Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 05:25 PM EDT

PDB ID	:	6II9
Title	:	Crystal structure of H7 hemagglutinin from A/Anhui/1/2013 in complex with a human neutralizing antibody L3A-44
Authors	:	Jiang, H.H.; Shi, Y.; Qi, J.; Gao, G.F.
Deposited on	:	2018-10-03
Resolution	:	3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

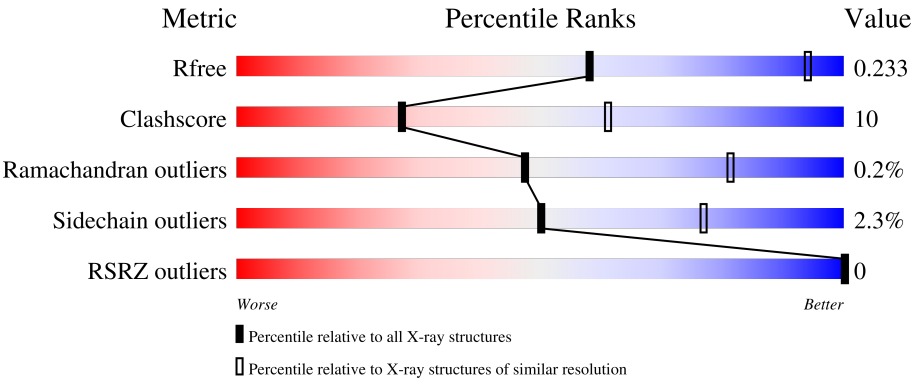
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	317	84% 16%
1	C	317	81% 18% .
1	E	317	79% 19% .
2	B	170	76% 22% .
2	D	170	91% 9% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	170	82% 16%
3	H	221	66% 30%
3	M	221	58% 36%
3	P	221	63% 32%
4	L	212	81% 19%
4	N	212	80% 19%
4	Q	212	76% 23%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	C	401	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 20939 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2420	1504	437	464	15			
1	C	317	Total	C	N	O	S	0	0	1
			2413	1498	437	463	15			
1	E	316	Total	C	N	O	S	0	0	0
			2412	1498	436	463	15			

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	170	Total	C	N	O	S	0	0	0
			1379	851	241	280	7			
2	D	170	Total	C	N	O	S	0	0	0
			1379	851	241	280	7			
2	F	170	Total	C	N	O	S	0	0	0
			1379	851	241	280	7			

- Molecule 3 is a protein called Heavy chain of L3A-44 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	216	Total	C	N	O	S	0	0	0
			1619	1029	266	320	4			
3	M	213	Total	C	N	O	S	0	0	0
			1603	1021	263	315	4			
3	P	216	Total	C	N	O	S	0	0	0
			1619	1029	266	320	4			

- Molecule 4 is a protein called Light chain of L3A-44 Fab.

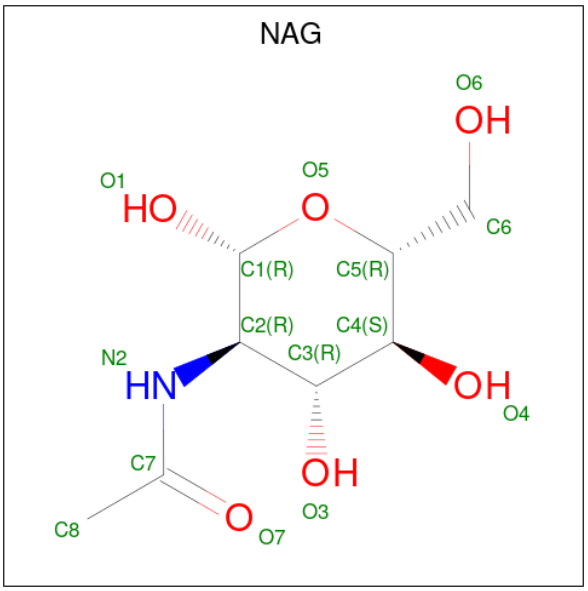
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	212	Total	C	N	O	S	0	0	0
			1558	977	260	317	4			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	212	Total	C	N	O	S	0	0	0
			1558	977	260	317	4			
4	Q	212	Total	C	N	O	S	0	0	0
			1558	977	260	317	4			

- 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).



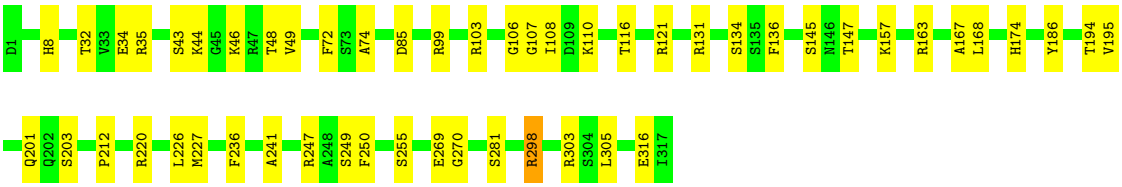
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		

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.

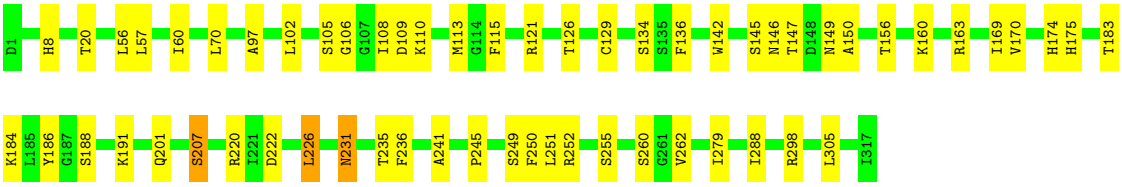
• Molecule 1: Hemagglutinin

Chain A:



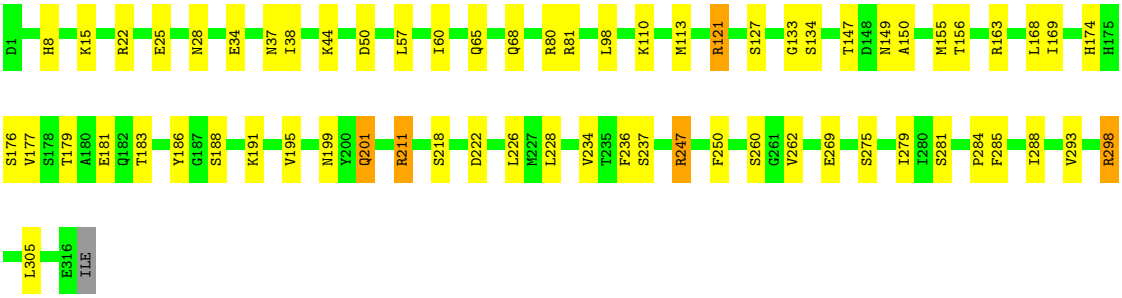
• Molecule 1: Hemagglutinin

Chain C:



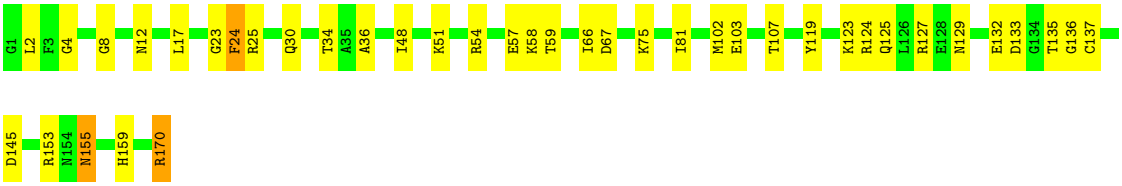
• Molecule 1: Hemagglutinin

Chain E:



• Molecule 2: Hemagglutinin

Chain B:

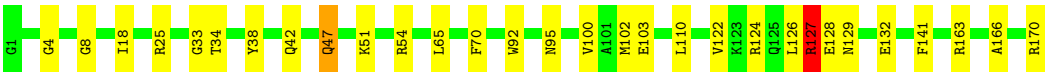


• Molecule 2: Hemagglutinin

Chain D:

• Molecule 2: Hemagglutinin

Chain F:

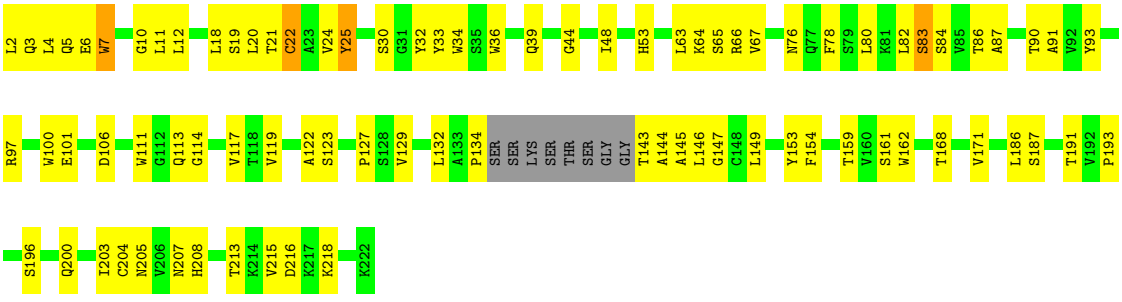


• Molecule 3: Heavy chain of L3A-44 Fab

Chain H:

