Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 05:17 PM EDT

PDB ID	:	6PZF
Title	:	Crystal structure of human NA-63 Fab in complex with neuraminidase from A/Hunan/02650/2016(H7N9)
Authors	:	Zhu, X.; Wilson, I.A.
Deposited on	:	2019-07-31
Resolution	:	2.80 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:

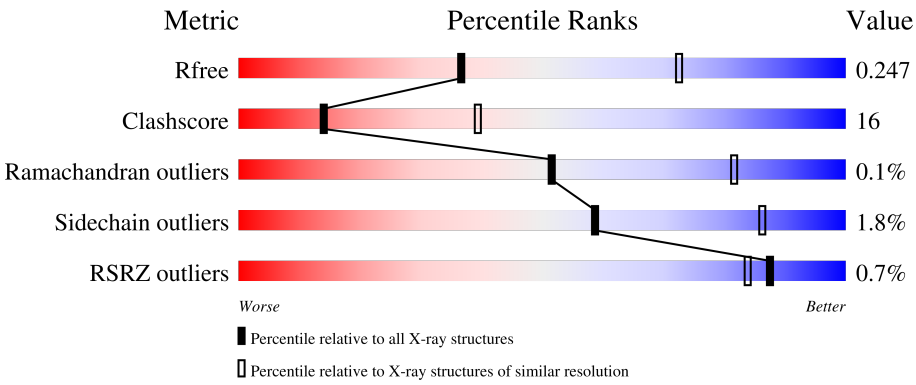
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	393	81% 17% •
1	B	393	77% 21% ••
2	E	216	2% 75% 23% •
2	L	216	4% 57% 41% •
3	F	228	61% 32% • 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	H	228	61% 30% • 7%
4	C	11	9% 91%
4	D	11	18% 82%
5	G	2	50% 50%

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
4	MAN	D	11	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 13026 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 Neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	388	3057	1902	543	589	23	0	1	0
1	A	388	3057	1902	543	589	23	0	1	0

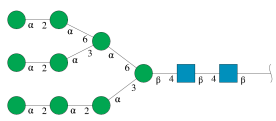
- Molecule 2 is a protein called NA-63 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	215	1646	1031	273	336	6	0	0	0
2	L	215	1646	1031	273	336	6	0	0	0

- Molecule 3 is a protein called NA-63 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	F	213	1606	1018	269	313	6	0	0	0
3	H	213	1606	1018	269	313	6	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

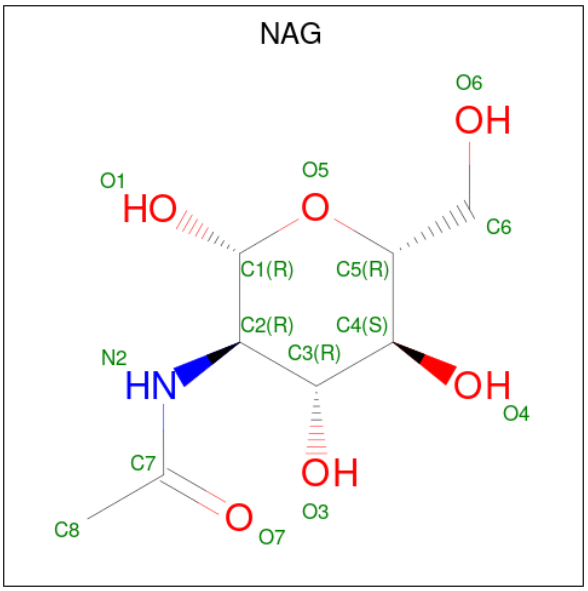


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	C	11	127	70	2	55	0	0	0
			Total	C	N	O			
4	D	11	127	70	2	55	0	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	G	2	28	16	2	10	0	0	0

- Molecule 6 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).

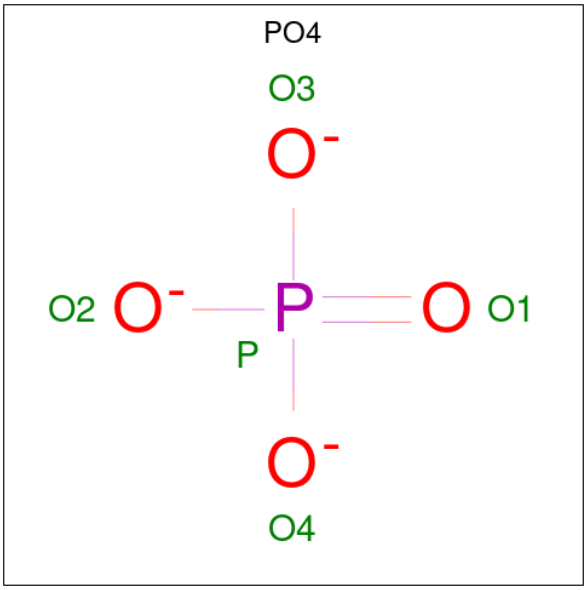


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	B	1	14	8	1	5	0	0
			Total	C	N	O		
6	B	1	14	8	1	5	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Ca 1 1	0	0
7	A	1	Total Ca 1 1	0	0

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total O P 5 4 1	0	0
8	B	1	Total O P 5 4 1	0	0
8	B	1	Total O P 5 4 1	0	0
8	A	1	Total O P 5 4 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	37	Total O 37 37	0	0
9	A	17	Total O 17 17	0	0
9	E	5	Total O 5 5	0	0

Continued on next page...

Continued from previous page...

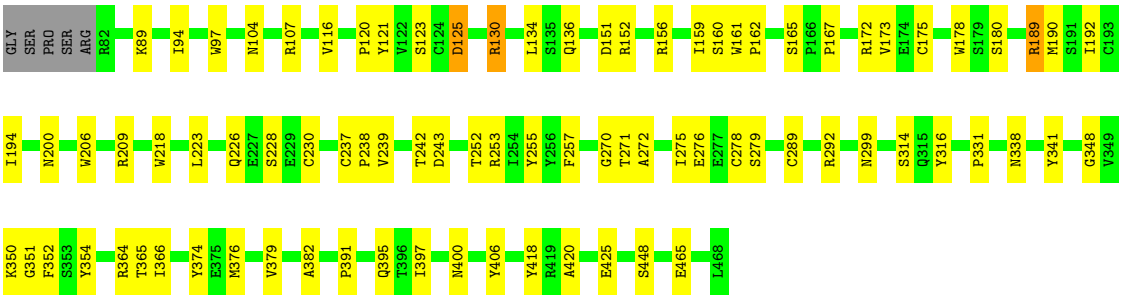
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	F	11	11	11	0	0
			Total	O		
9	L	4	4	4	0	0
			Total	O		
9	H	2	2	2	0	0

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.

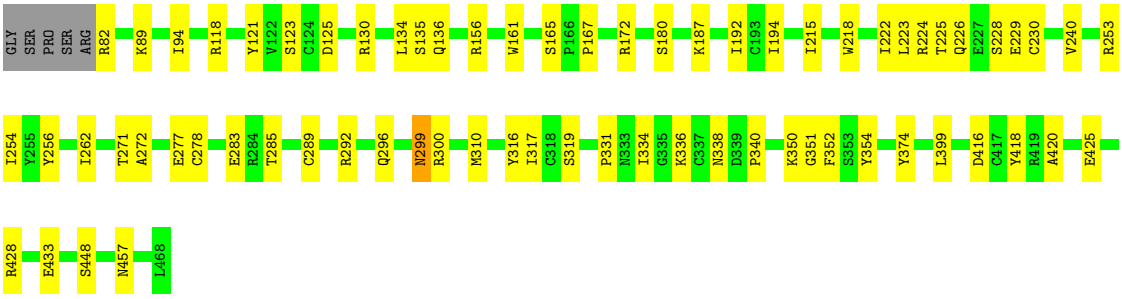
• Molecule 1: Neuraminidase

Chain B:



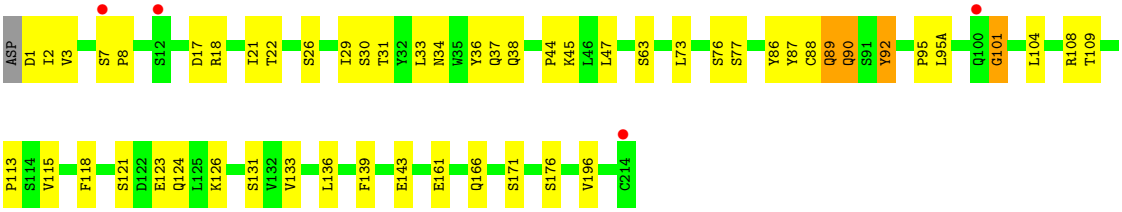
• Molecule 1: Neuraminidase

Chain A:



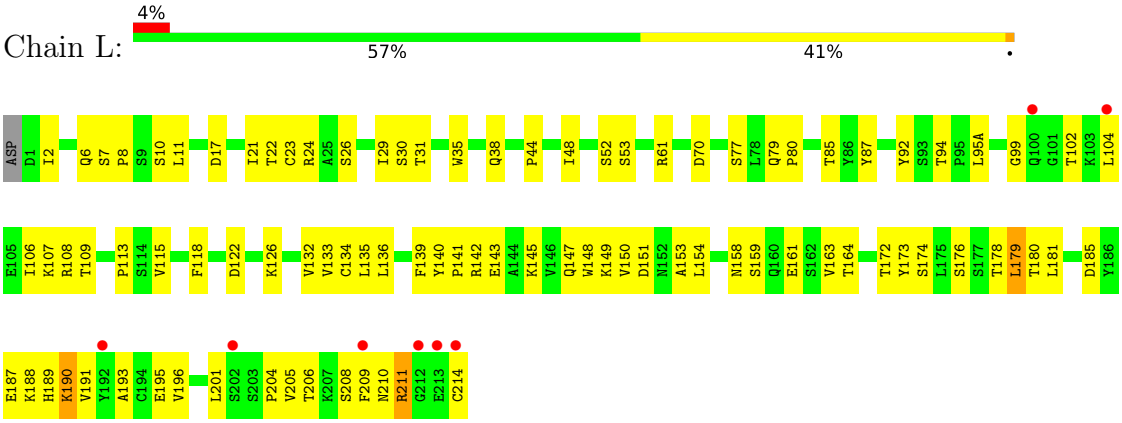
• Molecule 2: NA-63 Fab light chain

Chain E:



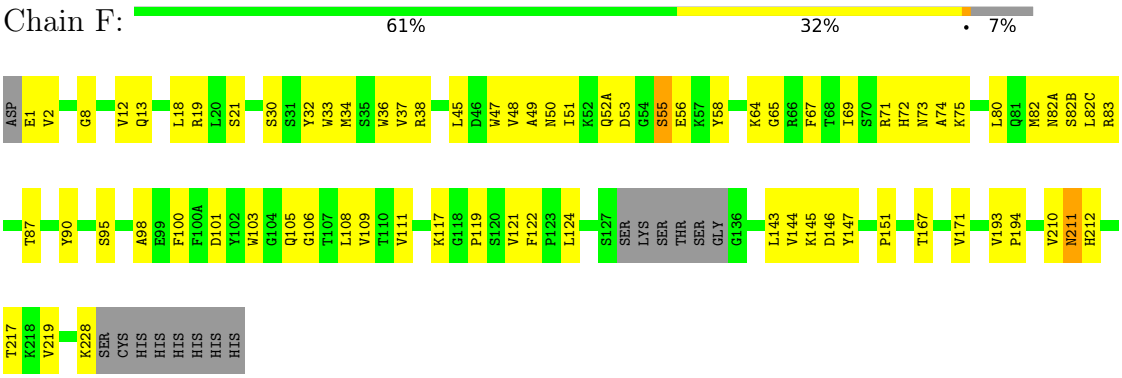
• Molecule 2: NA-63 Fab light chain

Chain L:



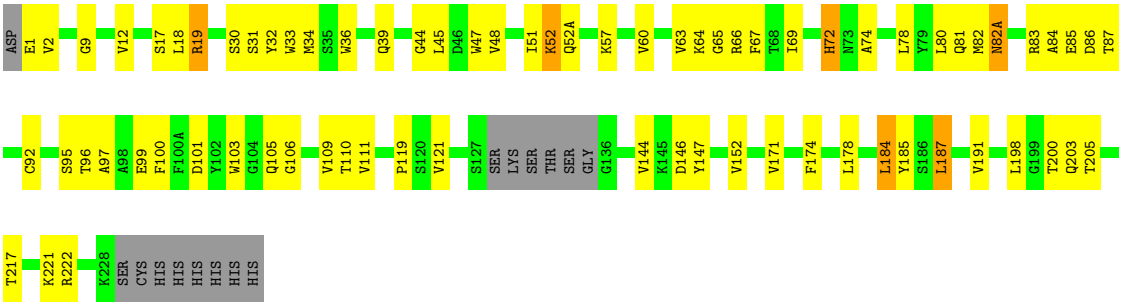
• Molecule 3: NA-63 Fab heavy chain

Chain F:



• Molecule 3: NA-63 Fab heavy chain

Chain H:

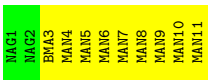


• Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

• Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 18% 82%



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 50% 50%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	164.58Å 164.58Å 192.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.80 – 2.80 49.80 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.4 (49.80-2.80) 96.4 (49.80-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.203 , 0.249 0.202 , 0.247	Depositor DCC
R_{free} test set	3291 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å^2)	59.1	Xtriage
Anisotropy	0.621	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 40.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13026	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% 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: BMA, PO4, MAN, CA, 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	0.39	0/3140	0.61	1/4277 (0.0%)
1	B	0.49	0/3140	0.70	3/4277 (0.1%)
2	E	0.41	0/1681	0.63	1/2283 (0.0%)
2	L	0.49	0/1681	0.74	0/2283
3	F	0.43	0/1646	0.66	0/2241
3	H	0.40	0/1646	0.62	1/2241 (0.0%)
All	All	0.44	0/12934	0.66	6/17602 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	200	ASN	CB-CA-C	7.41	125.21	110.40
2	E	101	GLY	N-CA-C	5.65	127.23	113.10
1	A	299	ASN	C-N-CA	-5.39	108.23	121.70
3	H	72	HIS	CB-CA-C	5.34	121.08	110.40
1	B	299	ASN	C-N-CA	-5.29	108.48	121.70
1	B	200	ASN	N-CA-CB	-5.06	101.50	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3057	0	2880	47	0
1	B	3057	0	2879	71	0
2	E	1646	0	1604	58	0
2	L	1646	0	1604	93	0
3	F	1606	0	1563	68	0
3	H	1606	0	1563	83	0
4	C	127	0	106	0	0
4	D	127	0	106	0	0
5	G	28	0	25	0	0
6	B	28	0	26	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	5	0	0	0	0
8	B	15	0	0	0	0
9	A	17	0	0	0	0
9	B	37	0	0	0	0
9	E	5	0	0	1	0
9	F	11	0	0	1	0
9	H	2	0	0	1	0
9	L	4	0	0	0	0
All	All	13026	0	12356	397	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 16.

