Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2025 – 12:43 pm GMT

PDB ID	:	9EQ6
Title	:	Cachd1 and FZD5 complex
Authors	:	Zhao, Y.; Ren, J.; Jones, E.Y.
Deposited on	:	2024-03-20
Resolution	:	2.72 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:

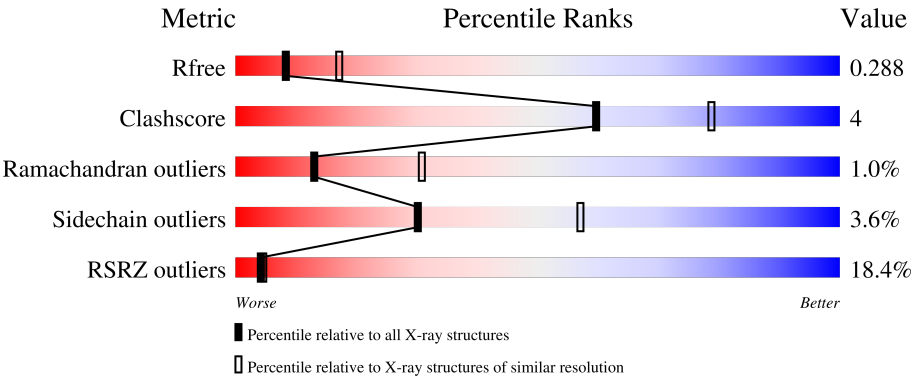
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.5

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 2.72 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}	164625	4050 (2.74-2.70)
Clashscore	180529	4439 (2.74-2.70)
Ramachandran outliers	177936	4374 (2.74-2.70)
Sidechain outliers	177891	4375 (2.74-2.70)
RSRZ outliers	164620	4050 (2.74-2.70)

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	B	140	9% 78% 7% • 14%
2	A	1102	18% 80% 12% • 6%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9193 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 Frizzled-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	120	965	610	167	172	16	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	24	GLU	-	expression tag	UNP Q9EQD0
B	25	THR	-	expression tag	UNP Q9EQD0
B	26	HIS	-	expression tag	UNP Q9EQD0
B	157	GLY	-	expression tag	UNP Q9EQD0
B	158	LEU	-	expression tag	UNP Q9EQD0
B	159	GLU	-	expression tag	UNP Q9EQD0
B	160	VAL	-	expression tag	UNP Q9EQD0
B	161	LEU	-	expression tag	UNP Q9EQD0
B	162	PHE	-	expression tag	UNP Q9EQD0
B	163	GLN	-	expression tag	UNP Q9EQD0

- Molecule 2 is a protein called VWFA and cache domain-containing protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	1038	8124	5109	1397	1559	59	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1095	THR	-	expression tag	UNP Q6PDJ1
A	1096	GLY	-	expression tag	UNP Q6PDJ1
A	1097	LEU	-	expression tag	UNP Q6PDJ1
A	1098	GLU	-	expression tag	UNP Q6PDJ1
A	1099	VAL	-	expression tag	UNP Q6PDJ1
A	1100	LEU	-	expression tag	UNP Q6PDJ1

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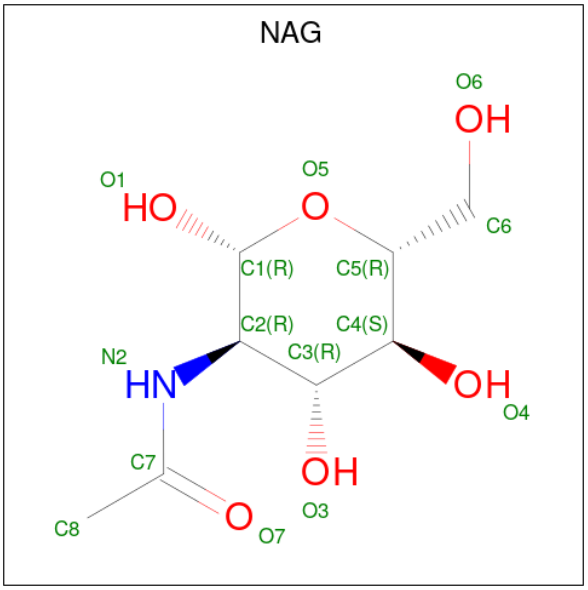
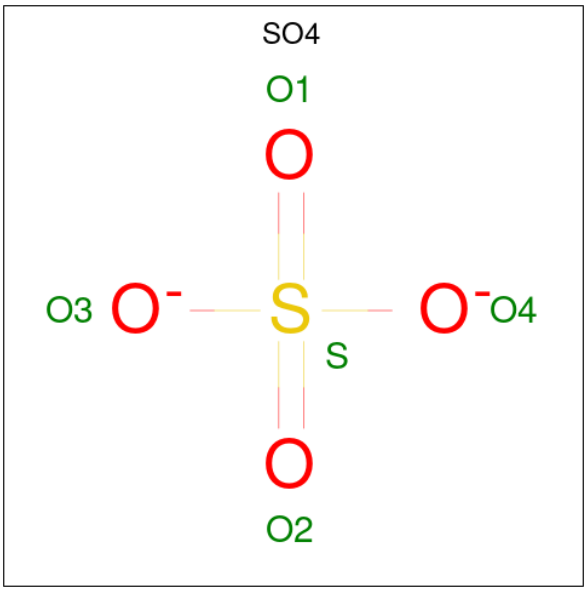
Chain	Residue	Modelled	Actual	Comment	Reference
A	1101	PHE	-	expression tag	UNP Q6PDJ1
A	1102	GLN	-	expression tag	UNP Q6PDJ1

- Molecule 3 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
3	B	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

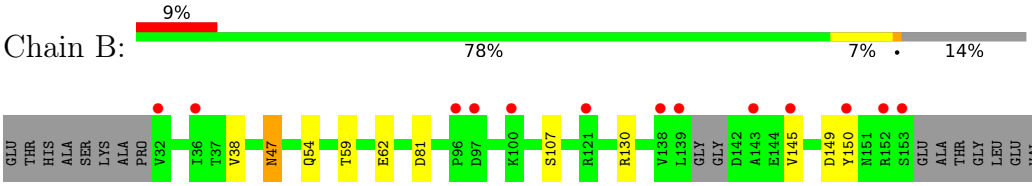
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