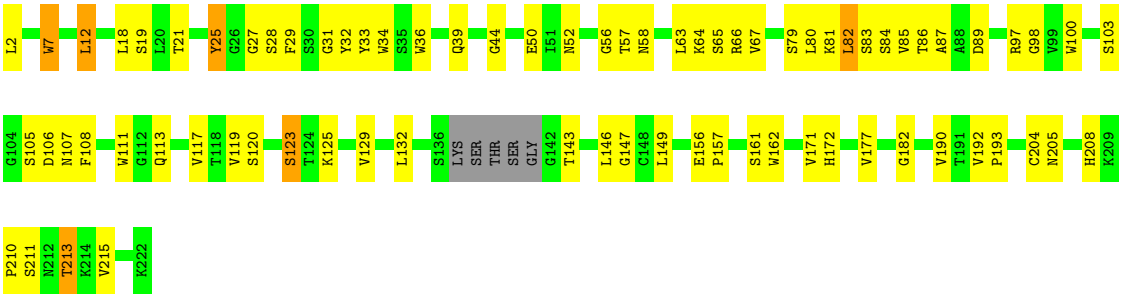
• Molecule 3: Heavy chain of L3A-44 Fab

Chain M:



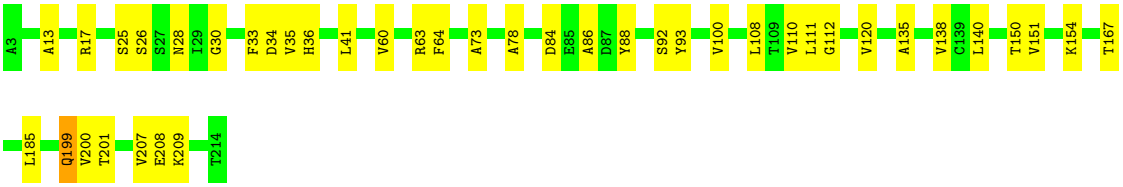
• Molecule 3: Heavy chain of L3A-44 Fab

Chain P:



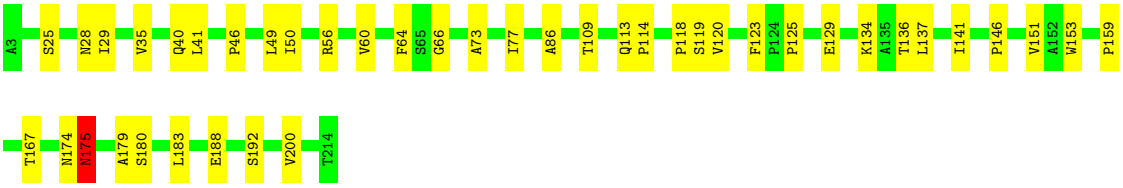
• Molecule 4: Light chain of L3A-44 Fab

Chain L:



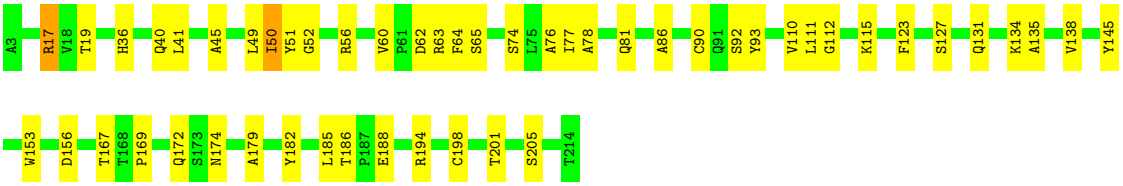
• Molecule 4: Light chain of L3A-44 Fab

Chain N:



• Molecule 4: Light chain of L3A-44 Fab

Chain Q:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	178.46Å 184.91Å 188.99Å 90.00° 106.47° 90.00°	Depositor
Resolution (Å)	43.84 – 3.50 43.84 – 3.48	Depositor EDS
% Data completeness (in resolution range)	96.9 (43.84-3.50) 96.9 (43.84-3.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.201 , 0.234 0.200 , 0.233	Depositor DCC
R_{free} test set	3688 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	86.2	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 28.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	20939	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.37	0/2466	0.55	1/3333 (0.0%)
1	C	0.37	0/2459	0.54	0/3324
1	E	0.39	0/2458	0.59	3/3322 (0.1%)
2	B	0.36	0/1403	0.49	0/1890
2	D	0.36	0/1403	0.48	0/1890
2	F	0.37	0/1403	0.56	0/1890
3	H	0.36	0/1663	0.59	0/2273
3	M	0.40	0/1647	0.95	4/2252 (0.2%)
3	P	0.38	0/1663	0.63	0/2273
4	L	0.34	0/1597	0.53	0/2181
4	N	0.39	1/1597 (0.1%)	0.67	3/2181 (0.1%)
4	Q	0.36	0/1597	0.56	0/2181
All	All	0.37	1/21356 (0.0%)	0.60	11/28990 (0.0%)

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
2	F	0	2
3	H	0	3
3	P	0	1
4	N	0	2
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	175	ASN	CG-ND2	5.39	1.46	1.32

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	200	GLN	CG-CD-OE1	26.77	175.15	121.60
3	M	200	GLN	CG-CD-NE2	-18.45	72.42	116.70
4	N	175	ASN	CB-CA-C	-12.69	85.02	110.40
1	E	247	ARG	NE-CZ-NH2	-10.12	115.24	120.30
4	N	175	ASN	N-CA-CB	7.46	124.02	110.60
3	M	200	GLN	OE1-CD-NE2	-7.39	104.89	121.90
1	A	226	LEU	CB-CG-CD2	-6.44	100.05	111.00
1	E	247	ARG	CG-CD-NE	-6.27	98.63	111.80
1	E	247	ARG	NE-CZ-NH1	6.14	123.37	120.30
4	N	174	ASN	C-N-CA	5.76	136.10	121.70
3	M	200	GLN	CB-CA-C	5.26	120.92	110.40

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	127	ARG	Peptide
2	F	47	GLN	Sidechain
3	H	102	GLY	Peptide
3	H	122	ALA	Peptide
3	H	82	LEU	Peptide
4	N	175	ASN	Mainchain,Sidechain
3	P	82	LEU	Peptide

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	2420	0	2385	30	0
1	C	2413	0	2373	41	0
1	E	2412	0	2372	43	0
2	B	1379	0	1281	28	0
2	D	1379	0	1281	12	0
2	F	1379	0	1280	30	0
3	H	1619	0	1565	43	0
3	M	1603	0	1552	59	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	1619	0	1565	65	0
4	L	1558	0	1509	31	0
4	N	1558	0	1509	30	0
4	Q	1558	0	1509	39	0
5	C	14	0	13	1	0
5	E	14	0	13	1	0
5	F	14	0	13	0	0
All	All	20939	0	20220	415	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 10.

