



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 02:28 PM UTC

PDB ID : 2CBI / pdb_00002cbi
Title : Structure of the Clostridium perfringens NagJ family 84 glycoside hydrolase, a homologue of human O-GlcNAcase
Authors : Rao, F.V.; Dorfmueller, H.C.; Villa, F.; Allwood, M.; Eggleston, I.M.; van Aalten, D.M.F.
Deposited on : 2006-01-04
Resolution : 2.25 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
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

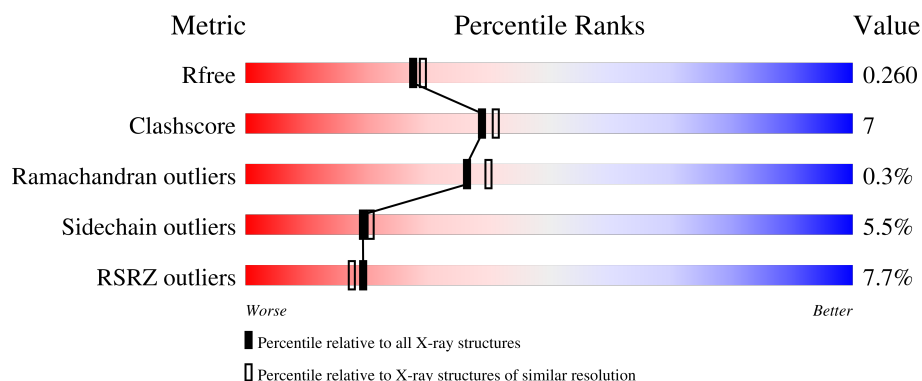
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	594	
1	B	594	

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
3	CL	A	1626	-	-	X	-
6	ZN	B	1625	-	-	-	X
6	ZN	B	1626	-	-	-	X
6	ZN	B	1628	-	-	-	X
6	ZN	B	1635	-	-	-	X
6	ZN	B	1636	-	-	-	X
6	ZN	B	1637	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9931 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 HYALURONIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	584	Total	C	N	O	S	0	0	0
			4620	2908	756	939	17			
1	B	584	Total	C	N	O	S	0	0	0
			4620	2908	756	939	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	196	GLN	LYS	conflict	UNP Q8XL08
A	234	SER	ASN	conflict	UNP Q8XL08
A	244	ASN	ASP	conflict	UNP Q8XL08
A	268	ASP	GLU	conflict	UNP Q8XL08
A	279	THR	ALA	conflict	UNP Q8XL08
A	348	ALA	THR	conflict	UNP Q8XL08
B	196	GLN	LYS	conflict	UNP Q8XL08
B	234	SER	ASN	conflict	UNP Q8XL08
B	244	ASN	ASP	conflict	UNP Q8XL08
B	268	ASP	GLU	conflict	UNP Q8XL08
B	279	THR	ALA	conflict	UNP Q8XL08
B	348	ALA	THR	conflict	UNP Q8XL08

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

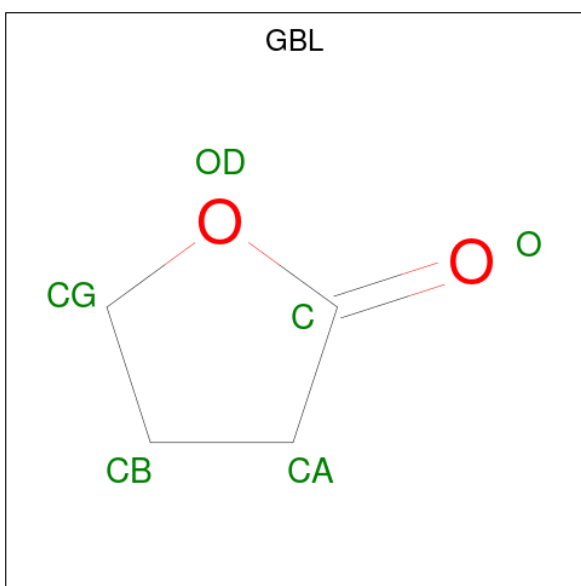


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is GAMMA-BUTYROLACTONE (CCD ID: GBL) (formula: C₄H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	4	2		
4	B	1	Total	C	O	0	0
			6	4	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	11	Total	Zn	0	0
			11	11		