All (397) 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:E:115:VAL:HG12	2:E:136:LEU:HD22	1.28	1.14
2:L:179:LEU:HD22	2:L:180:THR:N	1.69	1.08
2:L:149:LYS:HB2	2:L:193:ALA:HB3	1.34	1.05
2:L:95(A):LEU:HD23	3:H:47:TRP:CH2	1.99	0.98
3:H:63:VAL:HG11	3:H:67:PHE:HD2	1.27	0.97
2:E:36:TYR:HE2	2:E:89:GLN:HG2	1.31	0.95
3:H:187:LEU:HD12	3:H:187:LEU:O	1.72	0.90
2:L:190:LYS:HE3	2:L:191:VAL:H	1.36	0.88
1:A:399:LEU:HD11	1:A:457:ASN:CG	1.95	0.87
3:H:63:VAL:CG1	3:H:67:PHE:HD2	1.90	0.84
2:L:179:LEU:HD22	2:L:180:THR:H	1.40	0.83
2:L:151:ASP:HA	2:L:190:LYS:HE2	1.63	0.81
1:B:97:TRP:H	1:B:395:GLN:HE22	1.28	0.81
1:B:379:VAL:HG23	1:B:382:ALA:HB2	1.61	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:146:ASP:HA	3:H:184:LEU:HD13	1.64	0.79
2:L:95(A):LEU:HD23	3:H:47:TRP:HH2	1.46	0.78
3:F:64:LYS:HD3	3:F:65:GLY:N	1.99	0.77
2:L:185:ASP:HA	2:L:188:LYS:HB2	1.64	0.77
2:L:179:LEU:CD2	2:L:180:THR:H	1.98	0.76
2:E:115:VAL:CG1	2:E:136:LEU:HD22	2.13	0.76
3:F:67:PHE:CE2	3:F:82:MET:HE2	2.21	0.75
3:H:63:VAL:CG1	3:H:67:PHE:CD2	2.69	0.74
3:H:67:PHE:CE1	3:H:82:MET:HA	2.23	0.74
3:H:187:LEU:HD12	3:H:187:LEU:C	2.07	0.74
3:H:52:LYS:HG3	3:H:52(A):GLN:H	1.53	0.73
2:E:115:VAL:HG12	2:E:136:LEU:CD2	2.15	0.73
2:E:136:LEU:HD11	2:E:196:VAL:HG21	1.71	0.73
3:H:31:SER:OG	3:H:32:TYR:HD1	1.72	0.73
3:H:87:THR:HG23	3:H:110:THR:HA	1.71	0.72
1:A:399:LEU:HD11	1:A:457:ASN:OD1	1.88	0.72
2:L:133:VAL:HG12	2:L:178:THR:HB	1.72	0.71
2:L:190:LYS:HE3	2:L:191:VAL:N	2.05	0.71
3:H:121:VAL:O	3:H:221:LYS:NZ	2.21	0.71
1:A:428:ARG:NH1	1:A:433:GLU:OE1	2.23	0.71
2:E:95:PRO:HG2	3:F:58:TYR:CD2	2.25	0.70
3:F:121:VAL:HG11	3:F:210:VAL:HG11	1.73	0.70
2:L:8:PRO:HB2	2:L:11:LEU:HD21	1.73	0.70
3:F:13:GLN:H	3:F:13:GLN:CD	1.96	0.69
1:B:271:THR:HG21	1:B:338:ASN:HA	1.73	0.69
2:E:33:LEU:HD11	2:E:88:CYS:HB2	1.74	0.69
3:H:84:ALA:HA	3:H:111:VAL:HG21	1.75	0.69
3:H:119:PRO:HB3	3:H:147:TYR:HB3	1.75	0.69
3:F:87:THR:HG22	3:F:111:VAL:H	1.58	0.68
1:A:271:THR:HG21	1:A:338:ASN:HB3	1.73	0.68
1:B:194:ILE:HD13	1:B:223:LEU:HG	1.76	0.68
3:F:71:ARG:HD3	3:F:73:ASN:HD21	1.57	0.68
2:L:179:LEU:CD2	2:L:180:THR:N	2.49	0.68
3:H:121:VAL:HG12	3:H:144:VAL:HG22	1.75	0.68
2:E:95(A):LEU:HG	3:F:47:TRP:CH2	2.29	0.68
3:H:31:SER:OG	3:H:32:TYR:CD1	2.46	0.68
3:F:87:THR:HG23	3:F:111:VAL:HG22	1.75	0.68
2:E:95:PRO:HG3	3:F:33:TRP:HZ3	1.59	0.67
3:H:51:ILE:HB	3:H:69:ILE:HG21	1.77	0.66
1:A:194:ILE:HD13	1:A:223:LEU:HG	1.76	0.66
2:L:179:LEU:HD22	2:L:179:LEU:C	2.16	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:67:PHE:HE1	3:F:82(A):ASN:O	1.78	0.66
3:H:171:VAL:HG13	3:H:191:VAL:HG22	1.76	0.66
2:L:187:GLU:HA	2:L:211:ARG:NH1	2.11	0.66
2:L:190:LYS:HG2	2:L:191:VAL:HG23	1.77	0.65
2:L:151:ASP:OD1	2:L:190:LYS:HB3	1.97	0.65
3:H:67:PHE:CD1	3:H:82:MET:HA	2.31	0.65
1:A:399:LEU:CD1	1:A:457:ASN:OD1	2.45	0.64
1:B:242:THR:HG22	1:B:252:THR:HG23	1.79	0.64
2:E:90:GLN:HG2	2:E:92:TYR:H	1.62	0.63
2:E:87:TYR:CE1	2:E:101:GLY:HA3	2.32	0.63
3:H:84:ALA:HA	3:H:111:VAL:CG2	2.27	0.63
1:B:97:TRP:H	1:B:395:GLN:NE2	1.96	0.63
2:L:191:VAL:HG22	2:L:210:ASN:HB3	1.80	0.63
1:A:240:VAL:HG12	1:A:254:ILE:HG13	1.81	0.62
1:A:240:VAL:HG21	1:A:278:CYS:SG	2.40	0.62
2:L:30:SER:OG	2:L:31:THR:N	2.31	0.62
2:L:48:ILE:HD12	2:L:53:SER:O	2.00	0.62
2:L:190:LYS:HE3	2:L:191:VAL:HB	1.82	0.62
2:L:191:VAL:HG13	2:L:209:PHE:O	1.99	0.62
3:H:187:LEU:C	3:H:187:LEU:CD1	2.68	0.62
1:B:130:ARG:NH1	1:B:172:ARG:HH21	1.97	0.61
3:H:52:LYS:HG3	3:H:52(A):GLN:N	2.15	0.61
1:A:271:THR:HG21	1:A:338:ASN:CB	2.30	0.61
2:L:35:TRP:HB2	2:L:48:ILE:HG22	1.83	0.61
1:B:379:VAL:HG12	1:B:391:PRO:HA	1.83	0.61
2:L:29:ILE:HG23	2:L:92:TYR:HB2	1.82	0.61
1:B:94:ILE:HG13	1:B:448:SER:HB2	1.83	0.61
3:F:105:GLN:HG3	3:F:106:GLY:N	2.16	0.61
2:E:21:ILE:HD11	2:E:104:LEU:HD11	1.82	0.60
2:E:36:TYR:CE2	2:E:89:GLN:HG2	2.24	0.60
2:L:122:ASP:O	2:L:126:LYS:HG3	2.01	0.60
3:H:34:MET:O	3:H:51:ILE:HG22	2.01	0.60
2:L:35:TRP:HB2	2:L:48:ILE:CG2	2.32	0.60
2:L:108:ARG:HG2	2:L:109:THR:N	2.16	0.60
2:E:118:PHE:HB2	2:E:133:VAL:HG23	1.84	0.60
2:E:95(A):LEU:HG	3:F:47:TRP:HH2	1.65	0.59
3:F:72:HIS:CE1	3:F:74:ALA:HB3	2.37	0.59
2:E:95:PRO:HG3	3:F:33:TRP:CZ3	2.36	0.59
2:E:123:GLU:OE2	2:E:123:GLU:N	2.35	0.59
2:L:147:GLN:HG2	2:L:154:LEU:HD22	1.83	0.59
3:F:53:ASP:OD1	3:F:53:ASP:N	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:GLU:CG	1:A:285:THR:HG22	2.33	0.58
2:E:115:VAL:HG11	2:E:196:VAL:HG11	1.85	0.58
3:F:210:VAL:HG13	3:F:219:VAL:HG13	1.85	0.58
3:H:205:THR:HB	3:H:222:ARG:HH21	1.68	0.58
1:B:228:SER:HB3	1:B:350:LYS:HE2	1.84	0.58
3:F:82(A):ASN:O	3:F:82(B):SER:OG	2.19	0.58
1:B:190:MET:CE	1:B:237:CYS:HB2	2.33	0.58
3:H:144:VAL:HB	3:H:187:LEU:HD11	1.86	0.58
3:F:37:VAL:HG11	3:F:103:TRP:CZ3	2.39	0.58
2:E:108:ARG:NH1	2:E:109:THR:HG23	2.18	0.57
3:F:67:PHE:CD2	3:F:82:MET:HE2	2.38	0.57
3:H:1:GLU:HG3	3:H:2:VAL:H	1.68	0.57
1:B:130:ARG:CZ	1:B:172:ARG:HH21	2.18	0.57
3:H:63:VAL:HG12	3:H:63:VAL:O	2.04	0.57
1:B:123:SER:OG	1:B:189:ARG:NH2	2.34	0.57
1:A:228:SER:HB3	1:A:350:LYS:HE2	1.87	0.57
1:A:271:THR:HG21	1:A:338:ASN:CA	2.35	0.57
2:E:87:TYR:HE1	2:E:101:GLY:HA3	1.68	0.57
3:F:72:HIS:HE1	3:F:75:LYS:HG3	1.68	0.57
2:L:8:PRO:HB2	2:L:11:LEU:CD2	2.34	0.57
3:H:67:PHE:HE1	3:H:82:MET:HA	1.69	0.57
2:E:143:GLU:N	2:E:143:GLU:OE2	2.36	0.57
2:L:118:PHE:HB2	2:L:133:VAL:HG23	1.86	0.56
3:H:17:SER:HA	3:H:82:MET:O	2.05	0.56
3:H:34:MET:HB3	3:H:78:LEU:HD13	1.87	0.56
1:A:256:TYR:CG	1:A:310:MET:HG2	2.40	0.56
2:L:48:ILE:HD11	2:L:52:SER:C	2.25	0.56
3:H:63:VAL:HG11	3:H:67:PHE:CD2	2.19	0.56
2:L:195:GLU:OE1	2:L:206:THR:HB	2.05	0.56
1:B:218:TRP:CZ2	1:B:253:ARG:HG3	2.40	0.56
3:F:211:ASN:HD22	3:F:212:HIS:N	2.03	0.56
3:H:95:SER:HB2	3:H:100:PHE:O	2.05	0.56
1:B:271:THR:HG21	1:B:338:ASN:CA	2.36	0.56
1:B:226:GLN:HB3	1:B:278:CYS:O	2.06	0.56
2:L:61:ARG:HH12	2:L:79:GLN:HB2	1.69	0.56
1:A:218:TRP:CZ2	1:A:253:ARG:HG3	2.41	0.55
1:B:292:ARG:HE	1:B:348:GLY:HA3	1.71	0.55
2:L:193:ALA:HA	2:L:208:SER:OG	2.06	0.55
3:H:34:MET:CB	3:H:78:LEU:HD13	2.36	0.55
1:B:364:ARG:HG3	1:B:365:THR:O	2.06	0.55
1:B:94:ILE:HG13	1:B:448:SER:CB	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ARG:CZ	1:B:209:ARG:HB3	2.37	0.55
1:A:121:TYR:CG	1:A:228:SER:HA	2.41	0.55
2:E:126:LYS:N	2:E:126:LYS:HD2	2.20	0.55
2:L:80:PRO:HA	2:L:106:ILE:CD1	2.37	0.55
3:H:198:LEU:H	3:H:198:LEU:HD12	1.70	0.55
1:B:159:ILE:HG22	1:B:173:VAL:HG22	1.89	0.55
2:E:95:PRO:HG2	3:F:58:TYR:HD2	1.71	0.55
3:F:67:PHE:CD1	3:F:82:MET:HA	2.42	0.55
1:B:276:GLU:HB2	1:B:292:ARG:HB3	1.89	0.54
2:E:113:PRO:HB3	2:E:139:PHE:HB3	1.89	0.54
2:E:3:VAL:H	2:E:26:SER:HB3	1.71	0.54
3:H:66:ARG:NH2	3:H:86:ASP:OD2	2.40	0.54
2:E:30:SER:OG	2:E:31:THR:N	2.40	0.54
3:H:19:ARG:HB3	3:H:81:GLN:NE2	2.22	0.54
1:B:89:LYS:HD2	1:B:418:TYR:CE1	2.42	0.54
1:B:465:GLU:OE1	1:B:465:GLU:N	2.18	0.54
2:L:6:GLN:OE1	2:L:99:GLY:HA3	2.08	0.54
1:B:278:CYS:HB3	1:B:289:CYS:HB3	1.90	0.54
3:H:64:LYS:HD3	3:H:65:GLY:N	2.23	0.54
1:B:104:ASN:HD22	1:B:107:ARG:HD3	1.72	0.53
1:B:366:ILE:HG21	1:B:400:ASN:HB2	1.90	0.53
2:E:108:ARG:HG2	2:E:109:THR:N	2.22	0.53
2:L:44:PRO:HG2	3:H:103:TRP:CE3	2.44	0.53
2:L:151:ASP:CA	2:L:190:LYS:HE2	2.37	0.53
2:E:136:LEU:CD1	2:E:196:VAL:HG21	2.38	0.53
2:L:134:CYS:HB2	2:L:148:TRP:CH2	2.43	0.53
2:L:150:VAL:HG22	2:L:153:ALA:O	2.09	0.53
2:E:63:SER:O	2:E:73:LEU:HD12	2.09	0.53
2:L:159:SER:OG	2:L:179:LEU:HG	2.09	0.53
3:F:30:SER:O	3:F:52(A):GLN:HB3	2.08	0.53
1:A:278:CYS:HB3	1:A:289:CYS:HB3	1.91	0.53
1:B:94:ILE:HG21	1:B:97:TRP:CZ2	2.44	0.53
3:H:44:GLY:N	9:H:302:HOH:O	2.42	0.53
1:B:151:ASP:O	1:B:156:ARG:NH2	2.39	0.52
3:F:49:ALA:HB3	3:F:69:ILE:HD11	1.90	0.52
1:A:334:ILE:HD12	3:H:99:GLU:HB2	1.91	0.52
3:F:50:ASN:OD1	3:F:51:ILE:N	2.43	0.52
1:A:399:LEU:CD1	1:A:457:ASN:CG	2.74	0.52
3:F:95:SER:HB2	3:F:100:PHE:O	2.10	0.52
2:L:48:ILE:HD12	2:L:53:SER:C	2.31	0.52
2:E:38:GLN:NE2	2:E:44:PRO:HD3	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:SER:O	1:A:156:ARG:HD2	2.09	0.51
3:H:67:PHE:HE1	3:H:82:MET:CA	2.23	0.51
3:F:18:LEU:O	3:F:82:MET:HB2	2.10	0.51
2:L:151:ASP:HA	2:L:190:LYS:CE	2.37	0.51
3:H:18:LEU:O	3:H:82:MET:HB2	2.11	0.51
1:B:242:THR:HG21	1:B:275:ILE:O	2.09	0.51
1:B:272:ALA:HA	1:B:316:TYR:CE1	2.46	0.51
1:A:130:ARG:NH1	1:A:172:ARG:HH21	2.09	0.51
2:E:44:PRO:HG2	3:F:103:TRP:CE3	2.46	0.51
2:E:45:LYS:NZ	9:E:301:HOH:O	2.43	0.51
2:E:166:GLN:HG2	2:E:171:SER:HA	1.92	0.50
1:B:376:MET:HG2	1:B:397:ILE:HD11	1.93	0.50
3:F:82:MET:HE3	3:F:90:TYR:CE2	2.46	0.50
2:L:29:ILE:HD12	2:L:92:TYR:CB	2.42	0.50
2:L:164:THR:HG23	2:L:174:SER:O	2.12	0.50
2:E:34:ASN:ND2	2:E:89:GLN:OE1	2.42	0.50
2:L:29:ILE:HA	2:L:92:TYR:CD2	2.46	0.50
2:L:190:LYS:CE	2:L:191:VAL:H	2.16	0.50
2:L:38:GLN:HE21	2:L:87:TYR:HE2	1.59	0.50
3:H:200:THR:OG1	3:H:203:GLN:N	2.45	0.50
1:B:134:LEU:HB2	1:B:156:ARG:NH1	2.27	0.50
3:H:95:SER:OG	3:H:97:ALA:O	2.25	0.49
2:L:113:PRO:HB3	2:L:139:PHE:HB3	1.94	0.49
2:L:179:LEU:HD13	2:L:181:LEU:CD1	2.42	0.49
3:F:34:MET:HG3	3:F:71:ARG:NH2	2.28	0.49
3:F:38:ARG:HG3	3:F:48:VAL:HG21	1.94	0.49
3:F:71:ARG:HD3	3:F:73:ASN:ND2	2.26	0.49
3:F:124:LEU:HD11	3:F:143:LEU:HB2	1.94	0.49
1:B:120:PRO:HD3	1:B:425:GLU:OE2	2.13	0.49
