



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 07:04 PM UTC

PDB ID : 8P0L / pdb_00008p0l
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)

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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

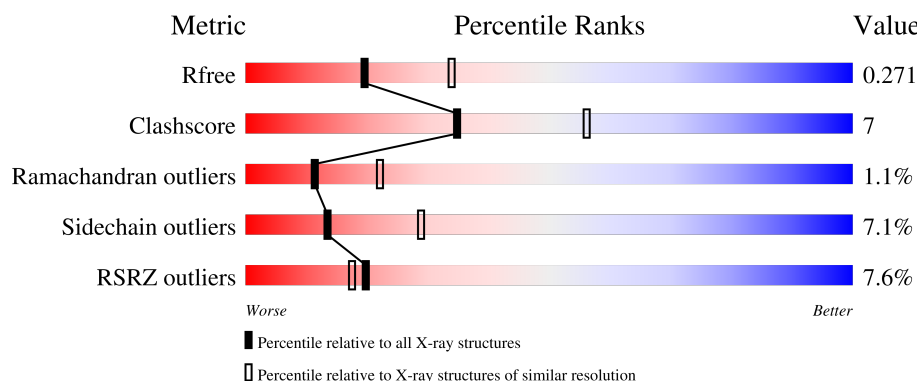
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 $\leq 5\%$. 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	4% 36% 10% • 52%
1	B	916	3% 41% 8% 51%

2 Entry composition [i](#)

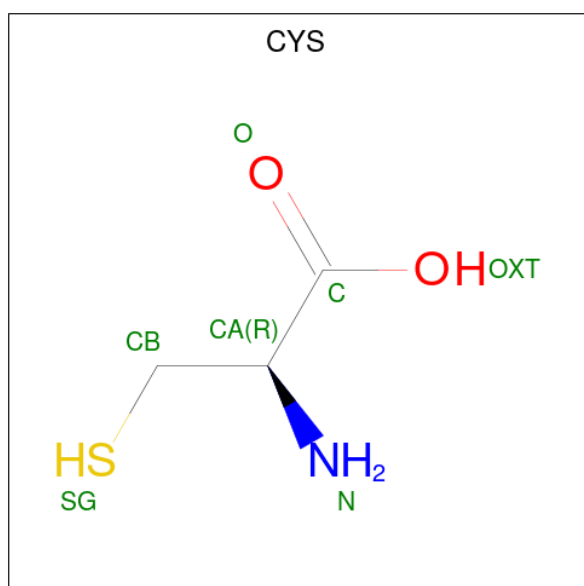
There are 5 unique types of molecules in this entry. The entry contains 13774 atoms, of which 6774 are hydrogens and 0 are deuteriums.

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.

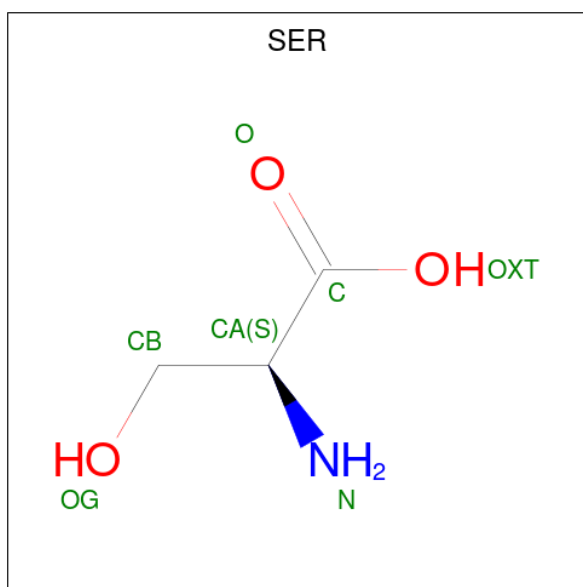
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	443	6709	2220	3301	552	616	20	142	0	0
1	B	453	6987	2308	3447	573	636	23	135	1	0

- Molecule 2 is CYSTEINE (CCD ID: CYS) (formula: $C_3H_7NO_2S$).