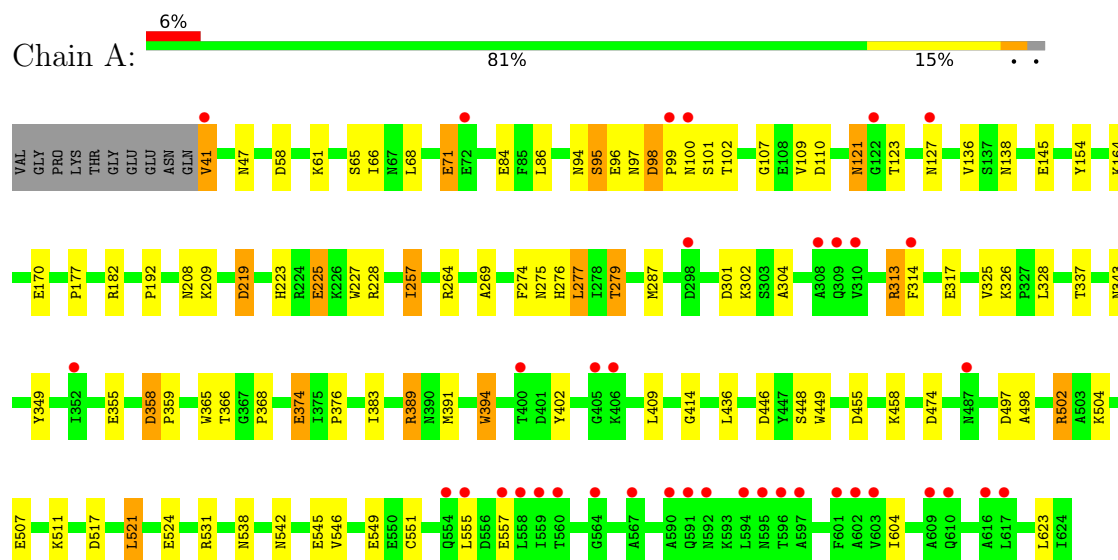
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	313	Total	O	0	0
			313	313		
7	B	337	Total	O	0	0
			337	337		

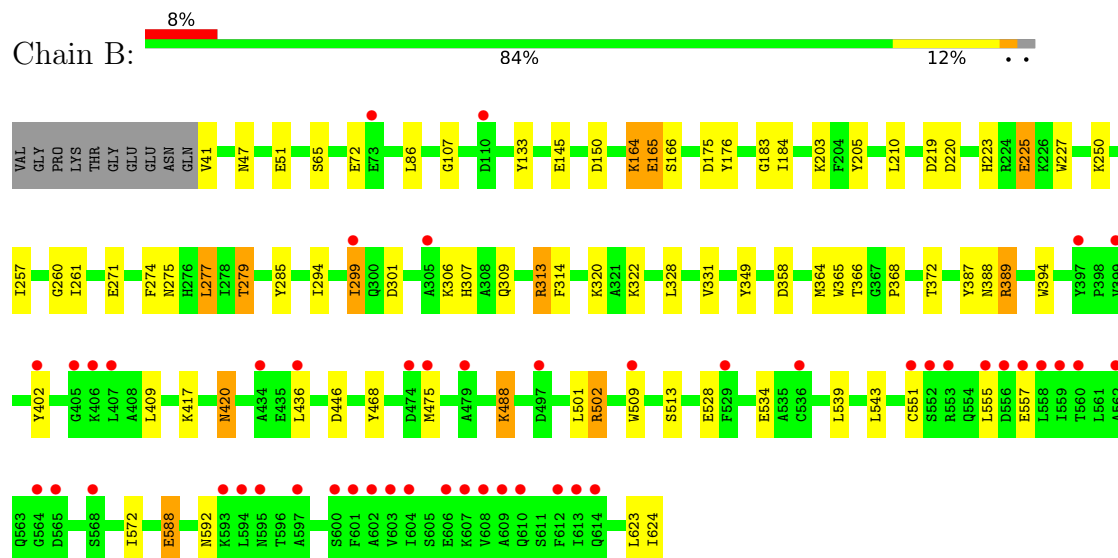
3 Residue-property plots [i](#)