3:F:87:THR:CG2	3:F:111:VAL:HG22	2.42	0.49
3:F:167:THR:O	3:F:171:VAL:HG12	2.13	0.49
2:L:158:ASN:HB2	2:L:179:LEU:HD21	1.92	0.49
2:L:190:LYS:CE	2:L:191:VAL:HB	2.42	0.49
3:F:83:ARG:O	3:F:111:VAL:HG21	2.13	0.49
2:L:107:LYS:HA	2:L:140:TYR:OH	2.13	0.49
3:F:38:ARG:CD	3:F:90:TYR:CZ	2.96	0.48
2:L:24:ARG:NH1	2:L:70:ASP:OD2	2.46	0.48
3:F:64:LYS:HD3	3:F:65:GLY:H	1.75	0.48
1:B:121:TYR:CG	1:B:228:SER:HA	2.48	0.48
3:F:67:PHE:CE1	3:F:82(A):ASN:N	2.81	0.48
2:L:85:THR:HA	2:L:102:THR:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:195:GLU:OE2	2:L:204:PRO:HB2	2.13	0.48
1:B:354:TYR:CZ	1:B:420:ALA:HB1	2.49	0.48
1:A:225:THR:OG1	1:A:226:GLN:N	2.45	0.48
3:H:105:GLN:HG3	3:H:106:GLY:N	2.28	0.48
3:F:83:ARG:HB2	9:F:306:HOH:O	2.13	0.48
2:L:148:TRP:O	2:L:154:LEU:HD23	2.13	0.48
3:H:152:VAL:CG2	3:H:187:LEU:HD21	2.44	0.48
1:B:379:VAL:CG2	1:B:382:ALA:HB2	2.38	0.48
3:F:13:GLN:CD	3:F:13:GLN:N	2.64	0.48
1:B:190:MET:HE1	1:B:237:CYS:HB2	1.94	0.47
2:E:124:GLN:HE22	2:E:131:SER:CB	2.27	0.47
3:F:119:PRO:HD2	3:F:217:THR:HG21	1.96	0.47
3:H:72:HIS:CE1	3:H:74:ALA:HB3	2.49	0.47
1:A:222:ILE:O	1:A:224:ARG:NH1	2.45	0.47
3:H:121:VAL:CG1	3:H:144:VAL:HG22	2.43	0.47
1:B:242:THR:HG22	1:B:252:THR:CG2	2.43	0.47
3:H:78:LEU:HD21	3:H:92:CYS:SG	2.54	0.47
3:H:147:TYR:O	3:H:184:LEU:HB2	2.13	0.47
1:B:209:ARG:HB3	1:B:209:ARG:NH1	2.30	0.47
2:L:179:LEU:CD2	2:L:179:LEU:C	2.81	0.47
1:B:116:VAL:HG12	1:B:136:GLN:HG3	1.96	0.47
1:A:136:GLN:CD	1:A:156:ARG:HD3	2.35	0.47
1:A:256:TYR:CD1	1:A:310:MET:HG2	2.50	0.47
3:F:117:LYS:HE3	3:F:146:ASP:O	2.15	0.47
1:B:175:CYS:HB3	1:B:206:TRP:NE1	2.30	0.47
1:B:354:TYR:CE2	1:B:420:ALA:HB1	2.49	0.47
2:E:21:ILE:CD1	2:E:104:LEU:HD11	2.45	0.47
2:L:6:GLN:HA	2:L:23:CYS:HA	1.96	0.47
2:L:142:ARG:HD2	2:L:142:ARG:O	2.14	0.47
2:E:18:ARG:HB2	2:E:76:SER:O	2.15	0.47
1:B:162:PRO:O	1:B:165[B]:SER:OG	2.31	0.47
1:B:228:SER:HB3	1:B:350:LYS:CE	2.45	0.47
1:A:336:LYS:HD3	3:H:96:THR:OG1	2.15	0.47
3:F:38:ARG:HD2	3:F:90:TYR:CZ	2.50	0.47
3:H:67:PHE:HE1	3:H:82:MET:CB	2.28	0.47
2:E:8:PRO:HG2	2:E:21:ILE:HG23	1.96	0.46
2:L:140:TYR:CG	2:L:141:PRO:HA	2.50	0.46
3:H:144:VAL:HB	3:H:187:LEU:CD1	2.44	0.46
1:A:272:ALA:HA	1:A:316:TYR:CE1	2.50	0.46
1:B:271:THR:HG21	1:B:338:ASN:CB	2.45	0.46
1:B:270:GLY:HA3	1:B:314:SER:HB3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:ALA:HA	1:B:316:TYR:HE1	1.81	0.46
1:B:341:TYR:HH	3:F:100:PHE:HZ	1.63	0.46
2:E:1:ASP:HB3	2:E:2:ILE:HD12	1.98	0.46
3:H:48:VAL:O	3:H:60:VAL:HG12	2.15	0.46
1:A:161:TRP:CE2	1:A:167:PRO:HB3	2.51	0.45
3:F:83:ARG:HB2	3:F:83:ARG:HE	1.34	0.45
2:L:188:LYS:HB3	2:L:189:HIS:ND1	2.30	0.45
2:L:61:ARG:NH1	2:L:79:GLN:HB2	2.32	0.45
2:E:124:GLN:HE22	2:E:131:SER:HB2	1.81	0.45
2:L:190:LYS:HE3	2:L:191:VAL:CA	2.46	0.45
3:H:9:GLY:HA2	3:H:109:VAL:HG12	1.98	0.45
3:H:82(A):ASN:N	3:H:82(A):ASN:HD22	2.13	0.45
3:H:85:GLU:H	3:H:85:GLU:CD	2.18	0.45
1:A:134:LEU:HD21	1:A:180:SER:HB3	1.99	0.45
1:A:161:TRP:NE1	1:A:165[A]:SER:O	2.49	0.45
1:B:271:THR:HG21	1:B:338:ASN:HB3	1.99	0.45
2:E:87:TYR:CD2	3:F:45:LEU:HD11	2.52	0.45
3:F:193:VAL:HG13	3:F:194:PRO:HD2	1.99	0.45
2:L:115:VAL:HA	2:L:135:LEU:O	2.17	0.45
1:B:161:TRP:CE2	1:B:167:PRO:HB3	2.52	0.45
1:A:283:GLU:HG3	1:A:285:THR:HG22	1.99	0.45
1:A:317:ILE:HG22	1:A:319:SER:H	1.81	0.45
3:H:63:VAL:HG13	3:H:67:PHE:CD2	2.49	0.45
2:L:142:ARG:HB2	2:L:173:TYR:CE2	2.52	0.45
2:L:176:SER:HB2	3:H:174:PHE:CG	2.52	0.45
1:A:118:ARG:HG2	1:A:118:ARG:HH11	1.82	0.44
3:H:119:PRO:HD2	3:H:217:THR:HG21	1.99	0.44
2:L:161:GLU:HA	2:L:176:SER:O	2.17	0.44
2:L:193:ALA:CB	2:L:208:SER:OG	2.65	0.44
3:H:66:ARG:CZ	3:H:83:ARG:HD2	2.47	0.44
1:B:125:ASP:OD1	1:B:125:ASP:N	2.51	0.44
1:B:134:LEU:HD21	1:B:180:SER:HB3	1.99	0.44
2:E:136:LEU:HD11	2:E:196:VAL:CG2	2.44	0.44
2:E:92:TYR:HD1	2:E:92:TYR:O	2.00	0.44
2:L:95(A):LEU:CD2	3:H:47:TRP:HH2	2.24	0.44
2:L:132:VAL:HG12	2:L:179:LEU:O	2.17	0.44
3:H:33:TRP:CZ2	3:H:52:LYS:HD3	2.52	0.44
1:B:350:LYS:HB3	1:B:406:TYR:CG	2.53	0.44
1:A:161:TRP:NE1	1:A:165[B]:SER:O	2.50	0.44
2:E:33:LEU:HD12	2:E:89:GLN:O	2.16	0.44
1:B:238:PRO:HA	1:B:255:TYR:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:143:GLU:OE2	2:L:143:GLU:N	2.48	0.44
1:B:465:GLU:H	1:B:465:GLU:CD	2.10	0.44
2:E:121:SER:OG	3:F:122:PHE:HB3	2.18	0.44
1:B:279:SER:OG	1:B:351:GLY:O	2.36	0.44
3:F:1:GLU:HG3	3:F:2:VAL:H	1.83	0.44
3:F:12:VAL:HG21	3:F:82(C):LEU:HD12	1.98	0.44
3:H:30:SER:O	3:H:52(A):GLN:HB3	2.18	0.44
1:A:118:ARG:NH1	1:A:425:GLU:OE1	2.51	0.43
2:L:140:TYR:CD1	2:L:141:PRO:HA	2.53	0.43
1:A:82:ARG:O	1:A:187:LYS:HE3	2.17	0.43
2:E:7:SER:HB3	2:E:22:THR:HB	1.99	0.43
1:B:152:ARG:HB3	1:B:178:TRP:CG	2.53	0.43
1:A:89:LYS:HD2	1:A:418:TYR:CE1	2.53	0.43
3:H:57:LYS:HD3	3:H:69:ILE:O	2.19	0.43
3:H:178:LEU:HD12	3:H:178:LEU:HA	1.83	0.43
1:A:352:PHE:HE1	1:A:374:TYR:HH	1.62	0.43
1:A:354:TYR:CZ	1:A:420:ALA:HB1	2.53	0.43
1:B:152:ARG:HB3	1:B:178:TRP:CD1	2.53	0.43
2:L:7:SER:HB3	2:L:22:THR:HB	2.00	0.43
2:L:211:ARG:HH11	2:L:211:ARG:HD2	1.68	0.43
2:E:29:ILE:HA	2:E:92:TYR:HD2	1.84	0.43
2:L:38:GLN:NE2	2:L:87:TYR:HE2	2.16	0.43
2:L:191:VAL:HG22	2:L:210:ASN:HA	2.00	0.43
1:B:130:ARG:HH21	1:B:160:SER:C	2.22	0.43
2:L:94:THR:HA	2:L:95(A):LEU:H	1.83	0.43
2:L:136:LEU:CD2	2:L:196:VAL:HG21	2.49	0.43
2:L:201:LEU:HD13	2:L:205:VAL:HG12	2.01	0.43
3:H:178:LEU:HD13	3:H:185:TYR:CE1	2.53	0.43
1:A:180:SER:HA	1:A:192:ILE:O	2.19	0.42
2:E:17:ASP:O	2:E:77:SER:HA	2.19	0.42
3:H:87:THR:OG1	3:H:111:VAL:HG22	2.19	0.42
2:L:142:ARG:HE	2:L:163:VAL:HG11	1.85	0.42
3:H:39:GLN:HG3	3:H:45:LEU:HD12	2.01	0.42
2:E:37:GLN:HB2	2:E:47:LEU:HD11	2.02	0.42
2:E:86:TYR:CD1	2:E:104:LEU:HD13	2.55	0.42
1:B:352:PHE:HE1	1:B:374:TYR:HH	1.67	0.42
2:E:131:SER:OG	3:F:145:LYS:HE3	2.19	0.42
3:F:119:PRO:HB3	3:F:147:TYR:HB3	2.02	0.42
2:L:17:ASP:O	2:L:77:SER:HA	2.18	0.42
3:H:1:GLU:CG	3:H:2:VAL:H	2.32	0.42
1:A:271:THR:HG21	1:A:338:ASN:HA	1.99	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:33:TRP:CH2	3:H:52:LYS:HD3	2.54	0.42
1:B:218:TRP:NE1	1:B:243:ASP:HB3	2.34	0.42
1:B:379:VAL:HG23	1:B:379:VAL:O	2.19	0.42
2:E:3:VAL:H	2:E:26:SER:CB	2.31	0.42
3:F:32:TYR:HE2	3:F:101:ASP:OD2	2.02	0.42
1:B:239:VAL:HB	1:B:257:PHE:HE1	1.84	0.42
3:H:78:LEU:HD23	3:H:78:LEU:H	1.84	0.42
3:F:72:HIS:CE1	3:F:75:LYS:HG3	2.50	0.42
2:L:44:PRO:HG2	3:H:103:TRP:CD2	2.55	0.42
1:A:94:ILE:HG12	1:A:448:SER:CB	2.50	0.41
2:E:87:TYR:HD2	3:F:45:LEU:HD11	1.84	0.41
3:H:12:VAL:O	3:H:111:VAL:HA	2.20	0.41
3:H:146:ASP:HA	3:H:184:LEU:CD1	2.44	0.41
3:H:119:PRO:HB2	3:H:144:VAL:HG13	2.02	0.41
1:A:277:GLU:OE1	1:A:292:ARG:NH1	2.53	0.41
2:E:95:PRO:HB3	3:F:98:ALA:HB1	2.02	0.41
2:L:139:PHE:N	2:L:172:THR:OG1	2.53	0.41
3:H:63:VAL:CG1	3:H:63:VAL:O	2.66	0.41
1:A:299:ASN:OD1	1:A:299:ASN:N	2.53	0.41
3:H:67:PHE:HE1	3:H:82:MET:HB3	1.85	0.41
3:H:82:MET:C	3:H:82(A):ASN:HD22	2.23	0.41
2:E:33:LEU:HD12	2:E:89:GLN:C	2.41	0.41
2:E:161:GLU:HA	2:E:176:SER:O	2.21	0.41
3:F:55:SER:OG	3:F:56:GLU:HG2	2.20	0.41
3:F:121:VAL:HG12	3:F:144:VAL:HG12	2.03	0.41
2:L:10:SER:O	2:L:11:LEU:HD22	2.20	0.41
1:B:134:LEU:HB2	1:B:156:ARG:HH11	1.85	0.41
1:B:136:GLN:HE21	1:B:156:ARG:CZ	2.33	0.41
1:A:123:SER:OG	1:A:229:GLU:HG3	2.20	0.41
3:F:12:VAL:O	3:F:111:VAL:HA	2.21	0.41
2:L:8:PRO:O	2:L:102:THR:HG23	2.20	0.41
2:L:190:LYS:HE3	2:L:191:VAL:CB	2.49	0.41
2:L:195:GLU:HB2	2:L:206:THR:HB	2.02	0.41
1:B:180:SER:HA	1:B:192:ILE:O	2.20	0.41
2:E:33:LEU:HG	2:E:34:ASN:N	2.35	0.41
3:F:108:LEU:HD23	3:F:151:PRO:HD3	2.01	0.41
1:B:190:MET:HE2	1:B:237:CYS:HB2	2.02	0.41
1:A:296:GLN:HG3	1:A:340:PRO:HG3	2.03	0.41
3:F:8:GLY:O	3:F:18:LEU:HD11	2.20	0.41
2:L:21:ILE:HD11	2:L:104:LEU:HD11	2.03	0.41
3:H:36:TRP:CE2	3:H:80:LEU:HB2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:64:LYS:HD3	3:H:65:GLY:H	1.86	0.41
3:F:36:TRP:NE1	3:F:80:LEU:HB2	2.36	0.41
2:L:6:GLN:HG2	2:L:23:CYS:HB2	2.03	0.41
2:L:191:VAL:HG22	2:L:210:ASN:CB	2.47	0.41
1:B:94:ILE:HG21	1:B:97:TRP:CE2	2.56	0.40
1:B:379:VAL:HG12	1:B:391:PRO:CA	2.49	0.40
1:A:300:ARG:CZ	1:A:351:GLY:HA3	2.51	0.40
3:F:67:PHE:CE1	3:F:82(A):ASN:O	2.67	0.40
2:L:95(A):LEU:CD2	3:H:47:TRP:CH2	2.88	0.40
2:E:95:PRO:HD2	3:F:58:TYR:HE2	1.86	0.40
3:F:108:LEU:HD12	3:F:109:VAL:N	2.36	0.40
1:A:215:ILE:HD11	1:A:262:ILE:HD11	2.04	0.40
2:L:2:ILE:HG21	2:L:2:ILE:HD13	1.83	0.40
1:B:331:PRO:HG3	1:B:341:TYR:CZ	2.57	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	387/393 (98%)	363 (94%)	23 (6%)	1 (0%)	41	72
1	B	387/393 (98%)	363 (94%)	24 (6%)	0	100	100
2	E	213/216 (99%)	206 (97%)	7 (3%)	0	100	100
2	L	213/216 (99%)	204 (96%)	8 (4%)	1 (0%)	29	61
3	F	209/228 (92%)	195 (93%)	14 (7%)	0	100	100
3	H	209/228 (92%)	195 (93%)	14 (7%)	0	100	100
All	All	1618/1674 (97%)	1526 (94%)	90 (6%)	2 (0%)	51	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	190	LYS
1	A	331	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	340/343 (99%)	337 (99%)	3 (1%)	78	94
1	B	340/343 (99%)	336 (99%)	4 (1%)	71	92
2	E	189/190 (100%)	186 (98%)	3 (2%)	62	88
2	L	189/190 (100%)	184 (97%)	5 (3%)	46	79
3	F	178/192 (93%)	173 (97%)	5 (3%)	43	77
3	H	178/192 (93%)	172 (97%)	6 (3%)	37	71
All	All	1414/1450 (98%)	1388 (98%)	26 (2%)	59	86