All (415) 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:F:47:GLN:HE21	2:F:110:LEU:HD11	1.17	1.04
2:F:47:GLN:NE2	2:F:110:LEU:HD11	1.80	0.96
2:B:25:ARG:HG3	2:B:34:THR:HG22	1.45	0.96
2:F:25:ARG:HE	2:F:34:THR:HG22	1.29	0.96
4:Q:111:LEU:HB3	4:Q:112:GLY:HA2	1.47	0.94
3:H:122:ALA:HB1	3:H:123:SER:HB3	1.50	0.94
3:P:177:VAL:HG12	4:Q:167:THR:HB	1.58	0.86
4:N:118:PRO:HA	4:N:119:SER:HB3	1.59	0.83
3:M:6:GLU:OE1	3:M:114:GLY:N	2.13	0.79
3:M:129:VAL:HG11	3:M:215:VAL:HG11	1.65	0.78
2:F:25:ARG:NE	2:F:34:THR:HG22	1.99	0.78
4:Q:36:HIS:CD2	4:Q:52:GLY:H	2.02	0.77
3:M:122:ALA:HB1	3:M:123:SER:HB3	1.67	0.77
3:M:48:ILE:HD11	3:M:80:LEU:HD11	1.66	0.74
1:A:194:THR:HG22	1:A:203:SER:HB3	1.69	0.74
4:N:151:VAL:HG12	4:N:200:VAL:HG22	1.70	0.73
3:M:82:LEU:HB2	3:M:83:SER:HB3	1.70	0.72
2:B:54:ARG:NH2	2:B:103:GLU:OE2	2.22	0.72
4:L:60:VAL:HG13	4:L:64:PHE:HD2	1.54	0.72
4:L:154:LYS:NZ	4:L:199:GLN:OE1	2.23	0.72
3:H:129:VAL:HG11	3:H:215:VAL:HG11	1.72	0.72
2:F:127:ARG:O	2:F:129:ASN:N	2.22	0.72
1:C:160:LYS:HD3	5:C:401:NAG:H83	1.70	0.71
3:H:197:LEU:N	3:H:198:GLY:HA3	2.04	0.71
4:L:138:VAL:HG12	4:L:140:LEU:CD1	2.20	0.71
3:P:129:VAL:HG11	3:P:215:VAL:HG11	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:110:LYS:HD2	1:E:247:ARG:HH21	1.55	0.71
1:A:44:LYS:HE2	1:A:269:GLU:HB2	1.72	0.71
3:M:18:LEU:HB3	3:M:82:LEU:O	1.91	0.71
3:P:161:SER:HB2	3:P:205:ASN:HB2	1.72	0.70
3:P:50:GLU:OE2	3:P:105:SER:OG	2.10	0.70
3:P:2:LEU:HA	3:P:25:TYR:HD1	1.57	0.69
2:D:54:ARG:NH2	2:D:103:GLU:OE2	2.25	0.69
3:H:33:TYR:CE2	3:H:104:GLY:HA2	2.26	0.69
3:P:57:THR:O	3:P:58:ASN:ND2	2.25	0.69
2:F:54:ARG:NH1	2:F:103:GLU:OE2	2.26	0.69
3:M:67:VAL:HG22	3:M:82:LEU:HD23	1.73	0.68
1:E:44:LYS:HE2	1:E:269:GLU:HB2	1.75	0.68
3:M:161:SER:HB2	3:M:205:ASN:HB2	1.76	0.68
1:E:121:ARG:HH22	3:P:103:SER:HB2	1.61	0.66
4:N:120:VAL:HG22	4:N:141:ILE:HG12	1.78	0.66
3:P:85:VAL:HG23	3:P:89:ASP:HB2	1.77	0.66
3:P:132:LEU:HD11	3:P:149:LEU:HB2	1.76	0.66
3:H:177:VAL:HG12	4:L:167:THR:HB	1.77	0.66
1:C:183:THR:HG22	1:C:188:SER:HA	1.78	0.65
2:F:25:ARG:HE	2:F:34:THR:CG2	2.07	0.65
1:C:231:ASN:O	1:C:231:ASN:ND2	2.30	0.65
4:N:113:GLN:NE2	4:N:175:ASN:OD1	2.29	0.64
1:E:80:ARG:NH2	1:E:262:VAL:O	2.30	0.64
3:M:39:GLN:HG3	3:M:44:GLY:O	1.98	0.64
1:E:121:ARG:NH2	3:P:33:TYR:OH	2.31	0.64
1:A:174:HIS:ND1	1:A:186:TYR:OH	2.27	0.64
1:E:133:GLY:HA3	3:P:31:GLY:HA3	1.81	0.63
1:C:147:THR:HG23	1:C:150:ALA:HB2	1.80	0.63
4:L:35:VAL:HG11	4:L:73:ALA:HB2	1.80	0.63
4:Q:64:PHE:HE1	4:Q:77:ILE:HG23	1.64	0.63
1:E:293:VAL:HG11	2:F:65:LEU:HD12	1.80	0.62
4:L:111:LEU:HB3	4:L:112:GLY:HA2	1.81	0.62
1:C:121:ARG:NH1	1:C:146:ASN:O	2.32	0.62
4:L:199:GLN:HA	4:L:207:VAL:O	1.98	0.62
1:C:186:TYR:HB2	1:C:191:LYS:HE3	1.79	0.62
1:A:212:PRO:HD3	1:C:235:THR:HB	1.81	0.62
4:Q:17:ARG:HG3	4:Q:78:ALA:HA	1.80	0.62
1:E:169:ILE:HB	1:E:226:LEU:HD23	1.81	0.62
4:L:120:VAL:O	4:L:209:LYS:NZ	2.26	0.62
3:M:143:THR:OG1	3:M:144:ALA:N	2.33	0.62
1:A:46:LYS:NZ	1:A:270:GLY:O	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:66:ARG:NH1	3:H:84:SER:O	2.33	0.61
4:L:17:ARG:HG3	4:L:78:ALA:HB2	1.82	0.61
3:M:32:TYR:CD2	3:M:97:ARG:HD2	2.36	0.61
3:H:3:GLN:HB2	3:H:25:TYR:HB3	1.83	0.60
4:Q:50:ILE:HD11	4:Q:64:PHE:HB3	1.83	0.60
1:A:298:ARG:HH22	2:B:59:THR:HG21	1.66	0.60
3:P:66:ARG:NH2	3:P:89:ASP:OD2	2.34	0.60
4:Q:41:LEU:HD23	4:Q:86:ALA:HB2	1.83	0.60
4:L:111:LEU:CB	4:L:112:GLY:HA2	2.32	0.60
3:M:7:TRP:NE1	3:M:21:THR:HG23	2.18	0.59
1:A:35:ARG:HD2	1:A:303:ARG:HH11	1.67	0.59
3:H:85:VAL:HG22	3:H:119:VAL:HG21	1.83	0.59
1:A:201:GLN:NE2	1:E:222:ASP:OD2	2.35	0.59
4:L:151:VAL:HG12	4:L:200:VAL:HG22	1.83	0.59
3:P:2:LEU:HA	3:P:25:TYR:CD1	2.38	0.59
3:M:132:LEU:HB2	3:M:147:GLY:O	2.03	0.58
4:N:175:ASN:CG	4:N:175:ASN:O	2.40	0.58
2:B:51:LYS:NZ	2:B:103:GLU:OE1	2.35	0.58
3:P:83:SER:OG	3:P:84:SER:N	2.36	0.58
3:M:7:TRP:HE1	3:M:21:THR:HG23	1.67	0.58
1:C:279:ILE:HG12	1:C:288:ILE:HD12	1.86	0.58
4:L:41:LEU:HD23	4:L:86:ALA:HB2	1.85	0.58
1:A:49:VAL:HG23	1:A:74:ALA:HB2	1.86	0.57
4:L:110:VAL:HG12	4:L:111:LEU:H	1.69	0.57
2:B:2:LEU:O	2:D:113:SER:OG	2.22	0.57
4:N:56:ARG:NH2	4:N:60:VAL:O	2.37	0.57
3:M:7:TRP:CD1	3:M:21:THR:HG23	2.39	0.57
3:P:87:ALA:HA	3:P:119:VAL:HG13	1.86	0.57
3:P:208:HIS:CD2	3:P:210:PRO:HD2	2.39	0.57
4:L:138:VAL:HG12	4:L:140:LEU:HD11	1.85	0.57
1:A:131:ARG:NH1	1:A:136:PHE:O	2.38	0.57
1:C:134:SER:HB2	3:M:100:TRP:HB3	1.87	0.57
1:A:85:ASP:OD2	1:A:99:ARG:NH2	2.37	0.56
3:H:160:VAL:HG11	3:H:188:SER:HB3	1.87	0.56
1:C:20:THR:OG1	2:F:47:GLN:HB3	2.05	0.56
2:F:25:ARG:NE	2:F:34:THR:CG2	2.66	0.56
3:M:5:GLN:O	3:M:22:CYS:HA	2.06	0.56
3:P:34:TRP:CZ3	3:P:97:ARG:HB2	2.41	0.56
3:P:64:LYS:HE3	3:P:65:SER:H	1.71	0.56
1:C:222:ASP:OD2	1:E:201:GLN:NE2	2.39	0.55
