Full wwPDB X-ray Structure Validation Report (i)

Nov 20, 2023 – 03:14 pm GMT

PDB ID	:	8P0L
Title	:	Crystal structure of human O-GlcNAcase in complex with an S-linked CKII peptide
Authors	:	Males, A.; Davies, G.J.; Calvelo, M.; Alteen, M.G.; Vocadlo, D.J.; Rovira, C.
Deposited on	:	2023-05-10
Resolution	:	2.50 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

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 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
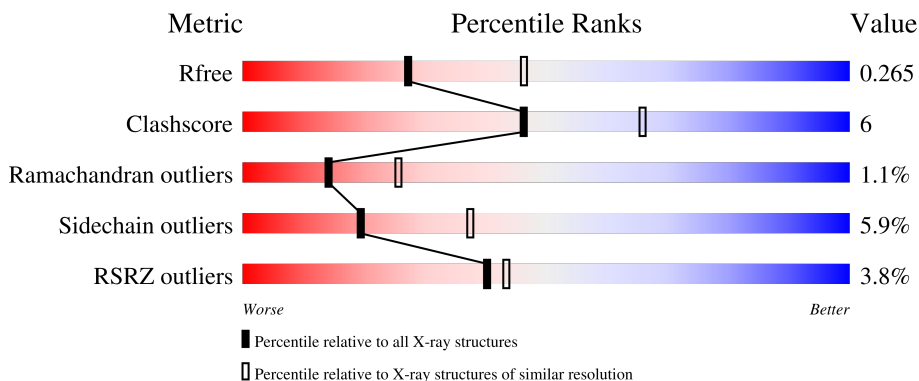
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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.

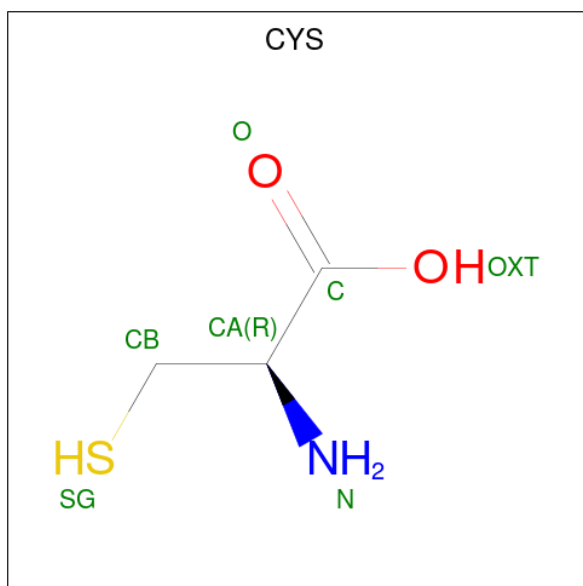| Mol	Chain	Length	Quality of chain
1	A	916	2% 38% 9% · 52%
1	B	916	% 42% 6% 51%

2   Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13774 atoms, of which 6774 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 Protein O-GlcNAcase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	443	Total	C	H	N	O	S	142	0	0
			6709	2220	3301	552	616	20			
1	B	453	Total	C	H	N	O	S	135	1	0
			6987	2308	3447	573	636	23			

- Molecule 2 is CYSTEINE (three-letter code: CYS) (formula: $C_3H_7NO_2S$).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	S	0	0
			13	3	7	1	1	1		

- Molecule 3 is SERINE (three-letter code: SER) (formula: $C_3H_7NO_3$).
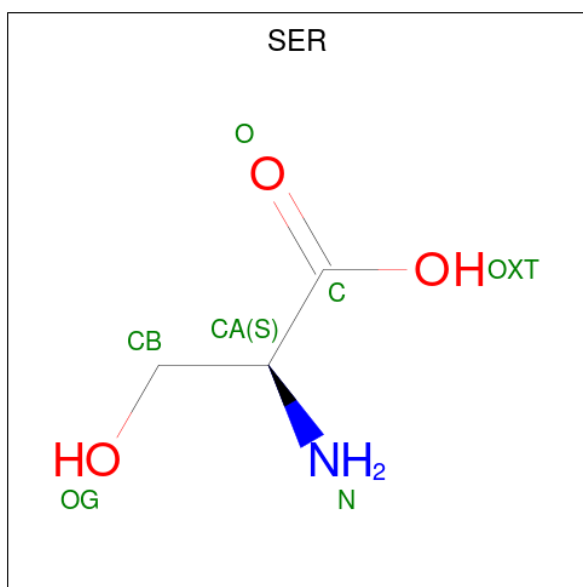
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total 11	C 3	H 5	N 1	O 2	1	0