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	125	ASP
1	B	130	ARG
1	B	189	ARG
1	B	230	CYS
1	A	125	ASP
1	A	230	CYS
1	A	416	ASP
2	E	89	GLN
2	E	90	GLN
2	E	92	TYR
3	F	19	ARG
3	F	21	SER
3	F	55	SER
3	F	211	ASN
3	F	228	LYS
2	L	26	SER
2	L	145	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	179	LEU
2	L	211	ARG
2	L	214	CYS
3	H	19	ARG
3	H	52	LYS
3	H	82(A)	ASN
3	H	101	ASP
3	H	184	LEU
3	H	187	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	104	ASN
1	B	136	GLN
1	B	345	ASN
1	B	395	GLN
2	E	38	GLN
2	E	124	GLN
2	E	147	GLN
3	F	39	GLN
3	F	72	HIS
3	F	73	ASN
3	F	211	ASN
2	L	38	GLN
3	H	39	GLN
3	H	72	HIS
3	H	82(A)	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)

24 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	C	1	1,4	14,14,15	0.46	0	17,19,21	1.09	2 (11%)
4	MAN	C	10	4	11,11,12	0.88	0	15,15,17	1.04	1 (6%)
4	MAN	C	11	4	11,11,12	1.14	2 (18%)	15,15,17	1.45	2 (13%)
4	NAG	C	2	4	14,14,15	0.27	0	17,19,21	0.60	0
4	BMA	C	3	4	11,11,12	0.76	0	15,15,17	1.04	1 (6%)
4	MAN	C	4	4	11,11,12	1.33	1 (9%)	15,15,17	1.93	4 (26%)
4	MAN	C	5	4	11,11,12	1.11	1 (9%)	15,15,17	1.12	2 (13%)
4	MAN	C	6	4	11,11,12	0.99	0	15,15,17	1.17	2 (13%)
4	MAN	C	7	4	11,11,12	1.08	1 (9%)	15,15,17	0.93	0
4	MAN	C	8	4	11,11,12	0.75	0	15,15,17	1.08	2 (13%)
4	MAN	C	9	4	11,11,12	1.32	1 (9%)	15,15,17	1.21	2 (13%)
4	NAG	D	1	1,4	14,14,15	0.41	0	17,19,21	0.52	0
4	MAN	D	10	4	11,11,12	1.00	2 (18%)	15,15,17	1.33	3 (20%)
4	MAN	D	11	4	11,11,12	1.32	2 (18%)	15,15,17	1.04	1 (6%)
4	NAG	D	2	4	14,14,15	0.23	0	17,19,21	0.52	0
4	BMA	D	3	4	11,11,12	0.63	0	15,15,17	1.23	2 (13%)
4	MAN	D	4	4	11,11,12	0.55	0	15,15,17	1.31	3 (20%)
4	MAN	D	5	4	11,11,12	1.37	2 (18%)	15,15,17	1.16	1 (6%)
4	MAN	D	6	4	11,11,12	1.29	2 (18%)	15,15,17	1.20	1 (6%)
4	MAN	D	7	4	11,11,12	1.34	2 (18%)	15,15,17	0.91	0
4	MAN	D	8	4	11,11,12	1.07	0	15,15,17	1.09	2 (13%)
4	MAN	D	9	4	11,11,12	1.03	1 (9%)	15,15,17	1.14	2 (13%)
5	NAG	G	1	5,1	14,14,15	0.36	0	17,19,21	0.59	0
5	NAG	G	2	5	14,14,15	0.75	1 (7%)	17,19,21	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1	1,4	-	0/6/23/26	0/1/1/1
4	MAN	C	10	4	-	0/2/19/22	0/1/1/1
4	MAN	C	11	4	-	1/2/19/22	0/1/1/1
4	NAG	C	2	4	-	0/6/23/26	0/1/1/1
4	BMA	C	3	4	-	0/2/19/22	0/1/1/1
4	MAN	C	4	4	-	0/2/19/22	0/1/1/1
4	MAN	C	5	4	-	0/2/19/22	0/1/1/1
4	MAN	C	6	4	-	0/2/19/22	0/1/1/1
4	MAN	C	7	4	-	0/2/19/22	0/1/1/1
4	MAN	C	8	4	-	0/2/19/22	0/1/1/1
4	MAN	C	9	4	-	0/2/19/22	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	MAN	D	10	4	-	1/2/19/22	0/1/1/1
4	MAN	D	11	4	-	2/2/19/22	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	0/2/19/22	0/1/1/1
4	MAN	D	5	4	-	0/2/19/22	0/1/1/1
4	MAN	D	6	4	-	0/2/19/22	0/1/1/1
4	MAN	D	7	4	-	0/2/19/22	0/1/1/1
4	MAN	D	8	4	-	1/2/19/22	0/1/1/1
4	MAN	D	9	4	-	0/2/19/22	0/1/1/1
5	NAG	G	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	1/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	4	MAN	C2-C3	3.89	1.58	1.52
4	D	7	MAN	C2-C3	3.11	1.57	1.52
4	D	6	MAN	O5-C1	-3.02	1.38	1.43
4	D	5	MAN	C2-C3	2.89	1.56	1.52
4	D	11	MAN	C2-C3	2.77	1.56	1.52
4	C	9	MAN	C1-C2	2.74	1.58	1.52
4	C	5	MAN	C2-C3	2.70	1.56	1.52
4	C	11	MAN	C1-C2	2.66	1.58	1.52
4	C	7	MAN	C2-C3	2.50	1.56	1.52
4	D	7	MAN	O5-C1	-2.47	1.39	1.43
4	D	10	MAN	O5-C5	2.32	1.48	1.43
4	D	5	MAN	O5-C1	2.31	1.47	1.43
4	D	6	MAN	O5-C5	2.29	1.48	1.43
4	C	11	MAN	O5-C5	2.24	1.48	1.43
5	G	2	NAG	O5-C1	-2.15	1.40	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	9	MAN	C1-C2	2.13	1.57	1.52
4	D	11	MAN	O5-C5	2.10	1.47	1.43
4	D	10	MAN	C4-C3	2.03	1.57	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	11	MAN	C1-O5-C5	4.20	117.88	112.19
4	C	4	MAN	C1-O5-C5	4.01	117.62	112.19
4	D	5	MAN	C1-O5-C5	3.77	117.30	112.19
4	C	4	MAN	C1-C2-C3	-3.69	105.13	109.67
4	C	4	MAN	O3-C3-C2	3.46	116.62	109.99
4	D	9	MAN	C1-O5-C5	3.27	116.62	112.19
4	D	4	MAN	C1-O5-C5	3.09	116.38	112.19
4	C	9	MAN	C1-O5-C5	3.08	116.37	112.19
4	D	10	MAN	C1-O5-C5	2.88	116.09	112.19
4	C	6	MAN	C1-C2-C3	-2.72	106.32	109.67
4	C	5	MAN	C1-O5-C5	2.72	115.87	112.19
4	D	3	BMA	C1-C2-C3	2.69	112.97	109.67
4	C	11	MAN	O2-C2-C3	-2.64	104.84	110.14
4	D	3	BMA	O2-C2-C3	-2.64	104.84	110.14
4	C	10	MAN	C1-O5-C5	2.62	115.74	112.19
4	C	4	MAN	C3-C4-C5	-2.57	105.65	110.24
4	D	8	MAN	C1-O5-C5	2.45	115.51	112.19
4	D	6	MAN	O2-C2-C1	2.44	114.15	109.15
4	C	8	MAN	C1-O5-C5	2.44	115.50	112.19
4	C	6	MAN	O2-C2-C3	-2.39	105.36	110.14
4	C	9	MAN	O2-C2-C3	-2.34	105.44	110.14
4	D	8	MAN	O2-C2-C3	-2.34	105.44	110.14
4	C	3	BMA	O2-C2-C3	-2.30	105.53	110.14
4	D	4	MAN	O3-C3-C2	2.24	114.29	109.99
4	C	1	NAG	O3-C3-C2	-2.22	104.86	109.47
4	C	1	NAG	O5-C5-C6	-2.22	103.72	107.20
4	D	10	MAN	O2-C2-C3	-2.18	105.77	110.14
4	C	8	MAN	C1-C2-C3	-2.14	107.03	109.67
4	D	11	MAN	C1-O5-C5	2.14	115.09	112.19
4	C	5	MAN	O3-C3-C2	2.14	114.08	109.99
4	D	10	MAN	C1-C2-C3	-2.13	107.05	109.67
4	D	9	MAN	O2-C2-C3	-2.05	106.03	110.14
4	D	4	MAN	O2-C2-C1	-2.01	105.05	109.15

There are no chirality outliers.

All (6) torsion outliers are listed below:

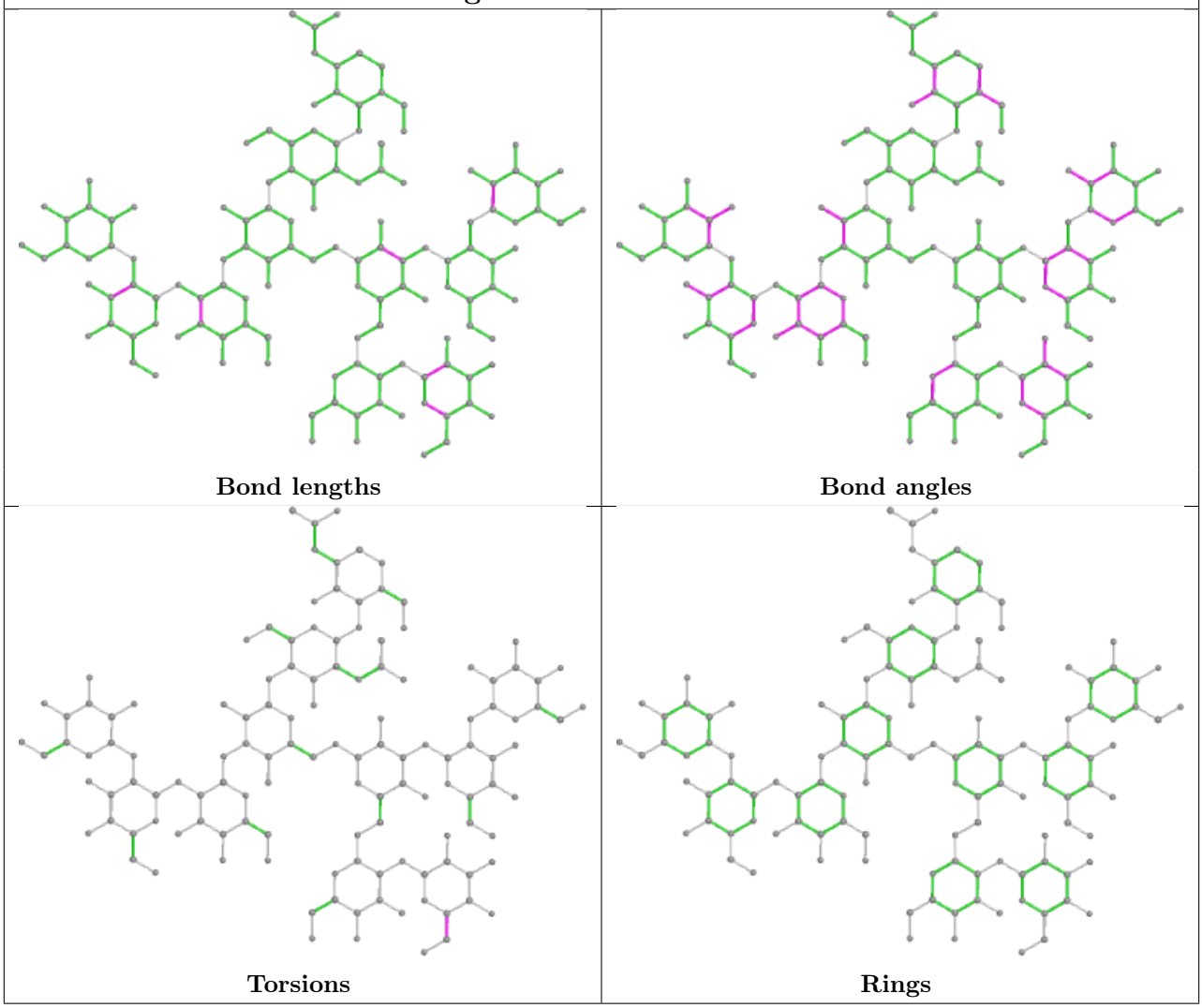
Mol	Chain	Res	Type	Atoms
4	D	11	MAN	C4-C5-C6-O6
4	D	11	MAN	O5-C5-C6-O6
4	C	11	MAN	C4-C5-C6-O6
4	D	10	MAN	O5-C5-C6-O6
4	D	8	MAN	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6

There are no ring outliers.

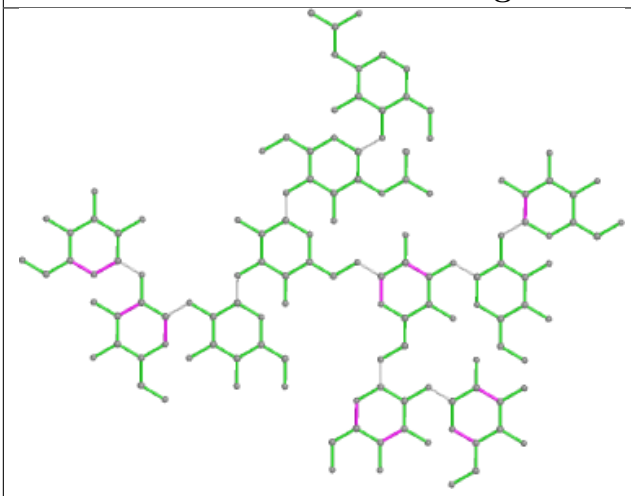
No monomer is involved in short contacts.