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: HYALURONIDASE



• Molecule 1: HYALURONIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	119.94Å 147.38Å 157.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.25 20.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.25) 99.7 (20.00-2.25)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.40 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.169 , 0.220 0.171 , 0.260	Depositor DCC
R_{free} test set	659 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.624	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 26.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	9931	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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: ZN, GBL, CL, GOL, 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	A	0.92	2/4716 (0.0%)	0.98	3/6403 (0.0%)
1	B	0.94	0/4716	0.99	4/6403 (0.1%)
All	All	0.93	2/9432 (0.0%)	0.98	7/12806 (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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	604	ILE	CA-CB	7.69	1.63	1.55
1	A	546	VAL	CA-CB	5.28	1.61	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	358	ASP	CA-C-N	6.77	127.32	119.47
1	B	358	ASP	C-N-CA	6.77	127.32	119.47
1	A	358	ASP	CA-C-N	5.55	125.91	119.47
1	A	358	ASP	C-N-CA	5.55	125.91	119.47
1	A	374	GLU	N-CA-C	5.34	116.40	108.60
1	B	220	ASP	CA-C-N	5.11	124.91	119.28
1	B	220	ASP	C-N-CA	5.11	124.91	119.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	97	ASN	Peptide
1	A	98	ASP	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	4620	0	4412	62	0
1	B	4620	0	4412	62	0
2	A	5	0	0	0	0
3	A	1	0	0	2	0
4	A	6	0	6	0	0
4	B	6	0	6	3	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	B	11	0	0	0	0
7	A	313	0	0	2	0
7	B	337	0	0	4	0
All	All	9931	0	8852	123	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 (123) 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:B:299:ILE:HD11	1:B:307:HIS:CE1	1.85	1.11
1:B:260:GLY:HA3	1:B:299:ILE:HG22	1.30	1.04
1:A:502:ARG:O	1:A:502:ARG:HD3	1.76	0.86
1:B:475:MET:HE2	1:B:539:LEU:HD22	1.60	0.84
1:A:455:ASP:HB3	1:A:458:LYS:HG2	1.58	0.83
1:B:502:ARG:O	1:B:502:ARG:HD3	1.79	0.82
1:B:260:GLY:CA	1:B:299:ILE:HG22	2.10	0.82
1:B:475:MET:CE	1:B:539:LEU:HD22	2.14	0.78
1:B:475:MET:CE	1:B:543:LEU:HD21	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:ARG:HD3	1:B:502:ARG:C	2.11	0.76
1:B:299:ILE:CD1	1:B:307:HIS:CE1	2.68	0.72
1:B:475:MET:HE2	1:B:539:LEU:CD2	2.22	0.70