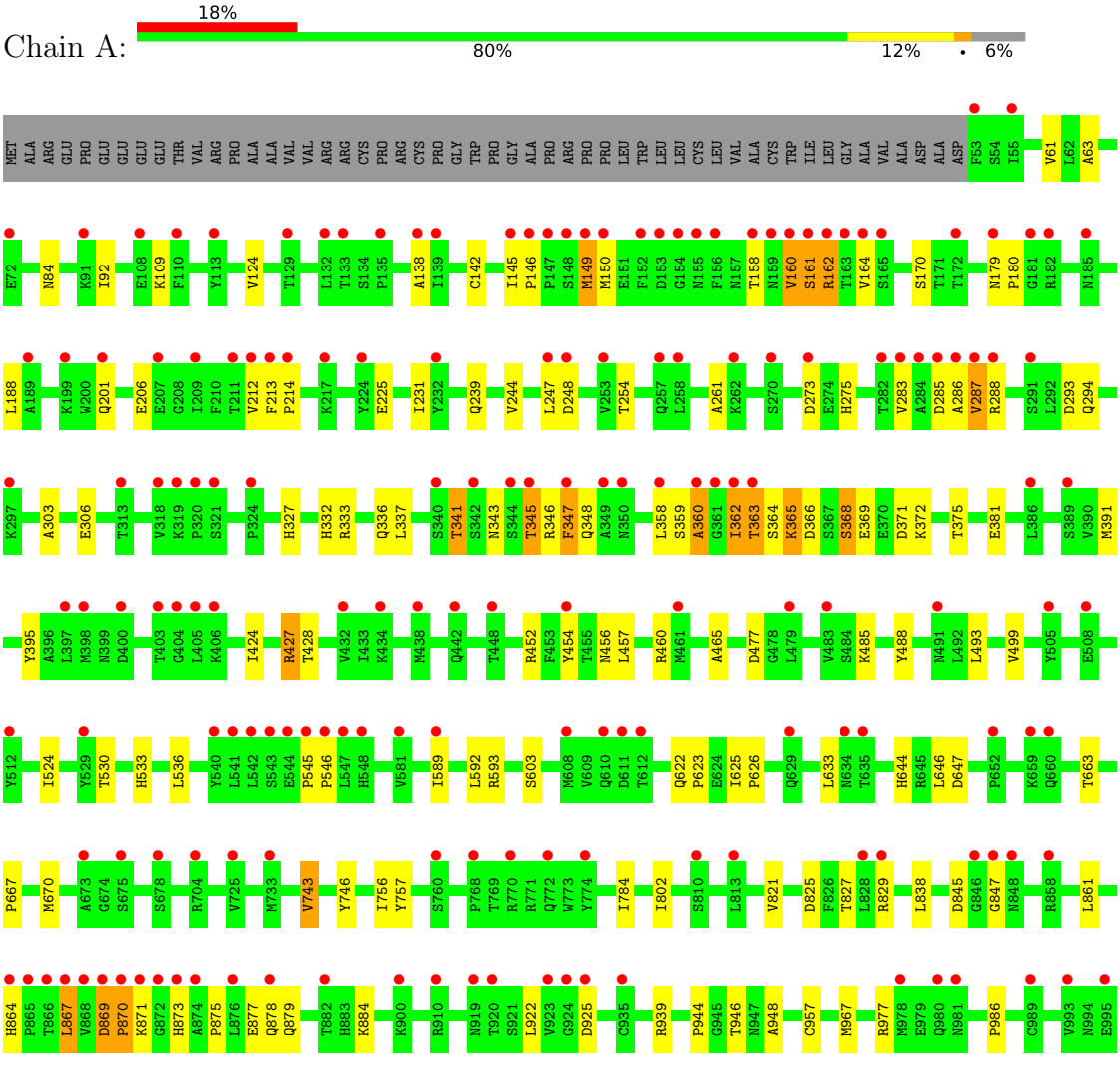
• Molecule 1: Frizzled-5

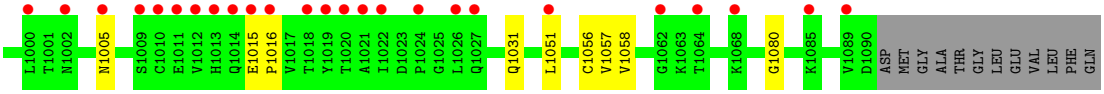
Chain B:



• Molecule 2: VWFA and cache domain-containing protein 1

Chain A:




L1000
T1001
N1002
N1005
S1009
C1010
E1011
V1012
H1013
Q1014
E1015
P1016
V1017
T1018
Y1019
T1020
A1021
I1022
D1023
P1024
G1025
L1026
Q1027
Q1031
L1051
C1056
V1057
V1058
G1062
K1063
T1064
K1068
G1080
K1085
V1089
D1090
ASP
MET
GLY
ALA
THR
GLY
LEU
GLU
VAL
LEU
PHE
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	123.11Å 123.11Å 367.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.91 – 2.72 91.91 – 2.72	Depositor EDS
% Data completeness (in resolution range)	95.6 (91.91-2.72) 95.8 (91.91-2.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.73Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.258 , 0.286 0.260 , 0.288	Depositor DCC
R_{free} test set	3854 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	72.2	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 90.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9193	wwPDB-VP
Average B, all atoms (Å^2)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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, SO4

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	B	0.23	0/994	0.40	0/1351
2	A	0.24	0/8293	0.44	0/11267
All	All	0.24	0/9287	0.43	0/12618

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	B	965	0	910	5	0
2	A	8124	0	7998	70	0
3	A	84	0	78	2	0
3	B	14	0	13	0	0
4	A	5	0	0	0	0
5	A	1	0	0	0	0
All	All	9193	0	8999	76	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 4.

All (76) 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:A:922:LEU:HA	3:A:1204:NAG:H82	1.57	0.86
2:A:247:LEU:HD11	2:A:261:ALA:HB1	1.74	0.70
2:A:946:THR:HG23	2:A:948:ALA:H	1.63	0.63
1:B:59:THR:HG23	1:B:62:GLU:H	1.66	0.61
2:A:188:LEU:HD13	2:A:213:PHE:HB2	1.81	0.61
2:A:454:TYR:HA	2:A:457:LEU:HD23	1.82	0.60
2:A:869:ASP:O	2:A:871:LYS:N	2.36	0.59
2:A:337:LEU:O	2:A:341:THR:OG1	2.21	0.58
2:A:864:HIS:CG	2:A:867:LEU:HB2	2.39	0.57
2:A:603:SER:HB2	2:A:623:PRO:HG3	1.87	0.55
2:A:358:LEU:HD23	2:A:395:TYR:HB2	1.89	0.55
2:A:465:ALA:HB2	2:A:485:LYS:HE3	1.90	0.54
2:A:161:SER:OG	2:A:162:ARG:NH1	2.41	0.53
2:A:593:ARG:NH1	2:A:622:GLN:O	2.41	0.53
2:A:391:MET:HE1	2:A:456:ASN:HB3	1.91	0.53
2:A:925:ASP:OD2	2:A:939:ARG:NH2	2.38	0.53
2:A:212:VAL:HG22	2:A:214:PRO:HD2	1.90	0.53
2:A:327:HIS:CE1	2:A:362:ILE:HG21	2.43	0.53
2:A:875:PRO:HG3	2:A:967:MET:HG2	1.91	0.53
2:A:1057:VAL:HG23	2:A:1058:VAL:HG23	1.91	0.53
2:A:138:ALA:O	2:A:179:ASN:ND2	2.43	0.52
2:A:589:ILE:HA	2:A:592:LEU:HD23	1.92	0.52
2:A:1015:GLU:N	2:A:1016:PRO:HD2	2.25	0.51
1:B:81:ASP:OD1	1:B:150:TYR:OH	2.26	0.50
2:A:63:ALA:HB2	2:A:944:PRO:HD2	1.94	0.50
2:A:622:GLN:HG2	2:A:625:ILE:HD12	1.94	0.50
2:A:306:GLU:OE1	2:A:306:GLU:N	2.41	0.49
2:A:327:HIS:NE2	2:A:362:ILE:HG21	2.27	0.49
2:A:488:TYR:HE1	2:A:493:LEU:HD12	1.77	0.49
2:A:533:HIS:HB3	2:A:536:LEU:HD13	1.95	0.48
3:A:1204:NAG:O7	3:A:1204:NAG:O3	2.30	0.48
1:B:54:GLN:HG2	1:B:130:ARG:HD3	1.96	0.48
2:A:829:ARG:HH21	2:A:864:HIS:HE1	1.61	0.48
2:A:343:ASN:HB3	2:A:346:ARG:HD3	1.95	0.48
2:A:746:TYR:HB3	2:A:756:ILE:HG22	1.95	0.47
2:A:61:VAL:HG12	2:A:838:LEU:HD12	1.96	0.46
2:A:784:ILE:HG23	2:A:802:ILE:HG23	1.97	0.46
2:A:869:ASP:N	2:A:870:PRO:HD2	2.31	0.46
2:A:644:HIS:CE1	2:A:670:MET:HG3	2.51	0.46
2:A:206:GLU:OE2	2:A:452:ARG:NH1	2.44	0.45
2:A:293:ASP:OD1	2:A:294:GLN:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:149:MET:HA	2:A:160:VAL:HG22	1.99	0.45
2:A:286:ALA:O	2:A:288:ARG:HG3	2.17	0.45
2:A:201:GLN:HB3	2:A:499:VAL:HG12	1.99	0.44
2:A:877:GLU:HG3	2:A:986:PRO:O	2.17	0.44
2:A:332:HIS:O	2:A:336:GLN:HG2	2.17	0.44
2:A:1005:ASN:O	2:A:1005:ASN:ND2	2.51	0.44
2:A:870:PRO:HA	2:A:878:GLN:HE22	1.82	0.44
2:A:231:ILE:HD12	2:A:231:ILE:H	1.83	0.44
2:A:646:LEU:HD21	2:A:663:THR:HG22	2.00	0.44
2:A:827:THR:HG21	2:A:1051:LEU:HA	1.98	0.43
1:B:47:ASN:OD1	1:B:47:ASN:N	2.49	0.43
2:A:381:GLU:HG2	2:A:427:ARG:NH1	2.34	0.43
2:A:524:ILE:HG22	2:A:530:THR:HA	2.00	0.43
2:A:545:PRO:HA	2:A:546:PRO:HD3	1.89	0.43
2:A:368:SER:O	2:A:372:LYS:HG3	2.18	0.43
2:A:743:VAL:HG22	2:A:825:ASP:HB2	1.99	0.43
2:A:283:VAL:HG13	2:A:285:ASP:H	1.83	0.42
2:A:273:ASP:O	2:A:303:ALA:HB3	2.20	0.42
2:A:845:ASP:O	2:A:847:GLY:N	2.47	0.42
2:A:213:PHE:HB3	2:A:214:PRO:HD3	2.01	0.42
2:A:239:GLN:HG2	2:A:460:ARG:NH2	2.35	0.41
2:A:861:LEU:HD12	2:A:884:LYS:HD3	2.02	0.41
2:A:870:PRO:HG3	2:A:879:GLN:HE22	1.85	0.41
2:A:170:SER:OG	2:A:225:GLU:OE1	2.32	0.41
2:A:667:PRO:HB3	2:A:757:TYR:HB2	2.01	0.41
1:B:107:SER:OG	1:B:149:ASP:OD2	2.26	0.41
2:A:109:LYS:HE3	2:A:109:LYS:HB2	1.91	0.41
2:A:345:THR:HB	2:A:347:PHE:HB3	2.01	0.41
2:A:359:SER:OG	2:A:360:ALA:N	2.52	0.41
2:A:371:ASP:O	2:A:375:THR:HG23	2.21	0.41
2:A:92:ILE:HD11	2:A:626:PRO:HG3	2.03	0.41
2:A:647:ASP:N	2:A:647:ASP:OD1	2.52	0.40
2:A:1056:CYS:HA	2:A:1080:GLY:HA2	2.03	0.40
2:A:149:MET:HB2	2:A:158:THR:HA	2.04	0.40
2:A:124:VAL:HG23	2:A:180:PRO:HG3	2.04	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	B	116/140 (83%)	112 (97%)	4 (3%)	0	100	100
2	A	1036/1102 (94%)	953 (92%)	72 (7%)	11 (1%)	12	28
All	All	1152/1242 (93%)	1065 (92%)	76 (7%)	11 (1%)	13	31

