Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 04:51 am GMT

PDB ID	:	1B9V
Title	:	NOVEL AROMATIC INHIBITORS OF INFLUENZA VIRUS NEU-RAMINIDASE MAKE SELECTIVE INTERACTIONS WITH CONSERVED RESIDUES AND WATER MOLECULES IN TEH ACTIVE SITE
Authors	:	Finley, J.B.; Atigadda, V.R.; Duarte, F.; Zahao, J.J.; Brouillette, W.J.; Air, G.M.; Luo, M.
Deposited on	:	1999-02-15
Resolution	:	2.35 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
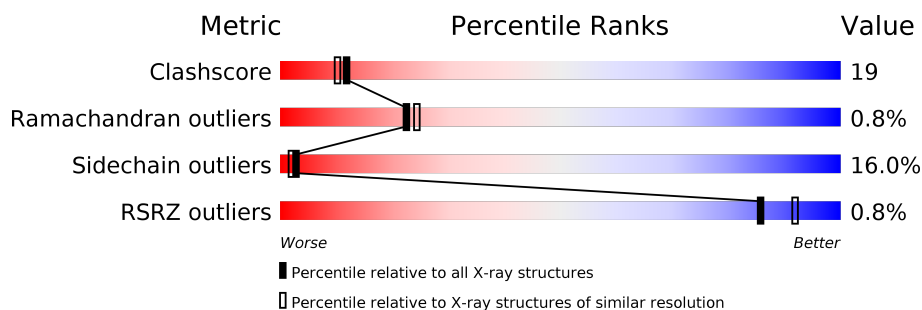with specific help available everywhere you see the ⓘ symbol.

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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 2.35 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	Percentile Ranks	Value
Clashscore		19
Ramachandran outliers		0.8%
Sidechain outliers		16.0%
RSRZ outliers		0.8%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	390	60% 33% 6%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 3188 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 PROTEIN (NEURAMINIDASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total 3040	C 1907	N 531	O 574	S 28	0	0	0

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
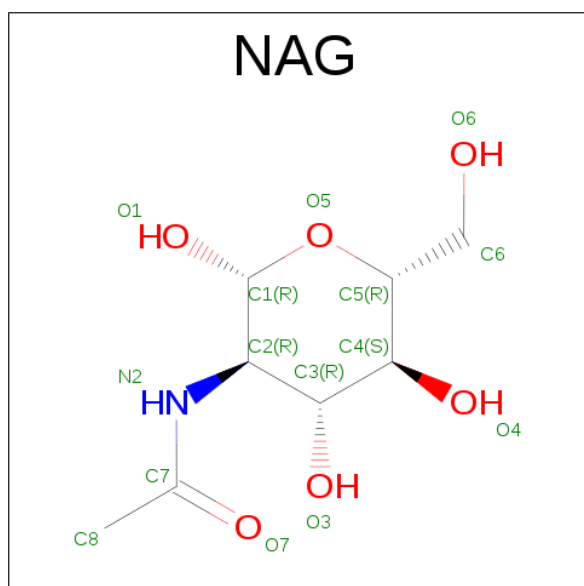
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 14	C 8	N 1	O 5	0	0