1:B:227:TRP:HB2	1:B:257:ILE:HD11	1.75	0.69
1:A:502:ARG:HD3	1:A:502:ARG:C	2.17	0.68
1:A:98:ASP:C	1:A:100:ASN:H	2.02	0.68
1:B:277:LEU:HD13	1:B:314:PHE:CD1	2.29	0.68
1:B:475:MET:HE3	1:B:543:LEU:HD21	1.76	0.67
1:B:260:GLY:HA3	1:B:299:ILE:CG2	2.17	0.66
1:B:47:ASN:HD21	1:B:446:ASP:HB2	1.60	0.66
1:B:475:MET:HE1	1:B:543:LEU:HD11	1.77	0.65
1:A:68:LEU:HG	1:A:71:GLU:HG3	1.80	0.64
1:A:66:ILE:HG22	1:A:102:THR:HB	1.79	0.63
1:A:264:ARG:HD2	1:A:269:ALA:HB1	1.82	0.61
1:A:504:LYS:HE2	1:A:524:GLU:OE2	2.01	0.61
1:A:274:PHE:CE2	1:A:313:ARG:HD2	2.36	0.61
1:B:366:THR:CG2	4:B:1629:GBL:HAC1	2.31	0.61
1:A:374:GLU:HB2	1:A:414:GLY:O	2.02	0.60
1:A:98:ASP:C	1:A:100:ASN:N	2.60	0.59
1:B:165:GLU:O	1:B:166:SER:HB2	2.02	0.58
1:A:274:PHE:CZ	1:A:313:ARG:HD2	2.38	0.58
1:B:299:ILE:HD11	1:B:307:HIS:HE1	1.60	0.58
1:A:302:LYS:CG	1:A:302:LYS:O	2.52	0.57
1:B:150:ASP:OD1	1:B:250:LYS:HD2	2.05	0.56
1:B:133:TYR:CE2	1:B:175:ASP:HB3	2.41	0.56
1:B:274:PHE:CE2	1:B:313:ARG:HD2	2.41	0.56
1:A:623:LEU:CD1	1:B:402:TYR:HA	2.36	0.56
1:B:275:ASN:O	1:B:279:THR:HG23	2.06	0.55
1:A:68:LEU:HG	1:A:71:GLU:CG	2.36	0.55
1:A:98:ASP:CG	1:A:98:ASP:O	2.51	0.53
1:A:389:ARG:HG2	1:A:389:ARG:HH11	1.73	0.53
1:B:274:PHE:CZ	1:B:313:ARG:HD2	2.42	0.53
1:A:41:VAL:HA	1:A:58:ASP:O	2.09	0.53
1:B:436:LEU:HD21	1:B:551:CYS:HB3	1.91	0.53
1:B:588:GLU:HG3	7:B:2304:HOH:O	2.08	0.53
1:A:227:TRP:HB2	1:A:257:ILE:HD11	1.91	0.53
1:A:192:PRO:HG3	1:A:219:ASP:HB3	1.90	0.52
1:B:387:TYR:O	1:B:389:ARG:HG3	2.09	0.52
1:A:337:THR:HB	1:A:368:PRO:HA	1.90	0.52
1:B:47:ASN:ND2	1:B:446:ASP:HB2	2.24	0.52
1:A:94:ASN:HB3	1:A:96:GLU:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:GLN:HG3	7:B:2115:HOH:O	2.09	0.52
1:B:368:PRO:HD2	1:B:372:THR:HG21	1.91	0.52
1:B:387:TYR:HB3	1:B:389:ARG:HD2	1.90	0.52
1:A:474:ASP:OD1	1:A:531:ARG:NH2	2.37	0.51
1:B:183:GLY:C	1:B:184:ILE:HD12	2.35	0.51
1:A:313:ARG:HD3	1:A:317:GLU:OE2	2.10	0.51
1:B:420:ASN:H	1:B:420:ASN:HD22	1.59	0.51
1:B:488:LYS:NZ	7:B:2221:HOH:O	2.43	0.51
1:B:501:LEU:HD13	1:B:528:GLU:HG2	1.91	0.51
1:B:475:MET:HE1	1:B:543:LEU:HD21	1.92	0.50
1:A:225:GLU:H	1:A:225:GLU:CD	2.19	0.50
1:A:98:ASP:OD1	1:A:100:ASN:HA	2.12	0.50
1:B:277:LEU:CD1	1:B:314:PHE:CD1	2.95	0.49
1:B:366:THR:HG21	4:B:1629:GBL:HAC1	1.94	0.48
1:A:275:ASN:O	1:A:279:THR:CG2	2.61	0.48
1:B:205:TYR:HB3	1:B:210:LEU:HB2	1.95	0.48
3:A:1626:CL:CL	7:A:2063:HOH:O	2.58	0.47
1:A:177:PRO:HB3	1:A:449:TRP:CE3	2.49	0.47
1:A:123:THR:OG1	1:A:136:VAL:HG21	2.15	0.47
1:A:228:ARG:HD3	1:A:276:HIS:CD2	2.50	0.47