- Molecule 4 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
4	B	1	Total 28	C 8	H 14	N 1	O 5	3	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	8	Total 8	O 8	0	0
5	B	18	Total 18	O 18	0	0

3 Residue-property plots ⓘ

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: Protein O-GlcNAcase

• Molecule 1: Protein O-GlcNAcase

%

Chain B:

42% 6% 51%

MET VAL GLN LYS GLU SER GLN GLN ALA THR LEU GLU GLU GLU ARG GLU SER GLU LEU SER SER ASN PRO ALA ALA SER ALA GLY ALA SER LEU GLU PRO PRO ALA ALA PRO ALA PRO GLY GLU ASP ASN PRO GLY ALA GLY GLY ALA VAL ALA GLY ALA ALA GLY GLY ALA ARG **R59**

M75 R83 A96 P97 D100 **Y101** K102 H103 S112 L122 Y135 A136 T144 N147 V151 S152 F169 A170 L171 H178 S189 S190 F191 A192 H193 E201 Y205 V247 W278 D285 R290 L291 F292 L293 P314 V323 T327 M336

V339 R340 LYS ASP VAL VAL MET THR ASP SER GLU SER THR VAL SER ILE GLN ILE LYS LEU GLU ASN GLU GLY SER GLU ASP ILE GLU SER LYS SER PRO ILE MET SER GLU THR ASP LYS GLY LEU ILE ALA ALA LEU SER GLU GLU PRO THR THR LEU THR LYS GLU GLU **D371** V372 GLU **H395** Q396 TYR SER SER ARG GLN VAL ALA HIS SER GLY ALA LYS ALA SER VAL ASP GLY THR PRO LEU VAL

ALA ALA PRO SER LEU ASN ALA THR THR VAL VAL THR VAL TYR GLN GLU PRO ILE MET SER GLN GLY ALA ALA LEU SER GLU GLU PRO THR THR LEU THR LYS GLU GLU MET SER MET GLU GLU CYS ILE SER ASP ILE ALA PRO MET ASP MET VAL GLU LYS GLN GLU GLU THR ASP HIS LYS

ASN ASP ASN GLN ILE LEU LEU SER GLU ILE VAL GLU ALA LYS MET ALA GLU GLU LEU LYS PRO MET ASP THR ASP LYS GLU SER ILE ALA GLU SER LYS SER PRO GLU MET SER MET GLU GLU ASP CYS ILE SER ASP ILE ALA PRO MET GLN THR ASP GLU GLN THR ASN LYS GLU **Q537**

P546 L547 Y548 T549 **L555** Q559 **F565 Y566 L567** P568 **E581** **S590** V591 V592 SER VAL ASN CYS LYS GLY LYS ASP SER SER GLU **K603** R608 S609 R610 S629 N630 R634 M640 K648 S649 S656 F657 V658 Q659 W660 C663 ARG SER HIS SER SER ALA GLN PHE

LEU ILE GLY ASP GLN **E677** P678 **F681** R682 **E688** L693 P694 I695 ASP GLY ALA ASN ASP SER LEU PHE PHE GLN PRO PRO **P707** **T711** S712 **Y715** THR ILE ARG PRO TYR PHE PRO LYS ASP GLU ALA SER VAL TYR LYS ILE CYS ARG GLU MET TYR ASP ASP GLY VAL GLY LEU

PRO PHE GLN SER GLN PRO ASP LEU ILE GLY ASP LYS LEU VAL GLY LEU LEU SER LEU ASP SER LEU ASP TYR CYS PHE VAL LEU GLU ASP GLU GLY THR GLU PHE LEU ALA ASN ASP SER VAL THR PRO PHE ILE LYS LYS CYS LYS ILE SER TRP ILE PRO PHE MET GLN

GLU LYS TYR THR LYS PRO ASN GLY ASP LYS GLU LEU SER GLU ALA GLU LYS ILE MET LEU SER PHE HIS GLU GLU GLN GLU VAL LEU PRO GLU THR PHE LEU ALA ASN PHE PRO SER LEU ILE LYS MET ASP ILE HIS LYS VAL THR VAL THR ASP PRO SER VAL ALA LYS SER MET MET ALA