- 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 1-[4-CARBOXY-2-(3-PENTYLAMINO)PHENYL]-5,5'-DI(HYDROXYMET

HYL)PYRROLIDIN-2-ONE (three-letter code: RA2) (formula: $C_{18}H_{26}N_2O_5$).
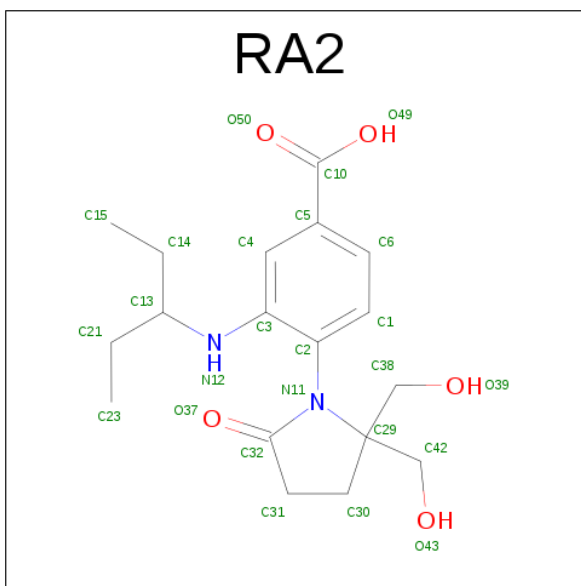
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	25	18	2	5	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	107	107	107	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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 (NEURAMINIDASE)
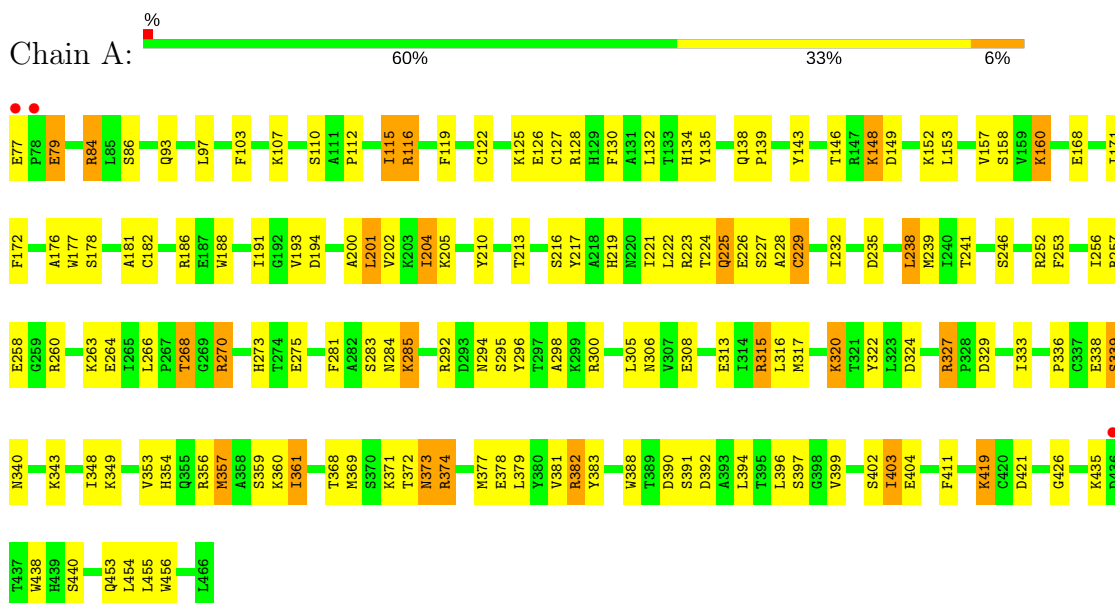
4   Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	124.70Å 124.70Å 71.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.35 31.18 – 2.28	Depositor EDS
% Data completeness (in resolution range)	70.2 (8.00-2.35) 72.4 (31.18-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 2.29Å)	Xtriage
Refinement program	X-PLOR 3.85	Depositor
R, R_{free}	0.183 , 0.271 0.187 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	19.5	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 60.6	EDS
L-test for twinning[2]	$< |L| > = 0.45, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3188	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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: CA, RA2, 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	0.34	0/3114	0.64	0/4210

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts Ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3040	0	2935	117	0
2	A	14	0	13	2	0
3	A	2	0	0	0	0
4	A	25	0	25	2	0
5	A	107	0	0	6	0
All	All	3188	0	2973	117	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 19.

