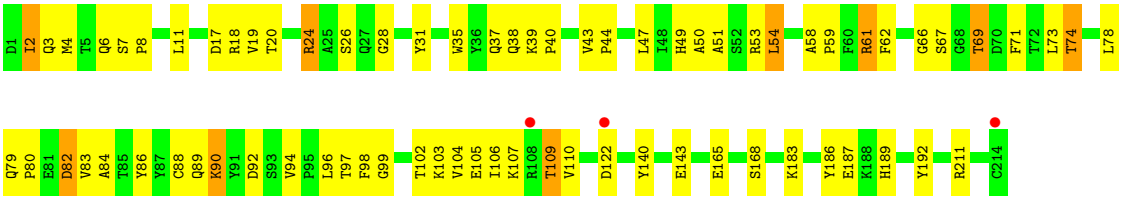
- Molecule 4: 429 B01 FAB light chain

Chain L:



- Molecule 4: 429 B01 FAB light chain

Chain I:


D1
I2
Q3
M4
T5
Q6
S7
P8
L11
D17
R18
V19
T20
R24
A25
S26
Q27
G28
Y31
W35
Y36
Q37
Q38
K39
P40
V43
P44
L47
I48
H49
A50
A51
S52
R53
L54
A58
P59
F60
R61
F62
G66
S67
G68
T69
D70
F71
T72
L73
T74
L78
Q79
P80
E81
D82
V83
A84
T85
Y86
Y87
C88
Q89
K90
Y91
D92
S93
V94
P95
L96
T97
F98
G99
T102
K103
V104
E105
I106
K107
R108
T109
V110
D122
Y140
E143
E165
S168
K183
Y186
E187
K188
H189
Y192
R211
C214

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	91.77Å 123.91Å 119.34Å 90.00° 112.00° 90.00°	Depositor
Resolution (Å)	42.23 – 2.95 42.22 – 2.93	Depositor EDS
% Data completeness (in resolution range)	93.5 (42.23-2.95) 86.0 (42.22-2.93)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 2.95Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.224 , 0.267 0.225 , 0.268	Depositor DCC
R_{free} test set	2510 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	81.8	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 42.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17212	wwPDB-VP
Average B, all atoms (Å^2)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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	0.32	0/2523	0.56	0/3438
1	E	0.29	0/2523	0.51	0/3438
2	B	0.32	0/1365	0.48	0/1834
2	F	0.32	0/1292	0.52	0/1736
3	G	0.32	0/1691	0.51	0/2308
3	H	0.32	0/1680	0.52	0/2294
4	I	0.28	0/1674	0.49	0/2273
4	L	0.28	0/1674	0.47	0/2273
All	All	0.31	0/14422	0.51	0/19594

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 (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	2467	0	2413	44	0
1	E	2467	0	2414	54	1
2	B	1343	0	1261	40	1
2	F	1271	0	1191	61	0
3	G	1654	679	1634	89	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1643	664	1619	96	0
4	I	1640	783	1599	63	1
4	L	1640	788	1599	51	1
5	A	56	0	52	3	0
5	B	14	0	13	0	0
5	E	42	0	39	0	0
5	F	14	0	13	1	0
5	G	14	0	13	0	0
5	H	14	0	13	2	0
6	A	8	0	0	1	0
6	B	1	0	0	0	0
6	E	1	0	0	1	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	3	0	0	0	0
6	L	4	0	0	1	0
All	All	14298	2914	13873	455	3

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 16.