CYS LEU LEU SER LEU LYS ALA ASN GLY SER ARG GLY ALA PHE CYS GLU VAL ARG PRO ASP ASP LYS ARG ILE LEU GLU PHE TYR SER LYS LEU GLY CYS PHE GLU ILE ALA LYS MET GLU GLY PHE PRO LYS ASP VAL VAL ILE LEU ARG SER LEU

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	101.50Å 101.50Å 284.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.78 – 2.50 95.60 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (95.78-2.50) 100.0 (95.60-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.216 , 0.271 0.219 , 0.265	Depositor DCC
R_{free} test set	1571 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å^2)	61.5	Xtriage
Anisotropy	0.643	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.1	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	13774	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.39	0/3501	0.73	2/4773 (0.0%)
1	B	0.42	0/3640	0.75	0/4955
All	All	0.41	0/7141	0.74	2/9728 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	4
All	All	0	8

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	142	ASP	CB-CA-C	-6.63	97.14	110.40
1	A	104	ARG	NE-CZ-NH1	-5.22	117.69	120.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	ARG	Sidechain
1	A	273	ARG	Sidechain
1	A	299	ARG	Sidechain
1	A	83	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	608	ARG	Sidechain
1	B	610	ARG	Sidechain
1	B	682	ARG	Sidechain
1	B	712	SER	Peptide

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	A	3408	3301	3187	54	0
1	B	3540	3447	3351	36	0
2	B	6	7	3	1	0
3	B	6	5	5	0	0
4	B	14	14	13	2	0
5	A	8	0	0	0	0
5	B	18	0	0	1	0
All	All	7000	6774	6559	85	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 6.