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	146	PRO
2	A	870	PRO
2	A	873	HIS
2	A	348	GLN
2	A	364	SER
2	A	365	LYS
2	A	161	SER
2	A	164	VAL
2	A	360	ALA
2	A	363	THR
2	A	287	VAL

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	B	110/124 (89%)	107 (97%)	3 (3%)	40	68
2	A	928/979 (95%)	894 (96%)	34 (4%)	29	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1038/1103 (94%)	1001 (96%)	37 (4%)	30 57

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	38	VAL
1	B	47	ASN
1	B	145	VAL
2	A	84	ASN
2	A	142	CYS
2	A	145	ILE
2	A	149	MET
2	A	150	MET
2	A	160	VAL
2	A	162	ARG
2	A	244	VAL
2	A	248	ASP
2	A	254	THR
2	A	275	HIS
2	A	287	VAL
2	A	333	ARG
2	A	341	THR
2	A	345	THR
2	A	347	PHE
2	A	362	ILE
2	A	363	THR
2	A	365	LYS
2	A	366	ASP
2	A	368	SER
2	A	369	GLU
2	A	424	ILE
2	A	427	ARG
2	A	428	THR
2	A	477	ASP
2	A	633	LEU
2	A	743	VAL
2	A	821	VAL
2	A	867	LEU
2	A	869	ASP
2	A	957	CYS
2	A	977	ARG
2	A	1031	GLN

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

Mol	Chain	Res	Type
2	A	848	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
3	NAG	A	1204	2	14,14,15	0.89	1 (7%)	17,19,21	0.95	1 (5%)
3	NAG	A	1206	2	14,14,15	0.26	0	17,19,21	0.41	0
4	SO4	A	1207	-	4,4,4	0.14	0	6,6,6	0.04	0
3	NAG	A	1201	2	14,14,15	0.26	0	17,19,21	0.37	0
3	NAG	A	1205	2	14,14,15	0.20	0	17,19,21	0.45	0
3	NAG	A	1203	2	14,14,15	0.38	0	17,19,21	0.62	0
3	NAG	A	1202	2	14,14,15	0.26	0	17,19,21	0.52	0
3	NAG	B	200	1	14,14,15	0.29	0	17,19,21	0.40	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
3	NAG	A	1204	2	-	3/6/23/26	0/1/1/1
3	NAG	A	1206	2	-	0/6/23/26	0/1/1/1
3	NAG	A	1201	2	-	0/6/23/26	0/1/1/1
3	NAG	A	1205	2	-	0/6/23/26	0/1/1/1
3	NAG	A	1203	2	-	1/6/23/26	0/1/1/1
3	NAG	A	1202	2	-	2/6/23/26	0/1/1/1
3	NAG	B	200	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)
3	A	1204	NAG	C1-C2	2.90	1.56	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1204	NAG	C1-O5-C5	3.19	116.51	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1204	NAG	C1-C2-N2-C7
3	A	1204	NAG	O5-C5-C6-O6
3	A	1202	NAG	C3-C2-N2-C7
3	A	1203	NAG	C3-C2-N2-C7
3	A	1204	NAG	C3-C2-N2-C7
3	A	1202	NAG	O5-C5-C6-O6

There are no ring outliers.

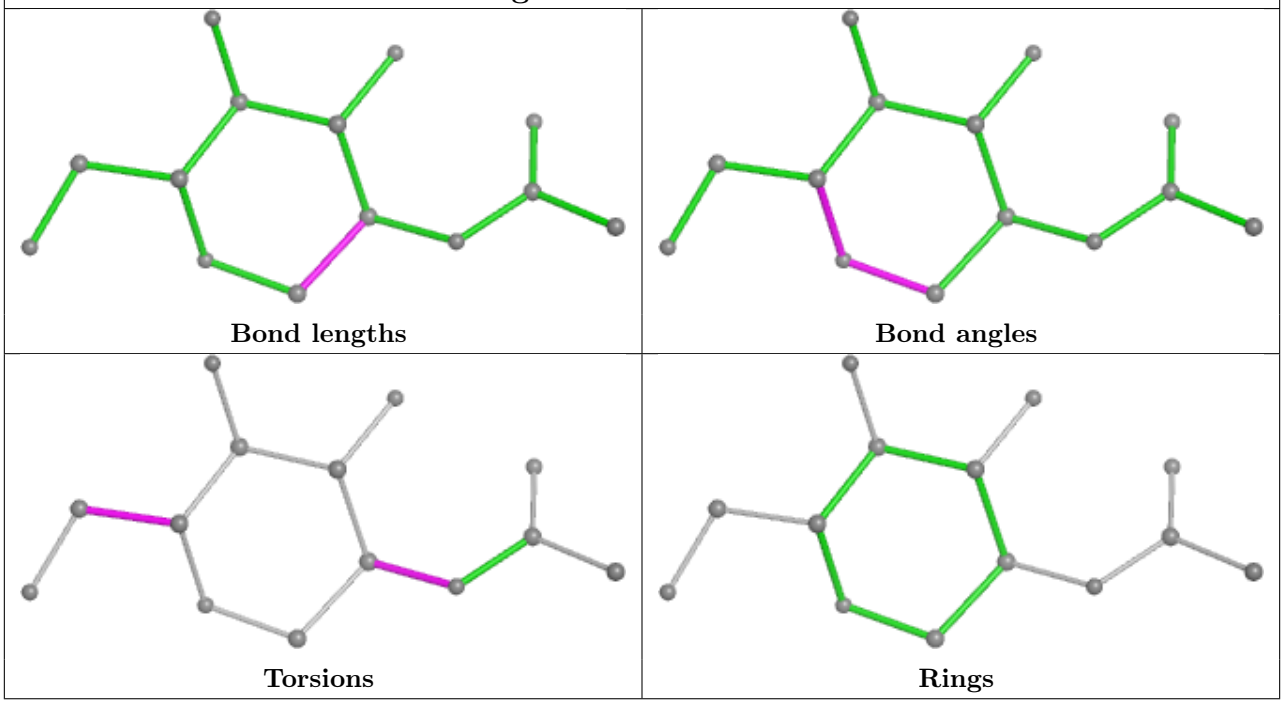
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1204	NAG	2	0

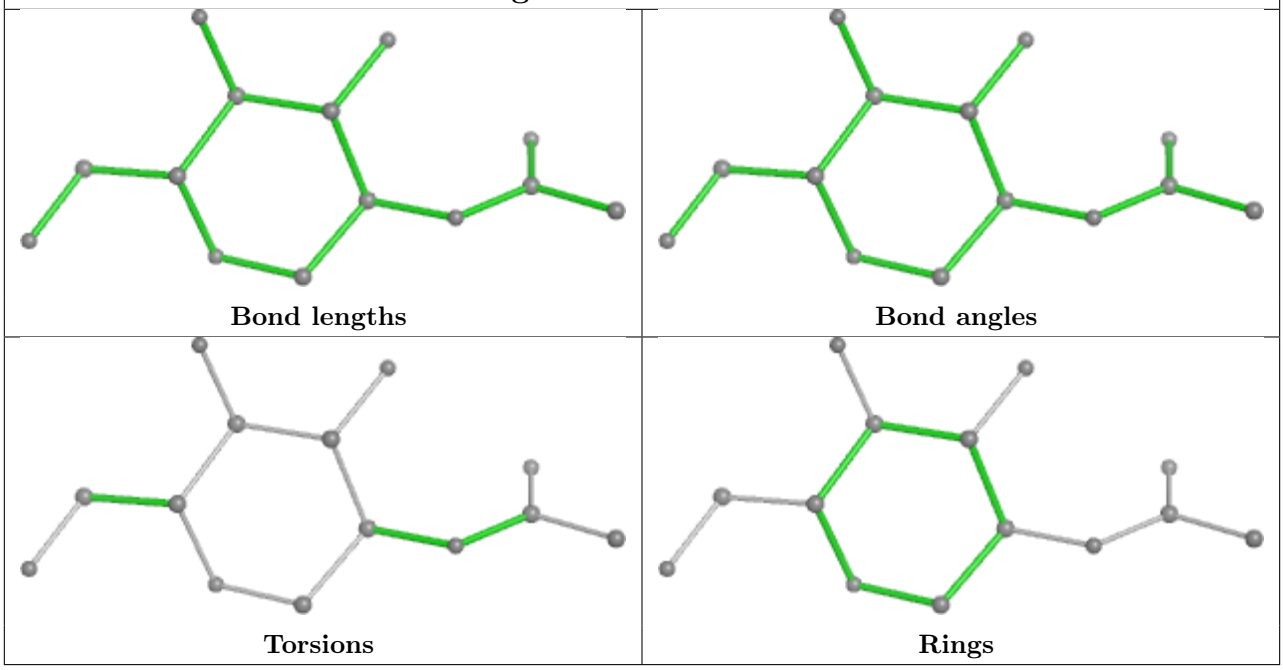
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