All (455) 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:B:17:MET:HE1	2:B:23:GLY:HA3	1.29	1.14
4:I:20:THR:HG22	4:I:74:THR:HG22	1.35	1.07
3:G:47:TRP:HZ2	3:G:50:VAL:HG23	1.32	0.94
4:L:83:VAL:HG22	4:L:106:ILE:HD13	1.50	0.93
1:E:99:PRO:HG2	1:E:226:LEU:HB2	1.50	0.93
3:H:12:VAL:HG21	3:H:18:LEU:HG	1.52	0.91
3:G:11:VAL:HG21	3:G:128:THR:HG22	1.51	0.89
3:H:64:VAL:HG13	3:H:68:PHE:CD1	2.10	0.86
1:E:221:PRO:O	1:E:229:ARG:NH1	2.08	0.86
3:H:64:VAL:HG22	3:H:68:PHE:CE1	2.10	0.86
3:H:47:TRP:HZ2	3:H:50:VAL:HG23	1.38	0.85
4:I:83:VAL:HG22	4:I:106:ILE:HD13	1.56	0.85
4:I:6:GLN:NE2	4:I:86:TYR:O	2.08	0.85
1:A:97:CYS:O	1:A:224:ARG:NH1	2.11	0.84
3:G:47:TRP:CZ2	3:G:50:VAL:HG23	2.12	0.83
3:H:11:VAL:HG23	3:H:159:PRO:HG3	1.60	0.83
3:G:97:ALA:HB1	3:G:112:MET:HG2	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:34:ILE:HG21	3:H:79:LEU:HD22	1.61	0.82
3:G:9:GLY:H	3:G:119:THR:HG21	1.42	0.82
1:A:29:ILE:HD13	2:B:102:LEU:HD23	1.62	0.82
2:F:27:GLN:HG3	2:F:32:THR:HG22	1.62	0.81
4:L:92:ASP:OD1	4:L:93:SER:N	2.13	0.81
3:H:86:LEU:HD23	3:H:123:VAL:HG12	1.62	0.81
2:F:141:TYR:HB2	2:F:165:GLU:OE2	1.81	0.81
4:I:59:PRO:HB2	4:I:61:ARG:HE	1.44	0.81
5:A:401:NAG:H62	3:H:104:GLY:H	1.46	0.81
1:E:325:GLU:HB2	2:F:15:GLU:HG3	1.63	0.81
3:H:9:GLY:H	3:H:119:THR:HG21	1.45	0.80
1:A:221:PRO:O	1:A:229:ARG:NH1	2.12	0.80
3:G:12:VAL:HG21	3:G:18:LEU:HG	1.64	0.80
1:A:27:LYS:HG2	1:A:32:ASP:O	1.82	0.79
3:H:47:TRP:CZ2	3:H:50:VAL:HG23	2.17	0.79
3:H:97:ALA:HB1	3:H:112:MET:HG2	1.63	0.79
3:H:31:THR:CG2	3:H:106:LEU:HD21	2.13	0.79
2:F:18:ILE:HG22	3:G:106:LEU:HB2	1.66	0.78
3:G:91:THR:HG22	3:G:123:VAL:H	1.46	0.78
3:H:31:THR:HG22	3:H:106:LEU:HD21	1.65	0.78
3:H:86:LEU:HB3	3:H:123:VAL:HG11	1.64	0.78
2:B:55:VAL:HG22	2:B:103:GLU:HG3	1.66	0.78
3:H:76:ASN:ND2	5:H:301:NAG:O7	2.17	0.78
4:I:61:ARG:NH2	4:I:82:ASP:OD1	2.17	0.76
2:B:51:LYS:HE2	2:B:107:THR:OG1	1.85	0.76
2:F:165:GLU:HG2	2:F:166:ALA:H	1.50	0.76
4:L:6:GLN:NE2	4:L:86:TYR:O	2.18	0.76
3:H:146:GLY:O	3:H:198:SER:OG	2.00	0.76
1:E:325:GLU:HB2	2:F:15:GLU:CG	2.16	0.76
1:E:119:GLU:OE1	1:E:261:ARG:NH2	2.19	0.76
3:G:31:THR:HG22	3:G:106:LEU:HD21	1.68	0.75
3:H:87:ARG:HB3	3:H:88:PRO:HD2	1.69	0.75
3:G:93:VAL:HG22	3:G:120:THR:HG22	1.69	0.74
1:E:310:LYS:HD3	2:F:90:ASP:OD1	1.88	0.73
2:B:27:GLN:HG3	2:B:32:THR:HG22	1.70	0.73
3:G:12:VAL:HG21	3:G:18:LEU:CG	2.18	0.73
3:H:12:VAL:HG21	3:H:18:LEU:CG	2.18	0.73
1:A:318:THR:O	1:A:318:THR:HG22	1.87	0.72
3:H:4:LEU:HD12	3:H:4:LEU:O	1.88	0.72
4:I:88:CYS:O	4:I:99:GLY:N	2.21	0.72
1:E:318:THR:HG22	1:E:318:THR:O	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:GLU:O	2:B:170:ARG:NH2	2.21	0.72
3:G:100:ILE:HG22	3:G:113:ASP:HB2	1.72	0.71
4:I:17:ASP:OD2	4:I:18:ARG:N	2.20	0.71
2:F:10:ILE:HG13	2:F:135:ASN:HA	1.71	0.71
2:B:172:GLN:O	2:B:173:ILE:HG13	1.91	0.71
1:E:288:ILE:HD13	1:E:297:VAL:HG11	1.73	0.71
2:F:18:ILE:CG2	3:G:106:LEU:HD13	2.21	0.70
2:F:56:ILE:HA	2:F:59:THR:OG1	1.91	0.70
1:E:195:TYR:O	1:E:196:VAL:HG22	1.90	0.70
3:G:16:ARG:NH1	3:G:16:ARG:HB3	2.06	0.70
3:H:93:VAL:HG22	3:H:120:THR:HG22	1.75	0.69
3:G:91:THR:HA	3:G:121:VAL:O	1.92	0.69
3:H:86:LEU:HD23	3:H:123:VAL:CG1	2.23	0.69
2:F:66:ILE:CD1	2:F:91:LEU:HD12	2.23	0.68
2:F:66:ILE:HD13	2:F:91:LEU:HD12	1.75	0.68
2:F:165:GLU:HG2	2:F:166:ALA:N	2.09	0.68
2:F:56:ILE:HA	2:F:59:THR:HG1	1.58	0.68
3:G:87:ARG:O	3:G:123:VAL:HG21	1.93	0.68
3:G:11:VAL:HG22	3:G:159:PRO:HG3	1.76	0.68
4:I:183:LYS:NZ	4:I:187:GLU:OE2	2.27	0.68
3:H:34:ILE:CG2	3:H:79:LEU:HD22	2.24	0.67
4:L:2:ILE:HG22	4:L:3:GLN:H	1.59	0.67
3:H:36:TRP:NE1	3:H:79:LEU:HD21	2.10	0.67
3:G:31:THR:CG2	3:G:106:LEU:HD21	2.24	0.67
2:B:19:ASP:OD1	2:B:19:ASP:N	2.27	0.67
4:L:79:GLN:HB3	4:L:80:PRO:HD2	1.77	0.66
3:G:16:ARG:HB3	3:G:16:ARG:HH11	1.58	0.66
2:B:62:LYS:HD2	2:B:95:ASN:ND2	2.10	0.66
4:L:33:LEU:HD13	4:L:71:PHE:CG	2.31	0.66
4:I:28:GLY:HA2	4:I:69:THR:HG22	1.76	0.66
3:H:39:GLN:O	3:H:92:ALA:HB1	1.96	0.66
2:B:17:MET:HE1	2:B:23:GLY:CA	2.18	0.65
4:L:38:GLN:HG3	4:L:44:PRO:HG3	1.78	0.65
2:F:54:ARG:NH1	2:F:103:GLU:OE1	2.30	0.65
4:I:20:THR:HG22	4:I:74:THR:CG2	2.21	0.65
3:H:51:ILE:HB	3:H:70:ILE:HG21	1.76	0.65
3:H:97:ALA:CB	3:H:112:MET:HG2	2.26	0.65
1:A:310:LYS:HD3	2:B:90:ASP:OD1	1.97	0.65
2:B:21:TRP:CD1	3:H:105:LEU:HD11	2.32	0.65
2:F:21:TRP:CD1	3:G:105:LEU:HD11	2.32	0.64
4:I:59:PRO:HG2	4:I:62:PHE:CD1	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ARG:HD3	6:A:502:HOH:O	1.98	0.64
3:H:48:LEU:HD22	3:H:64:VAL:HG21	1.79	0.64
3:G:5:VAL:HG23	3:G:23:ALA:HB3	1.79	0.64
1:A:111:LEU:HD11	1:A:236:ILE:HD11	1.80	0.64
2:B:25:ARG:NH2	2:B:34:GLN:OE1	2.27	0.64
1:E:99:PRO:HD3	1:E:226:LEU:HD12	1.80	0.64
3:G:51:ILE:HG21	3:G:79:LEU:HD11	1.80	0.64
4:I:80:PRO:O	4:I:83:VAL:HG23	1.96	0.64
4:L:83:VAL:CG2	4:L:106:ILE:HD13	2.26	0.64
3:H:9:GLY:N	3:H:119:THR:HG21	2.12	0.63
4:I:187:GLU:O	4:I:211:ARG:NH1	2.31	0.62
3:G:87:ARG:HB3	3:G:88:PRO:HD2	1.81	0.62
3:H:68:PHE:CE2	3:H:83:VAL:HG22	2.34	0.62
3:G:97:ALA:CB	3:G:112:MET:HG2	2.27	0.62
4:L:17:ASP:OD2	4:L:18:ARG:N	2.32	0.62
1:A:195:TYR:O	1:A:196:VAL:HG22	1.99	0.62
3:G:49:ALA:HB3	3:G:70:ILE:HD11	1.82	0.62
4:I:59:PRO:HG2	4:I:62:PHE:CE1	2.34	0.62
4:I:8:PRO:HG2	4:I:11:LEU:HD23	1.81	0.62
1:A:288:ILE:HD13	1:A:297:VAL:HG11	1.82	0.61
3:H:40:THR:HB	3:H:43:LYS:HB2	1.83	0.61
3:G:6:GLU:OE2	3:G:118:GLY:N	2.33	0.61
3:H:16:ARG:O	3:H:86:LEU:HD13	1.99	0.61
4:L:78:LEU:HD12	4:L:79:GLN:H	1.66	0.61
2:F:80:LEU:O	2:F:81:GLU:HB2	2.01	0.61
4:L:78:LEU:CD1	4:L:82:ASP:HB2	2.31	0.61
3:H:9:GLY:HA3	3:H:119:THR:HG22	1.82	0.61
3:H:22:CYS:HB3	3:H:79:LEU:HB3	1.81	0.61
3:H:52:SER:OG	3:H:54:ASP:OD2	2.16	0.61
4:I:79:GLN:HB3	4:I:80:PRO:HD2	1.83	0.60
2:B:67:GLU:O	2:B:71:SER:OG	2.18	0.60
3:H:35:HIS:ND1	3:H:50:VAL:HG22	2.17	0.60
4:L:189:HIS:O	4:L:211:ARG:NH1	2.35	0.60
3:G:72:ARG:HB3	3:G:79:LEU:HD12	1.82	0.60
2:F:18:ILE:HG21	3:G:106:LEU:HD22	1.83	0.60
4:L:43:VAL:HG13	4:L:44:PRO:HD2	1.84	0.60
3:G:35:HIS:ND1	3:G:50:VAL:HG22	2.17	0.60
1:E:99:PRO:CD	1:E:226:LEU:HD12	2.32	0.59
2:F:163:ARG:NH1	2:F:164:ASP:OD1	2.34	0.59
4:L:2:ILE:HG22	4:L:3:GLN:N	2.18	0.59
4:L:29:ILE:HG22	4:L:92:ASP:OD2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:50:GLY:HA2	4:I:31:TYR:CE2	2.38	0.59
3:G:64:VAL:HG13	3:G:64:VAL:O	2.01	0.59
3:H:87:ARG:O	3:H:123:VAL:HG21	2.03	0.59
3:G:91:THR:HG23	3:G:123:VAL:HG22	1.82	0.59
4:I:61:ARG:H	4:I:61:ARG:HD3	1.68	0.59
3:H:73:ASP:OD1	3:H:75:SER:OG	2.21	0.58
2:F:81:GLU:O	2:F:84:VAL:N	2.36	0.58
4:I:66:GLY:HA3	4:I:71:PHE:HA	1.85	0.58
4:I:54:LEU:HD22	4:I:58:ALA:HB3	1.84	0.58
5:A:401:NAG:H62	3:H:104:GLY:N	2.16	0.58
1:E:321:ARG:HG2	6:E:501:HOH:O	2.04	0.58
3:G:40:THR:HB	3:G:43:LYS:HB2	1.85	0.58
3:H:64:VAL:HG13	3:H:68:PHE:HD1	1.65	0.57
3:G:91:THR:HG22	3:G:123:VAL:N	2.18	0.57
2:F:55:VAL:HG22	2:F:103:GLU:HG3	1.86	0.57
3:H:77:ASN:OD1	3:H:77:ASN:N	2.37	0.57
4:I:2:ILE:O	4:I:3:GLN:HG2	2.05	0.57
3:H:98:ARG:NH2	3:H:113:ASP:OD2	2.37	0.57
1:E:309:VAL:HG13	1:E:311:GLN:OE1	2.05	0.57
4:I:43:VAL:HG13	4:I:44:PRO:HD2	1.86	0.57
4:L:72:THR:HG22	4:L:74:THR:CG2	2.35	0.56
4:L:94:VAL:HG13	4:L:95:PRO:HA	1.86	0.56
1:A:26:VAL:HG12	1:A:315:LYS:CB	2.35	0.56
1:E:311:GLN:HE21	2:F:97:GLU:HB2	1.70	0.56
3:G:68:PHE:HA	3:G:82:GLN:O	2.05	0.56
1:E:222:TRP:CZ3	1:E:227:SER:HB3	2.41	0.56
1:A:29:ILE:HD13	2:B:102:LEU:CD2	2.35	0.56
2:B:18:ILE:CG2	3:H:106:LEU:HD13	2.36	0.56
4:L:39:LYS:HA	4:L:84:ALA:HB2	1.86	0.56
4:L:151:ASP:OD2	4:L:190:LYS:N	2.38	0.56
3:G:197:PRO:O	3:G:199:SER:N	2.39	0.56
3:G:97:ALA:HB1	3:G:112:MET:CG	2.36	0.55
4:I:19:VAL:HG21	4:I:78:LEU:HD22	1.87	0.55
1:E:311:GLN:NE2	2:F:97:GLU:HB2	2.21	0.55
3:G:86:LEU:HD23	3:G:123:VAL:HG12	1.87	0.55
3:H:2:VAL:HG13	3:H:27:PHE:CD1	2.41	0.55
3:H:9:GLY:HA3	3:H:119:THR:CG2	2.36	0.55
1:A:285:ASN:ND2	5:A:404:NAG:O7	2.40	0.55
1:A:26:VAL:HG12	1:A:315:LYS:HB3	1.88	0.55
2:B:20:GLY:HA2	3:H:105:LEU:HD13	1.88	0.55
3:H:36:TRP:NE1	3:H:79:LEU:CD2	2.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:169:PRO:HB3	1:E:242:VAL:HG12	1.89	0.54
3:H:31:THR:HG23	3:H:106:LEU:HD21	1.88	0.54
4:L:50:ALA:O	4:L:51:ALA:HB3	2.06	0.54
4:L:78:LEU:HD12	4:L:79:GLN:N	2.22	0.54
3:G:34:ILE:HG21	3:G:79:LEU:HD22	1.89	0.54
3:G:86:LEU:HB3	3:G:123:VAL:HG11	1.88	0.54
3:H:49:ALA:HB3	3:H:70:ILE:HD11	1.90	0.54
2:F:20:GLY:HA2	3:G:105:LEU:HD13	1.90	0.54
1:E:20:VAL:HG13	1:E:21:PRO:HD2	1.89	0.54
1:E:18:HIS:CE1	3:G:105:LEU:HD21	2.43	0.54
3:H:68:PHE:CE2	3:H:83:VAL:HG13	2.43	0.54
1:E:127:TRP:CZ3	1:E:166:VAL:HG11	2.43	0.54
2:F:10:ILE:HG22	2:F:11:GLU:HG3	1.90	0.54
1:A:301:THR:HB	1:A:305:CYS:SG	2.48	0.54
1:A:280:GLU:HG3	1:A:304:ALA:H	1.73	0.54
4:L:78:LEU:HD11	4:L:82:ASP:HB2	1.90	0.53
2:F:147:ALA:O	5:F:201:NAG:O6	2.26	0.53
4:L:72:THR:HG22	4:L:74:THR:HG22	1.90	0.53
1:E:195:TYR:CZ	1:E:250:ASN:HA	2.43	0.53
1:E:325:GLU:HB2	2:F:15:GLU:HG2	1.91	0.53
4:I:78:LEU:HD12	4:I:79:GLN:N	2.24	0.53
2:F:62:LYS:HD2	2:F:95:ASN:ND2	2.24	0.53
4:I:24:ARG:HB2	4:I:24:ARG:HH11	1.73	0.53
3:G:91:THR:CG2	3:G:123:VAL:HG22	2.38	0.53
3:H:68:PHE:CD2	3:H:83:VAL:HG22	2.43	0.53
3:H:100:ILE:CG2	3:H:113:ASP:HB2	2.38	0.53
4:L:59:PRO:HG2	4:L:62:PHE:CD1	2.44	0.53
1:E:325:GLU:OE1	2:F:15:GLU:HB2	2.09	0.53
2:F:54:ARG:HA	2:F:57:GLU:HG2	1.90	0.53
1:E:67:ILE:HG13	1:E:105:TYR:CE2	2.44	0.52
2:F:54:ARG:NH1	2:F:103:GLU:OE2	2.42	0.52
1:E:10:THR:HG22	2:F:141:TYR:HA	1.91	0.52
1:A:213:ILE:HD12	1:A:233:TYR:OH	2.08	0.52
2:F:18:ILE:HG21	3:G:106:LEU:HD13	1.89	0.52
1:A:318:THR:CG2	3:H:103:PHE:CD1	2.92	0.52
3:H:36:TRP:HE1	3:H:79:LEU:HD21	1.74	0.52
2:F:17:MET:CE	2:F:23:GLY:HA3	2.39	0.52
2:B:10:ILE:HG22	2:B:11:GLU:HG3	1.92	0.52
2:F:91:LEU:HD13	2:F:91:LEU:O	2.08	0.52
2:F:163:ARG:HG3	2:F:164:ASP:N	2.25	0.52
1:A:310:LYS:HZ2	2:B:90:ASP:CG	2.12	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:66:GLY:HA3	4:L:71:PHE:HA	1.92	0.52
3:G:123:VAL:O	3:G:123:VAL:HG23	2.09	0.52