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

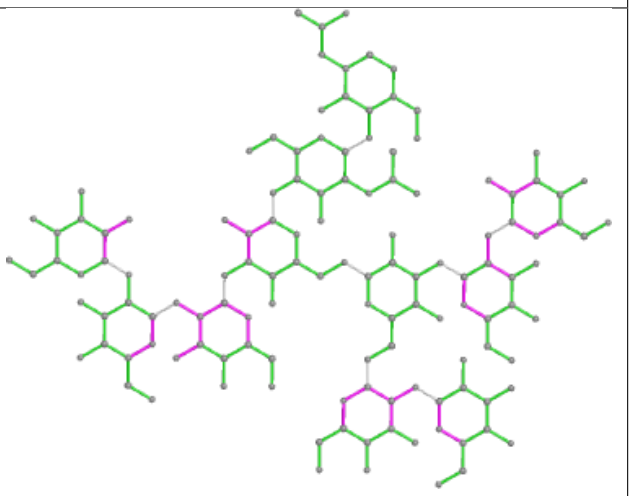
Oligosaccharide Chain C



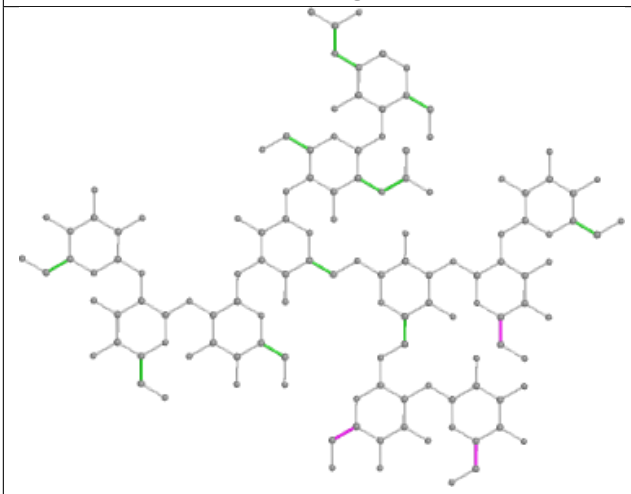
Oligosaccharide Chain D



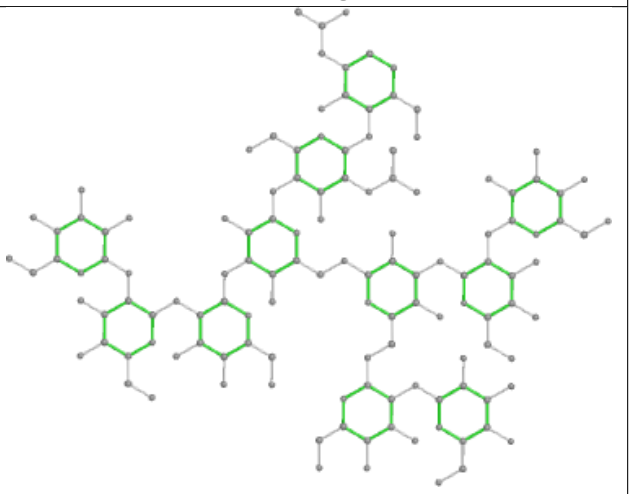
Bond lengths



Bond angles

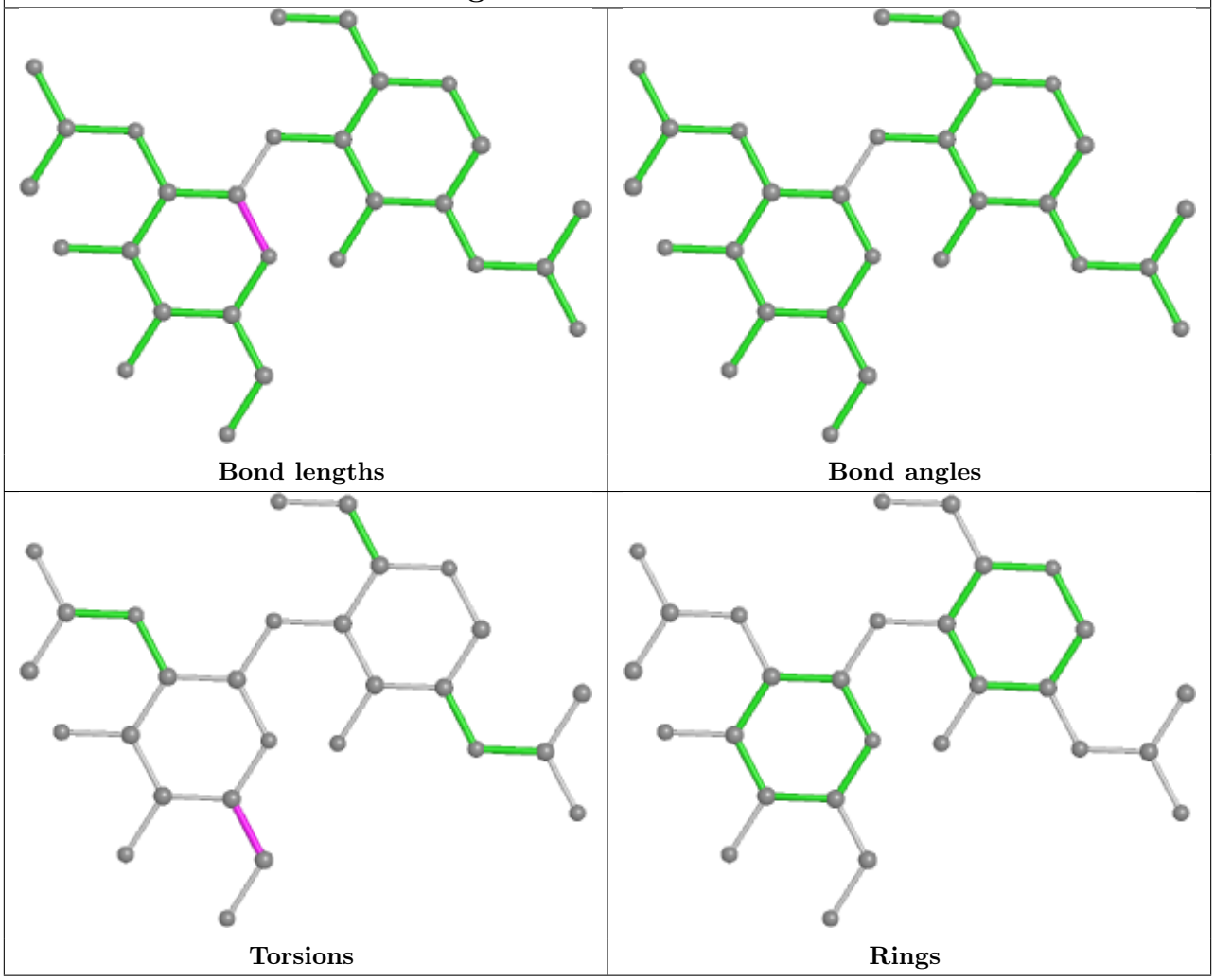


Torsions



Rings

Oligosaccharide Chain G



5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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	$\#\|Z\| > 2$
8	PO4	B	516	-	4,4,4	0.91	0	6,6,6	0.65	0
8	PO4	A	515	-	4,4,4	0.89	0	6,6,6	0.66	0
8	PO4	B	517	-	4,4,4	0.91	0	6,6,6	0.58	0
8	PO4	B	515	-	4,4,4	0.96	0	6,6,6	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	B	501	1	14,14,15	2.80	4 (28%)	17,19,21	1.54	4 (23%)
6	NAG	B	502	1	14,14,15	0.47	0	17,19,21	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	501	1	-	1/6/23/26	0/1/1/1
6	NAG	B	502	1	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	501	NAG	O5-C1	8.91	1.57	1.43
6	B	501	NAG	C1-C2	-3.70	1.46	1.52
6	B	501	NAG	C4-C5	2.34	1.58	1.53
6	B	501	NAG	C8-C7	-2.32	1.45	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	501	NAG	C4-C3-C2	-2.93	106.73	111.02
6	B	501	NAG	O5-C5-C4	2.63	117.22	110.83
6	B	501	NAG	O3-C3-C2	-2.36	104.58	109.47
6	B	501	NAG	C3-C4-C5	-2.24	106.24	110.24

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	502	NAG	O5-C5-C6-O6
6	B	502	NAG	C4-C5-C6-O6
6	B	501	NAG	O5-C5-C6-O6

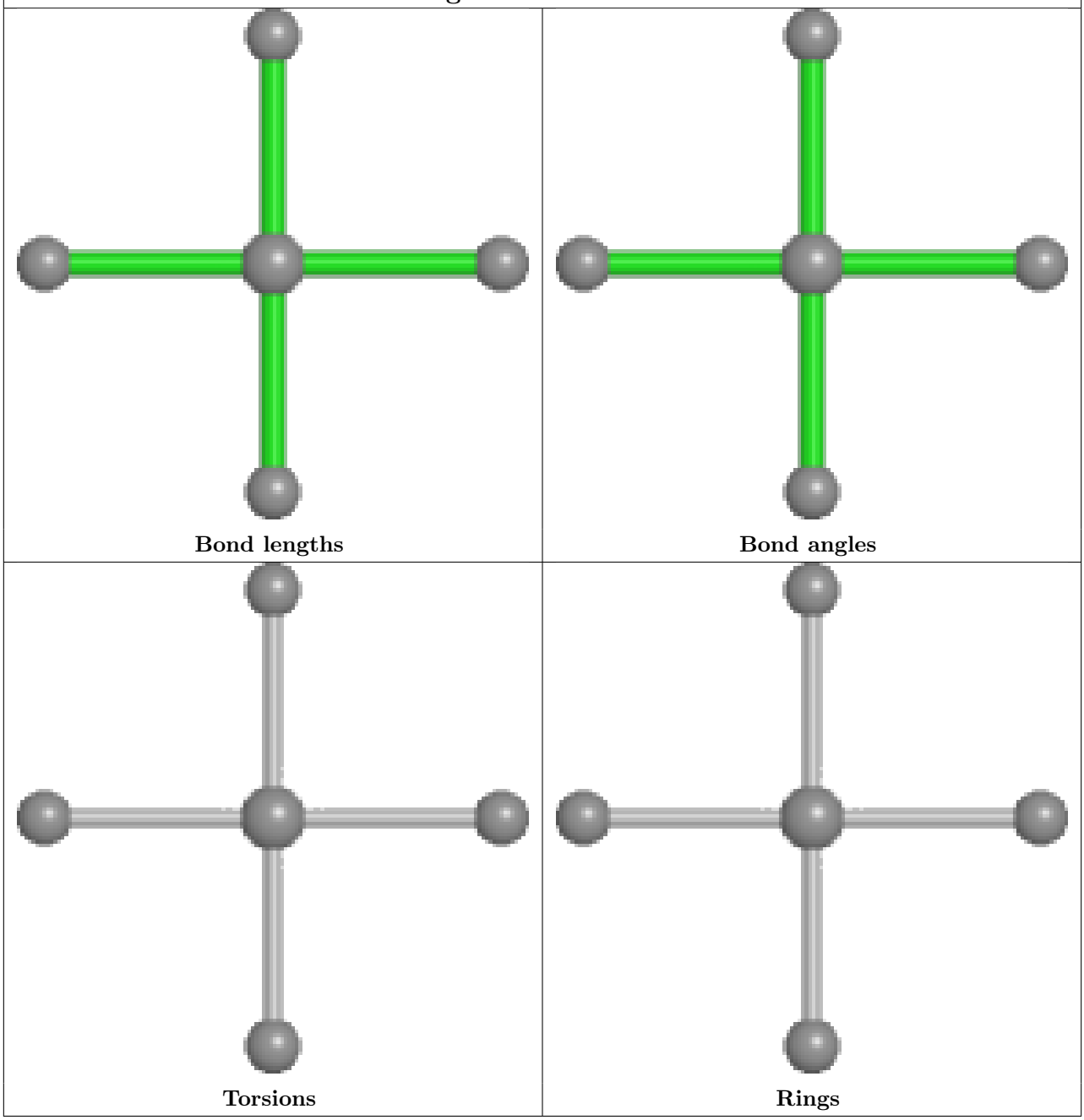
There are no ring outliers.

No monomer is involved in short contacts.

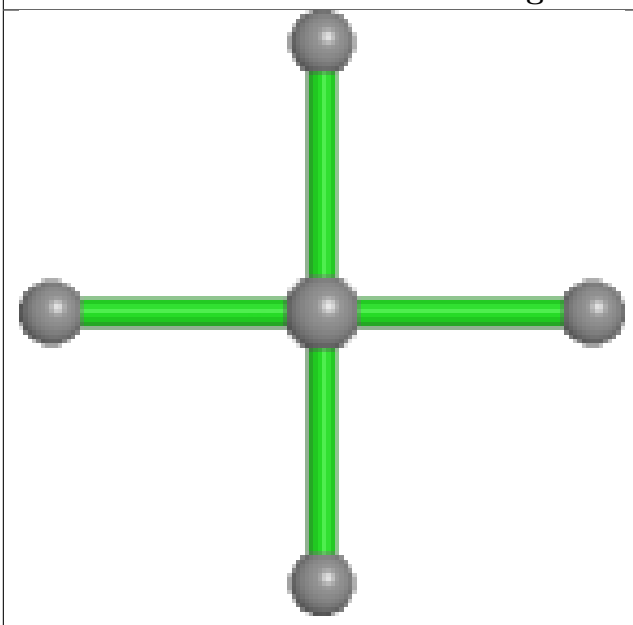
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

