WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Nov 25, 2024 – 03:16 PM EST

PDB ID	:	1IVB
Title	:	STRUCTURES OF AROMATIC INHIBITORS OF INFLUENZA VIRUS NEURAMINIDASE
Authors	:	Jedrzejas, M.J.; Luo, M.
Deposited on	:	1994-12-12
Resolution	:	2.40 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.40 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.
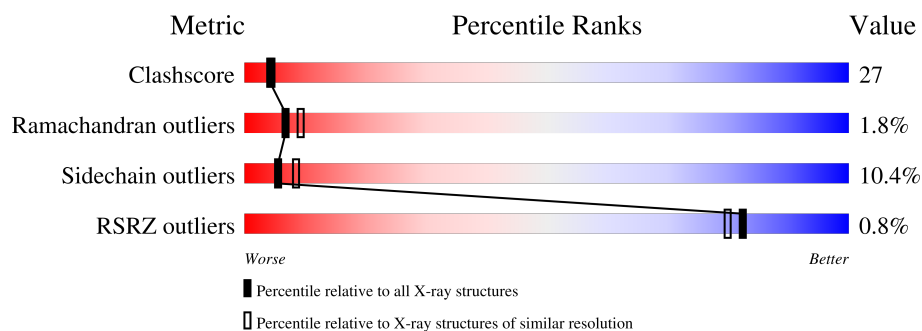
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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%

Mol	Chain	Length	Quality of chain
1	A	390	53% 39% 7% •

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 3785 atoms, of which 712 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.
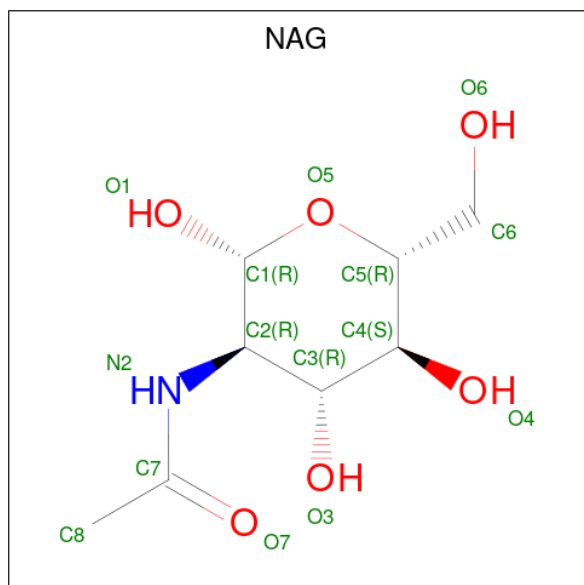
- Molecule 1 is a protein called INFLUENZA VIRUS B/LEE/40 NEURAMINIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	390	Total 3736	C 1907	H 696	N 531	O 574	S 28	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	382	ARG	LYS	conflict	UNP P03474

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 28	C 8	H 14	N 1	O 5	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Ca 2	0	0

- Molecule 4 is 4-(ACETYLAMINO)-3-HYDROXY-5-NITROBENZOIC ACID (three-letter code: ST1) (formula: $C_9H_8N_2O_6$).
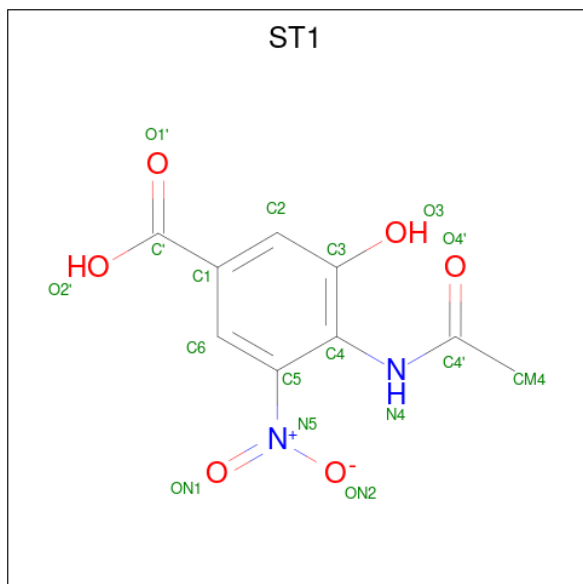
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
4	A	1	19	9	2	2	6	0	0