All (85) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ARG:HH22	1:A:142:ASP:HB2	1.26	1.00
2:B:1001:CYS:SG	4:B:1003:NAG:O6	2.42	0.77
1:B:285:ASP:OD1	4:B:1003:NAG:H61	1.88	0.73
1:A:108:ARG:HH22	1:A:142:ASP:CB	2.01	0.71
1:A:273:ARG:HG2	1:A:273:ARG:HH11	1.59	0.67
1:A:296:TYR:CE2	1:A:299:ARG:HG3	2.31	0.65
1:A:204:GLN:O	1:A:207:GLY:N	2.26	0.65
1:A:105:MET:CE	1:B:630:ASN:OD1	2.45	0.64
1:B:555:LEU:O	1:B:559:GLN:HG3	1.97	0.64
1:A:193:HIS:CD2	1:A:236:THR:HG21	2.33	0.63
1:A:105:MET:HE2	1:B:630:ASN:OD1	1.97	0.63
1:B:339:VAL:O	1:B:340:ARG:HB3	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:MET:SD	1:B:122:LEU:HD22	2.41	0.60
1:B:290:ARG:HD2	5:B:1116:HOH:O	2.01	0.59
1:A:544:GLU:HG2	1:B:144:THR:HG21	1.87	0.57
1:B:339:VAL:O	1:B:340:ARG:CB	2.52	0.57
1:A:108:ARG:NH2	1:A:142:ASP:HB2	2.10	0.56
1:A:296:TYR:CZ	1:A:299:ARG:HG3	2.41	0.56
1:A:684:GLY:CA	1:B:290:ARG:HD3	2.35	0.56
1:A:103:HIS:O	1:A:103:HIS:CG	2.59	0.56
1:A:625:PHE:HD1	1:A:644:VAL:HG12	1.70	0.55
1:A:60:PHE:CD2	1:A:332:TYR:CE1	2.94	0.55
1:B:97:PRO:HB2	1:B:100:ASP:HB2	1.87	0.55
1:A:654:VAL:HG22	1:B:693:LEU:HD21	1.89	0.54
1:B:101:TYR:CZ	1:B:102:LYS:HE3	2.42	0.54
1:A:220:CYS:HB3	1:A:250:THR:OG1	2.08	0.54
1:B:147:ASN:OD1	1:B:147:ASN:C	2.47	0.53
1:B:190:SER:OG	1:B:193:HIS:CD2	2.62	0.53
1:A:320:ALA:HB2	1:A:640:MET:CE	2.39	0.52
1:B:395:HIS:CD2	1:B:634:ARG:HB2	2.44	0.52
1:A:190:SER:O	1:A:193:HIS:N	2.42	0.51
1:A:320:ALA:CB	1:A:640:MET:HE1	2.40	0.51
1:A:271:ILE:O	1:A:273:ARG:NH1	2.45	0.50
1:B:581:GLU:OE2	1:B:610:ARG:NH1	2.44	0.50
1:A:685:LEU:O	1:A:686:ALA:C	2.49	0.50
1:B:323:VAL:O	1:B:327:THR:HG23	2.12	0.49
1:B:372:VAL:HG22	1:B:372:VAL:O	2.13	0.49
1:A:314:PRO:HG2	1:A:321:ASN:ND2	2.28	0.49
1:A:80:GLU:O	1:A:80:GLU:HG3	2.13	0.48
1:B:293:LEU:O	1:B:323:VAL:HG11	2.13	0.48
1:A:60:PHE:CE1	1:A:309:GLY:HA2	2.49	0.48
1:A:248:LEU:HA	1:A:276:VAL:O	2.13	0.48
1:A:143:ILE:HG23	1:A:143:ILE:O	2.13	0.47
1:B:581:GLU:OE1	1:B:610:ARG:HD2	2.13	0.47
1:A:162:SER:HB3	1:A:169:PHE:HZ	1.78	0.47
1:A:555:LEU:O	1:A:559:GLN:HB2	2.14	0.47
1:A:567:LEU:HB3	1:A:568:PRO:HD2	1.97	0.47
1:A:381:LYS:O	1:A:385:THR:HG23	2.16	0.46
1:A:300:SER:O	1:A:303:LEU:HB2	2.15	0.46
1:A:625:PHE:HD1	1:A:644:VAL:CG1	2.28	0.46
1:A:220:CYS:SG	1:A:223:PHE:CD1	3.08	0.46
1:A:259:ILE:O	1:A:303:LEU:HD21	2.16	0.46
1:A:105:MET:HE3	1:B:630:ASN:OD1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:648:LYS:HG3	1:B:649:SER:N	2.31	0.45
1:B:590:SER:O	1:B:592:VAL:N	2.49	0.45
1:A:86:GLN:HG3	1:A:129:TYR:O	2.17	0.45
1:B:103:HIS:HD2	1:B:136:ALA:O	1.99	0.44
1:A:171:LEU:HD12	1:A:199:THR:HA	1.98	0.44
1:A:304:ILE:HB	1:A:305:PRO:HD3	2.00	0.44
1:A:688:GLU:HG3	1:A:691:ARG:HH12	1.83	0.44
1:B:135:TYR:O	1:B:169:PHE:HA	2.18	0.44
1:A:320:ALA:HB2	1:A:640:MET:HE1	1.98	0.44
1:B:178:HIS:HA	1:B:191:PHE:CE2	2.52	0.44
1:B:205:TYR:CD1	1:B:205:TYR:C	2.91	0.44
1:A:581:GLU:OE2	1:A:610:ARG:HD2	2.19	0.43
1:A:102:LYS:HE2	1:A:109:GLU:HB3	2.00	0.43
1:B:103:HIS:CD2	1:B:136:ALA:O	2.72	0.43
1:A:591:VAL:HG12	1:A:591:VAL:O	2.18	0.43
1:A:60:PHE:CZ	1:A:309:GLY:HA2	2.54	0.43
1:A:96:ALA:N	1:A:97:PRO:CD	2.82	0.42
1:A:333:LYS:O	1:A:334:SER:C	2.57	0.42
1:B:293:LEU:HD11	1:B:640:MET:CE	2.49	0.42
1:B:567:LEU:HB3	1:B:568:PRO:HD2	2.00	0.42
1:B:293:LEU:HD11	1:B:640:MET:HE1	2.02	0.42
1:A:260:PRO:O	1:A:263:SER:OG	2.32	0.42
1:A:204:GLN:O	1:A:205:TYR:C	2.58	0.42
1:A:303:LEU:HD13	1:A:303:LEU:HA	1.94	0.41
1:B:190:SER:OG	1:B:193:HIS:HD2	2.03	0.41
1:A:385:THR:HG22	1:A:555:LEU:HD22	2.02	0.41
1:A:192:ALA:HB2	1:A:233:TYR:CD2	2.55	0.41
1:B:96:ALA:N	1:B:97:PRO:HD3	2.34	0.41
1:A:286:TYR:CD1	1:A:286:TYR:C	2.94	0.41
1:B:291:LEU:O	1:B:565:PHE:HB3	2.21	0.41
1:A:148:PRO:HA	1:A:151:VAL:HB	2.03	0.40
1:B:151:VAL:HG11	1:B:201:GLU:OE2	2.22	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	433/916 (47%)	396 (92%)	31 (7%)	6 (1%)	11	20
1	B	442/916 (48%)	414 (94%)	24 (5%)	4 (1%)	17	31
All	All	875/1832 (48%)	810 (93%)	55 (6%)	10 (1%)	14	26