4:I:50:ALA:O	4:I:51:ALA:HB3	2.10	0.52
3:H:64:VAL:CG1	3:H:64:VAL:O	2.57	0.52
4:L:106:ILE:H	4:L:166:GLN:HE22	1.57	0.52
1:E:27:LYS:HG2	1:E:32:ASP:O	2.10	0.52
2:B:68:LYS:HA	2:B:71:SER:OG	2.10	0.52
1:A:108:LEU:O	1:A:108:LEU:HD23	2.10	0.51
1:E:307:LYS:NZ	2:F:60:ASN:OD1	2.42	0.51
3:G:6:GLU:OE1	3:G:95:TYR:HA	2.10	0.51
4:L:80:PRO:O	4:L:83:VAL:HG23	2.10	0.51
1:A:51:ILE:HG22	1:A:58:ILE:CD1	2.41	0.51
4:I:69:THR:O	4:I:69:THR:OG1	2.20	0.51
4:L:21:ILE:HG12	4:L:102:THR:HG21	1.92	0.51
1:A:8:ASN:N	1:A:8:ASN:HD22	2.09	0.51
1:E:222:TRP:CH2	1:E:227:SER:HB3	2.45	0.51
4:I:78:LEU:HD12	4:I:79:GLN:H	1.76	0.51
4:I:186:TYR:O	4:I:192:TYR:OH	2.28	0.50
3:H:215:SER:HG	3:H:217:THR:HG1	1.59	0.50
1:E:52:CYS:HB3	1:E:277:CYS:O	2.12	0.50
3:H:21:SER:HA	3:H:79:LEU:O	2.11	0.50
3:G:24:ALA:HB2	3:G:29:PHE:CD1	2.46	0.50
3:H:115:TRP:HB2	4:L:43:VAL:HG11	1.93	0.50
4:I:39:LYS:HA	4:I:84:ALA:HB2	1.93	0.50
4:I:54:LEU:CD2	4:I:58:ALA:HB3	2.42	0.50
1:E:97:CYS:SG	1:E:98:TYR:N	2.83	0.50
3:H:4:LEU:HD13	3:H:96:CYS:HB2	1.94	0.50
3:H:36:TRP:HE1	3:H:79:LEU:CD2	2.25	0.50
3:H:190:LEU:O	3:H:191:SER:CB	2.60	0.50
2:F:19:ASP:OD1	3:G:108:ILE:HD13	2.12	0.50
3:H:38:ARG:HA	3:H:93:VAL:O	2.12	0.49
1:A:309:VAL:HG13	1:A:311:GLN:OE1	2.13	0.49
3:H:51:ILE:HD13	3:H:72:ARG:HD2	1.94	0.49
3:G:51:ILE:HB	3:G:70:ILE:HG21	1.94	0.49
4:I:2:ILE:HG22	4:I:3:GLN:N	2.27	0.49
3:G:39:GLN:O	3:G:92:ALA:HB1	2.13	0.49
4:L:103:LYS:HE2	4:L:105:GLU:OE2	2.12	0.49
3:G:77:ASN:O	3:G:77:ASN:ND2	2.46	0.49
3:G:70:ILE:HA	3:G:80:TYR:O	2.11	0.49
3:G:88:PRO:HA	3:G:123:VAL:CG2	2.42	0.49
3:H:86:LEU:HB3	3:H:123:VAL:CG1	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:42:ARG:NH1	6:L:301:HOH:O	2.45	0.49
3:H:6:GLU:H	3:H:117:GLN:HE22	1.61	0.49
3:G:38:ARG:HA	3:G:93:VAL:O	2.13	0.49
4:I:49:HIS:O	4:I:53:ARG:HB2	2.13	0.49
3:H:123:VAL:HG23	3:H:123:VAL:O	2.12	0.49
1:E:53:ASN:O	1:E:53:ASN:ND2	2.36	0.48
1:E:102:VAL:HG22	1:E:232:ILE:HB	1.95	0.48
3:G:97:ALA:HA	3:G:114:VAL:O	2.13	0.48
4:I:7:SER:HA	4:I:8:PRO:C	2.32	0.48
4:I:8:PRO:CG	4:I:11:LEU:HD23	2.42	0.48
1:A:52:CYS:HB3	1:A:277:CYS:O	2.13	0.48
3:G:100:ILE:CG2	3:G:113:ASP:HB2	2.41	0.48
4:I:103:LYS:HE2	4:I:105:GLU:OE2	2.13	0.48
1:A:14:CYS:SG	2:B:6:ILE:HG13	2.54	0.48
1:A:17:HIS:HA	2:B:21:TRP:O	2.13	0.48
1:E:108:LEU:HD23	1:E:108:LEU:O	2.14	0.48
1:E:318:THR:O	1:E:318:THR:CG2	2.60	0.48
2:F:54:ARG:NH1	2:F:103:GLU:CD	2.67	0.48
3:G:4:LEU:HD23	3:G:96:CYS:CB	2.43	0.48
4:I:20:THR:CG2	4:I:74:THR:HG22	2.25	0.48
4:I:107:LYS:HB3	4:I:140:TYR:OH	2.13	0.48
2:B:124:ARG:O	2:B:127:ARG:HG2	2.14	0.48
2:F:27:GLN:CG	2:F:32:THR:HG22	2.40	0.48
4:I:109:THR:HG22	4:I:110:VAL:O	2.14	0.48
2:F:17:MET:HE3	2:F:23:GLY:HA3	1.96	0.47
4:I:49:HIS:O	4:I:50:ALA:HB3	2.13	0.47
2:F:21:TRP:CZ3	2:F:45:ILE:HG13	2.50	0.47
1:A:196:VAL:CG2	1:A:197:GLN:N	2.77	0.47
4:L:33:LEU:C	4:L:33:LEU:HD23	2.34	0.47
3:G:21:SER:HA	3:G:79:LEU:O	2.14	0.47
3:G:83:VAL:HG12	3:G:86:LEU:HD12	1.95	0.47
4:L:2:ILE:HB	4:L:90:LYS:HE2	1.96	0.47
1:E:103:PRO:HD2	1:E:232:ILE:O	2.15	0.47
3:G:45:LEU:HD12	3:G:45:LEU:H	1.80	0.47
4:L:38:GLN:O	4:L:84:ALA:HB1	2.15	0.47
1:A:201:ARG:HB3	1:A:248:ASN:ND2	2.29	0.47
4:I:35:TRP:CD2	4:I:73:LEU:HB2	2.50	0.47
1:E:325:GLU:OE1	2:F:15:GLU:HG3	2.16	0.47
3:G:11:VAL:HG21	3:G:128:THR:CG2	2.36	0.47
4:L:59:PRO:HG2	4:L:62:PHE:CE1	2.51	0.46
3:G:36:TRP:HE1	3:G:79:LEU:CD2	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:59:TYR:HB3	4:I:94:VAL:HG11	1.96	0.46
3:H:70:ILE:HG22	3:H:71:SER:N	2.30	0.46
3:H:86:LEU:CD2	3:H:123:VAL:HG12	2.40	0.46
4:I:143:GLU:OE1	4:I:143:GLU:N	2.39	0.46
3:H:51:ILE:HD12	3:H:70:ILE:HG22	1.97	0.46
1:E:59:LEU:HD21	1:E:82:GLU:HG2	1.97	0.46
3:H:67:ARG:NH2	3:H:87:ARG:HD2	2.31	0.46
4:L:107:LYS:HA	4:L:140:TYR:OH	2.15	0.46
2:B:17:MET:CE	2:B:36:ALA:HA	2.46	0.46
3:H:89:GLU:O	3:H:89:GLU:HG2	2.16	0.46
3:H:76:ASN:CG	5:H:301:NAG:O7	2.54	0.46
3:G:107:ILE:HG23	3:G:109:ASN:H	1.80	0.46
4:I:122:ASP:OD2	4:I:122:ASP:N	2.48	0.46
3:H:190:LEU:O	3:H:191:SER:HB2	2.16	0.46
1:E:127:TRP:HB2	1:E:132:GLN:NE2	2.31	0.46
1:E:196:VAL:CG2	1:E:197:GLN:N	2.78	0.46
1:A:29:ILE:HG22	2:B:105:GLN:OE1	2.16	0.46
1:A:124:GLY:O	1:A:125:PHE:O	2.33	0.46
3:H:29:PHE:CD2	3:H:77:ASN:HA	2.51	0.46
2:F:54:ARG:HA	2:F:57:GLU:CG	2.45	0.46
2:F:81:GLU:O	2:F:82:LYS:C	2.54	0.45
3:G:19:ARG:O	3:G:19:ARG:HG2	2.16	0.45
4:I:97:THR:HG22	4:I:98:PHE:N	2.31	0.45
1:E:318:THR:CG2	3:G:103:PHE:CD1	3.00	0.45
3:H:6:GLU:OE1	3:H:118:GLY:N	2.49	0.45
3:G:68:PHE:N	3:G:68:PHE:CD1	2.84	0.45
4:L:11:LEU:HD12	4:L:11:LEU:C	2.37	0.45
3:G:64:VAL:O	3:G:64:VAL:CG1	2.61	0.45
4:I:11:LEU:HD11	4:I:104:VAL:HG13	1.99	0.45
4:I:38:GLN:O	4:I:84:ALA:HB1	2.16	0.45
1:A:26:VAL:HG12	1:A:315:LYS:HB2	1.99	0.45
2:F:133:MET:SD	2:F:139:LYS:HB2	2.57	0.45
3:G:12:VAL:HG21	3:G:18:LEU:CD1	2.47	0.45
2:F:54:ARG:HH11	2:F:103:GLU:CD	2.19	0.45
3:G:98:ARG:NH2	3:G:113:ASP:OD2	2.50	0.45
3:H:12:VAL:HG21	3:H:18:LEU:CD2	2.46	0.45
3:G:5:VAL:HA	3:G:117:GLN:OE1	2.17	0.45
4:L:49:HIS:O	4:L:50:ALA:HB3	2.17	0.45
1:E:87:PHE:O	1:E:267:ILE:HG13	2.16	0.45
1:A:318:THR:O	1:A:318:THR:CG2	2.58	0.44
2:B:51:LYS:HE2	2:B:107:THR:HG1	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:ILE:O	2:B:18:ILE:HG22	2.18	0.44
1:E:293:PRO:HG3	2:F:56:ILE:HD11	1.99	0.44
3:G:209:ASN:ND2	3:G:220:ASP:OD1	2.45	0.44
4:I:39:LYS:HA	4:I:84:ALA:CB	2.47	0.44
3:H:55:GLY:O	3:H:58:LYS:HE3	2.18	0.44
3:H:73:ASP:CG	3:H:76:ASN:HB2	2.38	0.44
3:G:86:LEU:HB3	3:G:123:VAL:CG1	2.46	0.44
3:H:19:ARG:O	3:H:19:ARG:HG2	2.18	0.44
3:H:97:ALA:HA	3:H:114:VAL:O	2.17	0.44
4:L:39:LYS:HA	4:L:84:ALA:CB	2.48	0.44
1:A:51:ILE:CG2	1:A:58:ILE:HD13	2.47	0.44
3:G:51:ILE:HB	3:G:70:ILE:CG2	2.48	0.44
1:E:26:VAL:HG12	1:E:315:LYS:HB3	1.99	0.44
2:F:165:GLU:CG	2:F:166:ALA:H	2.18	0.44
4:L:35:TRP:CD2	4:L:73:LEU:HB2	2.53	0.44
4:L:186:TYR:HA	4:L:192:TYR:OH	2.18	0.44
1:E:293:PRO:HB3	2:F:56:ILE:HD12	1.99	0.44
4:I:109:THR:HG22	4:I:110:VAL:N	2.33	0.44
1:A:8:ASN:N	1:A:8:ASN:ND2	2.65	0.44
1:A:164:LEU:O	1:A:246:ASN:HA	2.18	0.44
3:H:97:ALA:HB1	3:H:112:MET:CG	2.42	0.44
3:H:51:ILE:HB	3:H:70:ILE:CG2	2.45	0.44
4:I:96:LEU:HD23	4:I:96:LEU:N	2.33	0.43
2:B:18:ILE:HG21	3:H:106:LEU:HD13	2.00	0.43
3:H:100:ILE:HG23	3:H:113:ASP:HB2	1.99	0.43
3:G:22:CYS:HB3	3:G:79:LEU:HB3	1.99	0.43
3:G:83:VAL:HG12	3:G:86:LEU:CD1	2.48	0.43
4:I:2:ILE:HG22	4:I:3:GLN:H	1.83	0.43
1:A:316:LEU:HD11	2:B:55:VAL:HG21	2.00	0.43
3:G:88:PRO:HA	3:G:123:VAL:HG21	1.99	0.43
4:L:35:TRP:CE2	4:L:73:LEU:HB2	2.53	0.43
1:E:325:GLU:CB	2:F:15:GLU:HG3	2.41	0.43
3:G:16:ARG:O	3:G:86:LEU:HD13	2.18	0.43
1:A:295:GLN:OE1	1:A:297:VAL:HG12	2.18	0.43
2:B:67:GLU:HG2	2:B:88:LYS:HE3	2.00	0.43
2:B:172:GLN:O	2:B:173:ILE:CG1	2.63	0.43
4:L:13:ALA:O	4:L:107:LYS:N	2.48	0.43
3:G:68:PHE:N	3:G:68:PHE:HD1	2.16	0.43
4:I:4:MET:SD	4:I:90:LYS:HG2	2.59	0.43
1:A:196:VAL:HG23	1:A:197:GLN:N	2.33	0.43
3:H:2:VAL:HG13	3:H:27:PHE:HD1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:87:ARG:C	3:G:123:VAL:HG21	2.38	0.43
1:A:20:VAL:HG13	1:A:21:PRO:HD2	2.00	0.43
4:L:43:VAL:HG13	4:L:44:PRO:CD	2.48	0.43
1:E:124:GLY:O	1:E:125:PHE:O	2.37	0.43
2:F:18:ILE:HG22	3:G:106:LEU:CB	2.45	0.43
1:A:51:ILE:HG22	1:A:58:ILE:HD13	2.01	0.42
3:H:60:TYR:HB3	3:H:64:VAL:HG12	2.01	0.42
3:H:64:VAL:HG13	3:H:64:VAL:O	2.18	0.42
4:L:85:THR:HA	4:L:102:THR:O	2.19	0.42
3:G:89:GLU:O	3:G:89:GLU:HG2	2.19	0.42
2:B:67:GLU:OE2	2:B:88:LYS:NZ	2.46	0.42
3:G:4:LEU:HD23	3:G:96:CYS:HB2	2.01	0.42
3:H:64:VAL:O	3:H:68:PHE:HD1	2.02	0.42
2:B:18:ILE:HG22	3:H:106:LEU:HD13	2.01	0.42
1:E:20:VAL:CG1	1:E:21:PRO:HD2	2.49	0.42
1:E:323:VAL:HG23	2:F:13:GLY:HA3	2.02	0.42
3:G:3:GLN:HG2	3:G:4:LEU:H	1.83	0.42
2:F:91:LEU:HD13	2:F:91:LEU:C	2.40	0.42
3:G:45:LEU:HD12	3:G:45:LEU:N	2.34	0.42
1:E:167:THR:HA	1:E:243:LEU:O	2.19	0.42
1:E:50:LYS:HD3	1:E:275:ASP:HB2	2.02	0.42
2:F:54:ARG:HD2	2:F:58:LYS:NZ	2.35	0.42
3:G:24:ALA:CB	3:G:29:PHE:CD1	3.03	0.42
3:H:11:VAL:HG23	3:H:159:PRO:CG	2.42	0.42
1:E:270:SER:OG	1:E:284:PRO:O	2.27	0.42
4:I:189:HIS:O	4:I:211:ARG:NH1	2.52	0.42
1:E:196:VAL:HG23	1:E:197:GLN:N	2.35	0.42
4:L:54:LEU:HD12	4:L:62:PHE:O	2.20	0.42
1:E:169:PRO:HA	1:E:242:VAL:HA	2.01	0.42
4:I:40:PRO:HB3	4:I:165:GLU:OE1	2.20	0.42
1:A:20:VAL:N	1:A:322:ASN:OD1	2.45	0.41
3:H:22:CYS:O	3:H:78:THR:HA	2.20	0.41
3:H:196:VAL:HG11	3:H:206:TYR:CE1	2.54	0.41
4:L:4:MET:SD	4:L:90:LYS:HB2	2.60	0.41
4:I:80:PRO:HB2	4:I:168:SER:O	2.19	0.41
2:B:81:GLU:OE2	2:B:81:GLU:HA	2.20	0.41
2:F:52:LEU:C	2:F:52:LEU:HD23	2.41	0.41
3:H:138:PRO:HG3	3:H:149:ALA:O	2.20	0.41
4:I:2:ILE:HA	4:I:26:SER:HB3	2.02	0.41
4:I:37:GLN:HB2	4:I:47:LEU:HD11	2.01	0.41
2:B:168:ASN:O	2:B:172:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:83:VAL:CG2	4:I:106:ILE:HD13	2.39	0.41
4:I:28:GLY:CA	4:I:69:THR:HG22	2.47	0.41
3:H:4:LEU:CD1	3:H:96:CYS:HB2	2.51	0.41
1:E:301:THR:HB	1:E:305:CYS:SG	2.60	0.41
2:F:70:PHE:CE1	2:F:88:LYS:HB2	2.55	0.41
4:I:43:VAL:HG13	4:I:44:PRO:CD	2.51	0.41
1:A:29:ILE:CD1	2:B:102:LEU:CD2	2.99	0.41
1:A:99:PRO:HB2	1:A:229:ARG:HD3	2.03	0.41
1:A:325:GLU:HG3	2:B:12:ASN:OD1	2.19	0.41
2:B:47:GLN:O	2:B:51:LYS:HG3	2.21	0.41
4:L:2:ILE:O	4:L:3:GLN:HG2	2.21	0.41
3:G:11:VAL:CG2	3:G:128:THR:HG22	2.36	0.41
4:I:67:SER:HA	4:I:71:PHE:CE1	2.56	0.41
2:B:54:ARG:HD3	2:B:103:GLU:OE2	2.20	0.41
2:F:21:TRP:CH2	2:F:48:ILE:HD12	2.56	0.41
2:F:10:ILE:CG1	2:F:135:ASN:HA	2.47	0.40
3:G:40:THR:HG23	3:G:41:PRO:HD2	2.03	0.40
3:H:68:PHE:HE2	3:H:83:VAL:HG22	1.82	0.40
2:F:54:ARG:HA	2:F:57:GLU:CD	2.41	0.40
3:G:68:PHE:CE1	3:G:83:VAL:HG13	2.56	0.40
2:B:173:ILE:O	2:B:173:ILE:HG22	2.20	0.40
4:L:33:LEU:HD13	4:L:71:PHE:CD2	2.56	0.40
4:L:169:LYS:HG3	4:L:170:ASP:N	2.37	0.40
3:G:38:ARG:HG2	3:G:48:LEU:HD11	2.03	0.40
4:I:89:GLN:HE21	4:I:89:GLN:HB3	1.70	0.40
3:H:190:LEU:HD23	3:H:191:SER:N	2.35	0.40
4:L:50:ALA:O	4:L:51:ALA:CB	2.70	0.40
4:I:8:PRO:O	4:I:102:THR:HG23	2.22	0.40