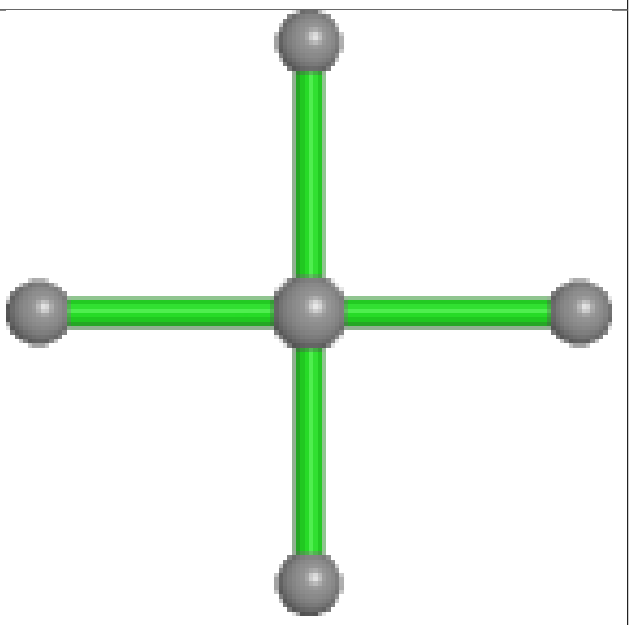
Ligand PO4 B 516



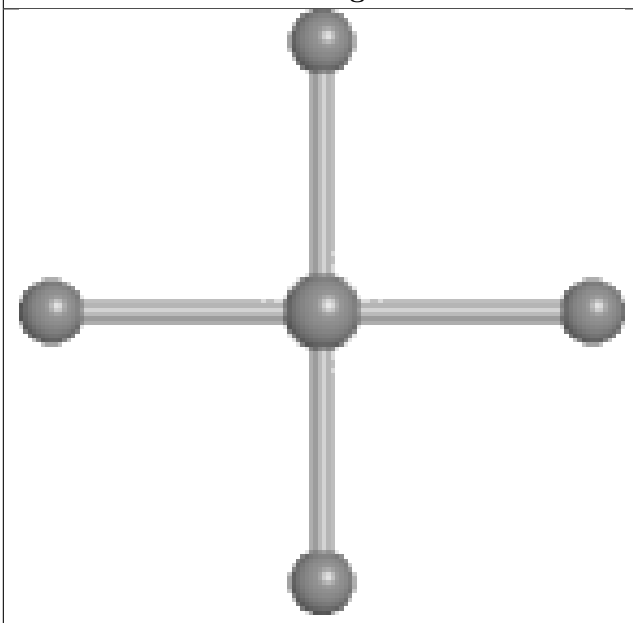
Ligand PO4 A 515



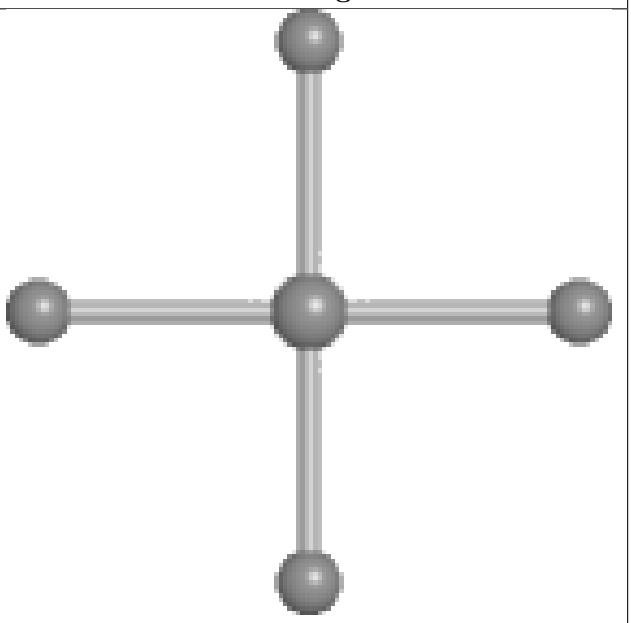
Bond lengths



Bond angles

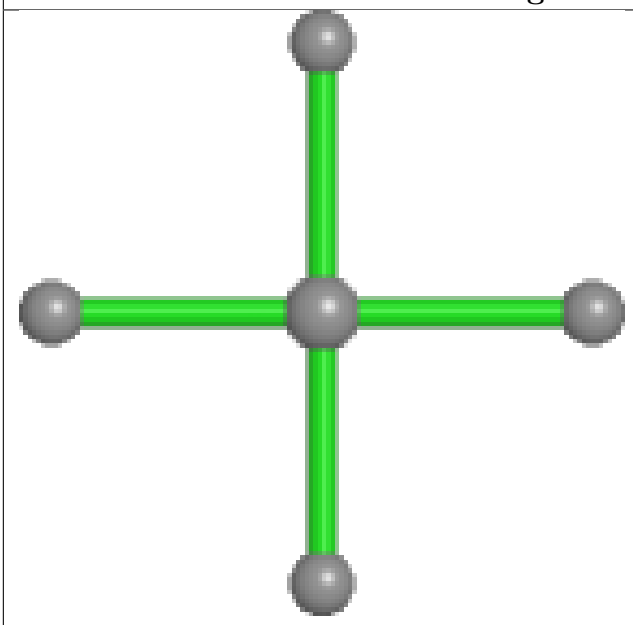


Torsions

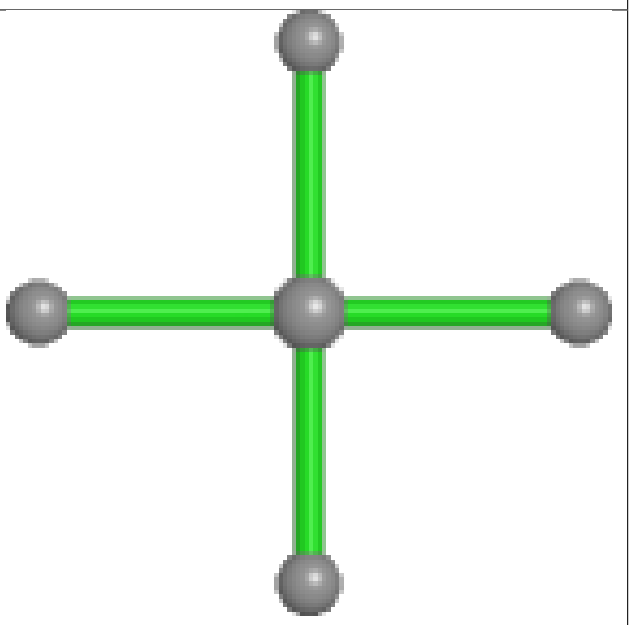


Rings

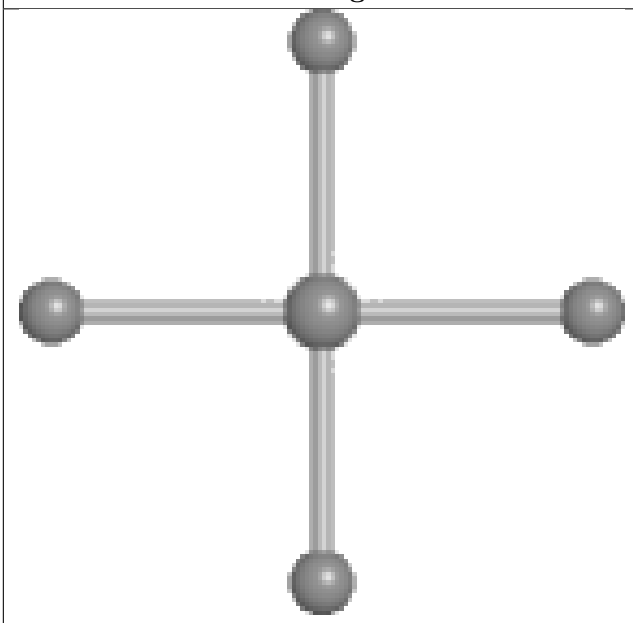
Ligand PO4 B 517



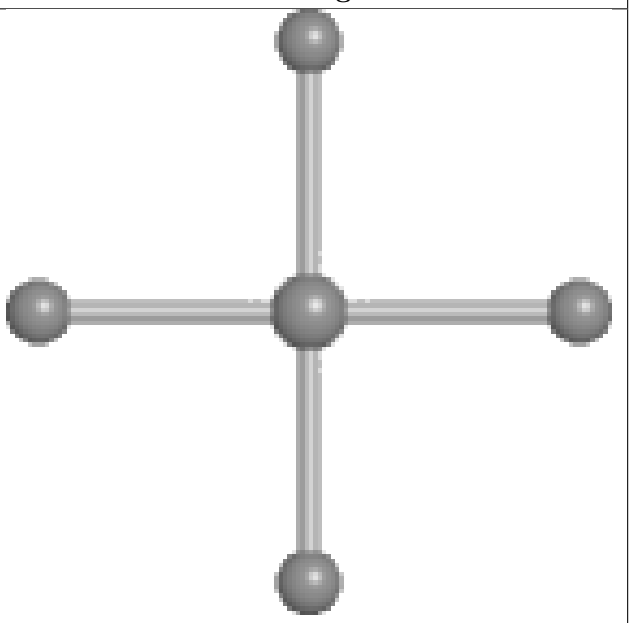
Bond lengths



Bond angles

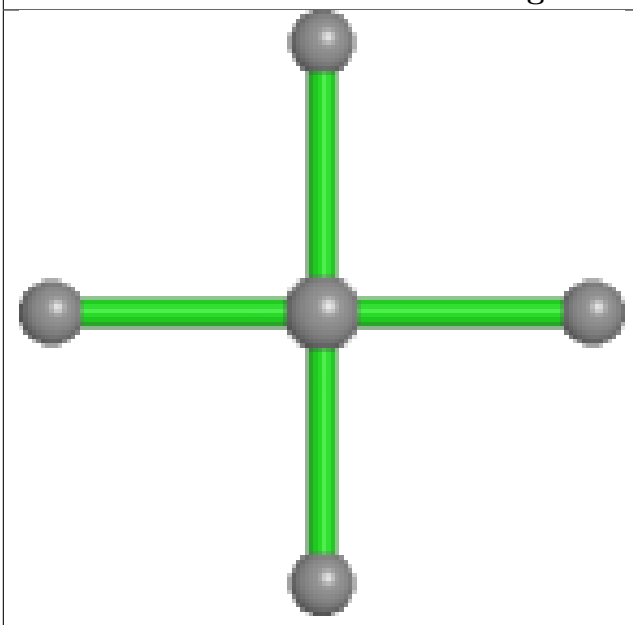


Torsions

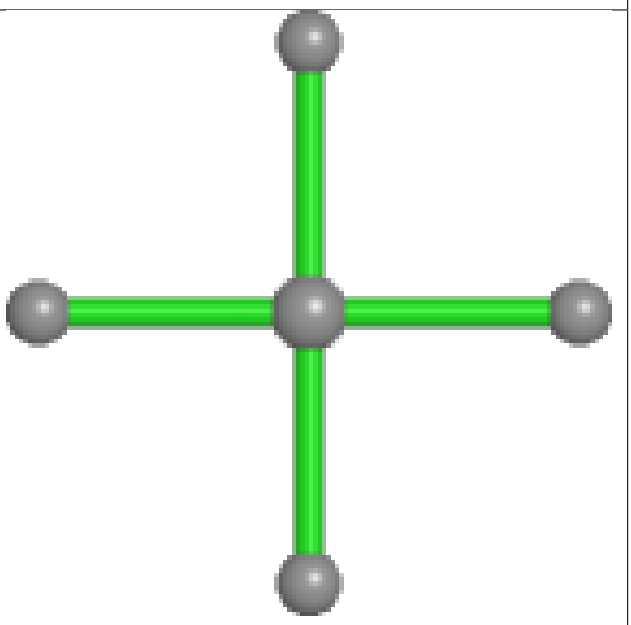


Rings

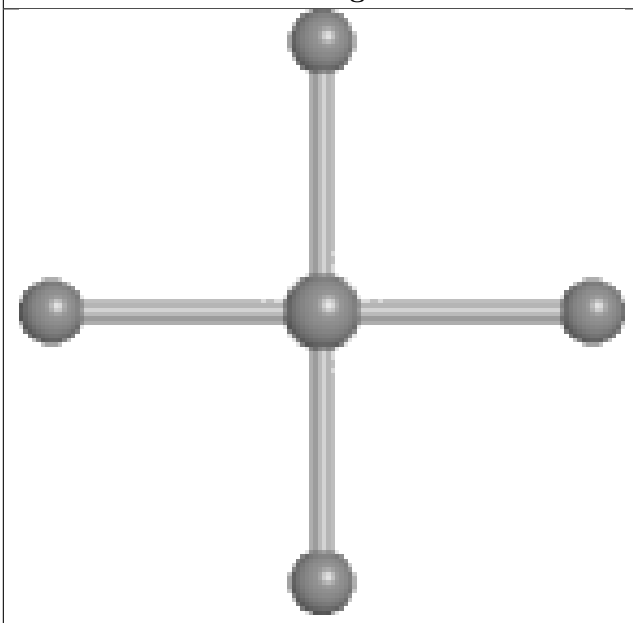
Ligand PO4 B 515



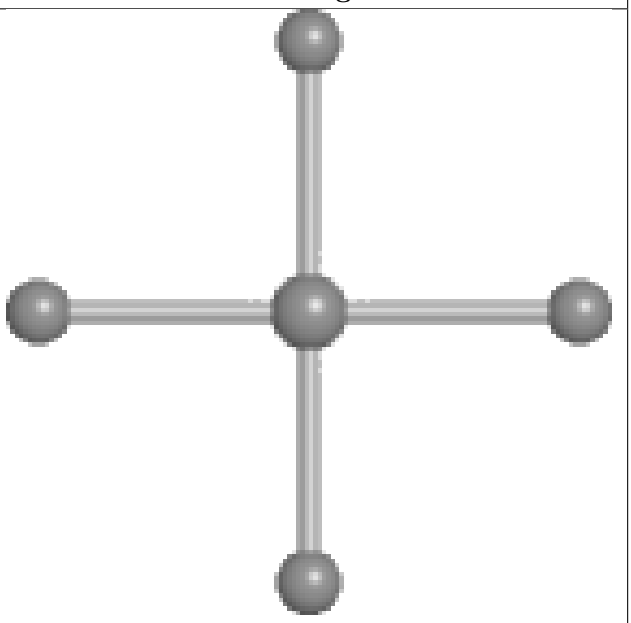
Bond lengths



Bond angles

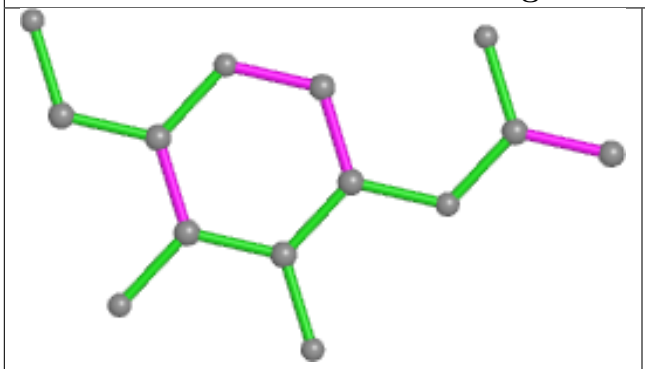


Torsions

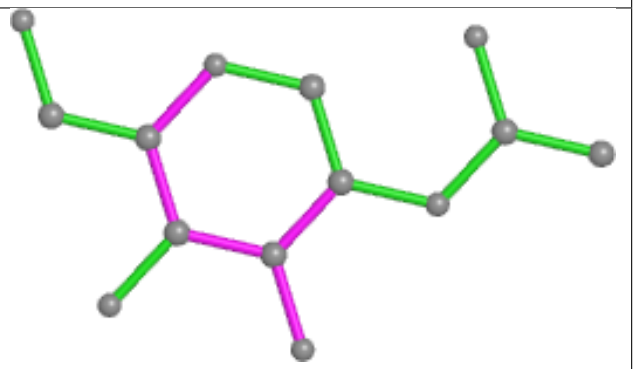


Rings

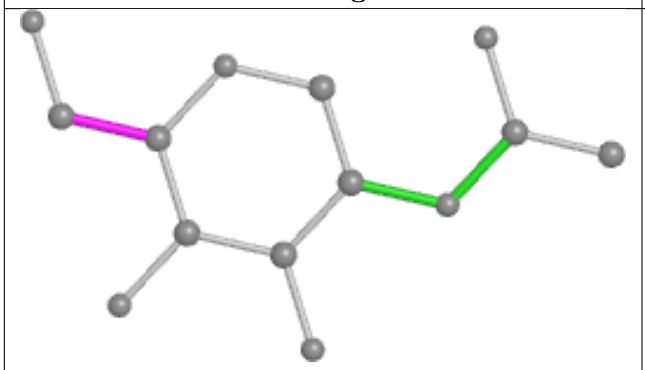
Ligand NAG B 501



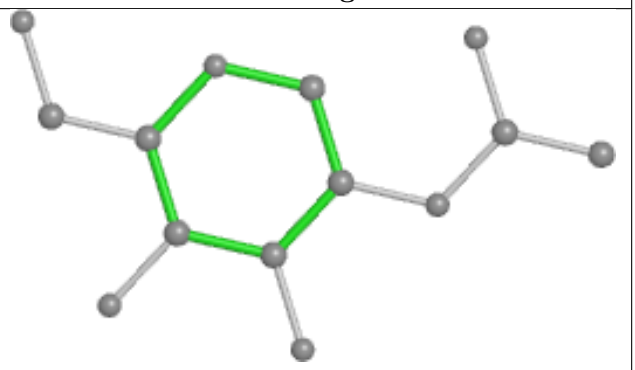
Bond lengths



Bond angles

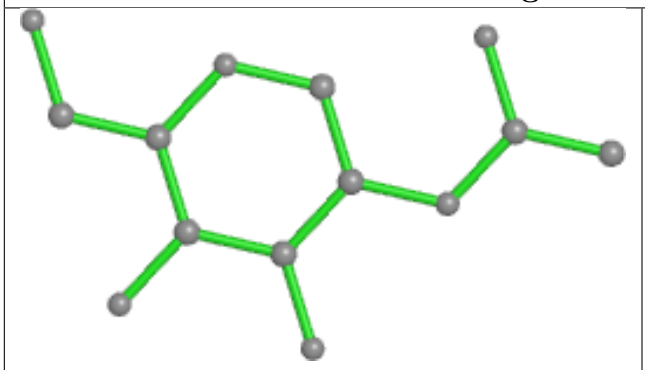


Torsions

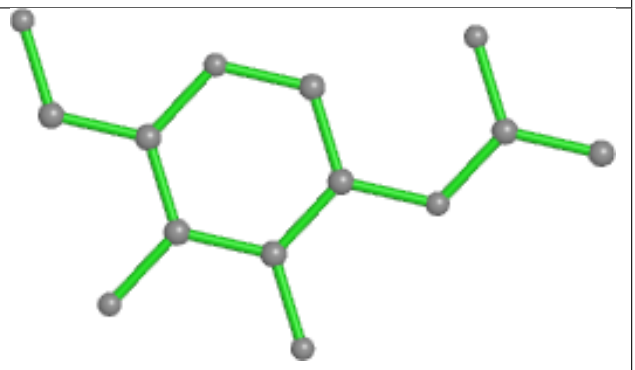


Rings

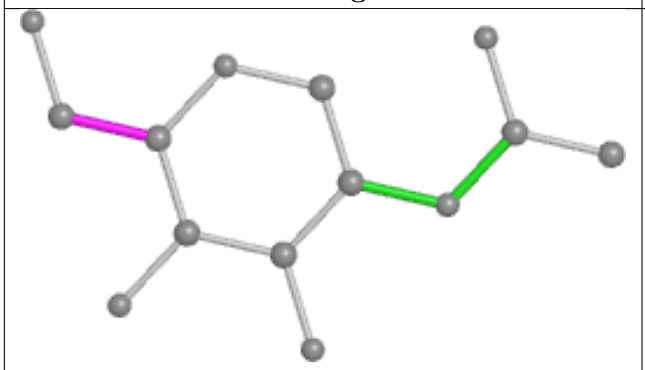
Ligand NAG B 502



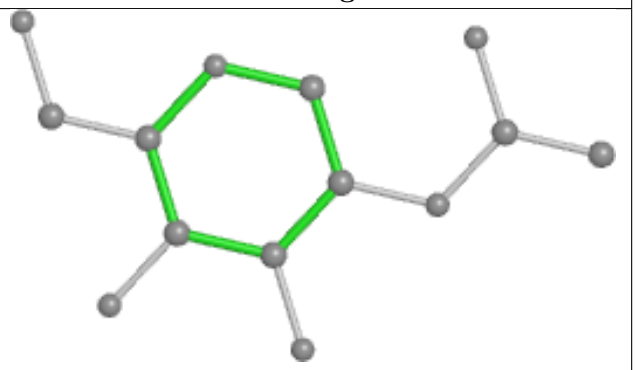
Bond lengths



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	388/393 (98%)	-0.28	0	100	100	47, 65, 83, 116	0
1	B	388/393 (98%)	-0.34	0	100	100	35, 51, 69, 92	0
2	E	215/216 (99%)	-0.04	4 (1%)	66	59	57, 88, 120, 160	0
2	L	215/216 (99%)	0.21	8 (3%)	41	31	61, 100, 160, 199	0
3	F	213/228 (93%)	-0.10	0	100	100	56, 85, 115, 136	0
3	H	213/228 (93%)	-0.22	0	100	100	64, 89, 120, 143	0
All	All	1632/1674 (97%)	-0.17	12 (0%)	87	84	35, 74, 120, 199	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	214	CYS	4.8
2	L	213	GLU	4.8
2	L	214	CYS	4.4
2	L	192	TYR	2.8
2	L	100	GLN	2.6
2	L	212	GLY	2.5
2	E	12	SER	2.2
2	E	7	SER	2.2
2	E	100	GLN	2.2
2	L	202	SER	2.1
2	L	209	PHE	2.1
2	L	104	LEU	2.0