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	395	HIS
1	B	591	VAL
1	A	205	TYR
1	A	394	PRO
1	A	104	ARG
1	A	239	GLU
1	B	112	SER
1	A	314	PRO
1	A	376	PRO
1	B	314	PRO

5.3.2 Protein sidechains ⓘ

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	340/797 (43%)	316 (93%)	24 (7%)	14	28
1	B	359/797 (45%)	342 (95%)	17 (5%)	26	49
All	All	699/1594 (44%)	658 (94%)	41 (6%)	19	37

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ARG
1	A	86	GLN

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Mol	Chain	Res	Type
1	A	100	ASP
1	A	101	TYR
1	A	142	ASP
1	A	176	ILE
1	A	177	ASP
1	A	208	GLU
1	A	273	ARG
1	A	288	GLN
1	A	299	ARG
1	A	301	THR
1	A	303	LEU
1	A	312	THR
1	A	375	SER
1	A	376	PRO
1	A	393	VAL
1	A	543	ASN
1	A	552	PRO
1	A	609	SER
1	A	634	ARG
1	A	648	LYS
1	A	656	SER
1	A	688	GLU
1	B	83	ARG
1	B	101	TYR
1	B	152	SER
1	B	171	LEU
1	B	189	SER
1	B	247	VAL
1	B	278	TRP
1	B	336	MET
1	B	340	ARG
1	B	372	VAL
1	B	395	HIS
1	B	549	THR
1	B	629	SER
1	B	656	SER
1	B	688	GLU
1	B	695	ILE
1	B	711	THR

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

Mol	Chain	Res	Type
1	A	86	GLN
1	A	103	HIS
1	A	193	HIS
1	A	204	GLN
1	A	288	GLN
1	A	326	HIS
1	A	335	ASN
1	A	583	GLN
1	A	630	ASN
1	B	103	HIS
1	B	163	GLN
1	B	193	HIS
1	B	395	HIS
1	B	583	GLN
1	B	659	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z|$ > 2	Counts	RMSZ	#$|Z|$ > 2
2	CYS	B	1001	4,3	4,5,6	0.83	0	1,5,7	0.40	0
3	SER	B	1002	2	4,5,6	0.89	0	0,5,7	-	-
4	NAG	B	1003	2	14,14,15	0.69	0	17,19,21	1.43	2 (11%)

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
2	CYS	B	1001	4,3	-	1/1/4/6	-
3	SER	B	1002	2	-	0/2/4/6	-
4	NAG	B	1003	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1003	NAG	C1-C2-N2	4.09	117.47	110.49
4	B	1003	NAG	C1-O5-C5	2.55	115.65	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1001	CYS	N-CA-CB-SG
4	B	1003	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	CYS	1	0
4	B	1003	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 B 1003