1:A:95:SER:HB2	1:A:96:GLU:HG3	1.96	0.47
1:A:47:ASN:OD1	1:A:446:ASP:HB2	2.15	0.47
1:B:164:LYS:HD3	1:B:165:GLU:HG2	1.96	0.47
1:A:302:LYS:O	1:A:302:LYS:HG2	2.13	0.47
1:A:507:GLU:HB3	1:A:521:LEU:HD21	1.97	0.47
1:A:402:TYR:HA	1:B:623:LEU:CD1	2.45	0.46
1:A:374:GLU:HG3	1:A:376:PRO:HD3	1.98	0.46
1:A:389:ARG:HG2	1:A:389:ARG:NH1	2.31	0.46
1:B:475:MET:HE1	1:B:539:LEU:HD22	1.96	0.46
1:B:225:GLU:H	1:B:225:GLU:CD	2.22	0.46
1:A:94:ASN:ND2	1:A:101:SER:OG	2.48	0.45
1:B:468:TYR:CE2	1:B:475:MET:HE3	2.51	0.45
1:A:545:GLU:O	1:A:549:GLU:HG2	2.16	0.45
1:B:51:GLU:HG2	1:B:176:TYR:CZ	2.52	0.45
1:A:304:ALA:HB2	1:A:349:TYR:CD1	2.52	0.45
1:B:388:ASN:C	1:B:389:ARG:HG3	2.41	0.45
1:B:349:TYR:CD2	1:B:349:TYR:C	2.95	0.44
1:B:274:PHE:CE1	1:B:313:ARG:HB3	2.52	0.44
1:A:127:ASN:HA	7:A:2027:HOH:O	2.17	0.44
1:A:182:ARG:HG2	1:A:448:SER:HB2	1.99	0.44
1:A:436:LEU:HD11	1:A:551:CYS:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:ASN:OD1	1:A:542:ASN:ND2	2.49	0.44
1:B:277:LEU:HD13	1:B:314:PHE:HD1	1.83	0.44
1:A:154:TYR:CE1	1:A:209:LYS:HA	2.53	0.43
1:A:517:ASP:C	1:A:517:ASP:OD1	2.61	0.43
1:B:502:ARG:C	1:B:502:ARG:CD	2.87	0.43
1:A:358:ASP:O	1:A:389:ARG:NH2	2.49	0.43
1:B:271:GLU:CD	1:B:313:ARG:HH22	2.26	0.43
1:A:107:GLY:O	1:A:145:GLU:HA	2.18	0.43
1:B:513:SER:HA	1:B:624:ILE:HD12	2.01	0.43
1:B:394:TRP:CD2	4:B:1629:GBL:HAC2	2.54	0.42
1:A:275:ASN:O	1:A:279:THR:HG22	2.20	0.42
1:A:511:LYS:HD2	1:A:521:LEU:HD22	2.00	0.42
1:B:592:ASN:ND2	7:B:2308:HOH:O	2.52	0.42
1:A:358:ASP:HA	1:A:359:PRO:HD3	1.94	0.42
1:A:497:ASP:O	1:A:498:ALA:C	2.62	0.42
1:A:109:VAL:O	1:A:110:ASP:HB2	2.20	0.42
1:B:277:LEU:HD13	1:B:314:PHE:CE1	2.54	0.42
1:B:331:VAL:HG22	1:B:364:MET:HB2	2.01	0.42
1:A:208:ASN:OD1	3:A:1626:CL:CL	2.75	0.41
1:A:275:ASN:O	1:A:279:THR:HG23	2.19	0.41
1:B:107:GLY:O	1:B:145:GLU:HA	2.21	0.41
1:A:65:SER:O	1:A:101:SER:HB2	2.21	0.41
1:A:325:VAL:HG12	1:A:326:LYS:O	2.19	0.41
1:A:138:ASN:HA	1:A:170:GLU:HG2	2.01	0.41
1:A:277:LEU:HD13	1:A:314:PHE:CD1	2.56	0.41
1:A:383:ILE:CG2	1:A:391:MET:HE2	2.51	0.41
1:A:383:ILE:HG22	1:A:391:MET:HE2	2.02	0.41
1:B:257:ILE:CG2	1:B:294:ILE:HG12	2.51	0.41
1:B:285:TYR:CZ	1:B:322:LYS:HD3	2.56	0.41
1:A:366:THR:HA	1:A:394:TRP:O	2.21	0.40
1:B:306:LYS:HA	1:B:309:GLN:HG2	2.02	0.40
1:B:509:TRP:CH2	1:B:572:ILE:HD11	2.57	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	582/594 (98%)	560 (96%)	19 (3%)	3 (0%)	24	24
1	B	582/594 (98%)	565 (97%)	16 (3%)	1 (0%)	43	50
All	All	1164/1188 (98%)	1125 (97%)	35 (3%)	4 (0%)	36	40