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

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

6.3 Carbohydrates (i)

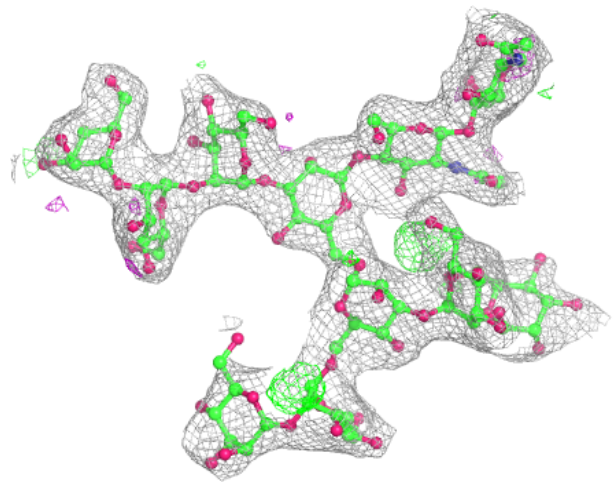
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

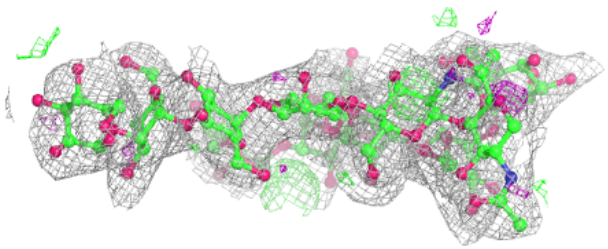
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MAN	D	11	11/12	0.75	0.40	116,122,126,127	0
4	MAN	D	10	11/12	0.80	0.28	98,102,106,111	0
4	MAN	C	11	11/12	0.85	0.22	114,120,123,124	0
4	MAN	C	9	11/12	0.88	0.27	96,100,102,102	0
4	MAN	D	7	11/12	0.89	0.15	79,85,92,96	0
5	NAG	G	2	14/15	0.91	0.28	101,112,118,118	0
4	MAN	D	9	11/12	0.92	0.26	106,109,111,111	0
5	NAG	G	1	14/15	0.92	0.18	71,84,89,99	0
4	MAN	C	10	11/12	0.92	0.18	91,94,101,103	0
4	MAN	D	8	11/12	0.93	0.17	85,95,98,102	0
4	MAN	C	7	11/12	0.94	0.11	56,61,76,86	0
4	MAN	D	6	11/12	0.95	0.12	73,75,78,79	0
4	MAN	C	6	11/12	0.95	0.14	57,66,72,76	0
4	NAG	C	1	14/15	0.95	0.15	43,47,55,59	0
4	MAN	C	8	11/12	0.95	0.16	64,72,77,87	0
4	BMA	D	3	11/12	0.96	0.10	67,73,83,85	0
4	MAN	D	5	11/12	0.96	0.13	64,66,71,75	0
4	BMA	C	3	11/12	0.96	0.12	58,62,68,75	0
4	NAG	D	1	14/15	0.96	0.15	57,66,76,78	0
4	NAG	D	2	14/15	0.96	0.13	63,66,69,73	0
4	MAN	C	4	11/12	0.97	0.11	50,57,61,69	0
4	MAN	C	5	11/12	0.97	0.10	47,52,57,59	0
4	MAN	D	4	11/12	0.97	0.09	60,63,67,70	0
4	NAG	C	2	14/15	0.97	0.14	40,48,62,66	0

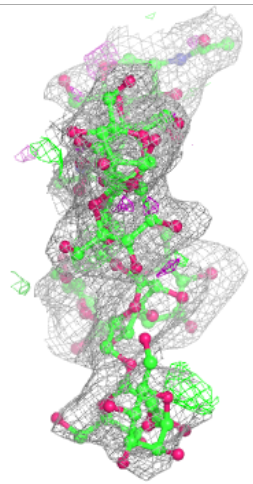
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

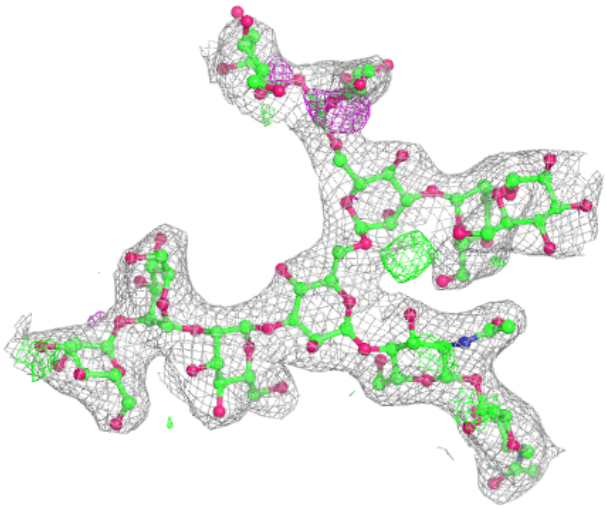


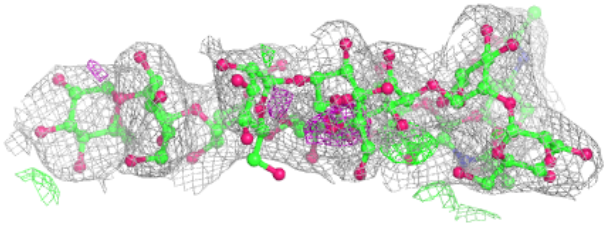


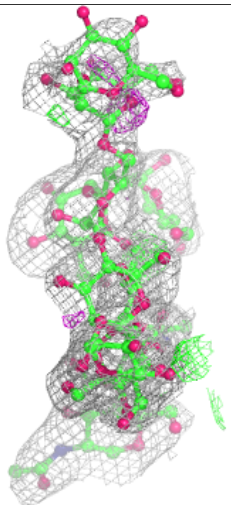


Electron density around Chain D:

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

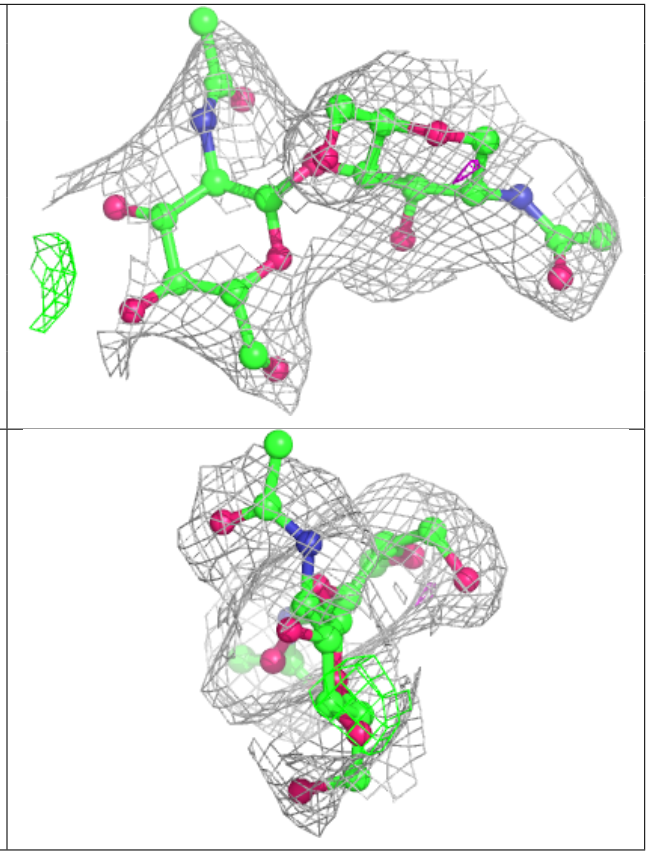






Electron density around Chain G:

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



6.4 Ligands (i)

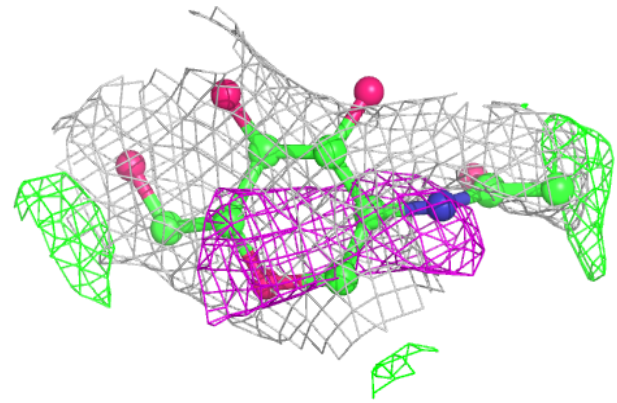
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

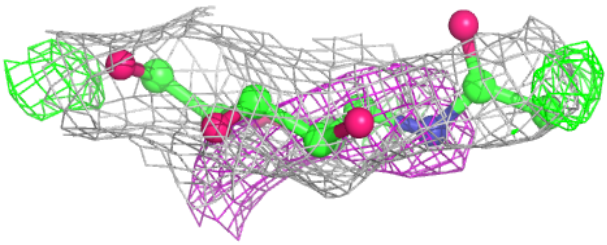
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	B	501	14/15	0.60	0.39	98,116,121,122	0
8	PO4	B	515	5/5	0.77	0.38	160,164,164,171	0
8	PO4	A	515	5/5	0.84	0.42	156,159,160,164	0
8	PO4	B	517	5/5	0.87	0.37	155,155,156,159	0
8	PO4	B	516	5/5	0.91	0.22	132,133,137,143	0
7	CA	A	512	1/1	0.92	0.17	111,111,111,111	0
6	NAG	B	502	14/15	0.95	0.19	45,67,80,89	0
7	CA	B	514	1/1	0.96	0.11	85,85,85,85	0

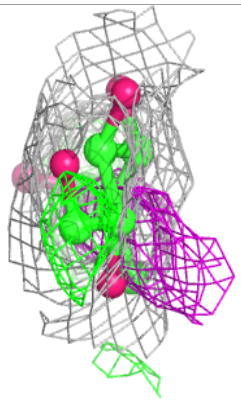
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG B 501:

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

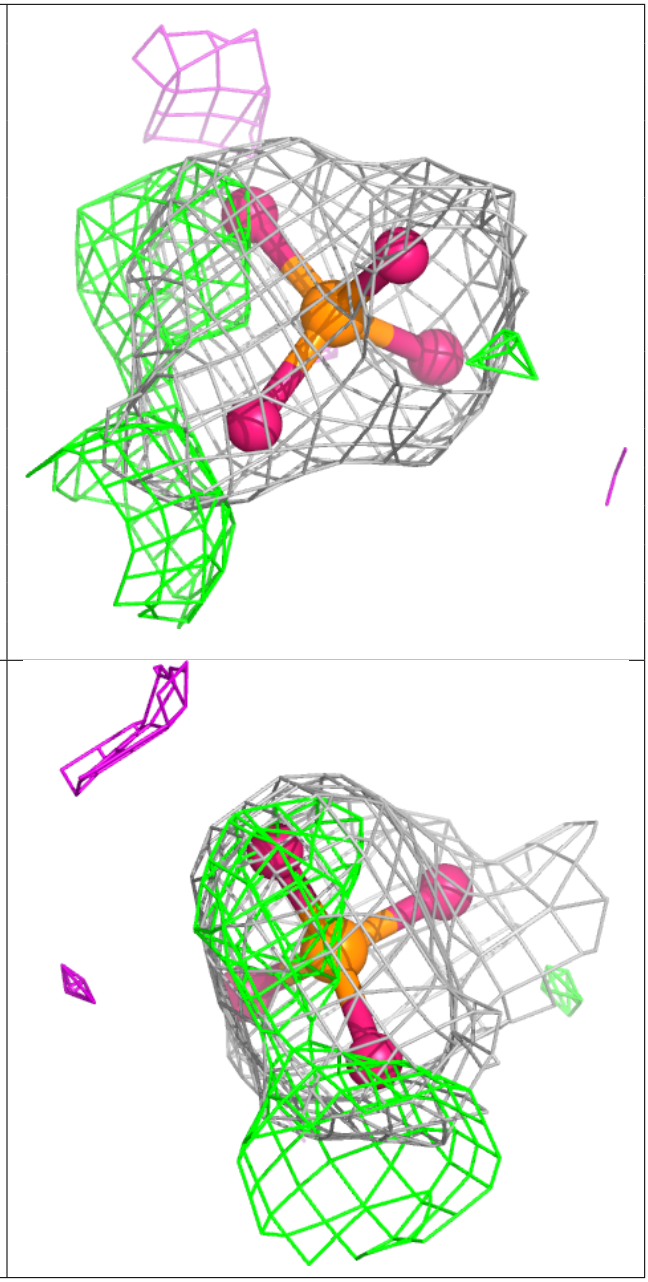






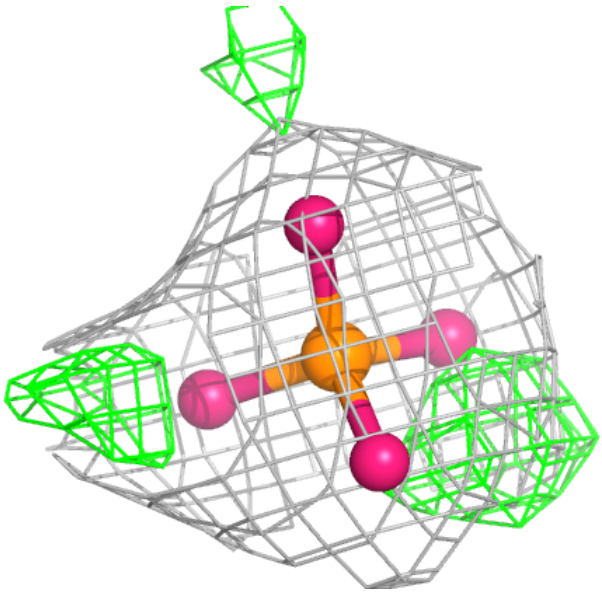
Electron density around PO4 B 515:

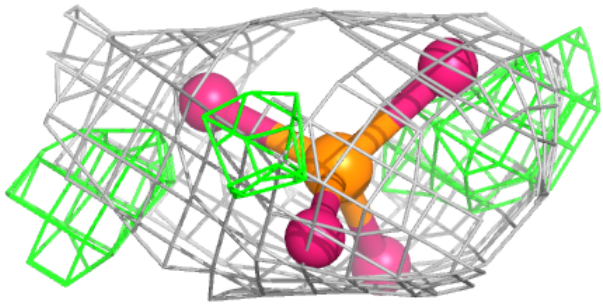
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