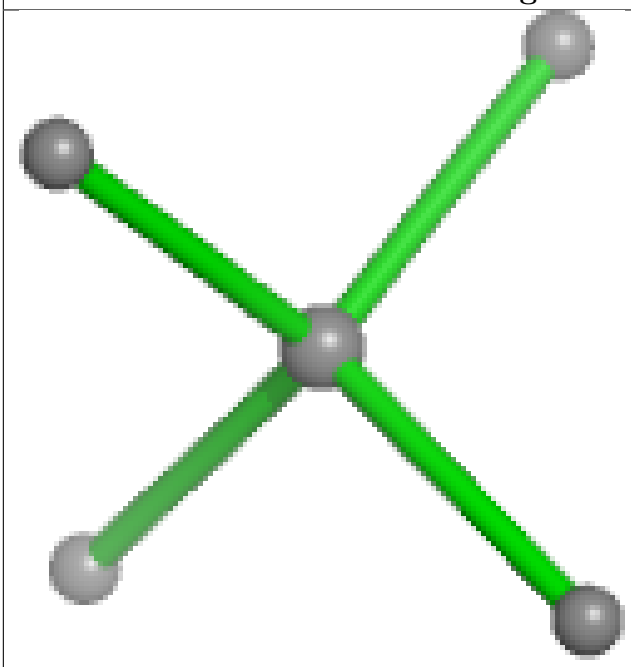
Ligand NAG A 1204



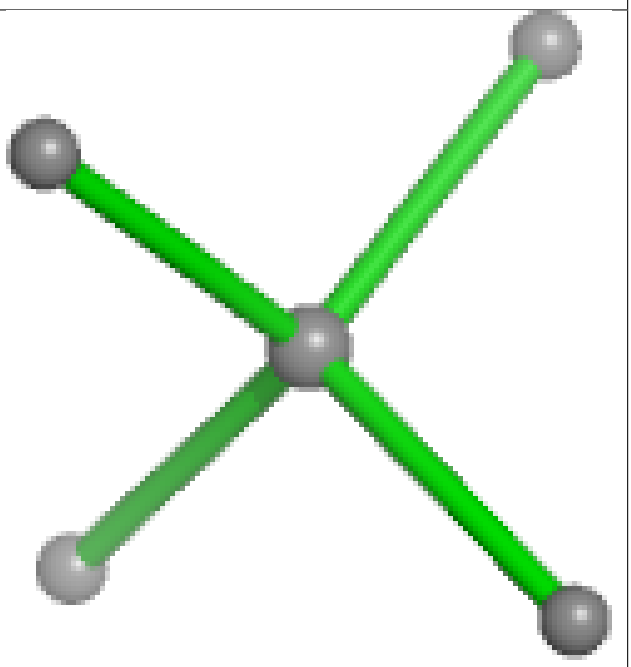
Ligand NAG A 1206



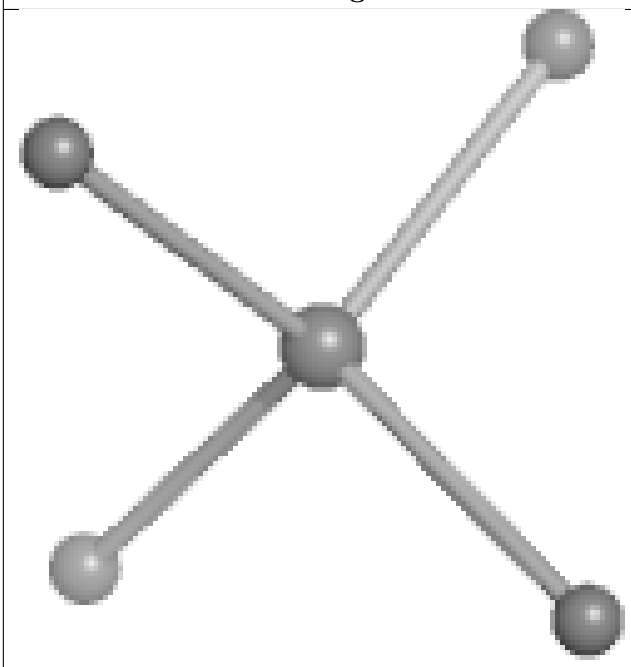
Ligand SO4 A 1207



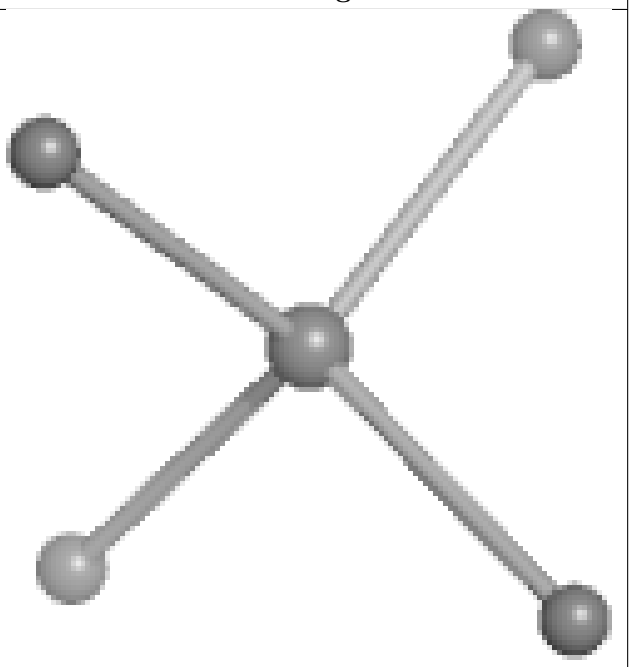
Bond lengths



Bond angles

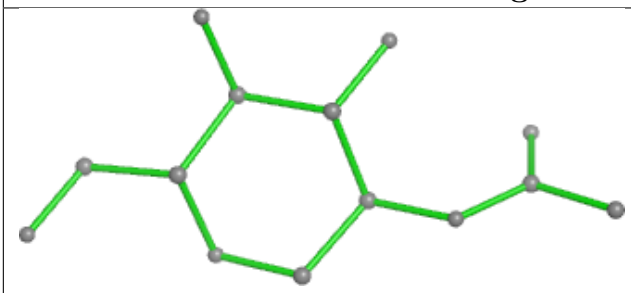


Torsions

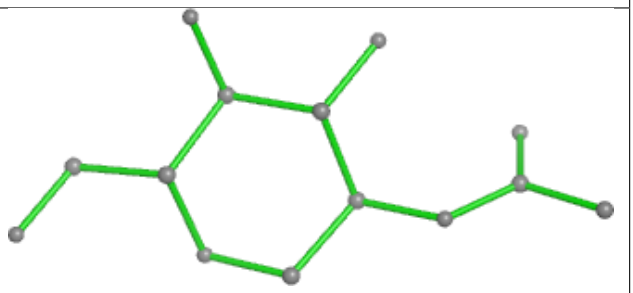


Rings

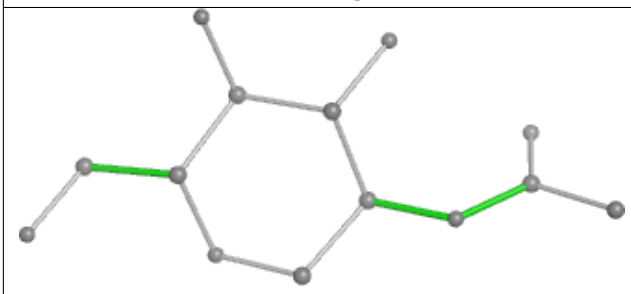
Ligand NAG A 1201



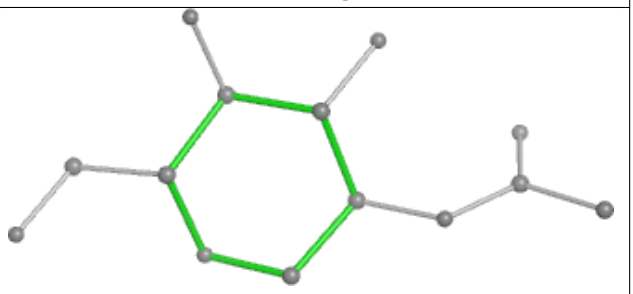
Bond lengths



Bond angles

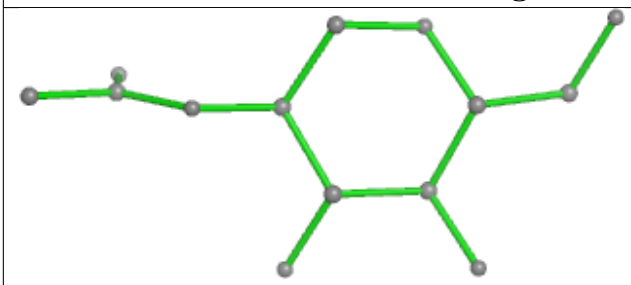


Torsions

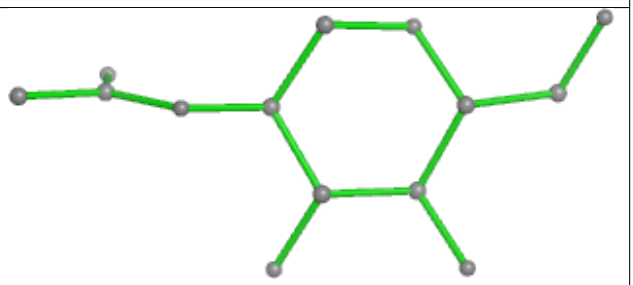


Rings

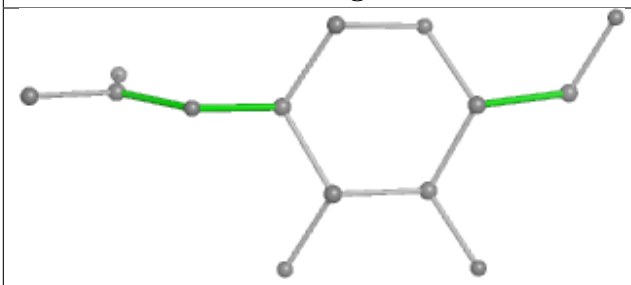
Ligand NAG A 1205



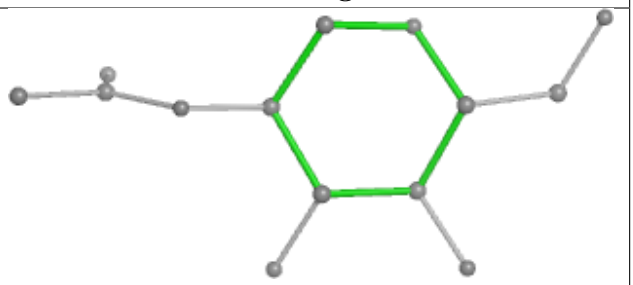
Bond lengths



Bond angles

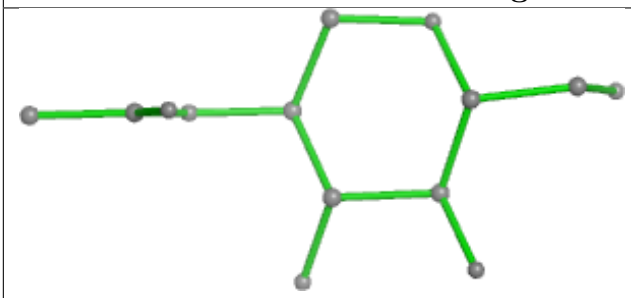


Torsions

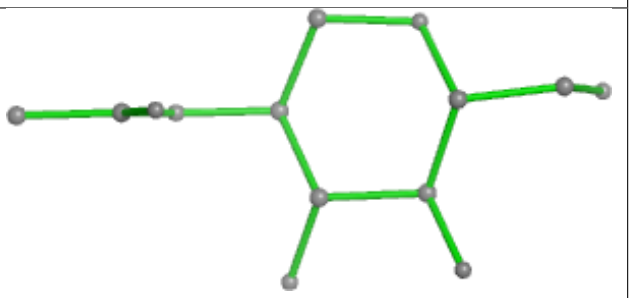


Rings

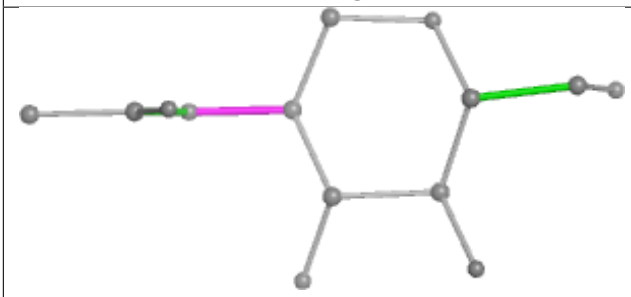
Ligand NAG A 1203



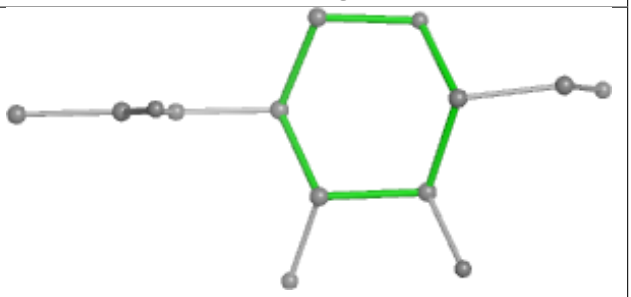
Bond lengths



Bond angles

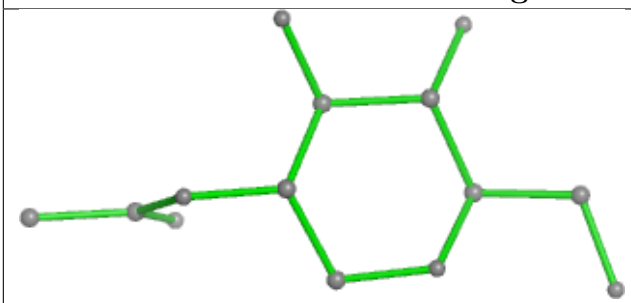


Torsions

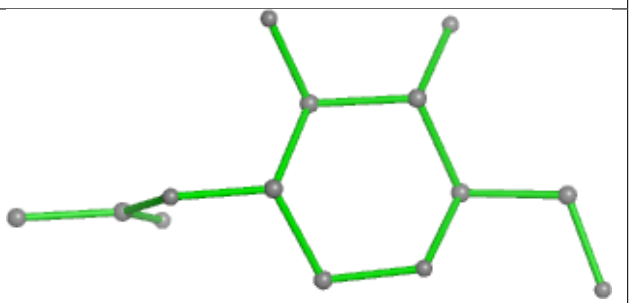


Rings

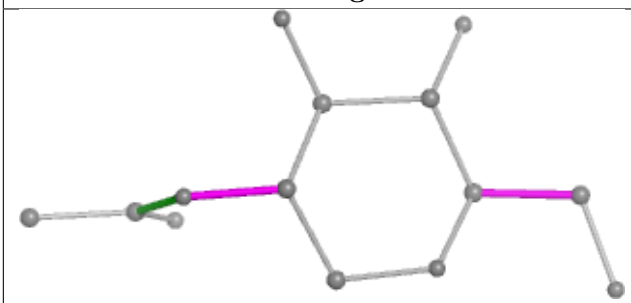
Ligand NAG A 1202



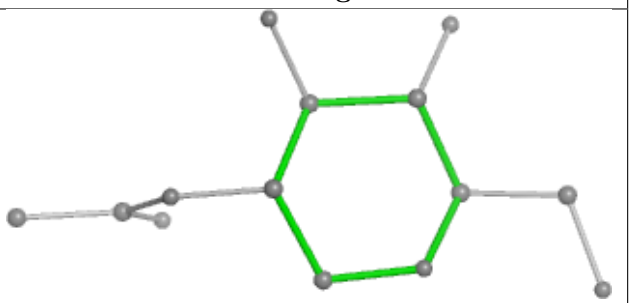
Bond lengths



Bond angles

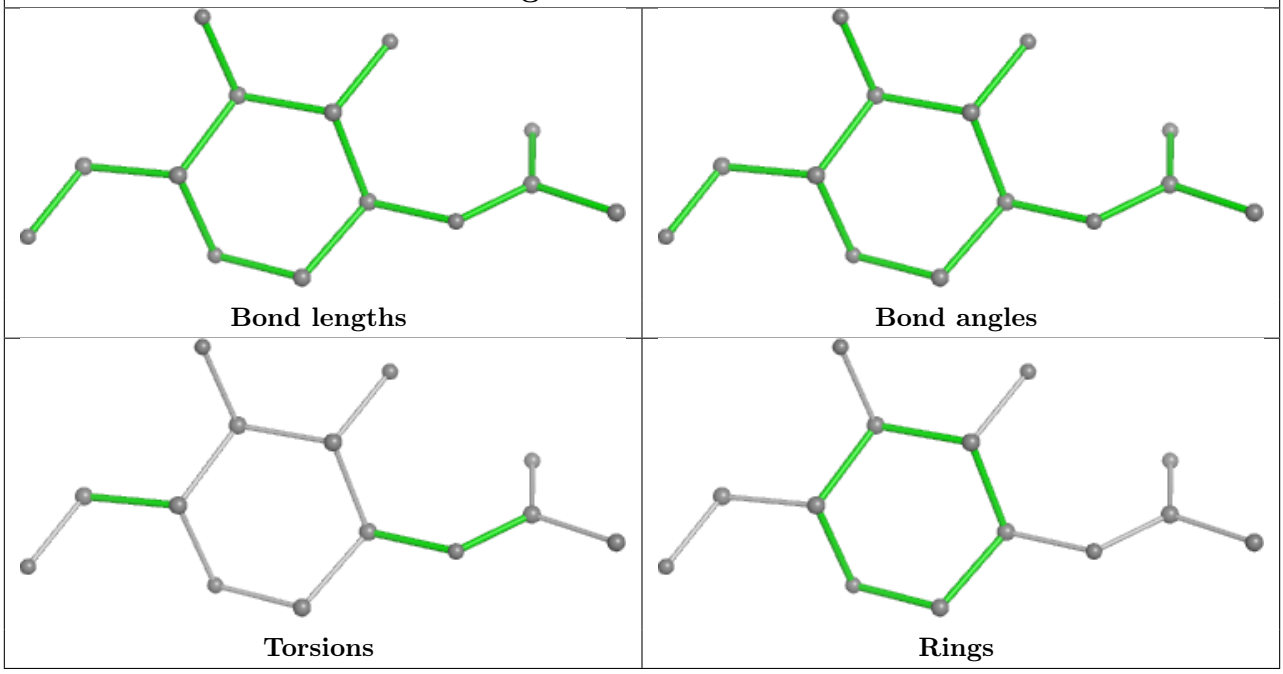


Torsions



Rings

Ligand NAG B 200



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	B	120/140 (85%)	0.83	13 (10%)	12	12	76, 98, 139, 174	0
2	A	1038/1102 (94%)	1.26	200 (19%)	4	4	62, 113, 176, 210	0
All	All	1158/1242 (93%)	1.21	213 (18%)	4	4	62, 110, 175, 210	0

All (213) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	284	ALA	11.4
2	A	868	VAL	8.6
2	A	870	PRO	7.1
2	A	160	VAL	6.8
2	A	53	PHE	6.7
2	A	673	ALA	6.2
1	B	139	LEU	5.9
2	A	152	PHE	5.8
2	A	347	PHE	5.8
2	A	113	TYR	5.7
2	A	139	ILE	5.6
2	A	148	SER	5.5
2	A	155	ASN	5.5
2	A	147	PRO	5.4