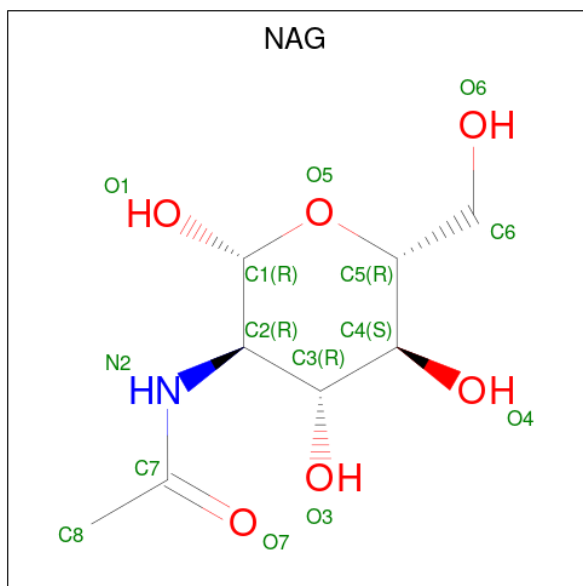
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
2	B	1	13	3	7	1	1	1	0	0

- Molecule 3 is SERINE (CCD ID: SER) (formula: $C_3H_7NO_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	H	N	O	1	0
			11	3	5	1	2		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).

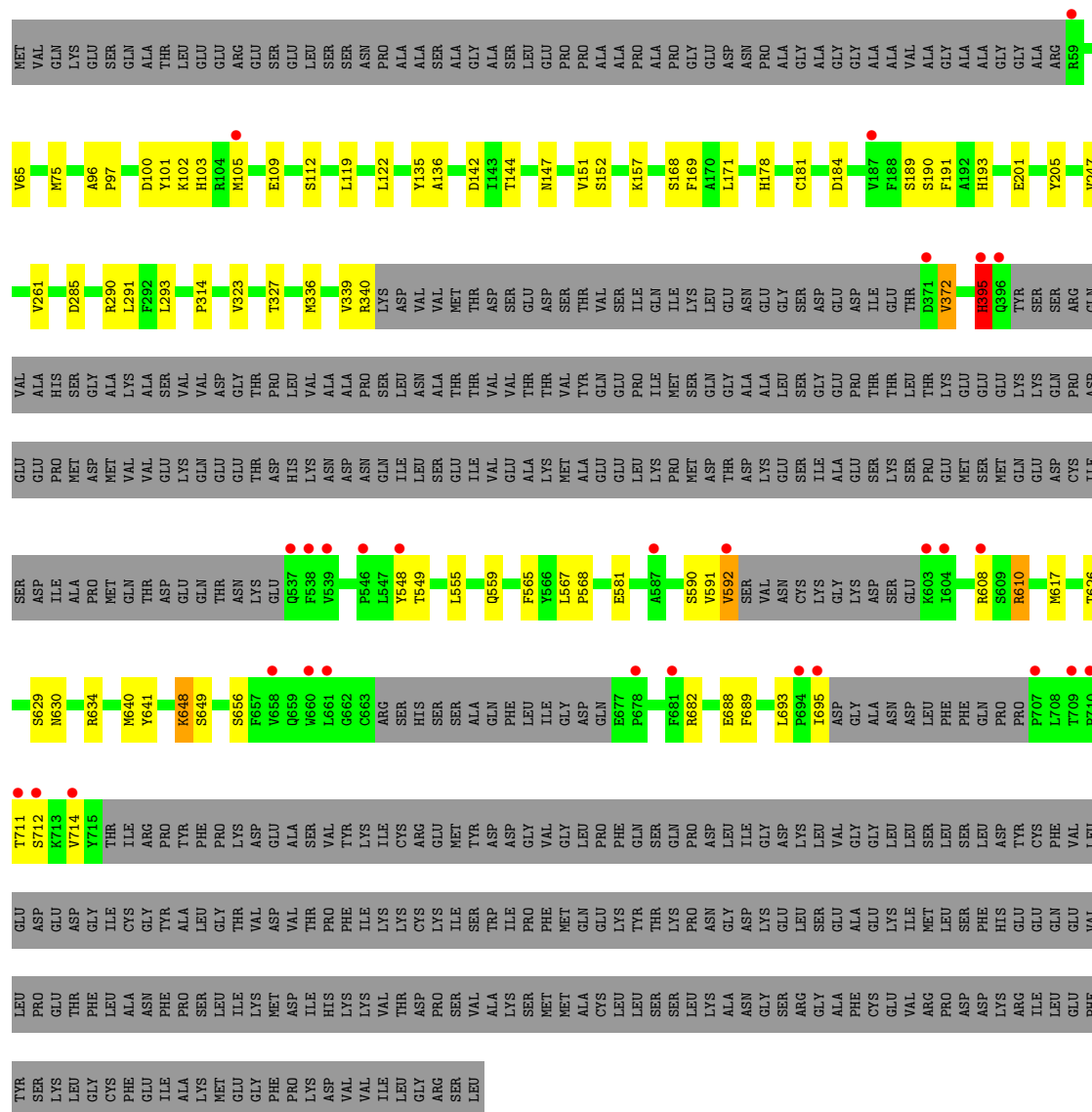
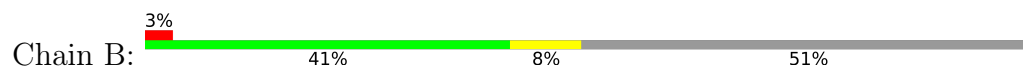