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. 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. 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: INFLUENZA VIRUS B/LEE/40 NEURAMINIDASE

Chain A:
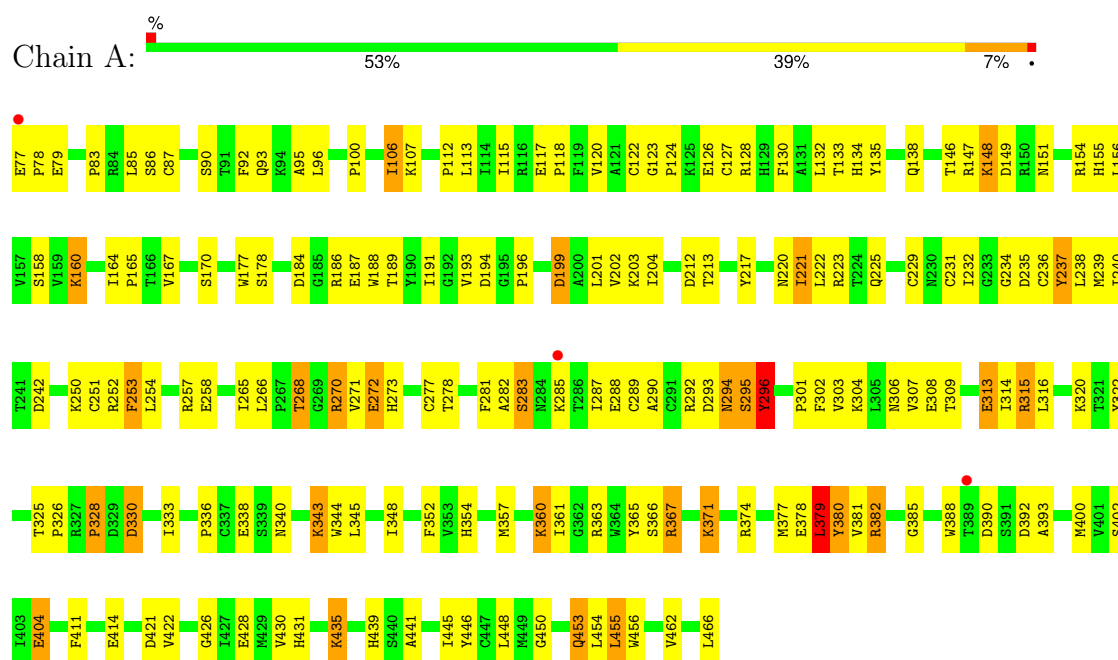
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	124.54Å 124.54Å 71.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.50 – 2.40 6.50 – 2.42	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.50-2.40) 63.6 (6.50-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.41Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.189 , (Not available) 0.251 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	11.7	Xtriage
Anisotropy	0.759	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 59.3	EDS
L-test for twinning[2]	$< |L| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.79	EDS
Total number of atoms	3785	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 4.72% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, ST1, CA

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	0.74	0/3114	0.99	8/4210 (0.2%)

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

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	379	LEU	CA-CB-CG	9.92	138.12	115.30
1	A	290	ALA	N-CA-C	-6.36	93.83	111.00
1	A	296	TYR	N-CA-C	6.15	127.61	111.00
1	A	96	LEU	CA-CB-CG	5.31	127.51	115.30
1	A	435	LYS	N-CA-C	5.24	125.14	111.00
1	A	371	LYS	CD-CE-NZ	5.17	123.58	111.70
1	A	330	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	A	189	THR	N-CA-C	-5.07	97.31	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	237	TYR	Sidechain
1	A	365	TYR	Sidechain

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	3040	696	2934	159	0
2	A	14	14	13	2	0
3	A	2	0	0	0	0
4	A	17	2	7	0	0
All	All	3073	712	2954	160	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 27.