2	A	161	SER	5.4
2	A	1089	VAL	5.2
2	A	864	HIS	5.1
2	A	214	PRO	4.9
2	A	162	ARG	4.7
2	A	154	GLY	4.7
2	A	163	THR	4.6
2	A	362	ILE	4.4
2	A	405	LEU	4.4
2	A	156	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
2	A	287	VAL	4.2
2	A	865	PRO	4.2
2	A	283	VAL	4.2
2	A	1026	LEU	4.2
2	A	869	ASP	4.2
2	A	876	LEU	4.1
2	A	345	THR	4.1
2	A	138	ALA	4.0
2	A	146	PRO	4.0
1	B	152	ARG	3.9
2	A	660	GLN	3.9
2	A	871	LYS	3.9
2	A	286	ALA	3.8
2	A	159	ASN	3.8
2	A	145	ILE	3.8
2	A	1016	PRO	3.8
2	A	1013	HIS	3.8
2	A	285	ASP	3.7
2	A	543	SER	3.7
2	A	149	MET	3.7
2	A	882	THR	3.7
1	B	145	VAL	3.6
2	A	217	LYS	3.6
2	A	321	SER	3.6
2	A	925	ASP	3.6
2	A	349	ALA	3.6
2	A	199	LYS	3.6
1	B	153	SER	3.5
2	A	813	LEU	3.5
2	A	867	LEU	3.5
2	A	1000	LEU	3.5
2	A	91	LYS	3.5
1	B	143	ALA	3.4
2	A	253	VAL	3.4
2	A	344	SER	3.3
2	A	207	GLU	3.3
2	A	224	TYR	3.3
2	A	529	TYR	3.3
2	A	1019	TYR	3.3
2	A	360	ALA	3.3
2	A	919	ASN	3.3
2	A	1014	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
2	A	434	LYS	3.3
2	A	846	GLY	3.3
2	A	448	THR	3.3
2	A	1015	GLU	3.3
1	B	32	VAL	3.3
2	A	181	GLY	3.3
2	A	920	THR	3.2
2	A	1051	LEU	3.2
2	A	324	PRO	3.2
2	A	540	TYR	3.2
2	A	659	LYS	3.2
2	A	874	ALA	3.2
2	A	1068	LYS	3.2
2	A	150	MET	3.2
2	A	1011	GLU	3.2
2	A	319	LYS	3.2
2	A	158	THR	3.1
2	A	129	THR	3.1
2	A	1064	THR	3.1
2	A	542	LEU	3.1
2	A	438	MET	3.1
2	A	262	LYS	3.1
2	A	611	ASP	3.0
2	A	1018	THR	3.0
2	A	172	THR	3.0
2	A	282	THR	3.0
2	A	1002	ASN	3.0
2	A	1021	ALA	3.0
2	A	866	THR	3.0
2	A	980	GLN	3.0
2	A	1005	ASN	3.0
2	A	993	VAL	2.9
2	A	135	PRO	2.9
2	A	342	SER	2.9
2	A	1009	SER	2.9
2	A	878	GLN	2.9
2	A	247	LEU	2.9
2	A	634	ASN	2.9
2	A	1024	PRO	2.8
2	A	318	VAL	2.8
2	A	774	TYR	2.8
2	A	461	MET	2.8

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Mol	Chain	Res	Type	RSRZ
2	A	389	SER	2.8
2	A	454	TYR	2.8
2	A	248	ASP	2.8
2	A	153	ASP	2.7
2	A	164	VAL	2.7
2	A	257	GLN	2.7
2	A	1022	ILE	2.7