3:H:159:THR:O	3:H:206:VAL:HA	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:98:GLY:HA2	3:P:108:PHE:HA	1.88	0.55
3:M:87:ALA:HA	3:M:119:VAL:HG13	1.88	0.55
3:M:132:LEU:HD11	3:M:149:LEU:HB2	1.88	0.55
3:H:107:ASN:HB3	4:L:36:HIS:CD2	2.42	0.55
1:E:211:ARG:NH1	1:E:218:SER:O	2.39	0.55
3:P:86:THR:O	3:P:119:VAL:HG11	2.07	0.55
3:H:143:THR:HG22	3:H:193:PRO:HA	1.89	0.55
4:N:35:VAL:HG11	4:N:73:ALA:HB2	1.89	0.55
3:H:4:LEU:HB3	3:H:112:GLY:HA2	1.90	0.54
3:P:34:TRP:CH2	3:P:97:ARG:HD3	2.42	0.54
4:Q:17:ARG:HA	4:Q:77:ILE:O	2.08	0.54
3:P:147:GLY:HA2	3:P:162:TRP:CH2	2.42	0.54
3:H:32:TYR:CD2	3:H:97:ARG:HD2	2.42	0.54
3:H:122:ALA:HB1	3:H:123:SER:CB	2.31	0.54
3:M:2:LEU:HA	3:M:25:TYR:HD1	1.72	0.53
4:N:64:PHE:CD1	4:N:77:ILE:HD12	2.43	0.53
3:H:127:PRO:HB3	3:H:153:TYR:HB3	1.90	0.53
4:L:138:VAL:HG12	4:L:140:LEU:HD13	1.89	0.53
1:E:260:SER:HA	1:E:275:SER:HA	1.90	0.53
3:P:50:GLU:HG2	3:P:58:ASN:HB2	1.89	0.53
3:H:64:LYS:NZ	3:H:65:SER:H	2.06	0.53
1:E:183:THR:HG22	1:E:188:SER:HA	1.91	0.53
3:M:82:LEU:O	3:M:82:LEU:HD12	2.09	0.53
4:L:150:THR:O	4:L:201:THR:OG1	2.26	0.53
3:P:63:LEU:O	3:P:67:VAL:HG23	2.08	0.53
1:A:106:GLY:HA2	1:A:255:SER:HB3	1.91	0.53
3:H:203:ILE:HG12	3:H:218:LYS:HG2	1.90	0.53
2:B:23:GLY:HA3	2:B:36:ALA:HA	1.91	0.53
1:E:110:LYS:HD2	1:E:247:ARG:NH2	2.23	0.53
2:F:47:GLN:NE2	2:F:110:LEU:CD1	2.65	0.52
4:N:167:THR:CG2	4:N:180:SER:H	2.22	0.52
4:Q:156:ASP:OD2	4:Q:194:ARG:N	2.40	0.52
1:E:156:THR:HA	1:E:236:PHE:O	2.10	0.52
3:M:83:SER:OG	3:M:84:SER:N	2.41	0.52
1:A:195:VAL:HG22	1:A:236:PHE:HD1	1.74	0.52
1:E:15:LYS:HG3	1:E:25:GLU:HG3	1.92	0.52
3:H:171:VAL:HA	3:H:190:VAL:HG22	1.91	0.52
1:A:32:THR:OG1	1:A:305:LEU:O	2.26	0.52
1:C:149:ASN:ND2	1:C:184:LYS:HA	2.24	0.52
1:E:176:SER:O	1:E:211:ARG:NH2	2.43	0.52
2:F:47:GLN:HE21	2:F:110:LEU:CD1	2.05	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:134:PRO:HG3	3:M:146:LEU:HD23	1.92	0.52
2:B:129:ASN:ND2	2:B:159:HIS:HB2	2.25	0.52
2:D:51:LYS:NZ	2:D:103:GLU:OE1	2.37	0.52
2:F:170:ARG:C	2:F:170:ARG:HD2	2.29	0.52
4:Q:64:PHE:CE1	4:Q:77:ILE:HG23	2.44	0.52
2:D:17:LEU:HD11	2:D:36:ALA:HB2	1.92	0.51
2:B:4:GLY:O	2:B:8:GLY:HA3	2.10	0.51
2:B:30:GLN:NE2	2:B:145:ASP:HB2	2.25	0.51
3:M:3:GLN:HB2	3:M:25:TYR:HB3	1.90	0.51
3:P:171:VAL:HA	3:P:190:VAL:HG22	1.92	0.51
1:E:50:ASP:OD1	1:E:80:ARG:NH1	2.43	0.51
4:N:41:LEU:HD23	4:N:86:ALA:HB2	1.92	0.51
3:P:82:LEU:O	3:P:82:LEU:HD12	2.11	0.51
3:P:106:ASP:O	4:Q:36:HIS:CE1	2.63	0.51
4:Q:201:THR:HA	4:Q:205:SER:O	2.09	0.51
2:F:25:ARG:NH2	2:F:34:THR:HG21	2.25	0.51
3:M:18:LEU:HD13	3:M:117:VAL:HG11	1.92	0.51
1:E:121:ARG:NH2	3:P:103:SER:HB2	2.24	0.51
1:A:116:THR:O	1:A:157:LYS:NZ	2.40	0.51
1:C:207:SER:O	1:C:207:SER:OG	2.25	0.51
3:H:129:VAL:CG1	3:H:215:VAL:HG11	2.38	0.51
3:P:7:TRP:CD1	3:P:21:THR:HG23	2.46	0.51
3:P:19:SER:OG	3:P:81:LYS:NZ	2.43	0.51
1:A:220:ARG:HD2	1:C:201:GLN:OE1	2.12	0.50
4:Q:135:ALA:HB3	4:Q:185:LEU:O	2.12	0.50
4:Q:169:PRO:HA	4:Q:179:ALA:HB2	1.93	0.50
2:B:66:ILE:HD13	2:B:81:ILE:HD13	1.92	0.50
1:C:105:SER:HB2	1:C:251:LEU:HD22	1.94	0.50
1:C:102:LEU:HA	1:C:105:SER:HB3	1.93	0.49
3:P:147:GLY:HA2	3:P:162:TRP:HH2	1.78	0.49
1:C:220:ARG:HG3	1:E:201:GLN:HG2	1.94	0.49
4:N:125:PRO:HD3	4:N:137:LEU:HG	1.95	0.49
3:P:32:TYR:CG	3:P:97:ARG:HD2	2.47	0.49
1:E:284:PRO:HG2	1:E:285:PHE:CD2	2.47	0.49
3:H:2:LEU:HB3	3:H:110:TYR:CD2	2.48	0.49
3:P:156:GLU:HG2	3:P:157:PRO:HA	1.95	0.49
1:A:108:ILE:HD12	1:A:110:LYS:HE3	1.95	0.49
3:P:39:GLN:HG3	3:P:44:GLY:O	2.12	0.49
1:E:28:ASN:OD1	5:E:401:NAG:H61	2.13	0.49
1:E:279:ILE:HG12	1:E:288:ILE:HD12	1.95	0.48
4:N:118:PRO:HB3	4:N:141:ILE:HG23	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:18:LEU:HD13	3:P:117:VAL:HG11	1.96	0.48
1:E:298:ARG:HG2	2:F:92:TRP:CE2	2.48	0.48
4:L:13:ALA:HA	4:L:111:LEU:HG	1.96	0.48
3:P:18:LEU:O	3:P:81:LYS:HA	2.14	0.48
3:P:34:TRP:HZ3	3:P:97:ARG:HB2	1.76	0.48
2:B:155:ASN:O	2:B:155:ASN:ND2	2.44	0.48
3:M:93:TYR:O	3:M:114:GLY:HA2	2.13	0.48
4:N:28:ASN:OD1	4:N:29:ILE:N	2.46	0.48
3:P:85:VAL:HG22	3:P:119:VAL:HG21	1.95	0.48
3:P:208:HIS:HB3	3:P:213:THR:HG23	1.95	0.48
3:M:203:ILE:HG12	3:M:218:LYS:HG2	1.96	0.48
4:N:153:TRP:O	4:N:159:PRO:HA	2.14	0.48
1:A:121:ARG:HD3	1:A:145:SER:O	2.13	0.47
1:C:56:LEU:HG	1:C:102:LEU:CD1	2.44	0.47
3:P:107:ASN:HB3	4:Q:36:HIS:ND1	2.28	0.47
4:Q:56:ARG:NH2	4:Q:60:VAL:O	2.47	0.47
2:B:17:LEU:HD11	2:B:36:ALA:HB2	1.96	0.47
2:D:155:ASN:O	2:D:155:ASN:ND2	2.38	0.47
3:H:132:LEU:HD11	3:H:149:LEU:HB2	1.96	0.47
3:M:63:LEU:O	3:M:67:VAL:HG23	2.14	0.47
3:M:101:GLU:HB3	3:M:106:ASP:HB2	1.96	0.47
3:M:127:PRO:HB3	3:M:153:TYR:HB3	1.96	0.47
4:N:25:SER:H	4:N:28:ASN:HD21	1.62	0.47
3:P:129:VAL:CG1	3:P:215:VAL:HG11	2.42	0.47