All (160) 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:296:TYR:HA	1:A:343:LYS:HG3	1.42	1.01
1:A:270:ARG:HH11	1:A:270:ARG:HG3	1.39	0.86
1:A:268:THR:HG22	1:A:313:GLU:HG2	1.58	0.86
1:A:77:GLU:HB2	1:A:78:PRO:HD2	1.61	0.81
1:A:336:PRO:HB2	1:A:338:GLU:OE1	1.81	0.80
1:A:292:ARG:HD2	1:A:348:ILE:N	2.00	0.77
1:A:202:VAL:HG23	1:A:222:LEU:HD21	1.64	0.76
1:A:225:GLN:HG2	1:A:277:CYS:O	1.87	0.73
1:A:270:ARG:HD3	1:A:270:ARG:O	1.89	0.73
1:A:378:GLU:HG3	1:A:380:TYR:CE1	2.23	0.72
1:A:357:MET:CE	1:A:360:LYS:HD2	2.21	0.71
1:A:282:ALA:O	1:A:283:SER:HB3	1.91	0.70
1:A:191:ILE:HD12	1:A:204:ILE:HD12	1.71	0.70
1:A:148:LYS:HD3	1:A:151:ASN:HD22	1.57	0.69
1:A:128:ARG:HG2	1:A:188:TRP:CZ2	2.29	0.67
1:A:196:PRO:HD2	1:A:199:ASP:O	1.95	0.67
1:A:357:MET:HE3	1:A:360:LYS:HD2	1.77	0.66
1:A:191:ILE:HG21	1:A:238:LEU:HD21	1.78	0.66
1:A:322:TYR:CZ	1:A:333:ILE:HD12	2.32	0.65
1:A:292:ARG:NH1	1:A:348:ILE:HA	2.12	0.65
1:A:306:ASN:HD21	1:A:308:GLU:HG2	1.62	0.65
1:A:278:THR:O	1:A:289:CYS:HA	1.98	0.64
1:A:314:ILE:O	1:A:315:ARG:HG2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:PHE:CD1	1:A:158:SER:HB3	2.33	0.64
1:A:201:LEU:HD11	1:A:213:THR:HB	1.80	0.64
1:A:250:LYS:HG2	1:A:271:VAL:O	1.99	0.63
1:A:352:PHE:HE1	1:A:363:ARG:HB3	1.63	0.63
1:A:232:ILE:HB	1:A:281:PHE:CZ	2.34	0.62
1:A:292:ARG:HH11	1:A:348:ILE:HA	1.63	0.62
1:A:430:VAL:HG22	1:A:441:ALA:HB2	1.80	0.62
1:A:296:TYR:CA	1:A:343:LYS:HG3	2.24	0.62
1:A:320:LYS:HD2	1:A:393:ALA:HB2	1.82	0.62
1:A:304:LYS:HE2	1:A:388:TRP:CE2	2.35	0.61
1:A:322:TYR:CE2	1:A:330:ASP:HA	2.35	0.61
1:A:304:LYS:HE2	1:A:388:TRP:CD2	2.35	0.61
1:A:221:ILE:O	1:A:223:ARG:HG3	2.00	0.60
1:A:354:HIS:CD2	1:A:361:ILE:HD11	2.37	0.60
1:A:377:MET:HG3	1:A:400:MET:HE3	1.83	0.59
1:A:411:PHE:CZ	1:A:426:GLY:HA3	2.37	0.58
1:A:92:PHE:HA	1:A:448:LEU:HA	1.84	0.58
1:A:221:ILE:O	1:A:221:ILE:HG22	2.03	0.58
1:A:314:ILE:C	1:A:315:ARG:HG2	2.22	0.58
1:A:381:VAL:HG22	1:A:382:ARG:H	1.68	0.58
1:A:270:ARG:HH11	1:A:270:ARG:CG	2.14	0.57
1:A:202:VAL:HG23	1:A:222:LEU:CD2	2.35	0.56
1:A:354:HIS:HD2	1:A:361:ILE:HD11	1.70	0.56
1:A:133:THR:O	1:A:154:ARG:HA	2.06	0.56
1:A:270:ARG:NH2	1:A:293:ASP:OD2	2.39	0.56
1:A:308:GLU:HG3	1:A:309:THR:HG23	1.87	0.56
1:A:240:ILE:O	1:A:251:CYS:HB2	2.06	0.55
1:A:315:ARG:HG3	1:A:388:TRP:CE2	2.40	0.55
1:A:232:ILE:HG21	1:A:307:VAL:HG11	1.89	0.55
1:A:93:GLN:HE22	1:A:455:LEU:H	1.52	0.55