2	A	848	ASN	2.7
1	B	138	VAL	2.7
2	A	432	VAL	2.7
2	A	1020	THR	2.7
2	A	291	SER	2.7
2	A	340	SER	2.7
2	A	361	GLY	2.6
1	B	36	ILE	2.6
2	A	297	LYS	2.6
2	A	829	ARG	2.6
2	A	548	HIS	2.6
2	A	72	GLU	2.5
2	A	400	ASP	2.5
2	A	1027	GLN	2.5
2	A	213	PHE	2.5
2	A	404	GLY	2.5
2	A	1012	VAL	2.5
2	A	406	LYS	2.5
2	A	828	LEU	2.5
1	B	96	PRO	2.5
2	A	725	VAL	2.5
2	A	981	ASN	2.5
2	A	544	GLU	2.5
2	A	675	SER	2.5
2	A	704	ARG	2.5
2	A	770	ARG	2.4
2	A	900	LYS	2.4
2	A	273	ASP	2.4
2	A	847	GLY	2.4
2	A	508	GLU	2.4
2	A	212	VAL	2.4
2	A	179	ASN	2.4
2	A	995	GLU	2.4
2	A	479	LEU	2.4
2	A	165	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	A	397	LEU	2.4
2	A	483	VAL	2.4
2	A	55	ILE	2.4
2	A	232	TYR	2.4
2	A	108	GLU	2.3
2	A	201	GLN	2.3
2	A	505	TYR	2.3
2	A	398	MET	2.3
2	A	810	SER	2.3
2	A	547	LEU	2.3
2	A	363	THR	2.3
1	B	121	ARG	2.3
2	A	110	PHE	2.3
2	A	132	LEU	2.3
2	A	189	ALA	2.3
2	A	1010	CYS	2.2
2	A	442	GLN	2.2
2	A	923	VAL	2.2
2	A	209	ILE	2.2
2	A	258	LEU	2.2
2	A	733	MET	2.2
2	A	182	ARG	2.2
2	A	350	ASN	2.2
2	A	873	HIS	2.2
2	A	288	ARG	2.2
2	A	858	ARG	2.2
2	A	760	SER	2.2
2	A	403	THR	2.2
2	A	546	PRO	2.2
2	A	612	THR	2.2
2	A	872	GLY	2.2
2	A	512	TYR	2.2
2	A	978	MET	2.2
2	A	1085	LYS	2.1
2	A	608	MET	2.1
2	A	545	PRO	2.1
2	A	270	SER	2.1
2	A	772	GLN	2.1
2	A	910	ARG	2.1
2	A	635	THR	2.1
2	A	589	ILE	2.1
2	A	491	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	97	ASP	2.1
2	A	541	LEU	2.1
2	A	652	PRO	2.1
1	B	100	LYS	2.1
2	A	313	THR	2.1
2	A	185	ASN	2.1
2	A	924	GLY	2.1
2	A	320	PRO	2.0
2	A	989	CYS	2.0
2	A	133	THR	2.0
2	A	581	VAL	2.0
2	A	610	GLN	2.0
2	A	386	LEU	2.0
2	A	1062	GLY	2.0
2	A	768	PRO	2.0
2	A	935	CYS	2.0
2	A	211	THR	2.0
2	A	358	LEU	2.0
2	A	629	GLN	2.0
2	A	678	SER	2.0
1	B	150	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
3	NAG	A	1201	14/15	0.47	0.16	171,185,202,207	0
3	NAG	A	1202	14/15	0.55	0.16	128,171,176,177	0