3:P:120:SER:OG	3:P:182:GLY:HA3	2.15	0.47
4:Q:172:GLN:HE21	4:Q:174:ASN:HB2	1.79	0.47
3:M:6:GLU:OE1	3:M:113:GLN:N	2.48	0.47
1:E:174:HIS:ND1	1:E:186:TYR:OH	2.42	0.47
1:E:179:THR:O	1:E:183:THR:HG23	2.14	0.47
3:M:4:LEU:HD12	3:M:24:VAL:HG12	1.97	0.47
4:N:113:GLN:HB3	4:N:114:PRO:HD2	1.96	0.47
1:A:43:SER:HB2	1:A:48:THR:HG21	1.96	0.47
4:L:111:LEU:HB3	4:L:112:GLY:CA	2.44	0.47
3:M:208:HIS:HB3	3:M:213:THR:HG23	1.96	0.47
2:D:134:GLY:HA2	2:F:124:ARG:HD3	1.96	0.47
3:M:19:SER:O	3:M:20:LEU:HD23	2.15	0.47
4:N:136:THR:HA	4:N:183:LEU:O	2.15	0.47
3:P:33:TYR:CD1	3:P:50:GLU:HG3	2.50	0.47
1:E:228:LEU:HD13	1:E:234:VAL:HB	1.98	0.46
3:P:64:LYS:HA	3:P:64:LYS:HD2	1.67	0.46
1:C:106:GLY:HA2	1:C:255:SER:HB3	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:ARG:HD3	1:C:250:PHE:CZ	2.50	0.46
3:P:12:LEU:O	3:P:119:VAL:HA	2.15	0.46
3:P:67:VAL:HG22	3:P:82:LEU:HD23	1.96	0.46
2:B:123:LYS:NZ	2:B:132:GLU:OE2	2.27	0.46
2:B:129:ASN:HD21	2:B:159:HIS:HB2	1.79	0.46
1:E:177:VAL:HG23	1:E:181:GLU:OE1	2.15	0.46
1:A:167:ALA:O	1:A:227:MET:HA	2.15	0.46
4:Q:111:LEU:CB	4:Q:112:GLY:HA2	2.29	0.46
3:H:125:LYS:HG2	3:H:126:GLY:H	1.80	0.46
3:M:111:TRP:CD2	4:N:46:PRO:HG2	2.49	0.46
3:P:208:HIS:ND1	3:P:211:SER:OG	2.45	0.46
4:L:138:VAL:CG1	4:L:140:LEU:HD11	2.46	0.46
3:M:159:THR:HB	3:M:207:ASN:HB3	1.97	0.46
2:B:170:ARG:C	2:B:170:ARG:HH11	2.19	0.46
4:L:25:SER:H	4:L:28:ASN:HD21	1.62	0.46
4:L:25:SER:OG	4:L:28:ASN:ND2	2.49	0.46
3:P:111:TRP:CD1	3:P:111:TRP:N	2.84	0.46
3:P:105:SER:O	3:P:106:ASP:HB3	2.15	0.45
1:C:20:THR:HG22	2:D:105:GLN:OE1	2.17	0.45
1:E:34:GLU:HG2	1:E:281:SER:HB2	1.98	0.45
3:M:91:ALA:HB3	3:M:93:TYR:CE1	2.51	0.45
4:N:188:GLU:O	4:N:192:SER:OG	2.27	0.45
1:C:170:VAL:O	1:C:245:PRO:HB3	2.15	0.45
3:H:86:THR:OG1	3:H:87:ALA:N	2.49	0.45
4:L:135:ALA:HB3	4:L:185:LEU:O	2.17	0.45
3:M:168:THR:O	3:M:171:VAL:HG12	2.16	0.45
2:B:127:ARG:HD3	2:B:159:HIS:NE2	2.31	0.45
2:B:133:ASP:OD2	2:B:135:THR:OG1	2.30	0.45
2:D:125:GLN:NE2	2:D:155:ASN:HA	2.32	0.45
2:D:131:GLU:CD	2:F:163:ARG:HH22	2.19	0.45
3:M:80:LEU:CD2	3:M:82:LEU:HG	2.47	0.45
4:N:40:GLN:O	4:N:86:ALA:HB1	2.17	0.45
4:N:141:ILE:HB	4:N:179:ALA:O	2.16	0.45
4:N:167:THR:HG22	4:N:180:SER:H	1.81	0.45
1:E:57:LEU:O	1:E:60:ILE:HG22	2.16	0.45
1:E:81:ARG:HB2	2:F:70:PHE:CE1	2.51	0.45
3:H:144:ALA:O	3:H:191:THR:HA	2.16	0.45
1:A:168:LEU:HB3	1:A:249:SER:HB2	1.98	0.45
1:E:147:THR:HG23	1:E:150:ALA:HB2	1.98	0.45
3:H:12:LEU:O	3:H:119:VAL:HA	2.16	0.45
3:H:85:VAL:HG23	3:H:89:ASP:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:79:SER:OG	3:H:80:LEU:N	2.50	0.45
3:M:12:LEU:O	3:M:119:VAL:HA	2.17	0.45
4:Q:92:SER:OG	4:Q:93:TYR:N	2.50	0.45
1:A:34:GLU:HG2	1:A:281:SER:HB2	1.98	0.45
1:C:57:LEU:O	1:C:60:ILE:HG22	2.16	0.45
3:H:36:TRP:CD2	3:H:80:LEU:HD12	2.52	0.45
4:L:33:PHE:CD1	4:L:93:TYR:HB3	2.52	0.45
4:N:118:PRO:HB2	4:N:120:VAL:HG23	1.98	0.45
4:Q:153:TRP:CZ3	4:Q:198:CYS:HB2	2.52	0.45
1:E:169:ILE:HB	1:E:226:LEU:CD2	2.45	0.45
3:M:145:ALA:HB2	3:M:191:THR:HG22	1.98	0.45
3:P:79:SER:OG	3:P:80:LEU:N	2.50	0.45
3:H:70:SER:OG	3:H:79:SER:HB3	2.16	0.44
3:P:63:LEU:O	3:P:66:ARG:HB2	2.17	0.44
1:E:37:ASN:OD1	1:E:38:ILE:N	2.50	0.44
1:E:149:ASN:HA	1:E:183:THR:O	2.17	0.44
2:F:129:ASN:N	2:F:129:ASN:OD1	2.50	0.44
4:L:92:SER:O	4:L:100:VAL:HG23	2.18	0.44
3:M:66:ARG:HB3	3:M:83:SER:HB2	1.99	0.44
1:C:136:PHE:CE2	1:C:142:TRP:HB2	2.52	0.44
1:E:155:MET:O	1:E:237:SER:HA	2.17	0.44
3:M:36:TRP:O	3:M:48:ILE:HG12	2.18	0.44
4:N:50:ILE:HG21	4:N:66:GLY:HA3	1.98	0.44
4:Q:111:LEU:HD22	4:Q:145:TYR:HE2	1.81	0.44
2:B:119:TYR:CE1	2:B:136:GLY:HA2	2.51	0.44
4:Q:81:GLN:O	4:Q:110:VAL:HG21	2.18	0.44
4:Q:127:SER:O	4:Q:131:GLN:HG3	2.17	0.44
1:C:70:LEU:O	1:C:110:LYS:NZ	2.36	0.44
2:F:18:ILE:H	2:F:18:ILE:HG13	1.62	0.44
3:H:17:THR:HG23	3:H:83:SER:HA	1.98	0.44
4:Q:115:LYS:HD2	4:Q:115:LYS:N	2.33	0.44
4:L:26:SER:HA	4:L:30:GLY:HA3	1.99	0.44
3:P:18:LEU:HB3	3:P:82:LEU:O	2.18	0.44
3:M:64:LYS:HD2	3:M:65:SER:H	1.82	0.43
4:L:34:ASP:HB2	4:L:36:HIS:HE1	1.83	0.43
3:M:129:VAL:CG1	3:M:215:VAL:HG11	2.44	0.43
4:N:64:PHE:HD1	4:N:77:ILE:HD12	1.80	0.43
3:P:113:GLN:HA	4:Q:45:ALA:HB2	2.00	0.43
3:M:30:SER:HB3	3:M:53:HIS:CG	2.53	0.43
3:M:153:TYR:OH	3:M:186:LEU:HD23	2.18	0.43
1:C:226:LEU:HD12	1:C:226:LEU:O	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:66:ARG:HG2	3:P:83:SER:OG	2.18	0.43
4:Q:138:VAL:HG13	4:Q:182:TYR:CE1	2.53	0.43
1:C:126:THR:HG23	1:C:129:CYS:H	1.83	0.43
1:C:174:HIS:ND1	1:C:186:TYR:OH	2.45	0.43
3:P:132:LEU:HD23	4:Q:123:PHE:CG	2.53	0.43
2:B:124:ARG:NH1	2:F:132:GLU:OE2	2.52	0.43
1:E:98:LEU:HD11	1:E:168:LEU:HD21	2.00	0.43
3:H:48:ILE:HD11	3:H:80:LEU:HD11	2.00	0.43
3:P:132:LEU:HD23	4:Q:123:PHE:CD2	2.53	0.43