Bond lengths

Bond angles

Torsions

Rings
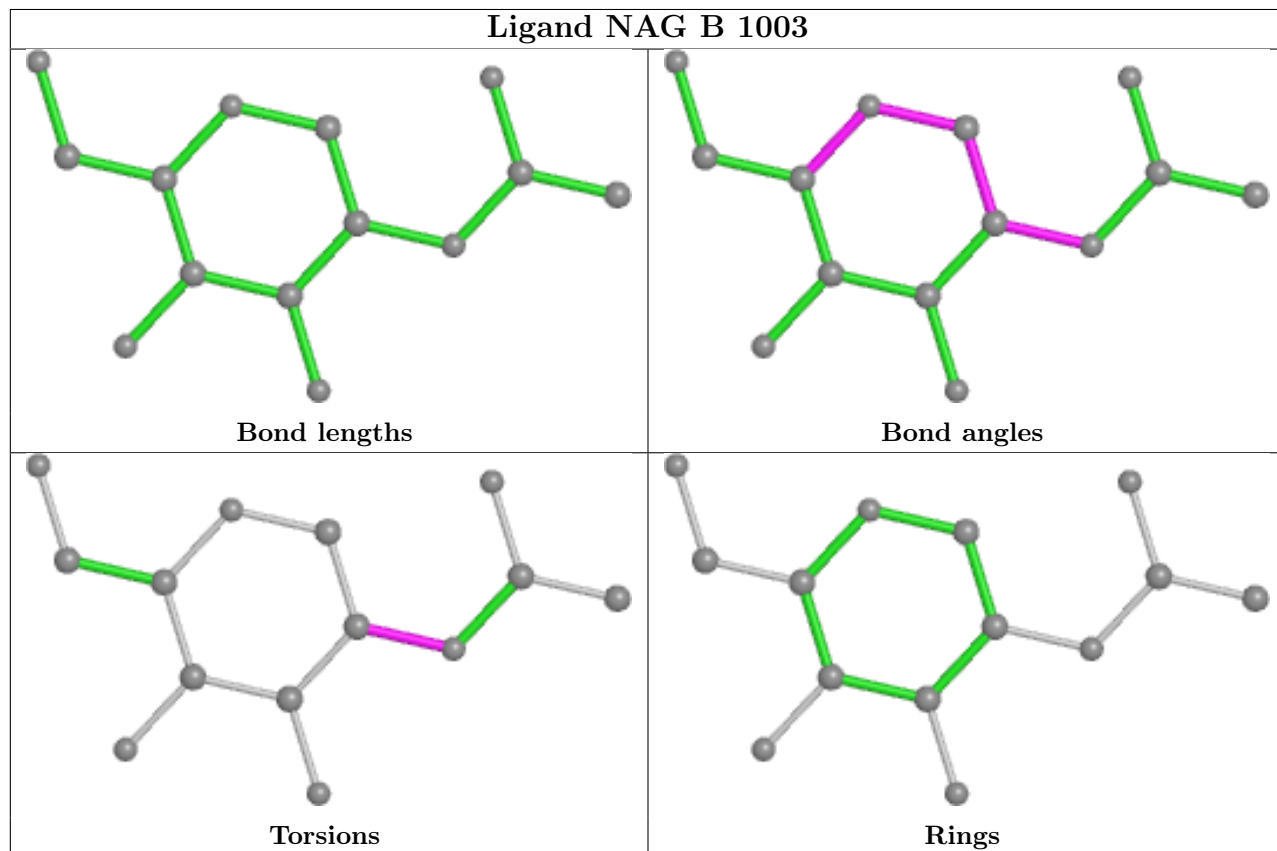
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å²)	Q<0.9
1	A	443/916 (48%)	0.47	22 (4%)	28	30	46, 76, 123, 163	0
1	B	453/916 (49%)	0.40	12 (2%)	56	59	42, 65, 114, 175	0
All	All	896/1832 (48%)	0.44	34 (3%)	40	43	42, 71, 119, 175	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	711	THR	8.6
1	B	537	GLN	5.9
1	A	660	TRP	4.1
1	B	694	PRO	3.5
1	A	538	PHE	3.2
1	A	611	ALA	3.2
1	B	548	TYR	3.0
1	B	660	TRP	3.0
1	A	325	ILE	3.0
1	A	591	VAL	2.8
1	A	607	TRP	2.8
1	A	604	ILE	2.8
1	A	223	PHE	2.7
1	A	657	PHE	2.6
1	B	678	PRO	2.6
1	B	547	LEU	2.5
1	A	608	ARG	2.5
1	B	681	PHE	2.5
1	A	372	VAL	2.4
1	A	621	VAL	2.4
1	A	650	ILE	2.4
1	A	620	LEU	2.3
1	B	715	TYR	2.3
1	B	608	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	658	VAL	2.2
1	A	281	ILE	2.2
1	A	647	ILE	2.2
1	A	645	TRP	2.2
1	A	254	VAL	2.1
1	A	540	PRO	2.1
1	A	188	PHE	2.1
1	B	658	VAL	2.1
1	A	539	VAL	2.0
1	B	546	PRO	2.0