All (3) 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)
2:B:160:ASP:OD2	3:G:16:ARG:NH2[2_646]	2.14	0.06
1:E:32:ASP:OD1	1:E:137:ASN:ND2[2_555]	2.14	0.06
4:L:211:ARG:HH21	4:I:187:GLU:O[2_656]	1.56	0.04

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	317/319 (99%)	305 (96%)	10 (3%)	2 (1%)	25	60
1	E	317/319 (99%)	303 (96%)	12 (4%)	2 (1%)	25	60
2	B	161/173 (93%)	155 (96%)	5 (3%)	1 (1%)	25	60
2	F	153/173 (88%)	147 (96%)	6 (4%)	0	100	100
3	G	217/228 (95%)	197 (91%)	17 (8%)	3 (1%)	11	39
3	H	216/228 (95%)	191 (88%)	22 (10%)	3 (1%)	11	39
4	I	212/214 (99%)	191 (90%)	19 (9%)	2 (1%)	17	51
4	L	212/214 (99%)	189 (89%)	23 (11%)	0	100	100
All	All	1805/1868 (97%)	1678 (93%)	114 (6%)	13 (1%)	22	56

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	PHE
1	E	125	PHE
3	G	64	VAL
3	G	198	SER
4	I	2	ILE
3	H	191	SER
1	A	62	ILE
2	B	172	GLN
1	E	62	ILE
3	G	199	SER
4	I	109	THR
3	H	139	SER
3	H	202	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	282/282 (100%)	280 (99%)	2 (1%)	84	93
1	E	282/282 (100%)	278 (99%)	4 (1%)	67	86
2	B	142/148 (96%)	139 (98%)	3 (2%)	53	80
2	F	134/148 (90%)	133 (99%)	1 (1%)	84	93
3	G	189/194 (97%)	181 (96%)	8 (4%)	30	63
3	H	187/194 (96%)	184 (98%)	3 (2%)	62	84
4	I	187/187 (100%)	179 (96%)	8 (4%)	29	62
4	L	187/187 (100%)	186 (100%)	1 (0%)	88	95
All	All	1590/1622 (98%)	1560 (98%)	30 (2%)	57	81

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	309	VAL
2	B	19	ASP
2	B	26	HIS
2	B	71	SER
3	H	64	VAL
3	H	77	ASN
3	H	101	THR
4	L	151	ASP
1	E	18	HIS
1	E	53	ASN
1	E	309	VAL
1	E	321	ARG
2	F	91	LEU
3	G	16	ARG
3	G	62	ASP
3	G	64	VAL
3	G	68	PHE
3	G	107	ILE

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Mol	Chain	Res	Type
3	G	119	THR
3	G	128	THR
3	G	140	SER
4	I	24	ARG
4	I	54	LEU
4	I	61	ARG
4	I	69	THR
4	I	74	THR
4	I	82	ASP
4	I	90	LYS
4	I	92	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

11 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	$\#\|Z\| > 2$
5	NAG	E	401	1	14,14,15	0.33	0	17,19,21	0.52	0
5	NAG	B	201	2	14,14,15	0.26	0	17,19,21	0.63	1 (5%)
5	NAG	E	402	1	14,14,15	0.38	0	17,19,21	0.46	0
5	NAG	H	301	3	14,14,15	0.29	0	17,19,21	1.43	3 (17%)
5	NAG	A	404	1	14,14,15	0.73	1 (7%)	17,19,21	0.76	1 (5%)
5	NAG	E	403	1	14,14,15	0.55	0	17,19,21	0.67	0
5	NAG	A	401	1	14,14,15	0.36	0	17,19,21	0.64	1 (5%)
5	NAG	F	201	2	14,14,15	0.23	0	17,19,21	0.47	0
5	NAG	G	301	3	14,14,15	0.38	0	17,19,21	0.38	0
5	NAG	A	403	1	14,14,15	0.31	0	17,19,21	0.36	0
5	NAG	A	402	1	14,14,15	0.39	0	17,19,21	0.76	1 (5%)

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	NAG	E	401	1	-	2/6/23/26	0/1/1/1
5	NAG	B	201	2	-	2/6/23/26	0/1/1/1
5	NAG	E	402	1	-	2/6/23/26	0/1/1/1
5	NAG	H	301	3	-	1/6/23/26	0/1/1/1
5	NAG	A	404	1	-	4/6/23/26	0/1/1/1
5	NAG	E	403	1	-	3/6/23/26	0/1/1/1
5	NAG	A	401	1	-	2/6/23/26	0/1/1/1
5	NAG	F	201	2	-	1/6/23/26	0/1/1/1
5	NAG	G	301	3	-	0/6/23/26	0/1/1/1
5	NAG	A	403	1	-	1/6/23/26	0/1/1/1
5	NAG	A	402	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	404	NAG	O5-C1	2.01	1.46	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	301	NAG	C1-O5-C5	3.50	116.93	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	301	NAG	C2-N2-C7	3.31	127.61	122.90
5	A	402	NAG	C1-O5-C5	2.74	115.90	112.19
5	H	301	NAG	C1-C2-N2	2.51	114.77	110.49
5	A	404	NAG	C1-O5-C5	2.50	115.58	112.19
5	B	201	NAG	C1-O5-C5	2.17	115.13	112.19
5	A	401	NAG	C1-O5-C5	2.16	115.11	112.19

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	404	NAG	C3-C2-N2-C7
5	H	301	NAG	C1-C2-N2-C7
5	E	401	NAG	C4-C5-C6-O6
5	E	401	NAG	O5-C5-C6-O6
5	A	402	NAG	O5-C5-C6-O6
5	E	402	NAG	O5-C5-C6-O6
5	A	401	NAG	C4-C5-C6-O6
5	B	201	NAG	C4-C5-C6-O6
5	A	401	NAG	O5-C5-C6-O6
5	A	404	NAG	C4-C5-C6-O6
5	E	403	NAG	C4-C5-C6-O6
5	B	201	NAG	O5-C5-C6-O6
5	A	404	NAG	O5-C5-C6-O6
5	E	403	NAG	O5-C5-C6-O6
5	E	403	NAG	C1-C2-N2-C7
5	E	402	NAG	C4-C5-C6-O6
5	A	402	NAG	C4-C5-C6-O6
5	A	403	NAG	O5-C5-C6-O6
5	F	201	NAG	C4-C5-C6-O6
5	A	404	NAG	C1-C2-N2-C7

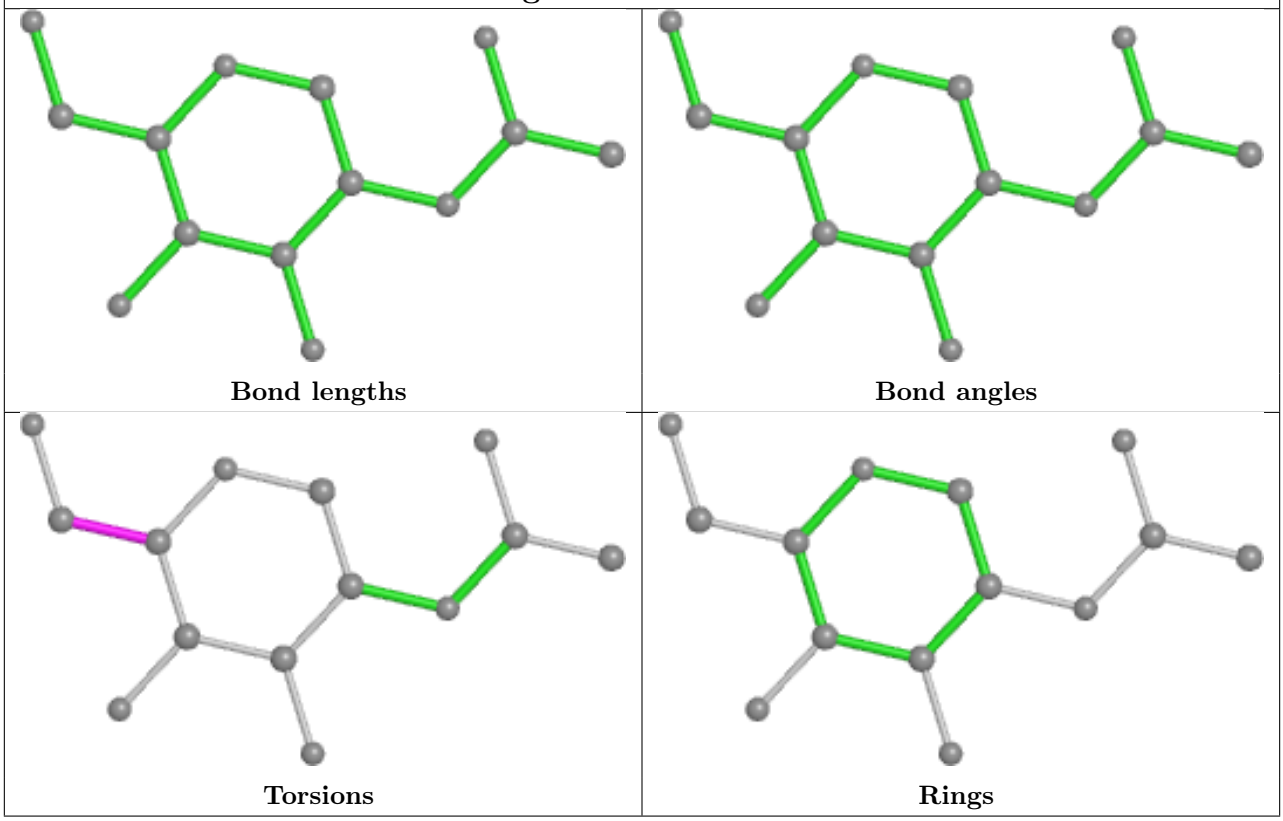
There are no ring outliers.

4 monomers are involved in 6 short contacts:

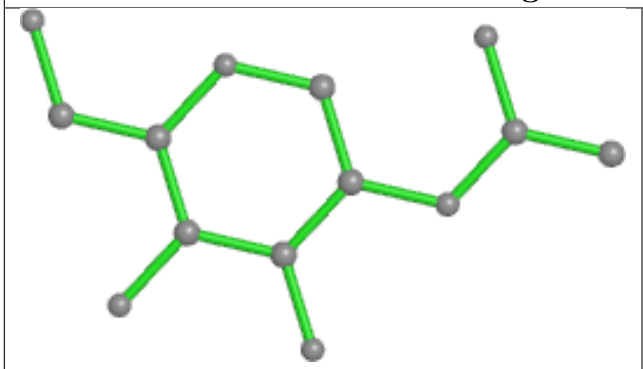
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	301	NAG	2	0
5	A	404	NAG	1	0
5	A	401	NAG	2	0
5	F	201	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