1:A:315:ARG:HG3	1:A:388:TRP:CD2	2.42	0.54
1:A:270:ARG:HG3	1:A:270:ARG:NH1	2.17	0.54
1:A:90:SER:N	1:A:450:GLY:O	2.40	0.54
1:A:132:LEU:HA	1:A:155:HIS:O	2.08	0.53
1:A:203:LYS:HG2	1:A:213:THR:HG22	1.89	0.53
1:A:126:GLU:HG2	1:A:127:CYS:N	2.24	0.53
1:A:147:ARG:HD2	1:A:439:HIS:CE1	2.44	0.53
1:A:252:ARG:HG2	1:A:266:LEU:HD13	1.91	0.52
1:A:431:HIS:CE1	1:A:462:VAL:HG21	2.45	0.52
1:A:77:GLU:HB2	1:A:78:PRO:CD	2.38	0.52
1:A:338:GLU:H	1:A:338:GLU:CD	2.11	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ILE:HG13	1:A:238:LEU:HD22	1.90	0.52
1:A:382:ARG:HH12	1:A:385:GLY:HA3	1.75	0.51
1:A:106:ILE:HD12	1:A:466:LEU:OXT	2.11	0.51
1:A:113:LEU:HD21	1:A:167:VAL:HG22	1.93	0.51
1:A:106:ILE:HD13	1:A:107:LYS:H	1.76	0.51
1:A:250:LYS:HD2	1:A:271:VAL:HG23	1.93	0.51
1:A:100:PRO:HG3	1:A:165:PRO:HD2	1.93	0.51
1:A:187:GLU:HG3	1:A:188:TRP:N	2.26	0.51
1:A:117:GLU:N	1:A:118:PRO:CD	2.74	0.51
1:A:148:LYS:HD3	1:A:151:ASN:ND2	2.23	0.51
1:A:268:THR:O	1:A:313:GLU:HA	2.10	0.51
1:A:325:THR:HB	1:A:348:ILE:HG21	1.93	0.50
1:A:381:VAL:HG22	1:A:382:ARG:N	2.26	0.50
1:A:382:ARG:HH11	1:A:382:ARG:HG2	1.77	0.50
1:A:281:PHE:CE1	1:A:287:ILE:HG12	2.47	0.50
1:A:320:LYS:O	1:A:330:ASP:HB3	2.12	0.49
1:A:306:ASN:ND2	1:A:308:GLU:HG2	2.26	0.49
1:A:253:PHE:CB	1:A:265:ILE:HB	2.43	0.49
1:A:315:ARG:HG3	1:A:388:TRP:CZ2	2.48	0.49
1:A:400:MET:HB3	1:A:446:TYR:CE1	2.48	0.49
1:A:315:ARG:HG3	1:A:388:TRP:CE3	2.48	0.49
1:A:83:PRO:O	2:A:467:NAG:N2	2.45	0.49
1:A:134:HIS:CE1	1:A:146:THR:O	2.66	0.49
1:A:270:ARG:CZ	1:A:272:GLU:HG2	2.43	0.49
1:A:414:GLU:HG2	1:A:421:ASP:HB3	1.94	0.49
1:A:322:TYR:O	1:A:367:ARG:NH2	2.46	0.48
1:A:78:PRO:HB2	1:A:186:ARG:HG2	1.95	0.48
1:A:118:PRO:HD2	1:A:428:GLU:OE2	2.14	0.48
1:A:378:GLU:HG3	1:A:380:TYR:HE1	1.75	0.48
1:A:87:CYS:SG	1:A:422:VAL:HG22	2.54	0.48
1:A:285:LYS:HG2	1:A:306:ASN:ND2	2.29	0.48
1:A:112:PRO:HD2	1:A:138:GLN:O	2.14	0.47
1:A:303:VAL:HG12	1:A:304:LYS:N	2.29	0.47
1:A:377:MET:HG3	1:A:400:MET:CE	2.44	0.47
1:A:123:GLY:N	1:A:126:GLU:O	2.48	0.47
1:A:285:LYS:HG2	1:A:306:ASN:HD21	1.78	0.47
1:A:122:CYS:HA	1:A:127:CYS:HA	1.97	0.47
1:A:292:ARG:HE	1:A:294:ASN:ND2	2.13	0.47
1:A:147:ARG:HD2	1:A:439:HIS:NE2	2.30	0.47
1:A:288:GLU:OE1	1:A:302:PHE:HE1	1.98	0.47
1:A:117:GLU:HB2	1:A:132:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:ARG:HH22	1:A:385:GLY:HA3	1.80	0.46
1:A:366:SER:HA	1:A:379:LEU:HA	1.95	0.46