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	3	0
			28	8	14	1	5		

- 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

- Molecule 1: Protein O-GlcNAcase



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
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.216 , 0.271 0.216 , 0.271	Depositor DCC
R_{free} test set	1571 reflections (2.42%)	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)	0.39 , 68.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.58	0/3501	1.06	4/4773 (0.1%)
1	B	0.60	0/3640	1.10	1/4955 (0.0%)
All	All	0.59	0/7141	1.08	5/9728 (0.1%)

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 (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	ASP	CB-CA-C	-7.68	97.14	109.13
1	A	142	ASP	CA-CB-CG	7.04	119.64	112.60
1	A	177	ASP	CB-CA-C	6.25	120.10	109.53
1	A	177	ASP	CA-CB-CG	5.41	118.01	112.60
1	B	142	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	273	ARG	Sidechain
1	A	299	ARG	Sidechain
1	A	83	ARG	Sidechain
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 [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	3408	3301	3187	65	0
1	B	3540	3447	3351	45	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	101	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 7.

All (101) 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:105:MET:HE3	1:B:630:ASN:OD1	1.91	0.70
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:MET:HE2	1:A:191:PHE:N	2.13	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:651:MET:HE1	1:B:689:PHE:CE1	2.34	0.63
1:A:630:ASN:ND2	1:B:105:MET:HE3	2.14	0.62
1:B:75:MET:SD	1:B:122:LEU:HD22	2.41	0.60
1:B:339:VAL:O	1:B:340:ARG:HB3	2.00	0.60
1:B:290:ARG:HD2	5:B:1116:HOH:O	2.01	0.59
1:B:147:ASN:OD1	1:B:147:ASN:C	2.47	0.58
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:651:MET:HE1	1:B:689:PHE:CZ	2.40	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:291:LEU:HD21	1:A:640:MET:HE1	1.87	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:685:LEU:O	1:A:686:ALA:C	2.49	0.54
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: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: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:B:323:VAL:O	1:B:327:THR:HG23	2.12	0.49
1:B:109:GLU:O	1:B:157:LYS:NZ	2.44	0.49
1:B:372:VAL:HG22	1:B:372:VAL:O	2.13	0.49
1:A:105:MET:HE1	1:B:548:TYR:HE2	1.77	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:205:TYR:C	1:B:205:TYR:CD1	2.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:581:GLU:OE1	1:B:610:ARG:HD2	2.13	0.47
1:A:333:LYS:O	1:A:334:SER:C	2.57	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:204:GLN:O	1:A:205:TYR:C	2.58	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:B:293:LEU:HD11	1:B:640:MET:HE1	1.98	0.46
1:A:286:TYR:CD1	1:A:286:TYR:C	2.94	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:320:ALA:CB	1:A:640:MET:HE1	2.47	0.45
1:B:291:LEU:HD21	1:B:640:MET:HE3	1.97	0.45
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:640:MET:O	1:B:641:TYR:C	2.59	0.44
1:A:190:SER:O	1:A:191:PHE:C	2.60	0.44
1:A:209:PRO:O	1:A:210:GLU:C	2.60	0.44
1:B:103:HIS:HD2	1:B:136:ALA:O	1.99	0.44
1:A:66:GLU:O	1:A:96:ALA:C	2.60	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:B:178:HIS:HA	1:B:191:PHE:CE2	2.52	0.44
1:A:581:GLU:OE2	1:A:610:ARG:HD2	2.19	0.43
1:A:105:MET:HE1	1:B:548:TYR:CE2	2.53	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:693:LEU:O	1:A:694:PRO:C	2.61	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: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:A:260:PRO:O	1:A:263:SER:OG	2.32	0.42
1:A:303:LEU:HD13	1:A:303:LEU:HA	1.94	0.41
1:A:100:ASP:O	1:A:101:TYR:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:168:SER:C	1:B:169:PHE:CD1	2.99	0.41
1:B:291:LEU:O	1:B:565:PHE:HB3	2.21	0.41
1:B:181:CYS:SG	1:B:184:ASP:OD2	2.79	0.40
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
1:A:284:ASN:OD1	1:A:284:ASN:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	9	17
1	B	442/916 (48%)	414 (94%)	24 (5%)	4 (1%)	14	27
All	All	875/1832 (48%)	810 (93%)	55 (6%)	10 (1%)	11	22