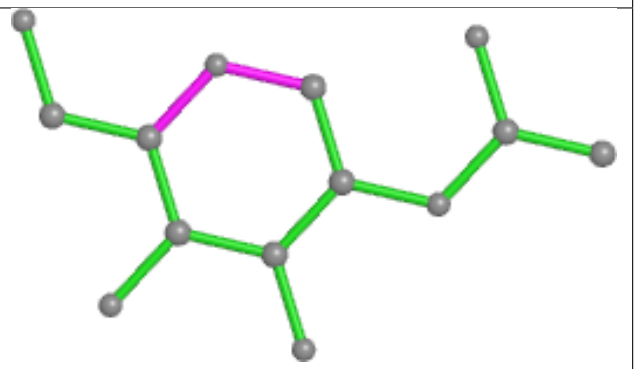
Ligand NAG E 401



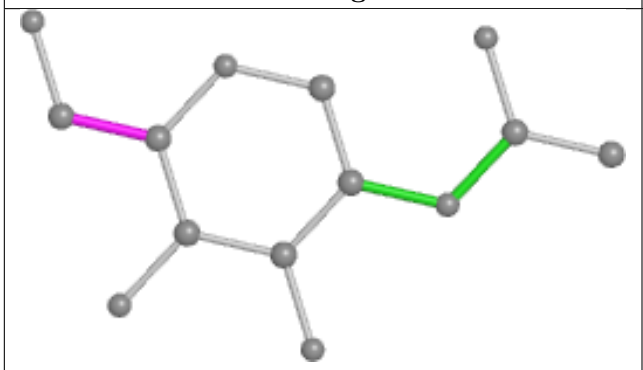
Ligand NAG B 201



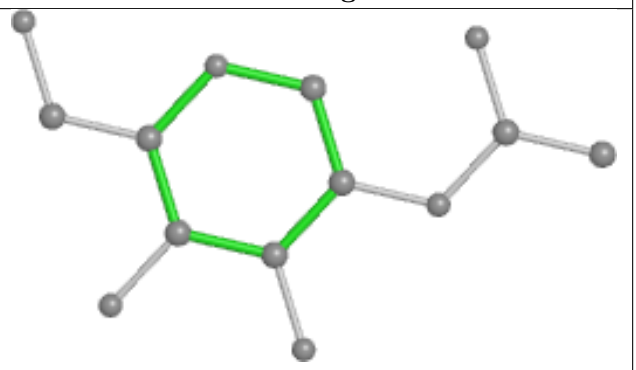
Bond lengths



Bond angles

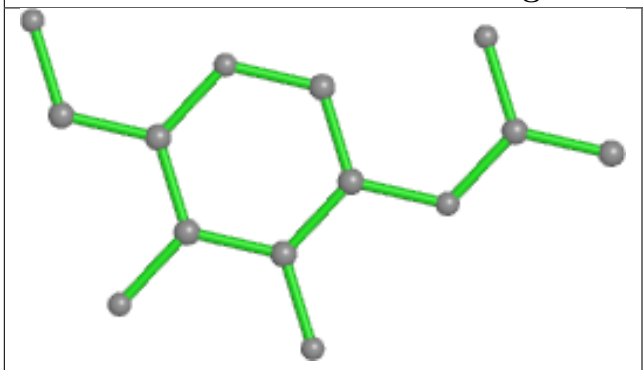


Torsions

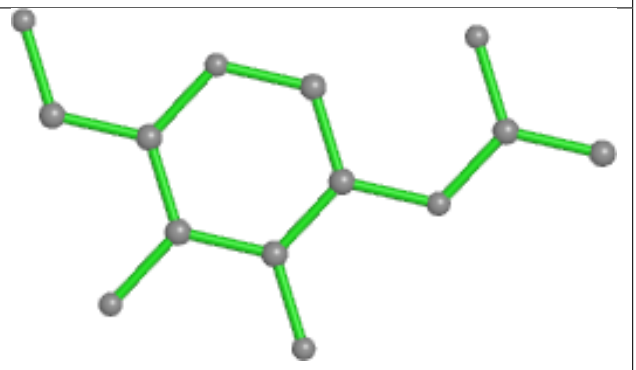


Rings

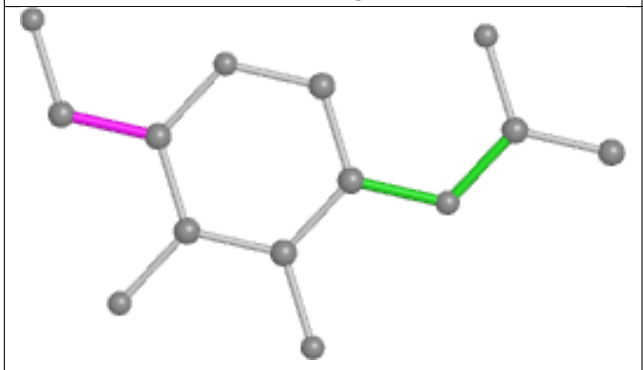
Ligand NAG E 402



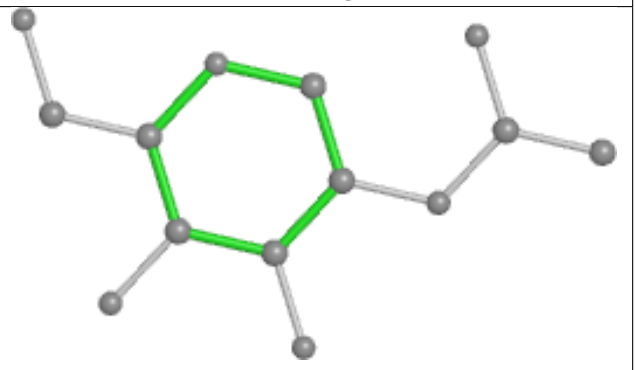
Bond lengths



Bond angles

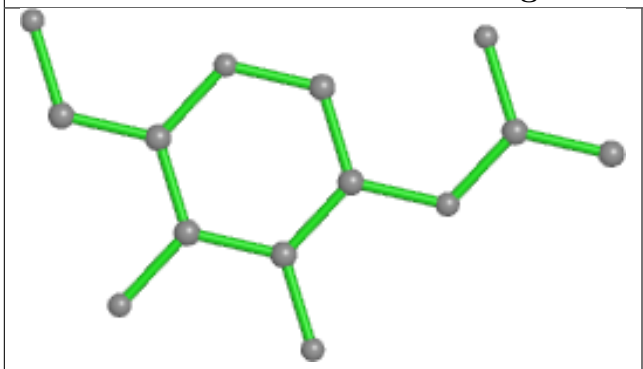


Torsions

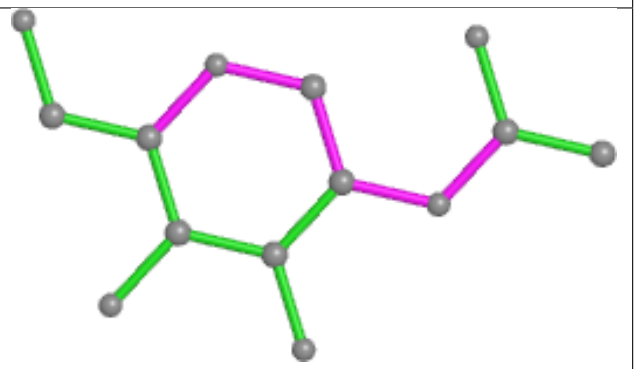


Rings

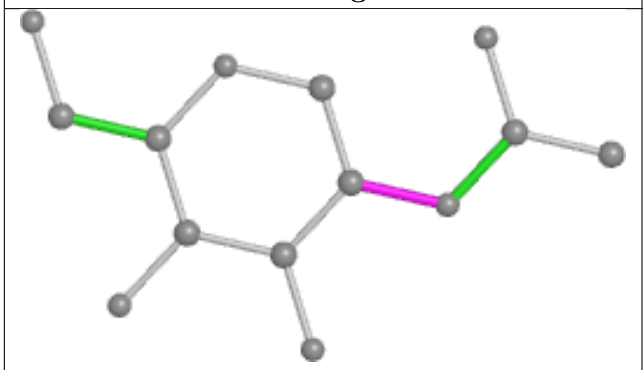
Ligand NAG H 301



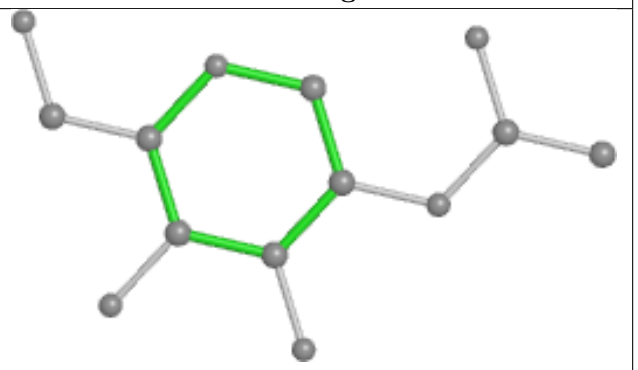
Bond lengths



Bond angles

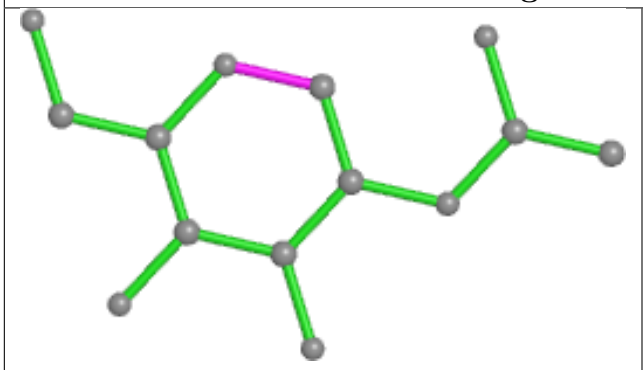


Torsions

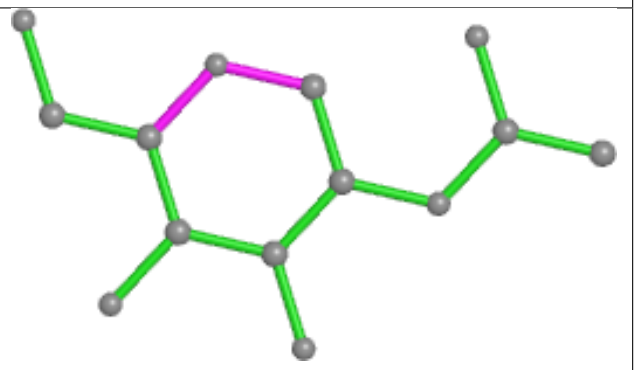


Rings

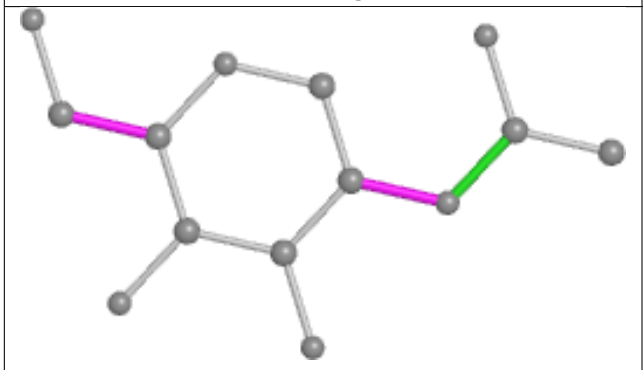
Ligand NAG A 404



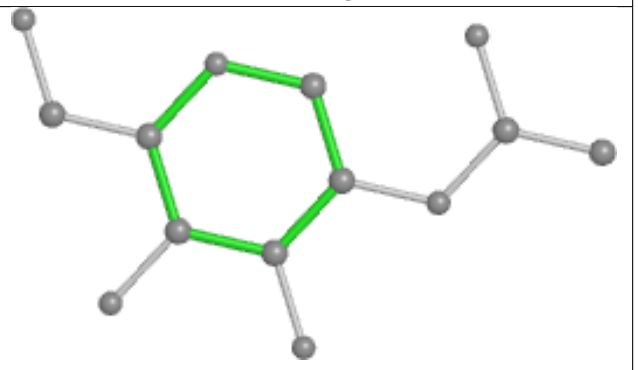
Bond lengths



Bond angles

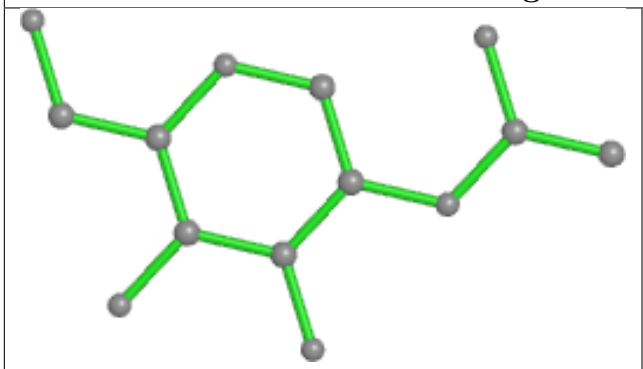


Torsions

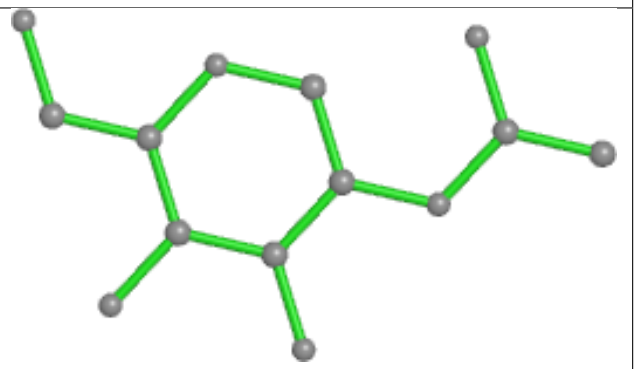


Rings

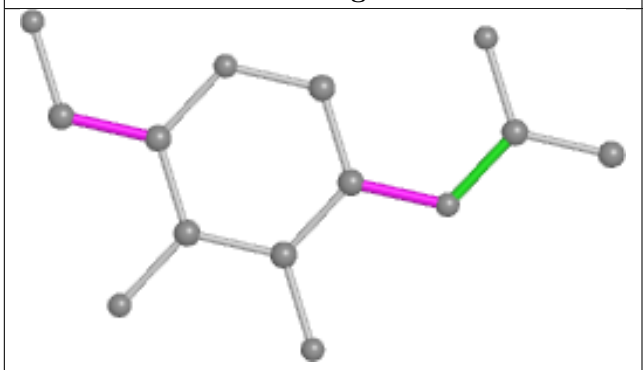
Ligand NAG E 403



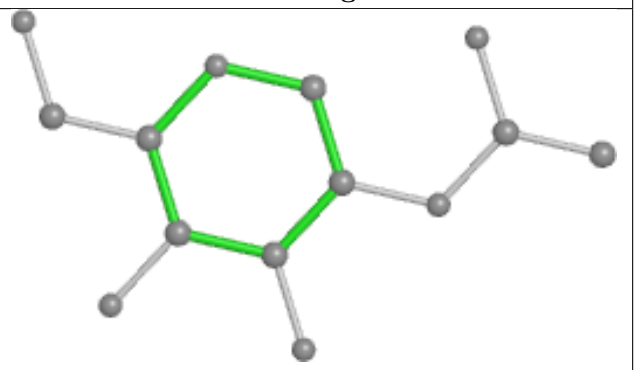
Bond lengths



Bond angles

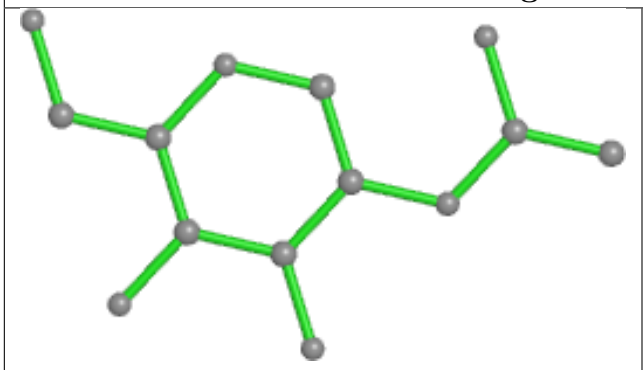


Torsions

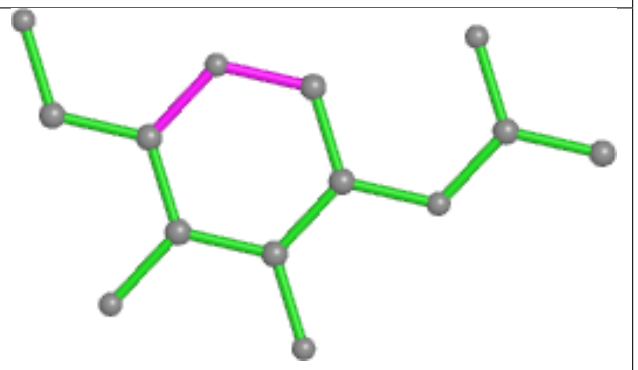


Rings

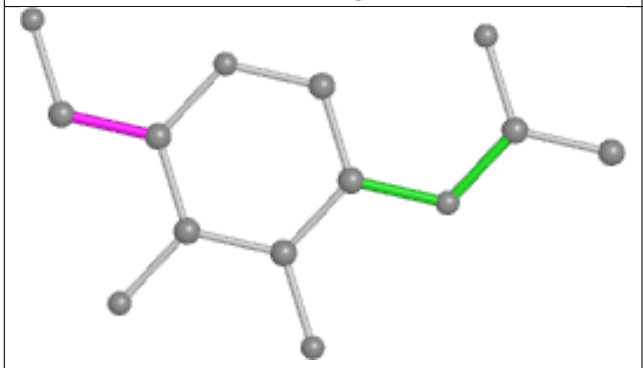
Ligand NAG A 401



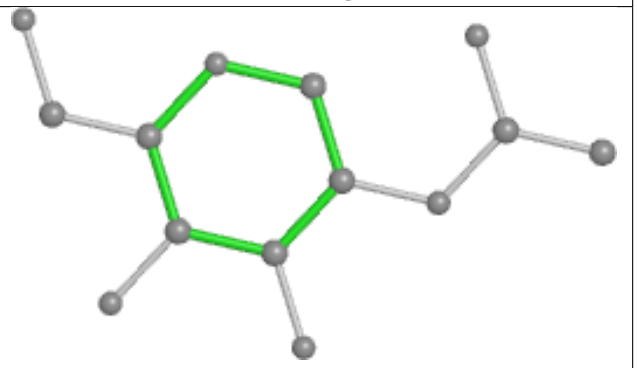
Bond lengths



Bond angles

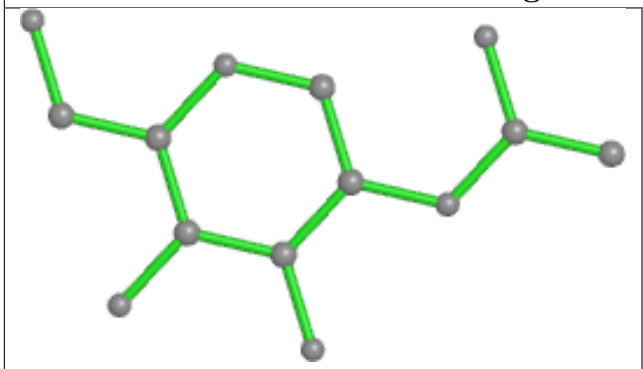


Torsions

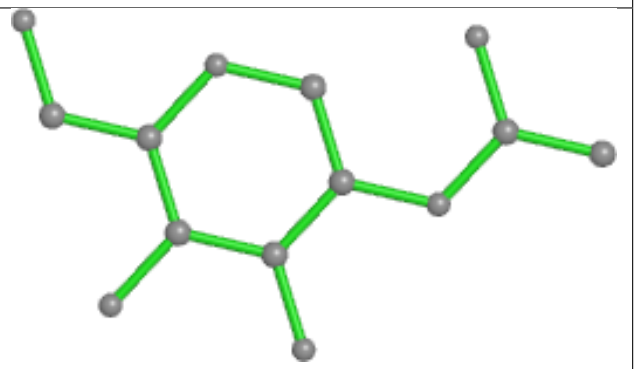


Rings

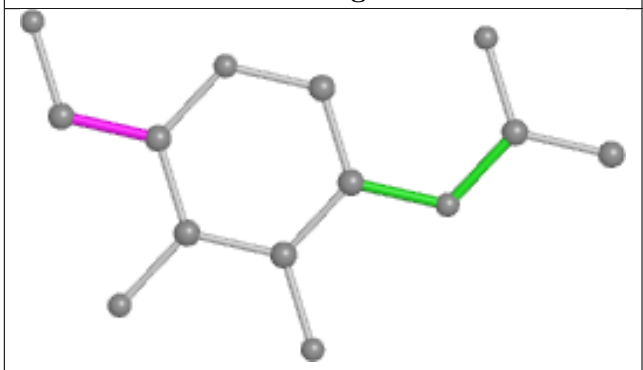
Ligand NAG F 201



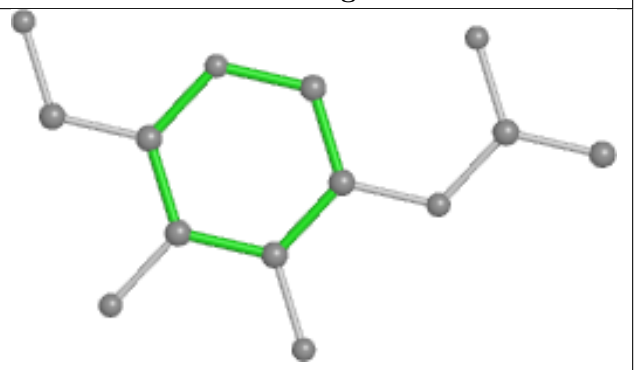
Bond lengths



Bond angles

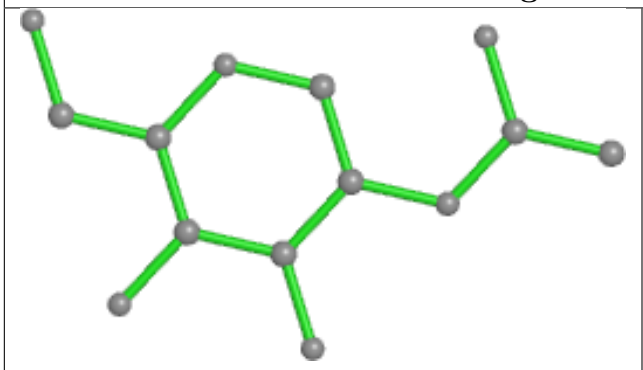


Torsions