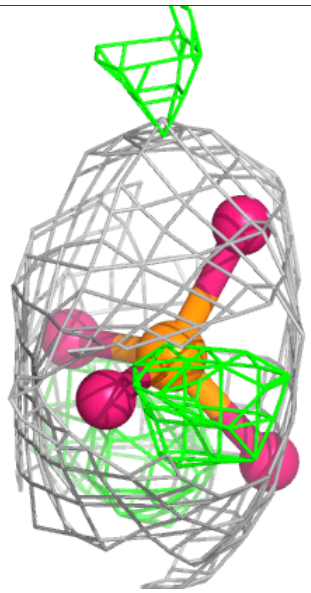


Electron density around PO4 A 515:

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

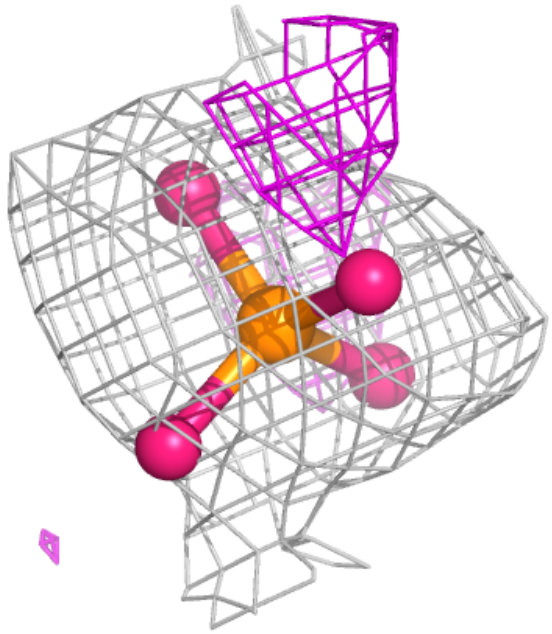


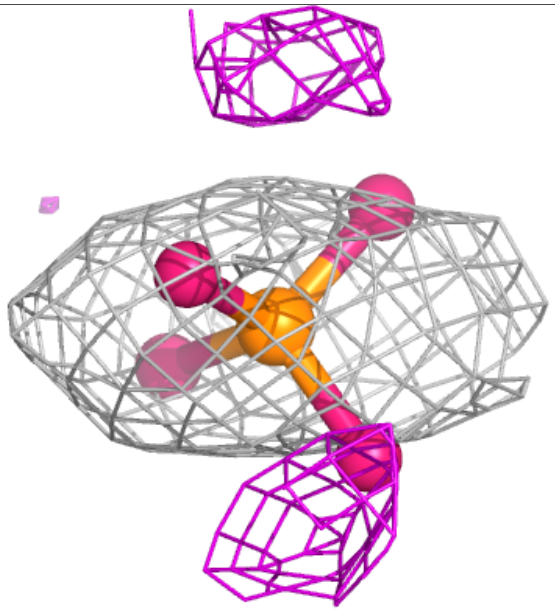


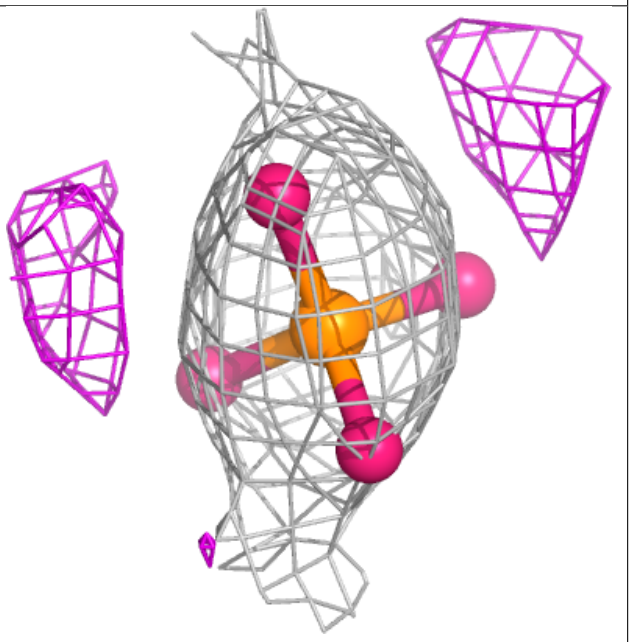


Electron density around PO4 B 517:

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

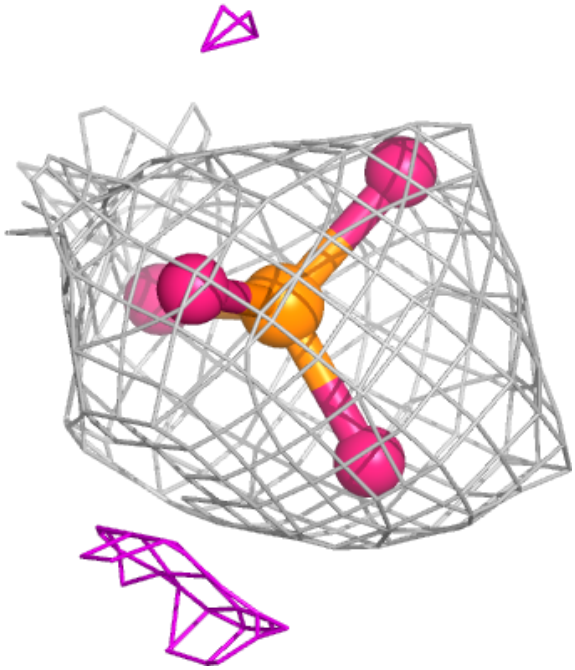


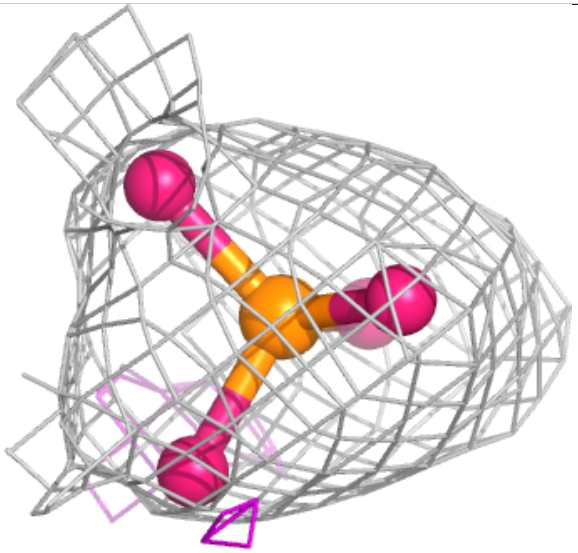


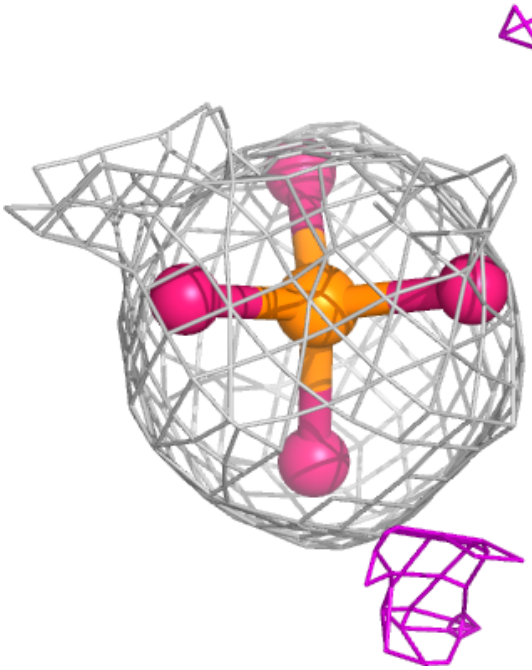


Electron density around PO4 B 516:

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

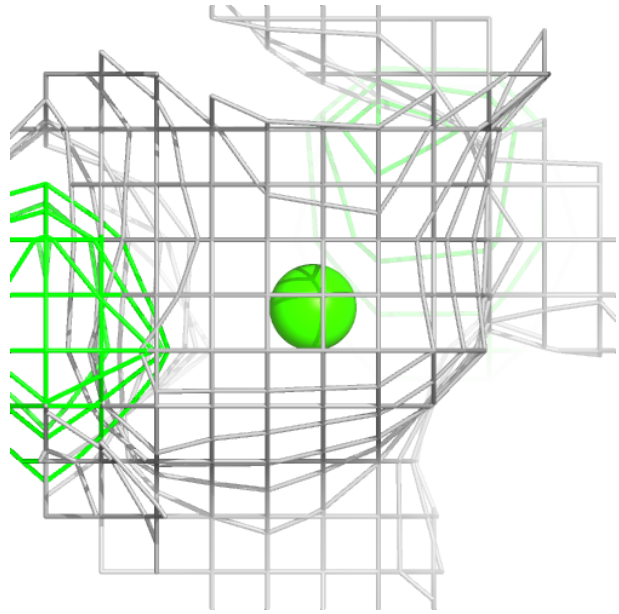


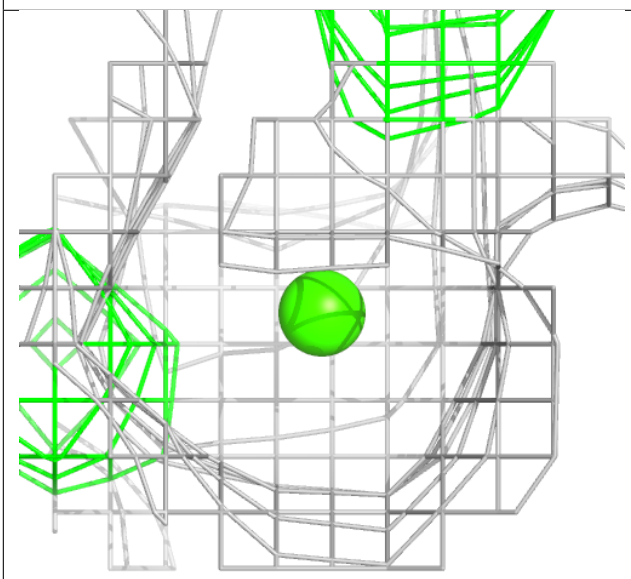


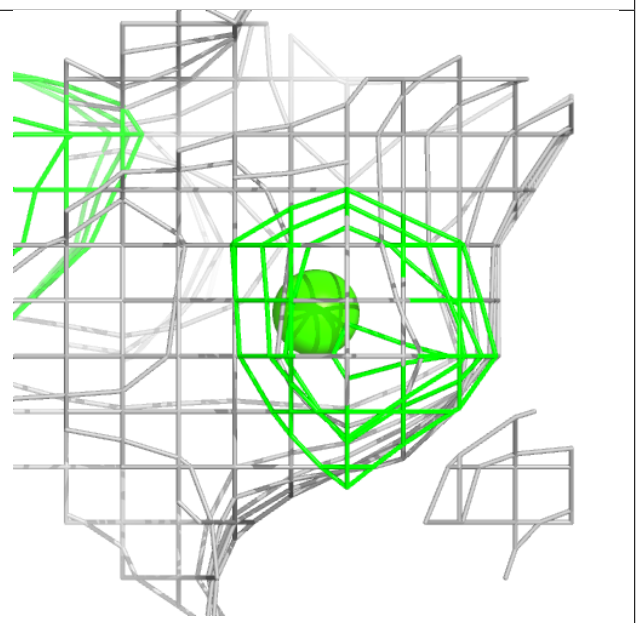


Electron density around CA A 512:

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

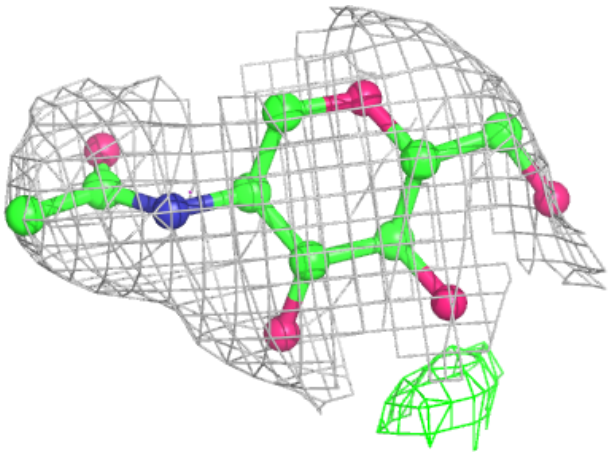


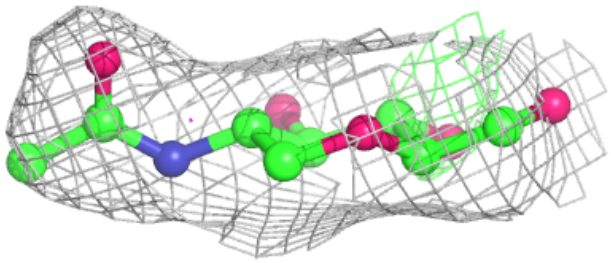


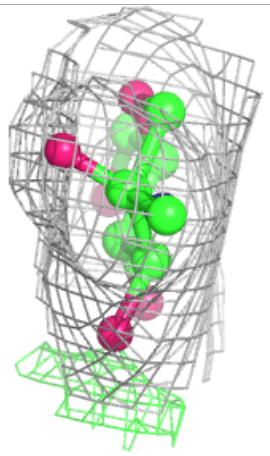


Electron density around NAG B 502:

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

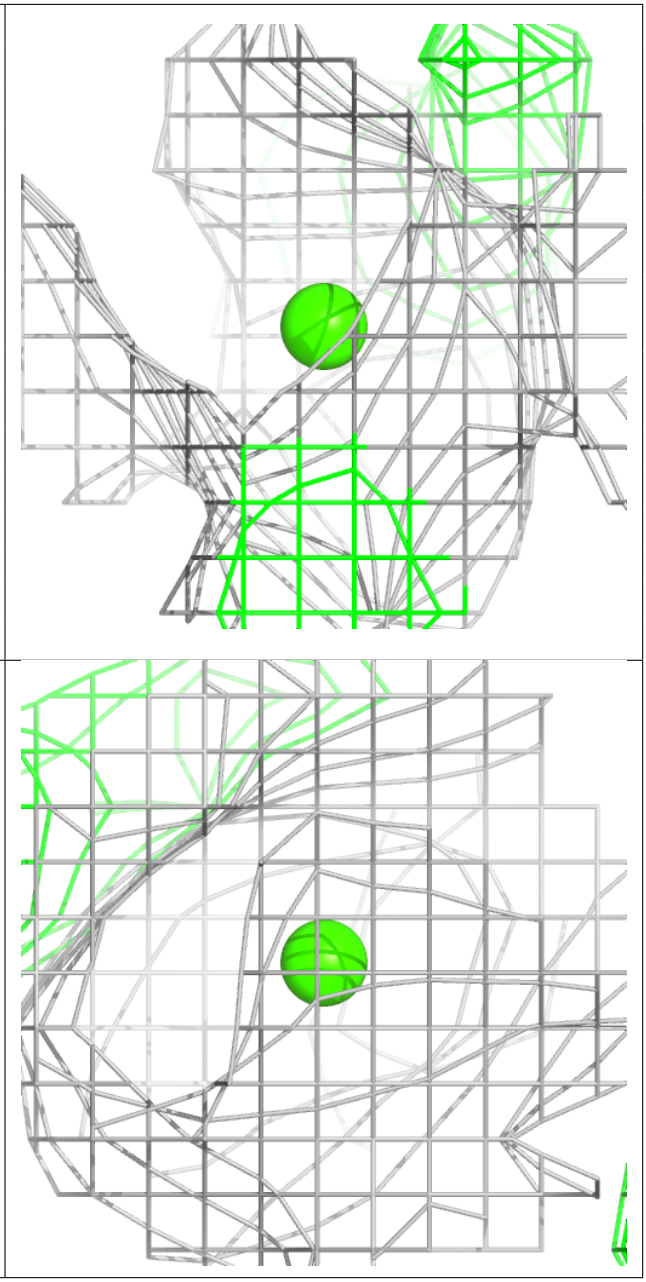






Electron density around CA B 514:

$2mF_o$-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.