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

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Mol	Chain	Res	Type
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%)	311 (92%)	29 (8%)	10	22
1	B	359/797 (45%)	338 (94%)	21 (6%)	18	38
All	All	699/1594 (44%)	649 (93%)	50 (7%)	13	28

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	A	100	ASP
1	A	142	ASP
1	A	176	ILE
1	A	177	ASP
1	A	208	GLU
1	A	222	THR
1	A	230	GLN
1	A	258	GLU
1	A	288	GLN
1	A	299	ARG
1	A	301	THR
1	A	303	LEU
1	A	312	THR
1	A	339	VAL
1	A	376	PRO
1	A	393	VAL
1	A	543	ASN
1	A	547	LEU
1	A	552	PRO
1	A	585	LEU

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Mol	Chain	Res	Type
1	A	609	SER
1	A	624	MET
1	A	644	VAL
1	A	648	LYS
1	A	650	ILE
1	A	655	LYS
1	A	656	SER
1	A	688	GLU
1	B	65	VAL
1	B	119	LEU
1	B	152	SER
1	B	171	LEU
1	B	189	SER
1	B	247	VAL
1	B	261	VAL
1	B	336	MET
1	B	372	VAL
1	B	395	HIS
1	B	549	THR
1	B	592	VAL
1	B	617	MET
1	B	626	THR
1	B	629	SER
1	B	648	LYS
1	B	656	SER
1	B	688	GLU
1	B	695	ILE
1	B	711	THR
1	B	714	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

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

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Mol	Chain	Res	Type
1	B	193	HIS
1	B	313	ASN
1	B	337	ASN
1	B	395	HIS
1	B	559	GLN
1	B	583	GLN
1	B	659	GLN

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](#)

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	3,4	4,5,6	0.87	0	1,5,7	0.42	0
4	NAG	B	1003	2	14,14,15	0.72	0	17,19,21	1.51	3 (17%)
3	SER	B	1002	2	4,5,6	0.93	0	1,5,7	0.06	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
2	CYS	B	1001	3,4	-	1/1/4/6	-
4	NAG	B	1003	2	-	1/6/23/26	0/1/1/1
3	SER	B	1002	2	-	0/2/4/6	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1003	NAG	C1-C2-N2	4.47	117.47	110.43
4	B	1003	NAG	C1-O5-C5	2.59	115.65	112.19
4	B	1003	NAG	C2-N2-C7	2.10	125.72	122.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