1:C:149:ASN:HA	1:C:183:THR:O	2.19	0.43
4:L:88:TYR:HE2	4:L:108:LEU:HD22	1.84	0.43
3:M:36:TRP:NE1	3:M:80:LEU:HB2	2.34	0.43
4:Q:36:HIS:O	4:Q:90:CYS:HA	2.19	0.43
1:A:99:ARG:O	1:A:103:ARG:HG3	2.19	0.43
3:H:134:PRO:HB3	3:H:146:LEU:HB3	2.00	0.43
4:L:154:LYS:NZ	4:L:208:GLU:OE2	2.44	0.43
3:P:2:LEU:HD22	3:P:97:ARG:HH21	1.84	0.43
1:A:163:ARG:HD3	1:A:250:PHE:CZ	2.54	0.43
1:A:110:LYS:HB2	1:A:247:ARG:NH2	2.34	0.42
3:H:4:LEU:CD1	3:H:24:VAL:HG12	2.49	0.42
3:M:24:VAL:HG22	3:M:76:ASN:O	2.19	0.42
1:A:72:PHE:CE2	1:A:107:GLY:HA2	2.54	0.42
1:C:113:MET:CE	1:C:115:PHE:CE2	3.03	0.42
1:C:186:TYR:CZ	1:C:241:ALA:HA	2.54	0.42
3:H:6:GLU:HA	3:H:22:CYS:HA	2.01	0.42
1:C:108:ILE:HD11	1:C:249:SER:OG	2.19	0.42
2:F:122:VAL:O	2:F:126:LEU:HB2	2.19	0.42
4:N:118:PRO:HA	4:N:119:SER:CB	2.38	0.42
4:Q:40:GLN:O	4:Q:86:ALA:HB1	2.19	0.42
3:M:90:THR:OG1	3:M:119:VAL:HG12	2.19	0.42
3:M:123:SER:O	3:M:154:PHE:HD2	2.03	0.42
3:P:28:SER:OG	3:P:29:PHE:N	2.51	0.42
3:P:123:SER:C	3:P:125:LYS:H	2.23	0.42
4:Q:19:THR:HG23	4:Q:74:SER:HB3	2.01	0.42
2:B:24:PHE:CD1	2:B:153:ARG:HG2	2.55	0.42
2:B:48:ILE:HD11	2:B:107:THR:HG23	2.02	0.42
4:N:141:ILE:HD11	4:N:200:VAL:HG21	2.01	0.42
1:C:109:ASP:HB2	1:C:252:ARG:CZ	2.50	0.42
1:E:186:TYR:HB2	1:E:191:LYS:HE3	2.01	0.42
3:M:147:GLY:HA2	3:M:162:TRP:CH2	2.55	0.42
2:B:58:LYS:HD2	2:B:58:LYS:HA	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:196:SER:C	3:H:198:GLY:HA3	2.40	0.42
3:P:192:VAL:HB	3:P:193:PRO:HD2	2.01	0.42
4:Q:65:SER:OG	4:Q:76:ALA:HB3	2.19	0.42
1:C:156:THR:HA	1:C:236:PHE:O	2.20	0.42
2:F:25:ARG:HA	2:F:33:GLY:O	2.19	0.42
2:B:66:ILE:HD12	2:B:67:ASP:N	2.33	0.42
2:B:129:ASN:OD1	2:B:129:ASN:N	2.53	0.42
2:D:170:ARG:HD2	2:D:170:ARG:C	2.41	0.42
3:H:120:SER:OG	3:H:182:GLY:HA3	2.20	0.42
3:P:36:TRP:CE2	3:P:80:LEU:HB2	2.55	0.41
1:C:169:ILE:HB	1:C:226:LEU:HD12	2.02	0.41
3:M:186:LEU:HD12	3:M:187:SER:N	2.35	0.41
1:C:260:SER:OG	1:C:262:VAL:HG22	2.20	0.41
1:C:305:LEU:HD23	1:C:305:LEU:HA	1.91	0.41
3:M:111:TRP:N	3:M:111:TRP:CD1	2.88	0.41
3:M:132:LEU:HB3	4:N:123:PHE:CE2	2.55	0.41
4:N:49:LEU:HD12	4:N:49:LEU:HA	1.76	0.41
1:E:134:SER:HB2	3:P:100:TRP:HB3	2.03	0.41
2:F:141:PHE:HB2	2:F:166:ALA:HB1	2.02	0.41
3:M:34:TRP:HB3	3:M:78:PHE:CZ	2.56	0.41
3:P:143:THR:HG22	3:P:193:PRO:HA	2.01	0.41
2:F:51:LYS:NZ	2:F:103:GLU:O	2.54	0.41
4:N:109:THR:HG21	4:N:146:PRO:HB3	2.03	0.41
4:Q:167:THR:HG23	4:Q:179:ALA:HB1	2.02	0.41
2:B:127:ARG:HD3	2:B:159:HIS:CD2	2.56	0.41
1:C:298:ARG:HG2	2:D:92:TRP:CE2	2.55	0.41
1:C:113:MET:HE1	1:C:245:PRO:HG2	2.01	0.41
1:E:163:ARG:HD3	1:E:250:PHE:CZ	2.55	0.41
2:B:125:GLN:OE1	2:B:155:ASN:HA	2.21	0.41
2:B:133:ASP:HB3	2:B:137:CYS:O	2.19	0.41
2:F:38:TYR:O	2:F:42:GLN:HB2	2.20	0.41
3:H:178:LEU:HD13	3:H:184:TYR:CZ	2.55	0.41
4:L:63:ARG:HB3	4:L:78:ALA:O	2.20	0.41
3:M:86:THR:OG1	3:M:87:ALA:N	2.53	0.41
4:Q:63:ARG:HB3	4:Q:78:ALA:O	2.20	0.41
1:A:121:ARG:NH1	1:A:147:THR:HA	2.36	0.41
1:A:134:SER:HB2	3:H:100:TRP:HB3	2.02	0.41
1:E:195:VAL:O	1:E:201:GLN:HA	2.21	0.41
1:E:305:LEU:HB3	2:F:100:VAL:HG21	2.03	0.41
4:Q:49:LEU:HB3	4:Q:50:ILE:HG12	2.02	0.41
4:Q:60:VAL:HG13	4:Q:64:PHE:HD2	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ARG:H	1:A:298:ARG:CD	2.33	0.40
2:F:4:GLY:O	2:F:8:GLY:HA3	2.21	0.40
3:P:52:ASN:OD1	3:P:56:GLY:N	2.50	0.40
2:D:94:TYR:CE2	2:F:95:ASN:HB3	2.55	0.40
3:H:200:GLN:OE1	3:H:201:THR:N	2.53	0.40
3:M:10:GLY:O	3:M:11:LEU:HD12	2.20	0.40
4:Q:50:ILE:HG12	4:Q:50:ILE:H	1.50	0.40
2:B:75:LYS:HB3	1:C:97:ALA:HB1	2.03	0.40
1:C:121:ARG:NH1	1:C:145:SER:O	2.54	0.40
1:E:65:GLN:O	1:E:68:GLN:NE2	2.54	0.40
2:F:25:ARG:HH21	2:F:34:THR:HG21	1.86	0.40
3:H:4:LEU:HD12	3:H:4:LEU:HA	1.78	0.40
4:L:84:ASP:O	4:L:108:LEU:HD23	2.21	0.40
1:A:186:TYR:CZ	1:A:241:ALA:HA	2.56	0.40
3:H:34:TRP:CH2	3:H:97:ARG:HD3	2.56	0.40
3:H:129:VAL:HA	3:H:149:LEU:O	2.22	0.40
4:Q:49:LEU:HB3	4:Q:50:ILE:H	1.50	0.40
3:M:193:PRO:HG2	3:M:196:SER:OG	2.21	0.40
3:P:27:GLY:HA3	3:P:28:SER:HA	1.62	0.40
4:Q:186:THR:OG1	4:Q:188:GLU:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	315/317 (99%)	307 (98%)	8 (2%)	0	100	100
1	C	315/317 (99%)	304 (96%)	11 (4%)	0	100	100
1	E	314/317 (99%)	300 (96%)	14 (4%)	0	100	100
2	B	168/170 (99%)	162 (96%)	6 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	D	168/170 (99%)	159 (95%)	9 (5%)	0	100 100
2	F	168/170 (99%)	160 (95%)	6 (4%)	2 (1%)	13 50
3	H	212/221 (96%)	191 (90%)	19 (9%)	2 (1%)	17 56
3	M	209/221 (95%)	186 (89%)	23 (11%)	0	100 100
3	P	212/221 (96%)	188 (89%)	24 (11%)	0	100 100
4	L	210/212 (99%)	191 (91%)	19 (9%)	0	100 100
4	N	210/212 (99%)	190 (90%)	20 (10%)	0	100 100
4	Q	210/212 (99%)	194 (92%)	14 (7%)	2 (1%)	15 54
All	All	2711/2760 (98%)	2532 (93%)	173 (6%)	6 (0%)	47 81