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

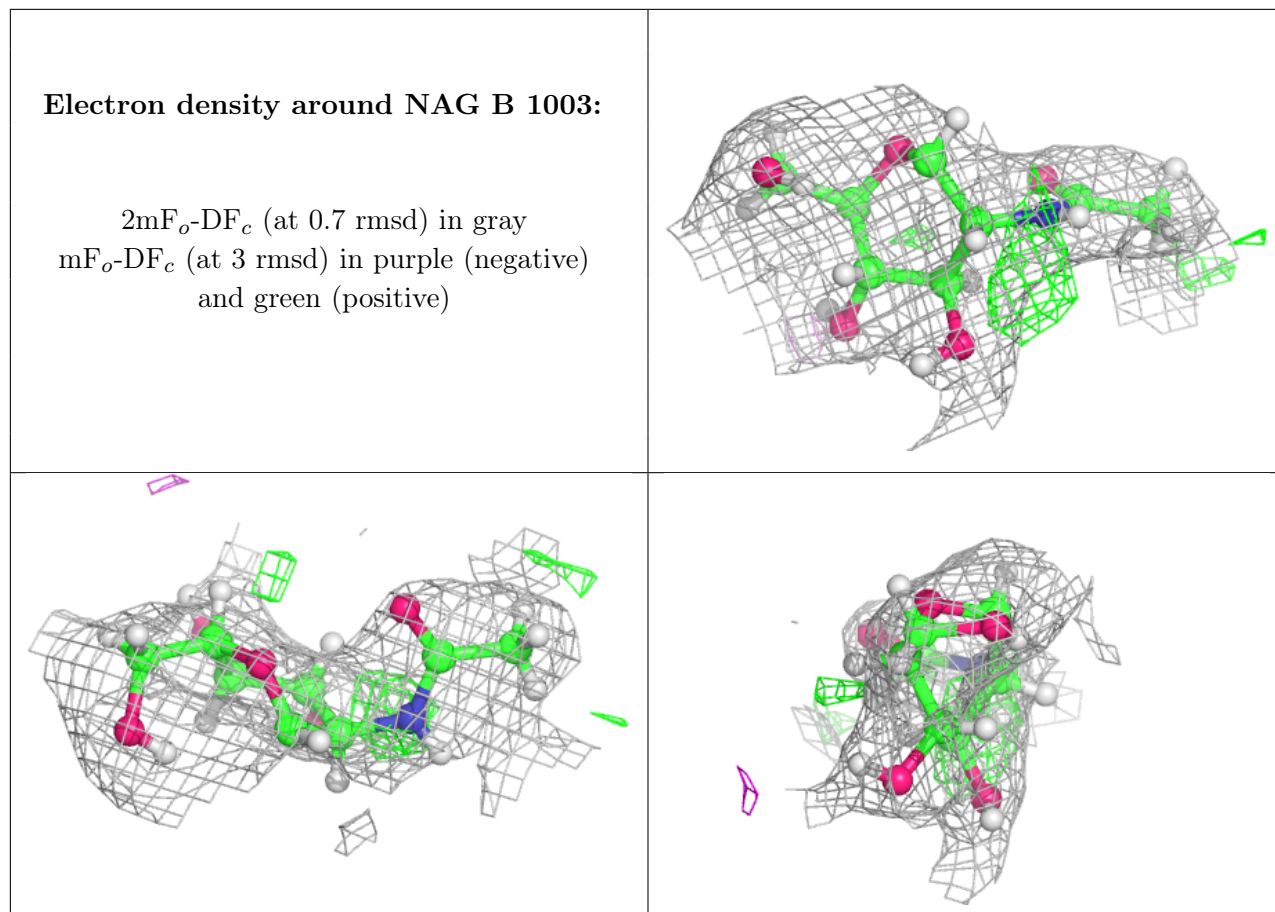There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
3	SER	B	1002	6/7	0.57	0.34	69,80,97,102	11
2	CYS	B	1001	6/7	0.62	0.37	69,82,91,95	13
4	NAG	B	1003	14/15	0.90	0.25	27,39,48,50	20

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 1003:

$2mF_o$-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 ⓘ

There are no such residues in this entry.