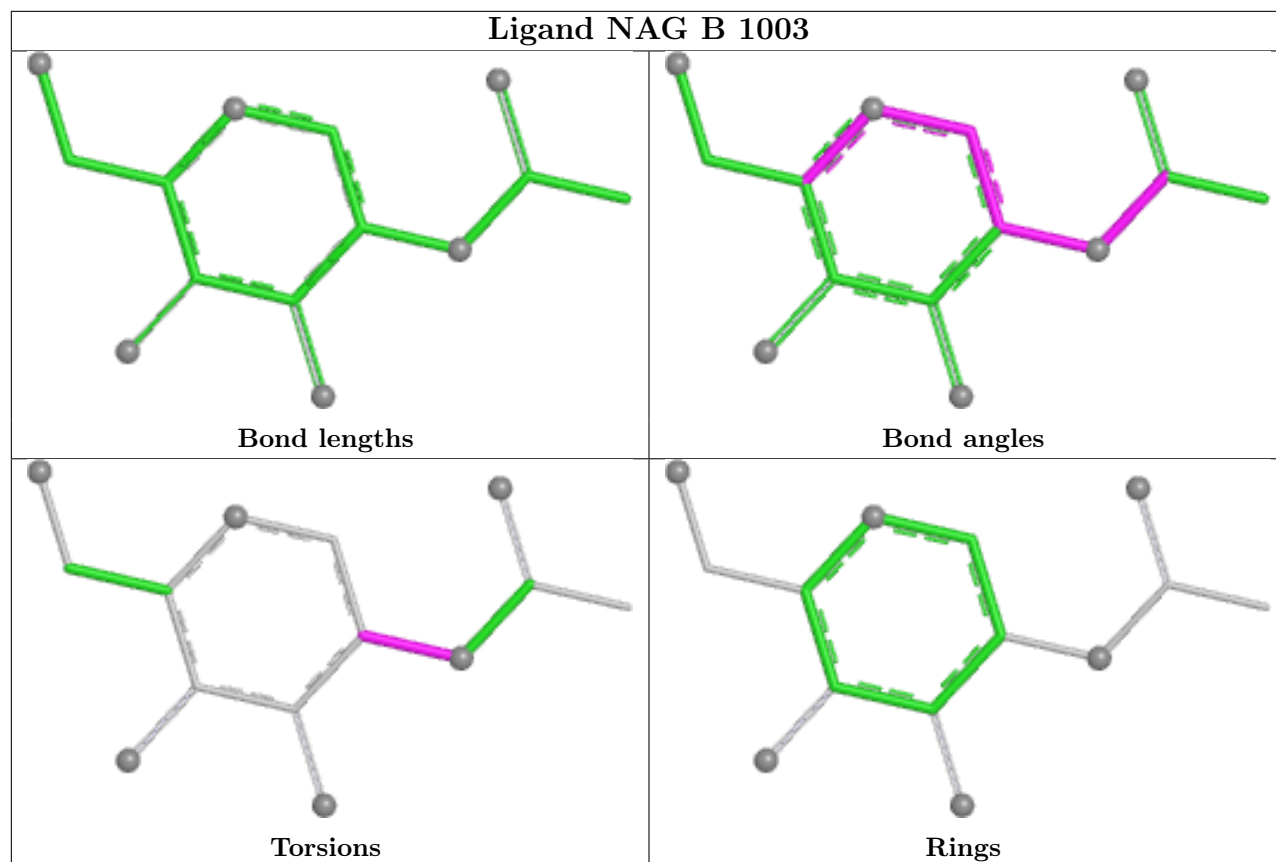
Mol	Chain	Res	Type	Atoms
2	B	1001	CYS	N-CA-CB-SG
4	B	1003	NAG	C3-C2-N2-C7

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 than 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.