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	301	ASP
1	B	261	ILE
1	A	99	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	499/507 (98%)	472 (95%)	27 (5%)	20	21
1	B	499/507 (98%)	471 (94%)	28 (6%)	19	20
All	All	998/1014 (98%)	943 (94%)	55 (6%)	19	20

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	VAL
1	A	61	LYS
1	A	71	GLU
1	A	84	GLU
1	A	86	LEU
1	A	95	SER
1	A	121	ASN
1	A	164	LYS

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Mol	Chain	Res	Type
1	A	219	ASP
1	A	223	HIS
1	A	225	GLU
1	A	257	ILE
1	A	277	LEU
1	A	279	THR
1	A	287	MET
1	A	313	ARG
1	A	328	LEU
1	A	343	ASN
1	A	355	GLU
1	A	365	TRP
1	A	389	ARG
1	A	394	TRP
1	A	409	LEU
1	A	502	ARG
1	A	521	LEU
1	A	555	LEU
1	A	557	GLU
1	B	41	VAL
1	B	65	SER
1	B	72	GLU
1	B	86	LEU
1	B	164	LYS
1	B	165	GLU
1	B	203	LYS
1	B	219	ASP
1	B	223	HIS
1	B	225	GLU
1	B	277	LEU
1	B	279	THR
1	B	299	ILE
1	B	301	ASP
1	B	313	ARG
1	B	320	LYS
1	B	328	LEU
1	B	365	TRP
1	B	389	ARG
1	B	409	LEU
1	B	417	LYS
1	B	420	ASN
1	B	488	LYS

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Mol	Chain	Res	Type
1	B	502	ARG
1	B	534	GLU
1	B	555	LEU
1	B	557	GLU
1	B	588	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	52	ASN
1	A	127	ASN
1	A	223	HIS
1	A	276	HIS
1	A	315	ASN
1	A	345	GLN
1	A	575	GLN
1	B	47	ASN
1	B	52	ASN
1	B	201	GLN
1	B	223	HIS
1	B	240	GLN
1	B	309	GLN
1	B	420	ASN
1	B	461	ASN
1	B	542	ASN
1	B	592	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 12 are monoatomic - leaving 5 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
4	GBL	A	1627	-	6,6,6	0.47	0	7,7,7	0.95	0
5	GOL	B	1630	-	5,5,5	0.55	0	5,5,5	0.51	0
5	GOL	A	1628	-	5,5,5	0.28	0	5,5,5	0.81	0
4	GBL	B	1629	-	6,6,6	0.91	0	7,7,7	1.02	0
2	SO4	A	1625	6	4,4,4	0.39	0	6,6,6	0.78	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	GBL	A	1627	-	-	-	0/1/1/1
4	GBL	B	1629	-	-	-	0/1/1/1
5	GOL	B	1630	-	-	0/4/4/4	-
5	GOL	A	1628	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1628	GOL	O1-C1-C2-O2
5	A	1628	GOL	O1-C1-C2-C3
5	A	1628	GOL	C1-C2-C3-O3
5	A	1628	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1629	GBL	3	0

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	573/594 (96%)	0.31	38 (6%) 24 23	-2, 15, 38, 53	1 (0%)
1	B	557/594 (93%)	0.61	49 (8%) 15 14	-5, 14, 34, 48	1 (0%)
All	All	1130/1188 (95%)	0.46	87 (7%) 19 17	-5, 14, 37, 53	2 (0%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	564	GLY	27.9
1	A	594	LEU	25.4
1	B	564	GLY	25.3
1	A	590	ALA	25.0
1	B	602	ALA	22.3
1	B	597	ALA	21.4
1	B	479	ALA	20.9
1	B	405	GLY	20.8
1	B	608	VAL	19.3
1	B	603	VAL	19.0
1	B	407	LEU	18.1
1	B	609	ALA	17.0
1	B	613	ILE	16.4
1	A	602	ALA	16.2
1	B	612	PHE	15.8
1	B	558	LEU	15.1
1	B	560	THR	14.9
1	A	595	ASN	14.3
1	A	558	LEU	14.0
1	A	592	ASN	12.6
1	B	553	ARG	12.5
1	B	594	LEU	11.3
1	B	601	PHE	11.3
1	B	559	ILE	10.5