1:A:402:SER:OG	1:A:404:GLU:HG2	2.15	0.46
1:A:234:GLY:O	1:A:257:ARG:HG3	2.14	0.46
1:A:270:ARG:NE	1:A:272:GLU:HG2	2.31	0.46
1:A:217:TYR:CE1	1:A:242:ASP:HB3	2.50	0.46
1:A:270:ARG:HD3	1:A:270:ARG:C	2.36	0.46
1:A:178:SER:HB3	1:A:193:VAL:HB	1.98	0.45
1:A:380:TYR:CD1	1:A:380:TYR:N	2.82	0.45
1:A:315:ARG:HG3	1:A:388:TRP:CH2	2.51	0.45
1:A:315:ARG:HG3	1:A:388:TRP:CZ3	2.51	0.45
1:A:120:VAL:HA	1:A:128:ARG:O	2.17	0.45
1:A:177:TRP:CE2	1:A:194:ASP:HA	2.52	0.45
1:A:278:THR:HG21	1:A:352:PHE:H	1.82	0.45
1:A:316:LEU:HD11	1:A:340:ASN:ND2	2.32	0.45
1:A:288:GLU:OE1	1:A:302:PHE:CE1	2.71	0.44
1:A:134:HIS:HD2	1:A:151:ASN:HD21	1.65	0.44
1:A:164:ILE:HA	1:A:165:PRO:HD3	1.80	0.44
1:A:231:CYS:HA	1:A:236:CYS:HA	1.99	0.44
1:A:357:MET:HB2	1:A:360:LYS:O	2.17	0.44
1:A:106:ILE:HD13	1:A:107:LYS:N	2.32	0.44
1:A:235:ASP:OD1	1:A:257:ARG:HD2	2.18	0.44
1:A:322:TYR:CD2	1:A:330:ASP:HA	2.53	0.44
1:A:414:GLU:CG	1:A:421:ASP:HB3	2.48	0.44
1:A:86:SER:HA	1:A:421:ASP:O	2.18	0.43
1:A:253:PHE:HB3	1:A:265:ILE:HB	2.00	0.43
1:A:147:ARG:HD2	1:A:439:HIS:CD2	2.53	0.43
1:A:414:GLU:HA	1:A:422:VAL:O	2.18	0.43
1:A:328:PRO:HB3	1:A:344:TRP:CZ2	2.53	0.43
2:A:467:NAG:C7	2:A:467:NAG:O3	2.66	0.43
1:A:352:PHE:CZ	1:A:363:ARG:HD3	2.54	0.43
1:A:453:GLN:NE2	1:A:453:GLN:HA	2.34	0.43
1:A:85:LEU:HA	1:A:85:LEU:HD23	1.60	0.43
1:A:184:ASP:C	1:A:186:ARG:H	2.21	0.43
1:A:431:HIS:HE1	1:A:462:VAL:HG21	1.81	0.43
1:A:270:ARG:HG2	1:A:272:GLU:OE1	2.19	0.43
1:A:454:LEU:HD23	1:A:454:LEU:C	2.39	0.42
1:A:270:ARG:CG	1:A:270:ARG:NH1	2.77	0.42
1:A:292:ARG:HH11	1:A:348:ILE:CA	2.32	0.42
1:A:237:TYR:CE1	1:A:307:VAL:HG13	2.55	0.41
1:A:296:TYR:N	1:A:343:LYS:HG3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:PRO:HA	1:A:316:LEU:HA	2.02	0.41
1:A:295:SER:HB2	1:A:296:TYR:H	1.60	0.41
1:A:95:ALA:HB3	1:A:445:ILE:HG22	2.02	0.41
1:A:187:GLU:HG3	1:A:188:TRP:H	1.86	0.41
1:A:303:VAL:HG22	1:A:314:ILE:HG12	2.02	0.41
1:A:431:HIS:CD2	1:A:431:HIS:N	2.88	0.41
1:A:160:LYS:HE3	1:A:160:LYS:HB2	1.88	0.41
1:A:366:SER:HA	1:A:378:GLU:O	2.21	0.41
1:A:348:ILE:HD12	1:A:374:ARG:NE	2.35	0.41
1:A:149:ASP:O	1:A:154:ARG:HD2	2.21	0.41
1:A:273:HIS:CD2	1:A:294:ASN:H	2.39	0.40
1:A:237:TYR:HA	1:A:254:LEU:O	2.22	0.40
1:A:316:LEU:HD11	1:A:340:ASN:HD22	1.85	0.40
1:A:326:PRO:HA	1:A:371:LYS:O	2.22	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	388/390 (100%)	346 (89%)	35 (9%)	7 (2%)	7	9