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

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(Å ²)	Q<0.9
1	A	443/916 (48%)	0.56	39 (8%)	15 14	44, 74, 116, 146	0
1	B	453/916 (49%)	0.19	29 (6%)	25 22	38, 63, 111, 159	1 (0%)
All	All	896/1832 (48%)	0.37	68 (7%)	20 17	38, 69, 115, 159	1 (0%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	711	THR	6.6
1	A	601	SER	5.3
1	B	538	PHE	5.3
1	B	603	LYS	5.2
1	A	59	ARG	4.9
1	A	677	GLU	4.8
1	A	679	TRP	4.8
1	B	592	VAL	4.8
1	A	537	GLN	4.6
1	B	604	ILE	4.5
1	A	603	LYS	4.4
1	B	395	HIS	4.3
1	A	339	VAL	4.3
1	B	695	ILE	4.3
1	B	707	PRO	4.2
1	A	372	VAL	4.1
1	A	337	ASN	4.0
1	A	602	GLU	3.9
1	A	660	TRP	3.9
1	B	537	GLN	3.8
1	A	611	ALA	3.7
1	B	710	PRO	3.6
1	B	396	GLN	3.6
1	A	225	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	660	TRP	3.3
1	B	681	PHE	3.2
1	A	605	GLU	3.2
1	A	678	PRO	3.2
1	A	620	LEU	3.2
1	B	694	PRO	3.2
1	B	105	MET	3.1
1	B	59	ARG	2.9
1	B	678	PRO	2.9
1	A	547	LEU	2.9
1	B	548	TYR	2.9
1	A	262	GLU	2.9
1	A	593	SER	2.9
1	B	187	VAL	2.8
1	A	395	HIS	2.8
1	A	324	ALA	2.8
1	A	661	LEU	2.7
1	A	607	TRP	2.7
1	A	377	GLN	2.7
1	B	608	ARG	2.7
1	A	223	PHE	2.7
1	A	538	PHE	2.7
1	B	539	VAL	2.6
1	A	548	TYR	2.6
1	A	294	GLY	2.6
1	B	709	THR	2.5
1	A	584	TRP	2.5
1	B	712	SER	2.5
1	B	546	PRO	2.4
1	B	371	ASP	2.4
1	A	373	LEU	2.4
1	B	658	VAL	2.4
1	B	587	ALA	2.4
1	A	591	VAL	2.3
1	A	302	GLU	2.3
1	A	663	CYS	2.3
1	A	662	GLY	2.3
1	A	393	VAL	2.2
1	B	714	VAL	2.2
1	A	542	PRO	2.2
1	A	150	GLU	2.1
1	A	178	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	661	LEU	2.0
1	A	261	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

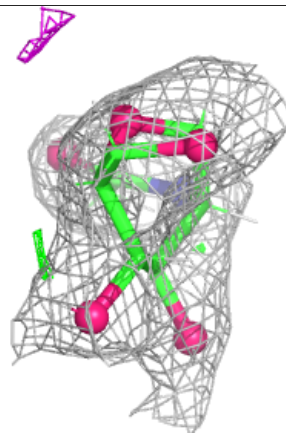
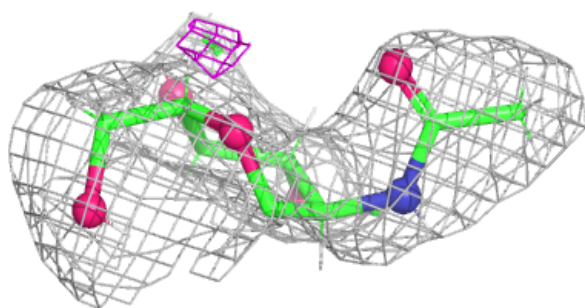
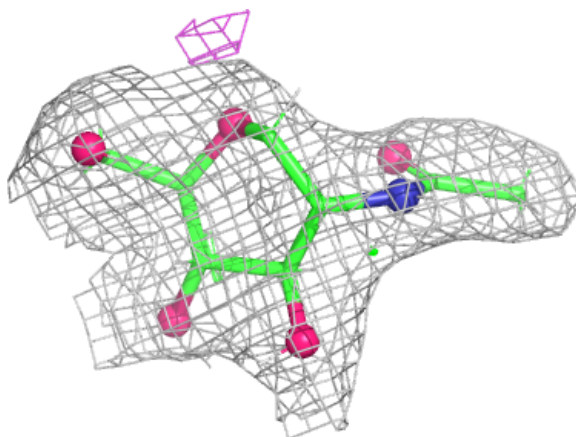
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CYS	B	1001	6/7	0.84	0.23	69,82,91,95	13
3	SER	B	1002	6/7	0.87	0.24	69,80,97,102	11
4	NAG	B	1003	14/15	0.93	0.15	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 [i](#)

There are no such residues in this entry.