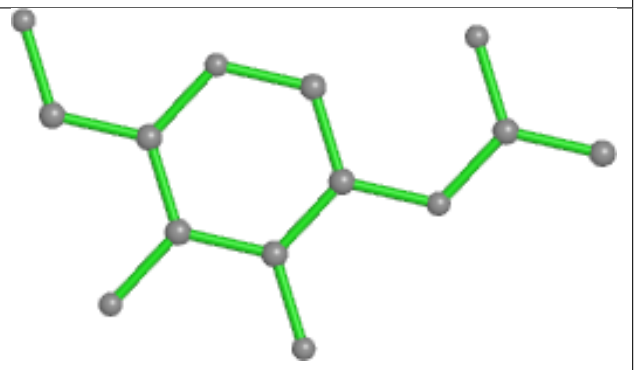


Rings

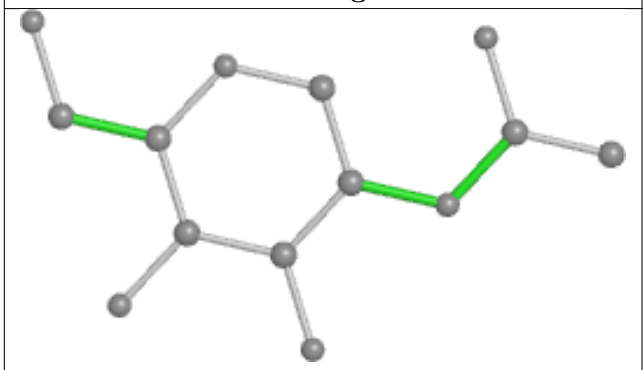
Ligand NAG G 301



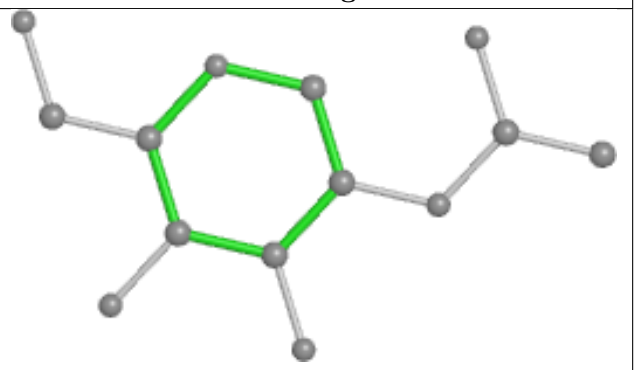
Bond lengths



Bond angles

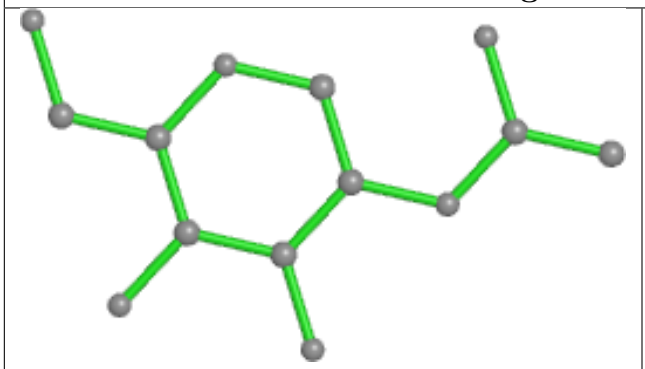


Torsions

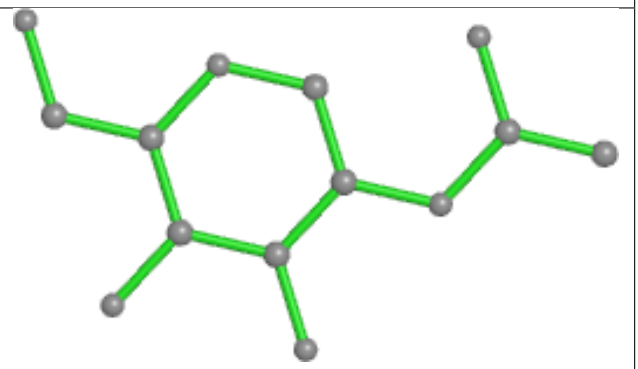


Rings

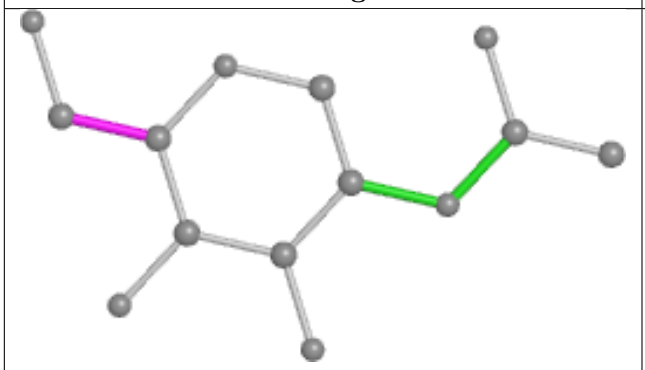
Ligand NAG A 403



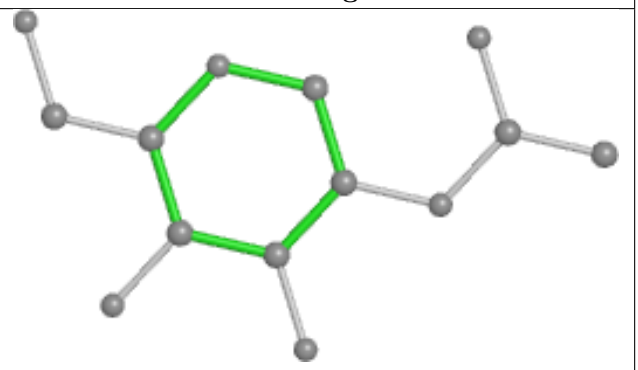
Bond lengths



Bond angles

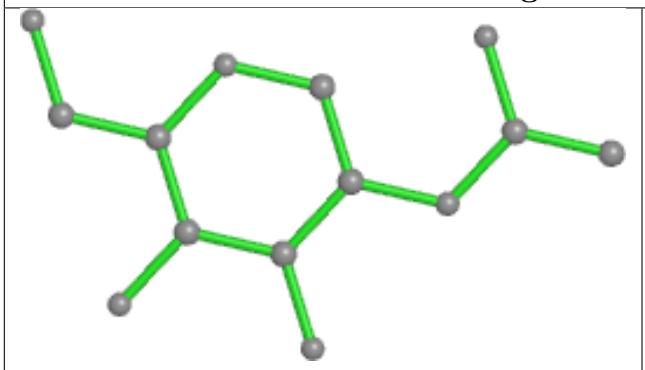


Torsions

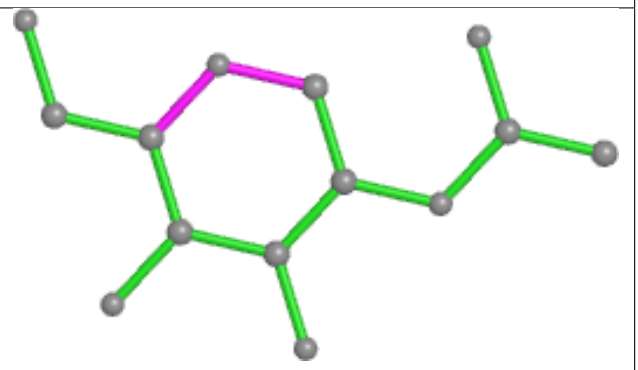


Rings

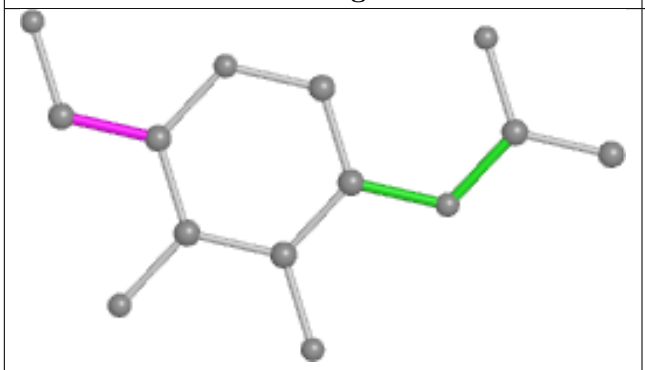
Ligand NAG A 402



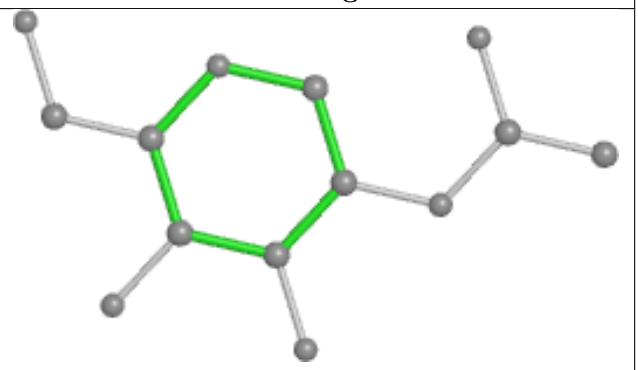
Bond lengths



Bond angles



Torsions



Rings

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	319/319 (100%)	-0.15	1 (0%)	94	87	60, 87, 128, 155	6 (1%)
1	E	319/319 (100%)	0.31	18 (5%)	24	15	85, 130, 208, 279	6 (1%)
2	B	165/173 (95%)	-0.03	2 (1%)	79	63	60, 87, 140, 219	3 (1%)
2	F	157/173 (90%)	0.32	7 (4%)	33	21	85, 125, 177, 249	2 (1%)
3	G	221/228 (96%)	0.16	5 (2%)	60	43	67, 98, 164, 220	0
3	H	220/228 (96%)	0.27	5 (2%)	60	43	65, 130, 168, 206	0
4	I	214/214 (100%)	0.09	3 (1%)	75	59	77, 111, 158, 202	0
4	L	214/214 (100%)	0.17	4 (1%)	66	49	66, 131, 198, 243	0
All	All	1829/1868 (97%)	0.14	45 (2%)	57	40	60, 109, 179, 279	17 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	L	214	CYS	9.1
1	E	223	VAL	7.1
1	E	213	ILE	6.6
2	F	5	ALA	6.5
2	F	4	GLY	5.5
1	E	214	ILE	5.4
3	H	225	PRO	5.4
3	G	1	GLN	5.4
1	E	224	ARG	5.0
1	E	225	GLY	4.2
2	F	6	ILE	4.2
1	A	326	LYS	4.1
1	E	222	TRP	4.0
2	B	4	GLY	3.9
1	E	127	TRP	3.9
4	I	214	CYS	3.8

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Mol	Chain	Res	Type	RSRZ