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	SER
1	A	296	TYR
1	A	345	LEU
1	A	392	ASP
1	A	328	PRO
1	A	124	PRO
1	A	221	ILE

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	326/326 (100%)	292 (90%)	34 (10%)	5 8

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	GLU
1	A	106	ILE
1	A	115	ILE
1	A	135	TYR
1	A	148	LYS
1	A	156	LEU
1	A	160	LYS
1	A	170	SER
1	A	199	ASP
1	A	212	ASP
1	A	220	ASN
1	A	229	CYS
1	A	239	MET
1	A	253	PHE
1	A	258	GLU
1	A	268	THR
1	A	270	ARG
1	A	272	GLU
1	A	294	ASN
1	A	295	SER
1	A	313	GLU
1	A	315	ARG
1	A	343	LYS
1	A	360	LYS
1	A	367	ARG
1	A	379	LEU
1	A	380	TYR
1	A	382	ARG
1	A	390	ASP
1	A	404	GLU

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Mol	Chain	Res	Type
1	A	435	LYS
1	A	453	GLN
1	A	455	LEU
1	A	456	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	134	HIS
1	A	169	ASN
1	A	220	ASN
1	A	294	ASN
1	A	340	ASN
1	A	439	HIS

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	ST1	A	471	-	17,17,17	1.75	2 (11%)	19,24,24	1.98	6 (31%)
2	NAG	A	467	1	14,14,15	3.14	3 (21%)	17,19,21	2.37	6 (35%)

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	ST1	A	471	-	-	4/10/12/12	0/1/1/1
2	NAG	A	467	1	-	1/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	467	NAG	O5-C1	9.46	1.59	1.43
2	A	467	NAG	C4-C5	4.60	1.62	1.53
4	A	471	ST1	C1-C'	-4.39	1.40	1.49
2	A	467	NAG	C4-C3	3.86	1.62	1.52
4	A	471	ST1	C5-N5	-3.59	1.39	1.45

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	467	NAG	O5-C1-C2	4.78	118.68	111.29
4	A	471	ST1	ON1-N5-C5	-4.75	110.90	119.03
2	A	467	NAG	C2-N2-C7	-4.56	116.78	122.90
4	A	471	ST1	C4-N4-C4'	-4.14	115.75	122.82
2	A	467	NAG	C1-O5-C5	3.89	117.40	112.19
2	A	467	NAG	C8-C7-N2	3.72	122.29	116.12
2	A	467	NAG	O7-C7-C8	-3.09	116.55	122.05
4	A	471	ST1	C1-C6-C5	2.77	122.58	119.06
4	A	471	ST1	O2'-C'-C1	2.59	121.48	114.84
4	A	471	ST1	C6-C5-C4	-2.49	119.13	121.96
4	A	471	ST1	CM4-C4'-N4	2.13	118.16	114.95
2	A	467	NAG	C1-C2-N2	2.01	113.60	110.43

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	471	ST1	O4'-C4'-N4-C4
4	A	471	ST1	CM4-C4'-N4-C4
4	A	471	ST1	C4-C5-N5-ON1
4	A	471	ST1	C6-C5-N5-ON1
2	A	467	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
2	A	467	NAG	2	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

Warning: The R factor obtained from EDS is 0.2519, which does not match the depositor's R factor of 0.189. Please interpret the results in this section carefully.

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	390/390 (100%)	-0.01	3 (0%)	82 80	15, 15, 15, 15	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	77	GLU	3.2
1	A	285	LYS	2.1
1	A	389	THR	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, 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
2	NAG	A	467	14/15	0.85	0.12	15,15,15,15	0
4	ST1	A	471	17/17	0.89	0.10	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	CA	A	501	1/1	0.95	0.21	15,15,15,15	1
3	CA	A	500	1/1	0.98	0.02	15,15,15,15	0

6.5 Other polymers ⓘ

There are no such residues in this entry.