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Mol	Chain	Res	Type	RSRZ
1	B	497	ASP	9.5
1	B	604	ILE	9.1
1	B	610	GLN	8.8
1	A	405	GLY	8.8
1	B	529	PHE	8.4
1	A	406	LYS	7.8
1	B	551	CYS	6.9
1	B	475	MET	6.8
1	A	591	GLN	6.8
1	A	617	LEU	6.7
1	A	609	ALA	6.4
1	A	122	GLY	6.4
1	B	557	GLU	6.3
1	B	606	GLU	6.2
1	A	400	THR	6.0
1	B	406	LYS	5.5
1	B	607	LYS	5.5
1	B	565	ASP	4.8
1	A	99	PRO	4.8
1	A	560	THR	4.6
1	A	100	ASN	4.5
1	B	536	CYS	4.4
1	A	72	GLU	4.2
1	B	509	TRP	4.2
1	B	556	ASP	4.1
1	B	593	LYS	4.1
1	A	487	ASN	3.9
1	B	614	GLN	3.8
1	B	552	SER	3.6
1	A	559	ILE	3.5
1	A	567	ALA	3.5
1	B	299	ILE	3.5
1	B	73	GLU	3.4
1	A	557	GLU	3.3
1	B	562	ALA	3.2
1	A	555	LEU	3.1
1	B	436	LEU	3.0
1	B	305	ALA	2.8
1	A	554	GLN	2.8
1	A	610	GLN	2.7
1	B	434	ALA	2.7
1	B	402	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	603	VAL	2.6
1	B	555	LEU	2.5
1	A	352	ILE	2.5
1	B	568	SER	2.5
1	B	600	SER	2.5
1	B	110	ASP	2.5
1	A	616	ALA	2.5
1	B	397	TYR	2.4
1	A	41	VAL	2.4
1	A	601	PHE	2.4
1	B	399	VAL	2.3
1	A	127	ASN	2.3
1	A	308	ALA	2.3
1	A	309	GLN	2.3
1	A	597	ALA	2.2
1	B	474	ASP	2.2
1	A	596	THR	2.2
1	A	310	VAL	2.1
1	A	298	ASP	2.1
1	B	595	ASN	2.1
1	A	314	PHE	2.1

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
6	ZN	B	1625	1/1	-0.69	1.30	-4,-4,-4,-4	1
6	ZN	B	1628	1/1	0.05	0.55	27,27,27,27	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	ZN	B	1635	1/1	0.38	0.57	42,42,42,42	1
6	ZN	B	1634	1/1	0.41	0.24	23,23,23,23	1
6	ZN	B	1637	1/1	0.49	1.08	183,183,183,183	1
6	ZN	B	1631	1/1	0.60	0.33	41,41,41,41	1
6	ZN	B	1632	1/1	0.65	0.26	40,40,40,40	1
6	ZN	B	1626	1/1	0.70	0.56	25,25,25,25	1
6	ZN	B	1636	1/1	0.71	0.77	48,48,48,48	1
6	ZN	B	1633	1/1	0.74	0.40	25,25,25,25	1
6	ZN	B	1627	1/1	0.80	0.36	15,15,15,15	1
2	SO4	A	1625	5/5	0.87	0.10	35,41,46,48	0
5	GOL	A	1628	6/6	0.90	0.11	9,17,25,30	0
3	CL	A	1626	1/1	0.91	0.10	31,31,31,31	0
4	GBL	A	1627	6/6	0.92	0.08	6,8,13,13	0
5	GOL	B	1630	6/6	0.94	0.07	2,13,16,16	0
4	GBL	B	1629	6/6	0.94	0.09	13,15,20,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.