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	Q	50	ILE
2	F	128	GLU
3	H	103	SER
3	H	104	GLY
2	F	127	ARG
4	Q	51	TYR

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	266/266 (100%)	263 (99%)	3 (1%)	73 88
1	C	265/266 (100%)	260 (98%)	5 (2%)	57 80
1	E	265/266 (100%)	256 (97%)	9 (3%)	37 68
2	B	145/145 (100%)	139 (96%)	6 (4%)	30 63
2	D	145/145 (100%)	142 (98%)	3 (2%)	53 79
2	F	145/145 (100%)	144 (99%)	1 (1%)	84 93
3	H	182/186 (98%)	179 (98%)	3 (2%)	62 83

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	M	180/186 (97%)	173 (96%)	7 (4%)	32 64
3	P	182/186 (98%)	174 (96%)	8 (4%)	28 62
4	L	173/173 (100%)	172 (99%)	1 (1%)	86 94
4	N	173/173 (100%)	170 (98%)	3 (2%)	60 82
4	Q	173/173 (100%)	170 (98%)	3 (2%)	60 82
All	All	2294/2310 (99%)	2242 (98%)	52 (2%)	50 77

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	298	ARG
1	A	316	GLU
2	B	12	ASN
2	B	24	PHE
2	B	57	GLU
2	B	102	MET
2	B	155	ASN
2	B	170	ARG
1	C	8	HIS
1	C	175	HIS
1	C	207	SER
1	C	226	LEU
1	C	231	ASN
2	D	57	GLU
2	D	148	CYS
2	D	155	ASN
1	E	8	HIS
1	E	22	ARG
1	E	113	MET
1	E	121	ARG
1	E	127	SER
1	E	199	ASN
1	E	201	GLN
1	E	211	ARG
1	E	298	ARG
2	F	102	MET
3	H	6	GLU
3	H	12	LEU
3	H	172	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	L	199	GLN
3	M	7	TRP
3	M	22	CYS
3	M	25	TYR
3	M	33	TYR
3	M	83	SER
3	M	204	CYS
3	M	216	ASP
4	N	129	GLU
4	N	134	LYS
4	N	175	ASN
3	P	7	TRP
3	P	12	LEU
3	P	25	TYR
3	P	123	SER
3	P	146	LEU
3	P	172	HIS
3	P	204	CYS
3	P	213	THR
4	Q	17	ARG
4	Q	62	ASP
4	Q	134	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	GLN
1	C	175	HIS
2	F	47	GLN
3	M	200	GLN
4	N	113	GLN
4	N	175	ASN
4	Q	36	HIS
4	Q	174	ASN

5.3.3 RNA

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)

3 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	C	401	1	14,14,15	0.61	0	17,19,21	0.41	0
5	NAG	F	301	2	14,14,15	0.51	0	17,19,21	0.50	0
5	NAG	E	401	1	14,14,15	1.36	1 (7%)	17,19,21	1.61	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	C	401	1	-	2/6/23/26	0/1/1/1
5	NAG	F	301	2	-	2/6/23/26	0/1/1/1
5	NAG	E	401	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	401	NAG	O5-C1	4.95	1.51	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	401	NAG	C1-O5-C5	6.38	120.83	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	401	NAG	O5-C5-C6-O6
5	F	301	NAG	O5-C5-C6-O6
5	C	401	NAG	C4-C5-C6-O6
5	F	301	NAG	C4-C5-C6-O6

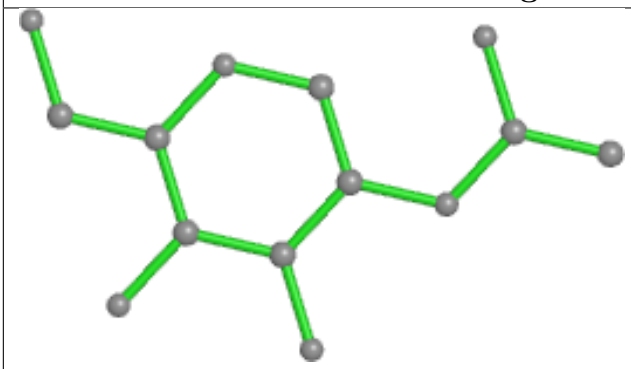
There are no ring outliers.