3	G	201	LEU	3.7
1	E	251	LEU	3.7
1	E	220	ARG	3.6
2	F	141	TYR	3.5
3	H	137	ALA	3.5
2	F	7	ALA	3.4
1	E	160	THR	3.4
1	E	163	VAL	3.3
2	B	171	PHE	3.2
3	H	18	LEU	3.1
4	I	122	ASP	3.1
4	L	202	SER	3.0
3	G	196	VAL	2.9
2	F	138	PHE	2.9
1	E	226	LEU	2.9
2	F	73	VAL	2.8
1	E	161	TYR	2.8
3	G	227	SER	2.6
1	E	130	VAL	2.6
4	I	108	ARG	2.5
4	L	208	SER	2.4
3	H	213	LYS	2.4
3	G	2	VAL	2.3
4	L	116	PHE	2.2
3	H	201	LEU	2.2
1	E	32	ASP	2.1
1	E	212	THR	2.1
1	E	162	PRO	2.1
1	E	216	ASN	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)

There are no monosaccharides in this entry.

6.4 Ligands (i)

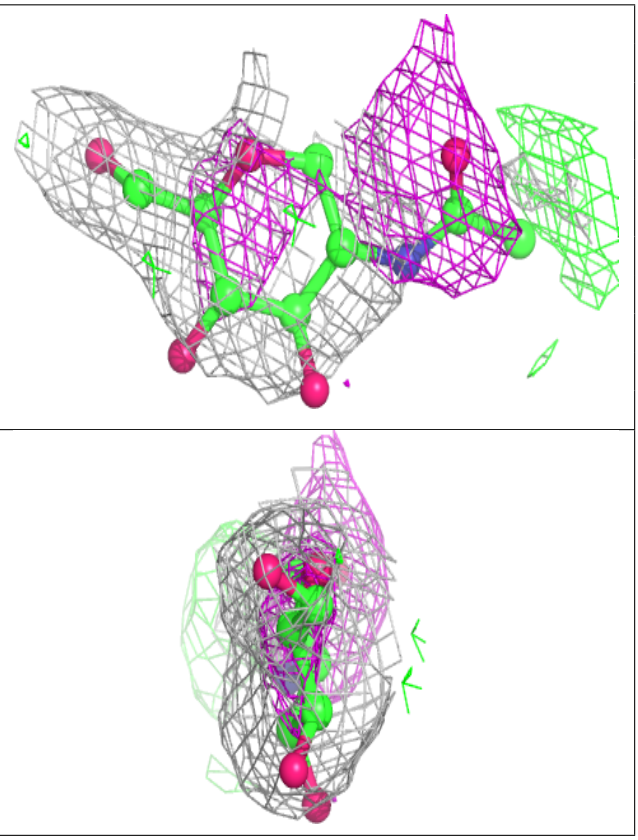
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	A	404	14/15	0.70	0.38	88,94,97,98	0
5	NAG	H	301	14/15	0.73	0.31	233,236,240,241	0
5	NAG	E	402	14/15	0.81	0.31	88,96,97,97	0
5	NAG	E	401	14/15	0.86	0.20	88,92,95,97	0
5	NAG	A	403	14/15	0.86	0.26	88,93,96,96	0
5	NAG	E	403	14/15	0.87	0.22	88,93,96,100	0
5	NAG	F	201	14/15	0.88	0.16	88,93,94,95	0
5	NAG	G	301	14/15	0.88	0.48	88,94,96,97	0
5	NAG	A	401	14/15	0.89	0.21	88,91,95,97	0
5	NAG	A	402	14/15	0.90	0.24	88,93,95,96	0
5	NAG	B	201	14/15	0.90	0.17	88,93,94,94	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

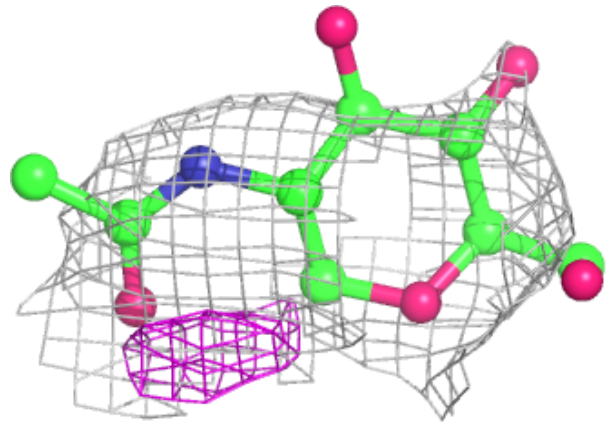
Electron density around NAG A 404:

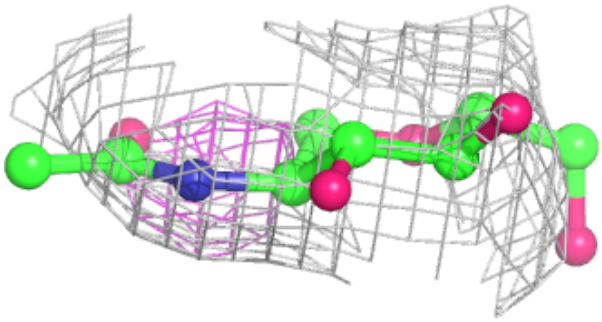
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

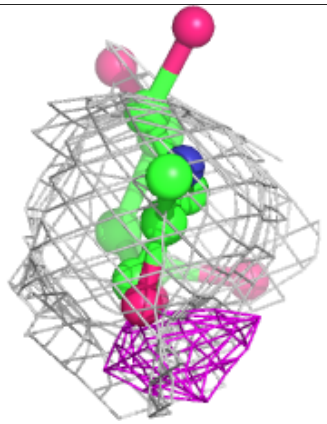


Electron density around NAG H 301:

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

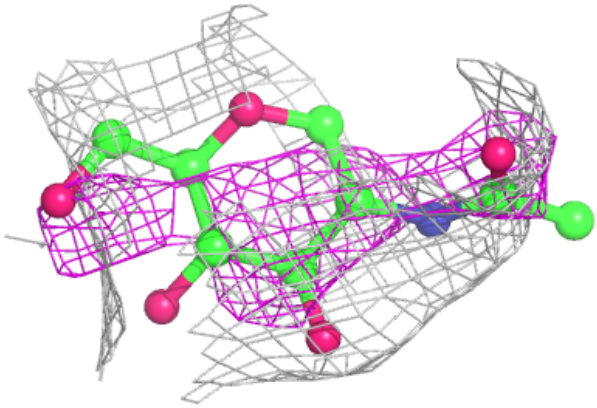


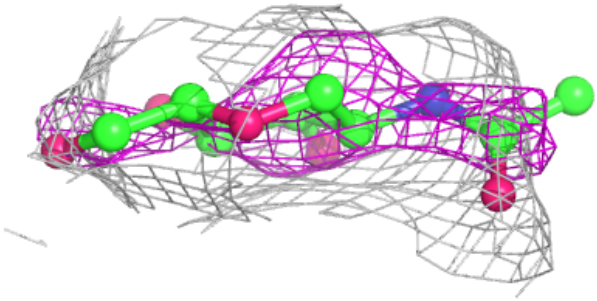


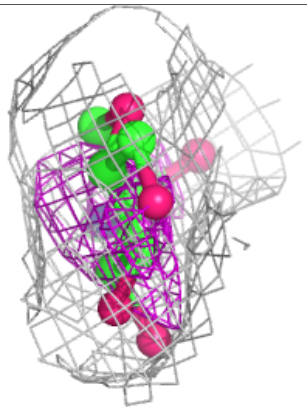


Electron density around NAG E 402:

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

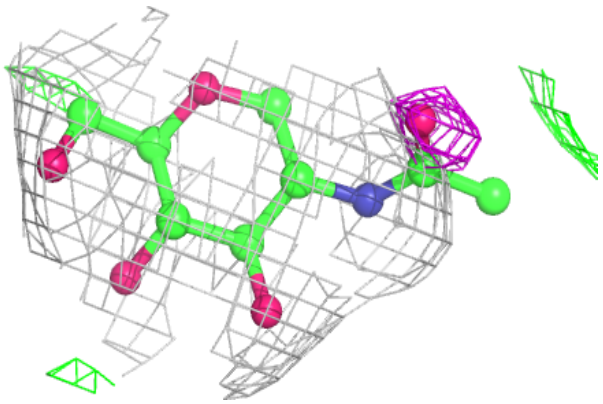


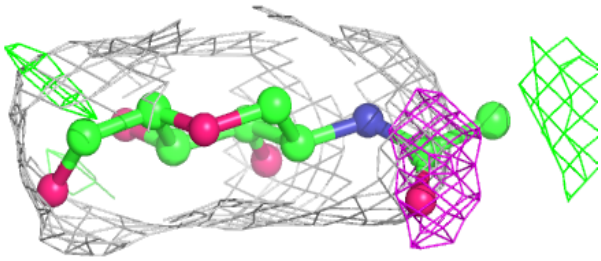


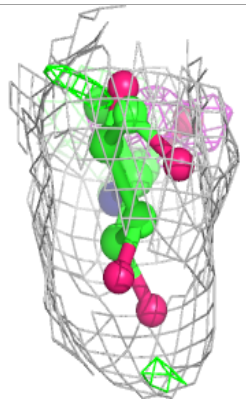


Electron density around NAG E 401:

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

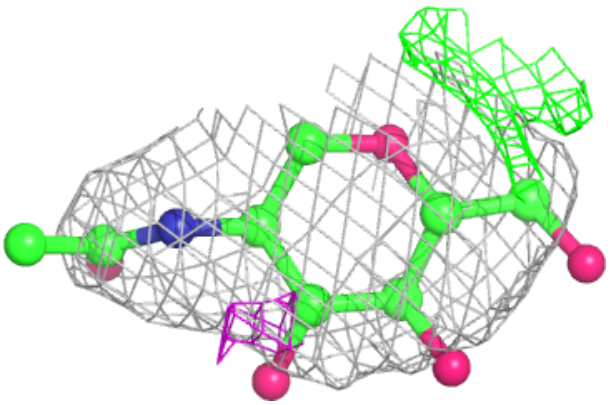


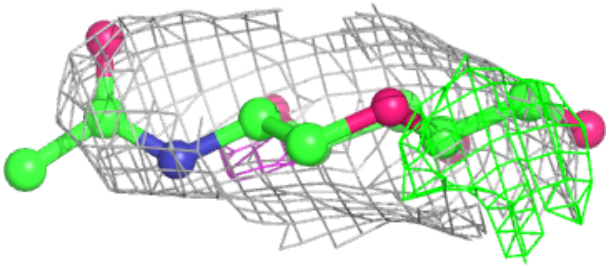


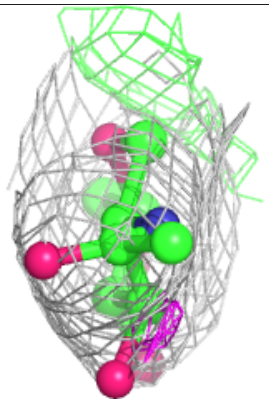


Electron density around NAG A 403:

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

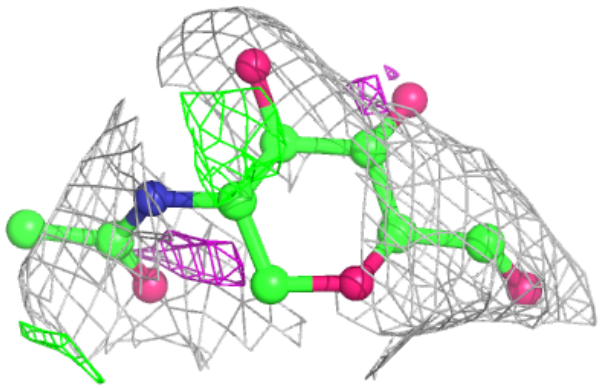


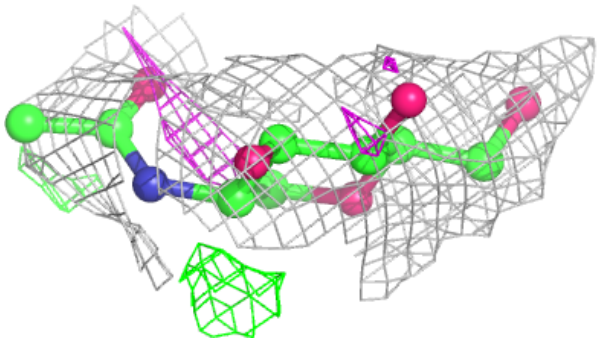


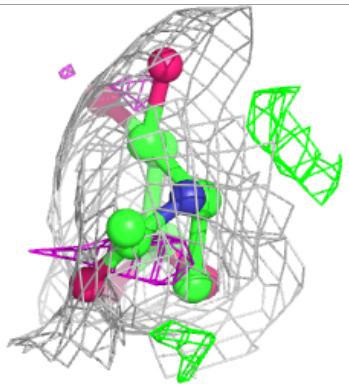


Electron density around NAG E 403:

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

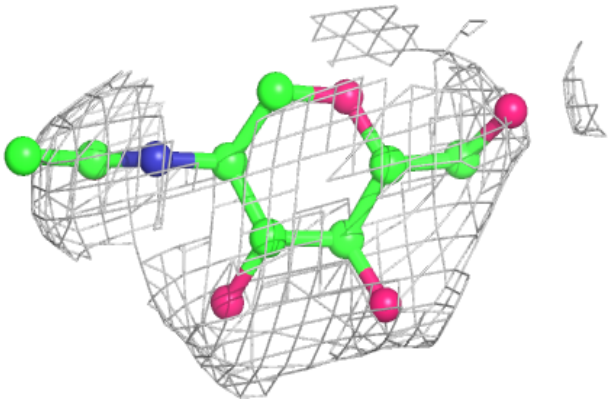


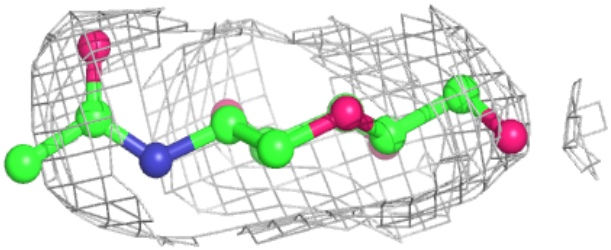


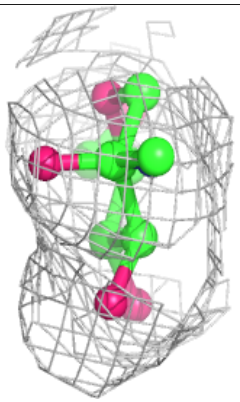


Electron density around NAG F 201:

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

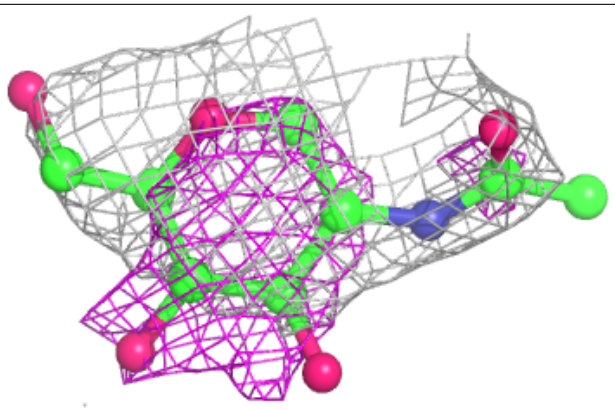


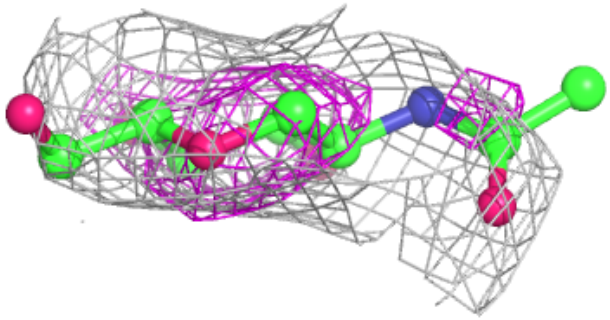


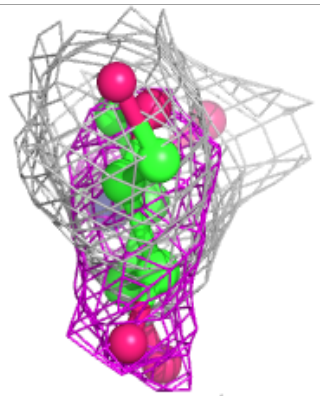


Electron density around NAG G 301:

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

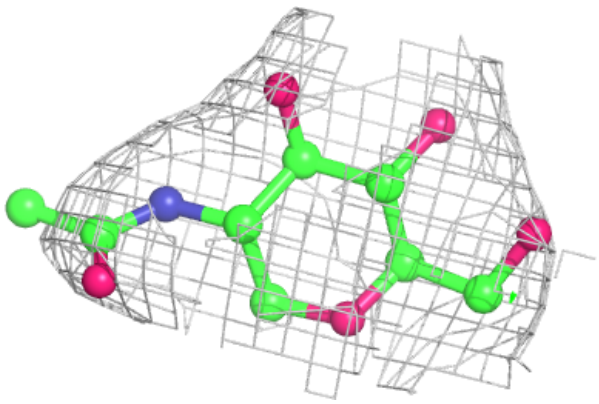


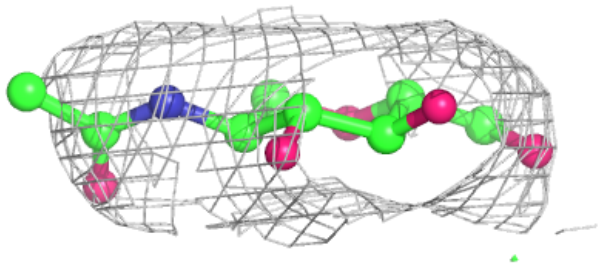


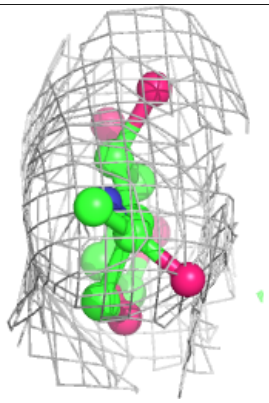


Electron density around NAG A 401:

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

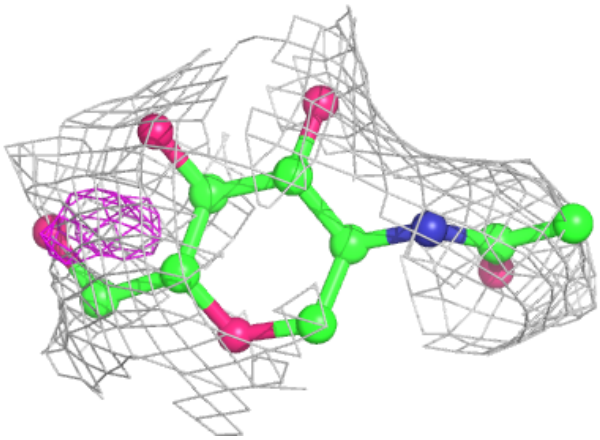


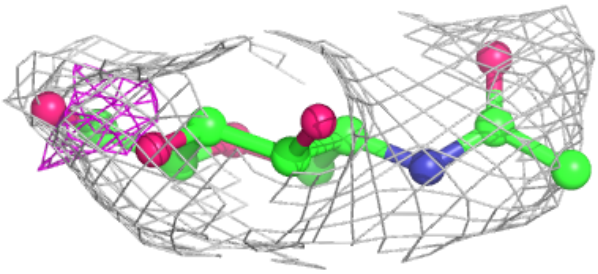


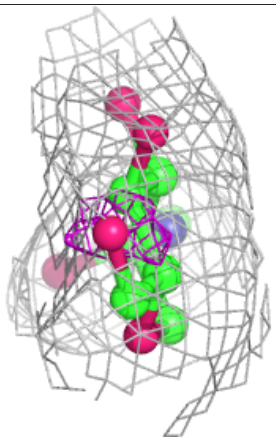


Electron density around NAG A 402:

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

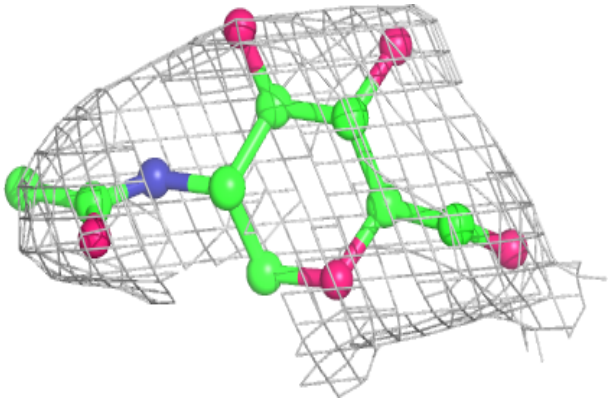


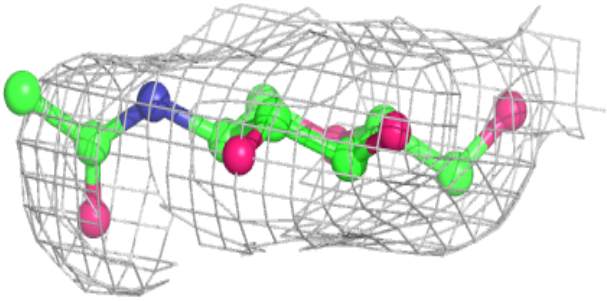




Electron density around NAG B 201:

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





6.5 Other polymers (i)

There are no such residues in this entry.