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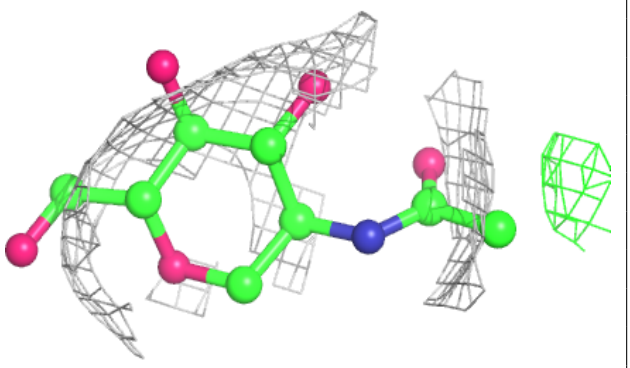
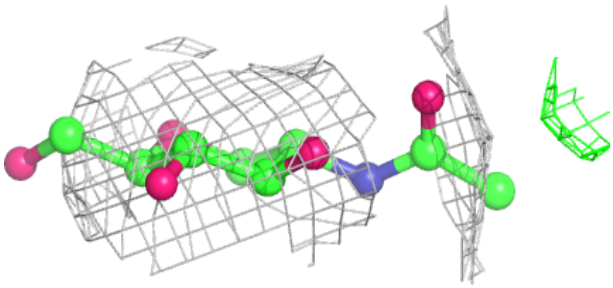
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	A	1206	14/15	0.58	0.20	147,179,200,200	0
4	SO4	A	1207	5/5	0.65	0.12	138,138,178,196	0
3	NAG	B	200	14/15	0.73	0.13	121,155,164,166	0
3	NAG	A	1204	14/15	0.77	0.15	94,132,144,147	0
3	NAG	A	1203	14/15	0.82	0.13	115,133,146,149	0
3	NAG	A	1205	14/15	0.87	0.13	112,128,134,140	0

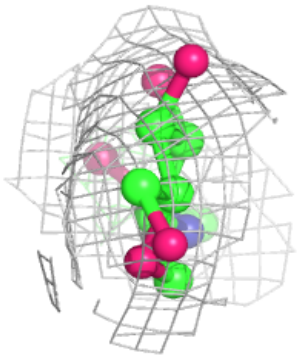
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG A 1201:

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

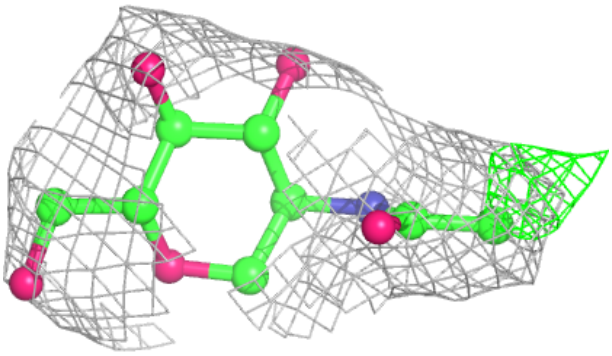


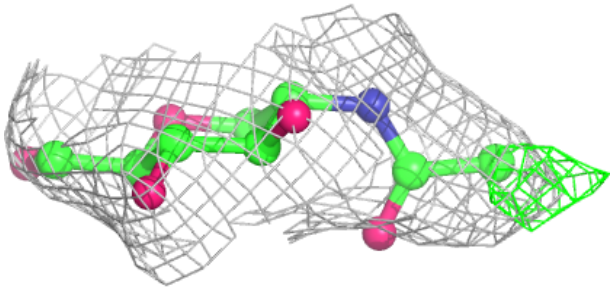


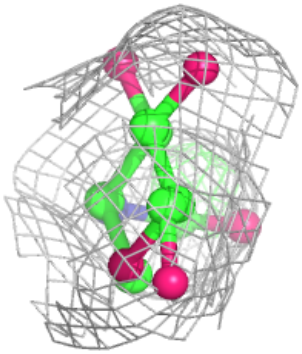


Electron density around NAG A 1202:

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

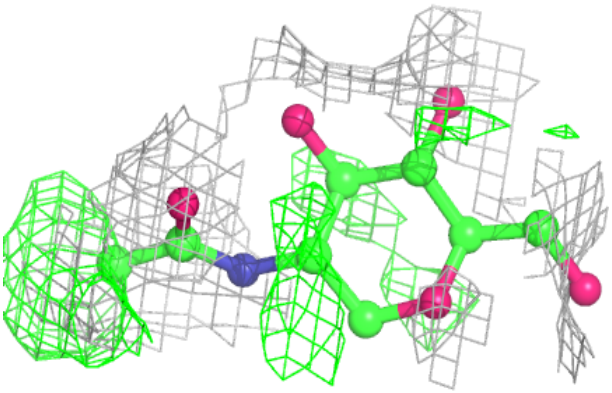


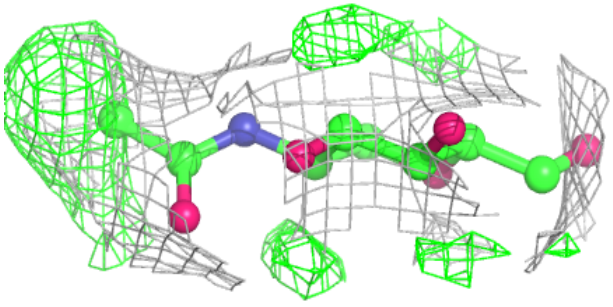


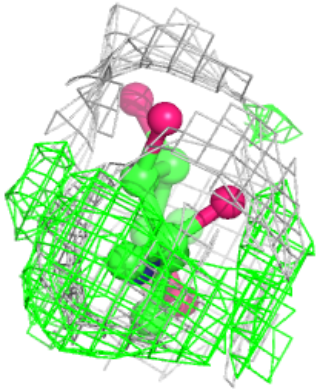


Electron density around NAG A 1206:

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

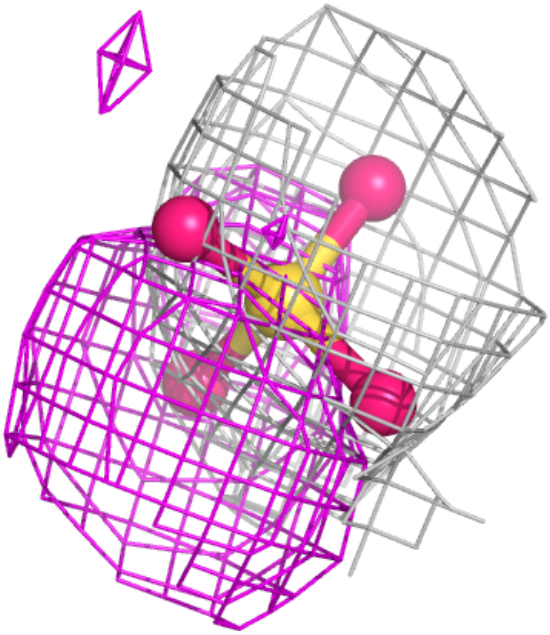


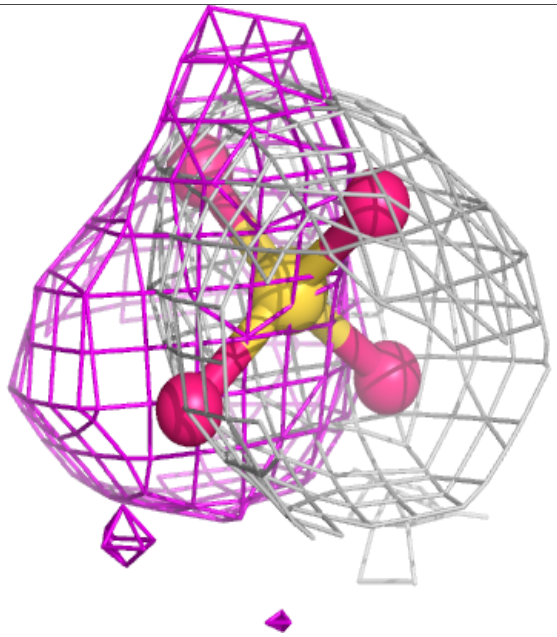


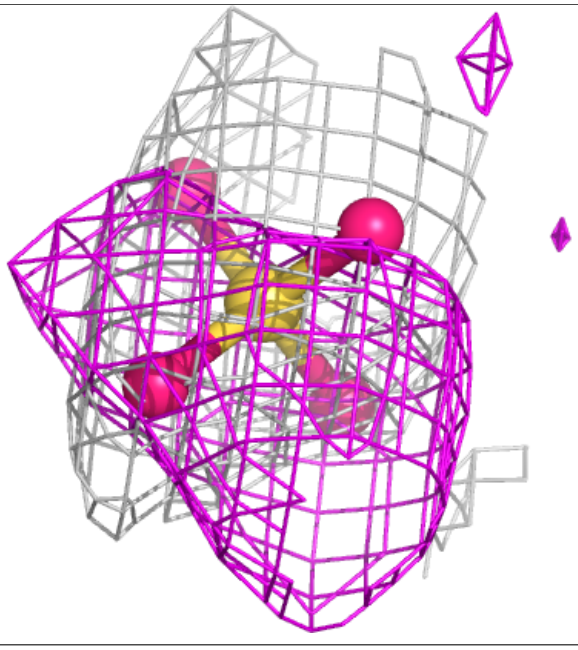


Electron density around SO4 A 1207:

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

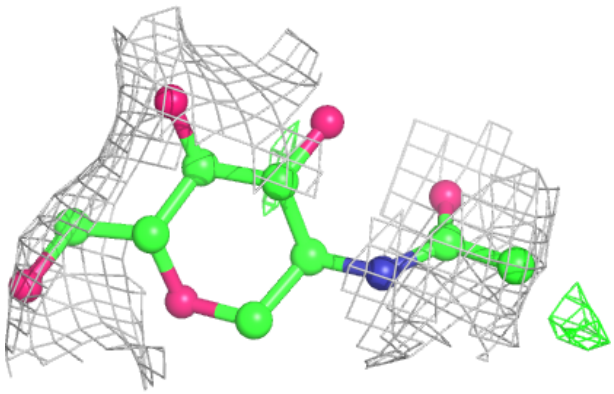


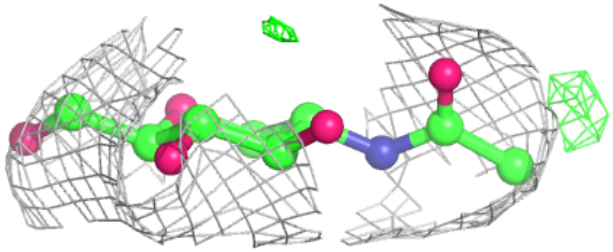


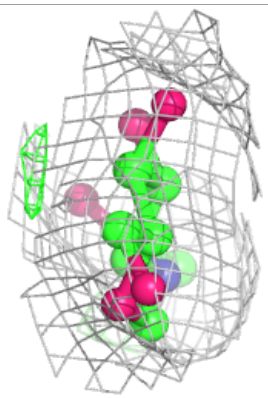


Electron density around NAG B 200:

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

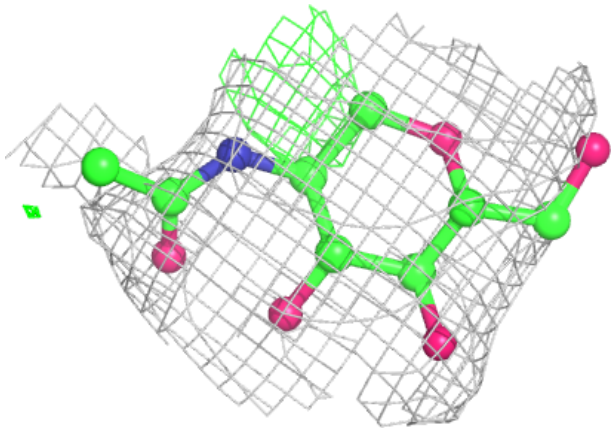


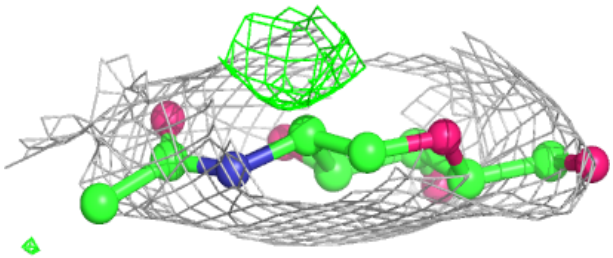


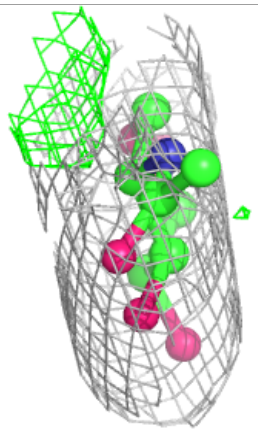


Electron density around NAG A 1204:

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

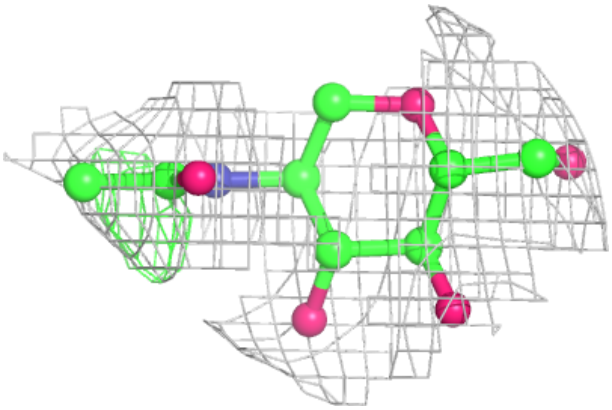


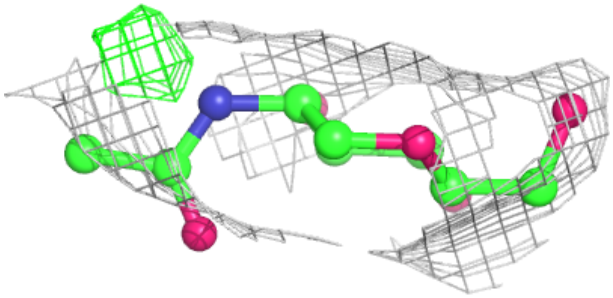


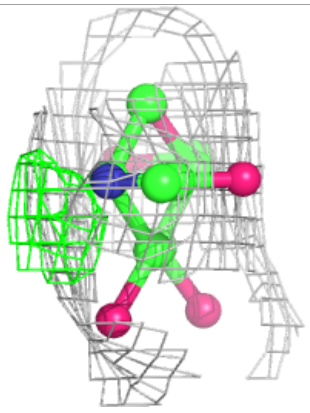


Electron density around NAG A 1203:

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

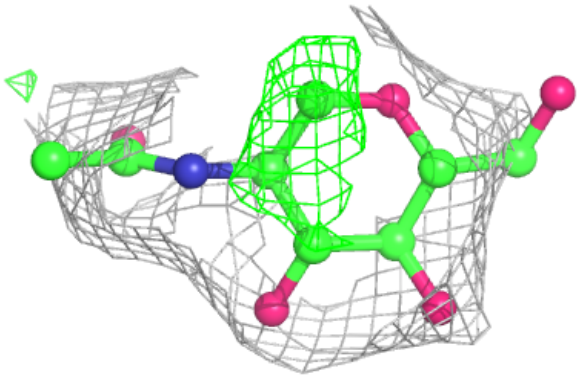


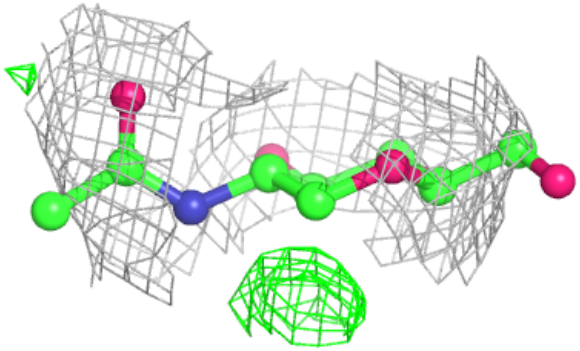


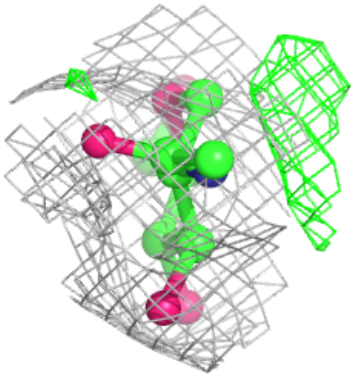


Electron density around NAG A 1205:

$2mF_o$-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.