2 monomers are involved in 2 short contacts:

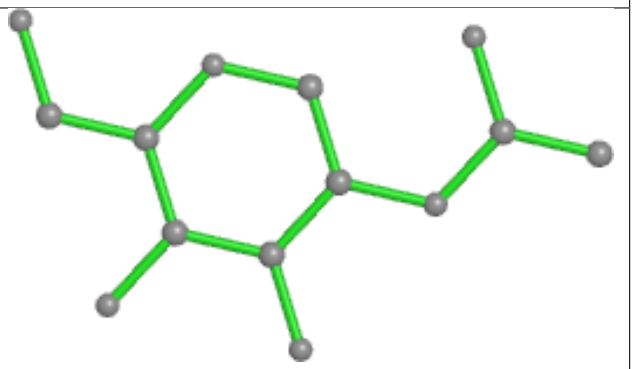
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	401	NAG	1	0
5	E	401	NAG	1	0

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.

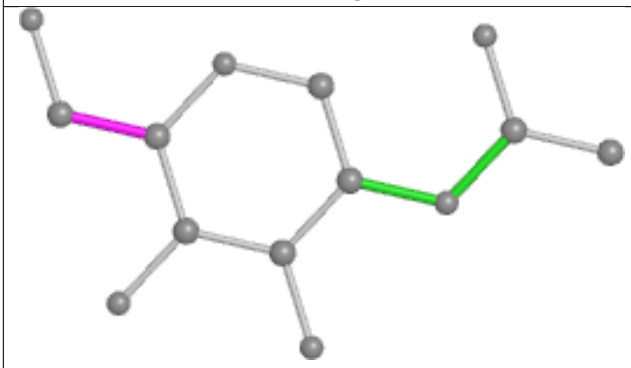
Ligand NAG C 401



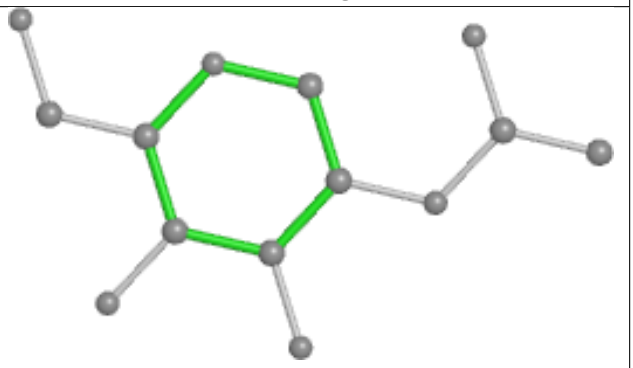
Bond lengths



Bond angles

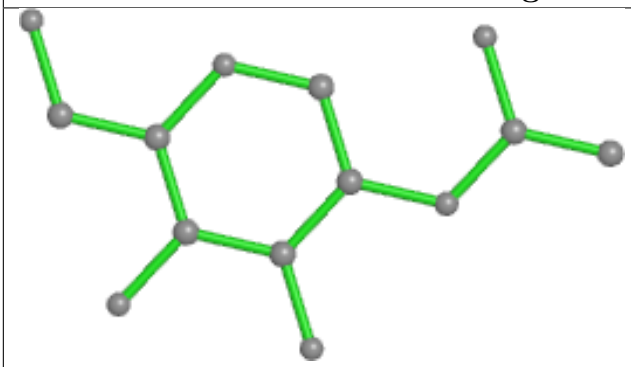


Torsions

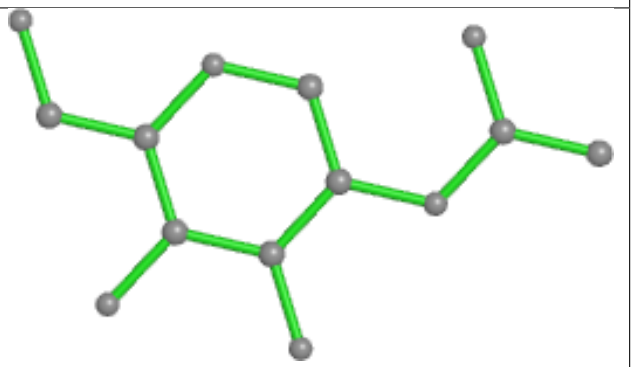


Rings

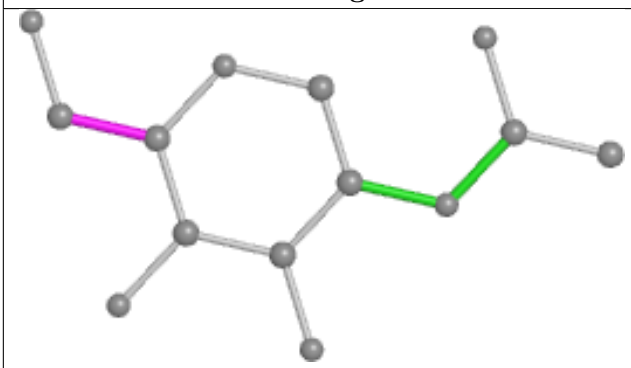
Ligand NAG F 301



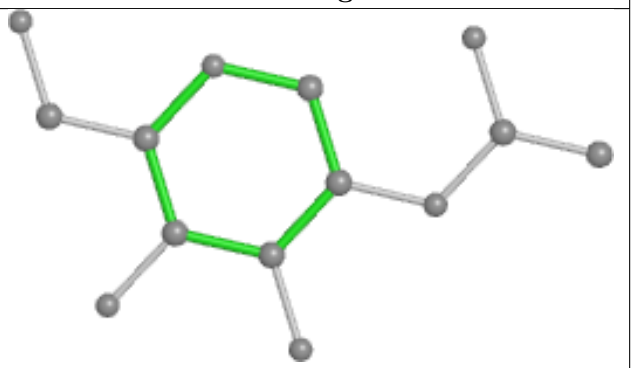
Bond lengths



Bond angles

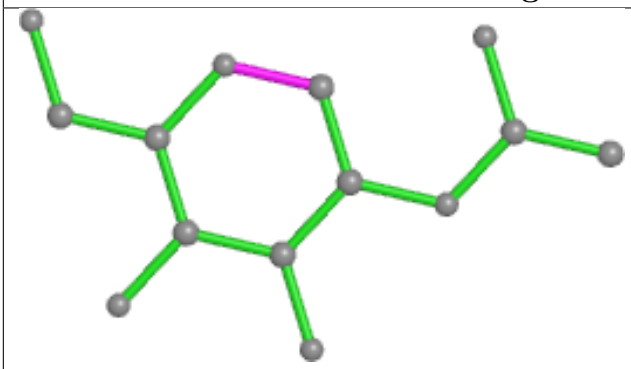


Torsions

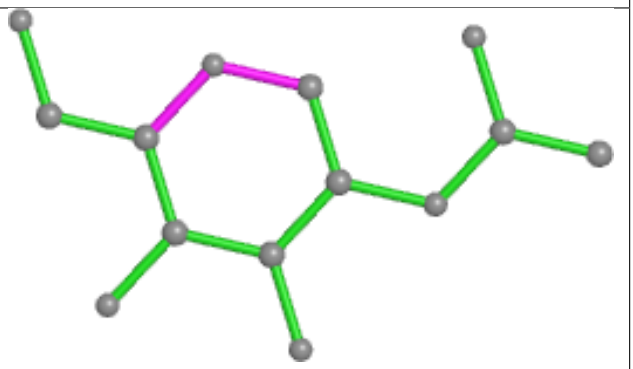


Rings

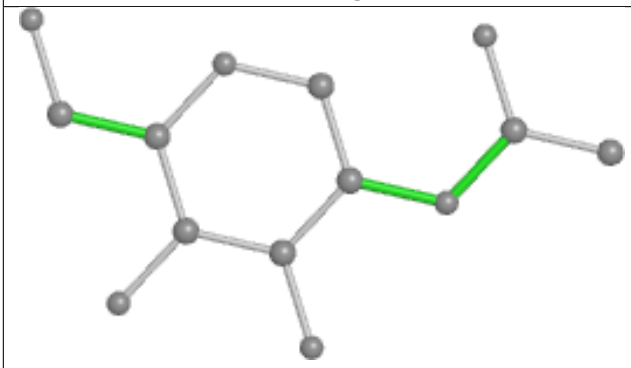
Ligand NAG E 401



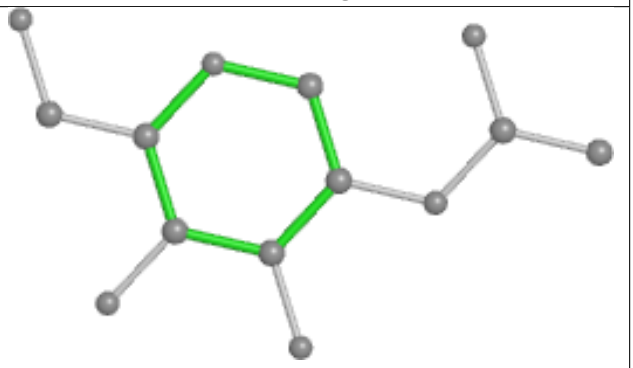
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	317/317 (100%)	-0.53	0	100	100	51, 77, 107, 141	1 (0%)
1	C	317/317 (100%)	-0.55	0	100	100	42, 80, 116, 159	1 (0%)
1	E	316/317 (99%)	-0.55	0	100	100	42, 74, 116, 154	1 (0%)
2	B	170/170 (100%)	-0.46	0	100	100	46, 96, 127, 162	0
2	D	170/170 (100%)	-0.47	0	100	100	42, 108, 151, 189	0
2	F	170/170 (100%)	-0.43	0	100	100	46, 116, 153, 173	0
3	H	216/221 (97%)	-0.48	0	100	100	65, 105, 158, 188	0
3	M	213/221 (96%)	-0.43	0	100	100	54, 95, 162, 224	0
3	P	216/221 (97%)	-0.52	0	100	100	53, 90, 142, 188	0
4	L	212/212 (100%)	-0.40	0	100	100	65, 109, 148, 201	0
4	N	212/212 (100%)	-0.44	0	100	100	55, 105, 156, 204	0
4	Q	212/212 (100%)	-0.47	0	100	100	49, 95, 138, 160	0
All	All	2741/2760 (99%)	-0.49	0	100	100	42, 92, 144, 224	3 (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

There are no monosaccharides in this entry.

6.4 Ligands

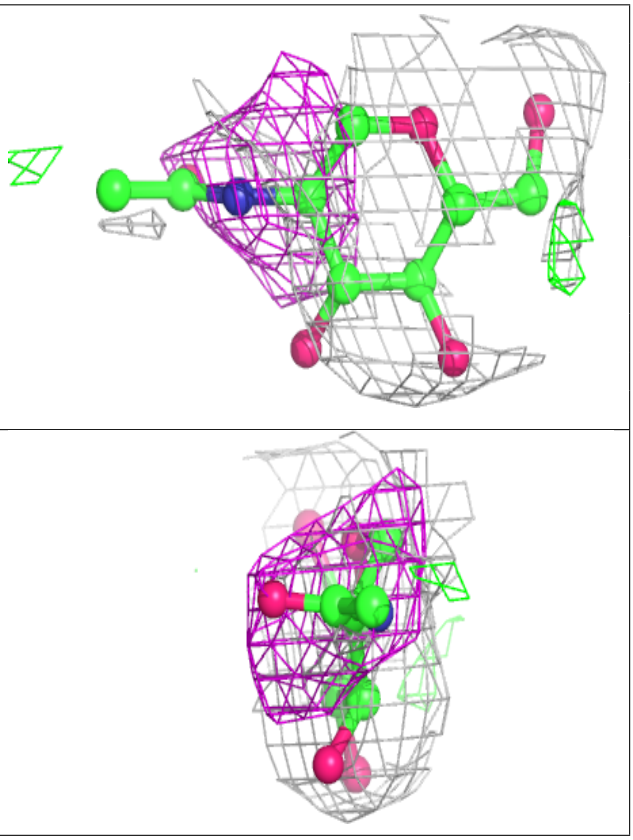
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

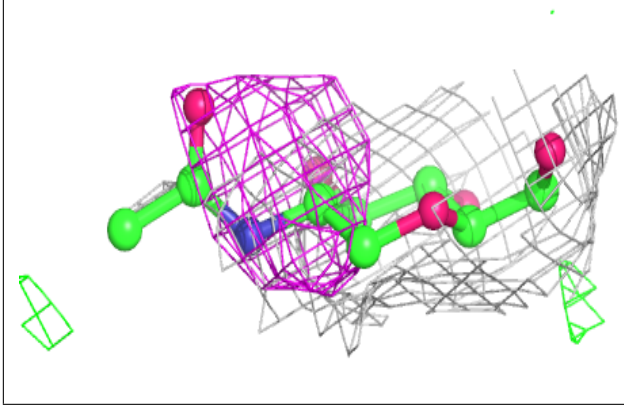
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	C	401	14/15	0.66	0.43	111,144,154,154	0
5	NAG	E	401	14/15	0.78	0.24	112,136,145,145	0
5	NAG	F	301	14/15	0.90	0.18	90,103,112,114	0

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 C 401:

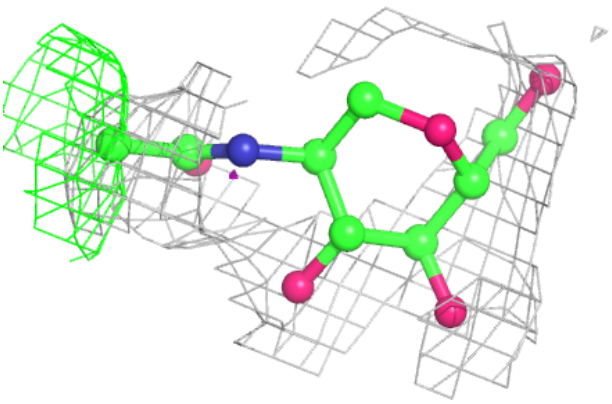
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

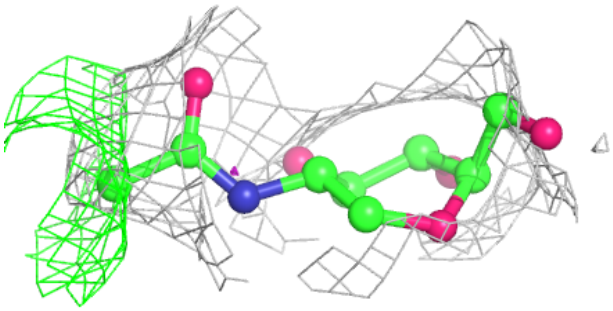


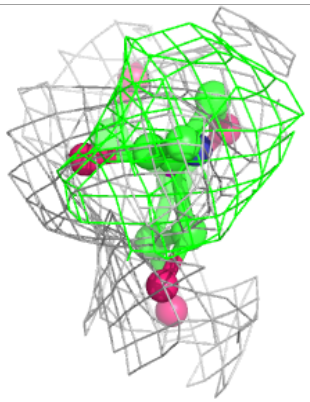


Electron density around NAG E 401:

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

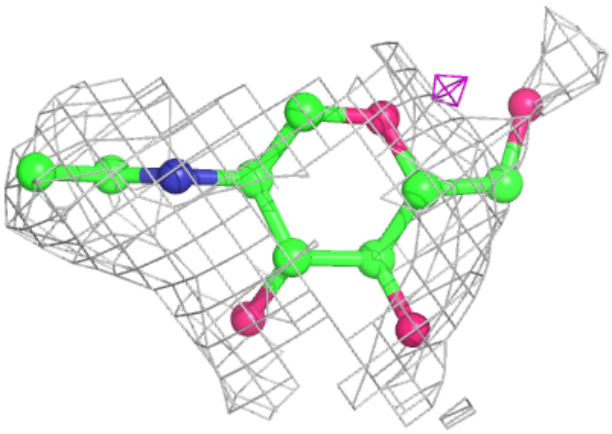


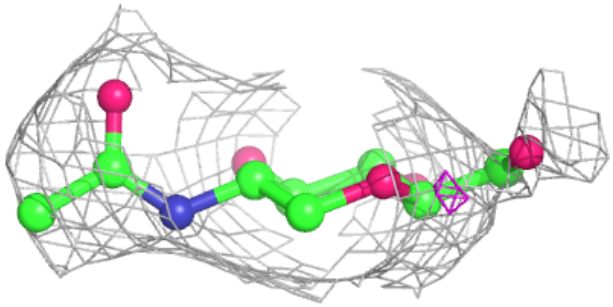


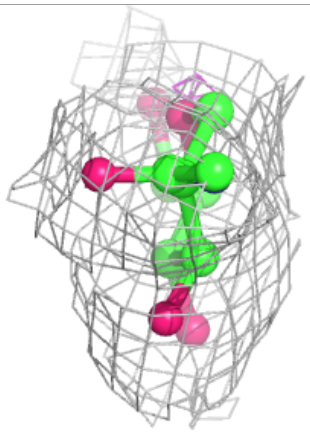


Electron density around NAG F 301:

$2mF_o$-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.