All (117) 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:201:LEU:HD11	1:A:213:THR:HB	1.47	0.96
1:A:348:ILE:HD12	1:A:374:ARG:HD2	1.57	0.83
1:A:246:SER:HA	1:A:295:SER:HB3	1.62	0.81
1:A:284:ASN:HD21	2:A:467:NAG:C1	1.93	0.81
1:A:268:THR:HG22	1:A:313:GLU:HG3	1.69	0.74
1:A:316:LEU:HD11	1:A:340:ASN:ND2	2.05	0.71
1:A:139:PRO:HA	1:A:143:TYR:OH	1.91	0.70
1:A:284:ASN:ND2	2:A:467:NAG:C1	2.54	0.69
1:A:223:ARG:HG3	1:A:241:THR:HG22	1.73	0.69
1:A:357:MET:HG3	1:A:360:LYS:HB3	1.74	0.69
1:A:122:CYS:HB3	5:A:623:HOH:O	1.94	0.68
1:A:320:LYS:HG2	1:A:391:SER:O	1.93	0.68
1:A:285:LYS:HG2	1:A:308:GLU:HG3	1.74	0.68
1:A:232:ILE:HB	1:A:281:PHE:CZ	2.31	0.65
1:A:148:LYS:HD3	1:A:149:ASP:H	1.61	0.65
1:A:327:ARG:NH1	1:A:371:LYS:HG2	2.12	0.65
1:A:217:TYR:CE2	1:A:252:ARG:HD2	2.32	0.64
1:A:368:THR:HG22	1:A:377:MET:HE1	1.79	0.64
1:A:112:PRO:HD2	1:A:138:GLN:O	1.98	0.63
1:A:148:LYS:HD3	1:A:149:ASP:N	2.13	0.63
1:A:348:ILE:HD12	1:A:374:ARG:CD	2.28	0.62
1:A:438:TRP:HZ3	1:A:440:SER:HB3	1.63	0.62
1:A:403:ILE:HB	5:A:973:HOH:O	2.00	0.62
1:A:201:LEU:CD1	1:A:213:THR:HB	2.26	0.60
1:A:193:VAL:HG11	1:A:222:LEU:O	2.01	0.60
1:A:315:ARG:HG3	1:A:315:ARG:NH1	2.16	0.60
1:A:270:ARG:HD3	1:A:316:LEU:HG	1.84	0.59
1:A:177:TRP:NE1	1:A:194:ASP:HA	2.18	0.59
1:A:84:ARG:O	1:A:356:ARG:NH1	2.33	0.59
1:A:193:VAL:HG22	1:A:202:VAL:HG22	1.84	0.59
1:A:285:LYS:HZ1	1:A:308:GLU:HB2	1.67	0.58
1:A:239:MET:CE	1:A:275:GLU:HA	2.33	0.58
1:A:336:PRO:HD2	1:A:339:SER:OG	2.04	0.58
1:A:322:TYR:CZ	1:A:333:ILE:HG12	2.39	0.58
1:A:157:VAL:HG12	1:A:172:PHE:HA	1.85	0.57
1:A:239:MET:CE	1:A:241:THR:HB	2.35	0.57
1:A:373:ASN:N	1:A:373:ASN:HD22	2.03	0.56
1:A:205:LYS:HE3	1:A:210:TYR:CZ	2.41	0.56
1:A:296:TYR:O	1:A:343:LYS:HA	2.06	0.56
1:A:107:LYS:HG2	5:A:966:HOH:O	2.04	0.56
1:A:191:ILE:CD1	1:A:204:ILE:HD13	2.36	0.56
1:A:239:MET:HE2	1:A:241:THR:HB	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:ARG:HG3	1:A:315:ARG:HH11	1.69	0.55
1:A:128:ARG:HG3	1:A:188:TRP:CZ2	2.41	0.55
1:A:369:MET:SD	1:A:403:ILE:CG2	2.94	0.55
1:A:273:HIS:CD2	1:A:294:ASN:H	2.25	0.55
1:A:182:CYS:HB3	1:A:229:CYS:O	2.07	0.54
1:A:235:ASP:OD1	1:A:257:ARG:HD2	2.06	0.54
1:A:191:ILE:HD12	1:A:204:ILE:HD13	1.90	0.54
1:A:368:THR:HA	1:A:377:MET:HE2	1.89	0.54
1:A:152:LYS:HG3	5:A:970:HOH:O	2.08	0.53
1:A:128:ARG:NH1	1:A:158:SER:OG	2.42	0.53
1:A:411:PHE:CZ	1:A:426:GLY:HA3	2.43	0.53
1:A:126:GLU:HG2	1:A:127:CYS:N	2.23	0.52
1:A:315:ARG:HB2	1:A:388:TRP:CE2	2.45	0.52
1:A:369:MET:CE	1:A:399:VAL:HG13	2.40	0.52
1:A:361:ILE:HG23	1:A:361:ILE:O	2.09	0.52
1:A:369:MET:SD	1:A:403:ILE:HG22	2.50	0.52
1:A:239:MET:HB2	1:A:253:PHE:CZ	2.44	0.52
1:A:369:MET:HE3	1:A:399:VAL:HG13	1.92	0.52
1:A:226:GLU:OE1	1:A:226:GLU:HA	2.10	0.51
1:A:315:ARG:CG	1:A:315:ARG:HH11	2.22	0.51
1:A:285:LYS:NZ	1:A:308:GLU:HB2	2.25	0.51
1:A:223:ARG:HG3	1:A:241:THR:CG2	2.41	0.51
1:A:134:HIS:CD2	1:A:146:THR:HA	2.45	0.50
1:A:201:LEU:HD11	1:A:213:THR:CB	2.29	0.50
1:A:372:THR:C	1:A:373:ASN:HD22	2.15	0.50
1:A:285:LYS:NZ	1:A:306:ASN:HD21	2.09	0.50
1:A:298:ALA:O	1:A:324:ASP:HB2	2.12	0.50
1:A:396:LEU:HD12	1:A:397:SER:H	1.76	0.49
1:A:77:GLU:HB3	1:A:186:ARG:NH2	2.27	0.49
1:A:225:GLN:O	1:A:226:GLU:HB2	2.11	0.49
1:A:360:LYS:HD3	1:A:383:TYR:CD2	2.47	0.49
1:A:177:TRP:CE2	1:A:194:ASP:HA	2.47	0.49
1:A:372:THR:OG1	1:A:373:ASN:ND2	2.45	0.49
1:A:239:MET:HE3	1:A:275:GLU:HA	1.95	0.48
1:A:216:SER:OG	1:A:219:HIS:HA	2.13	0.48
1:A:178:SER:HB3	1:A:193:VAL:HB	1.95	0.48
1:A:369:MET:CB	1:A:403:ILE:HG22	2.43	0.48
1:A:239:MET:HE1	1:A:275:GLU:HA	1.95	0.47
1:A:438:TRP:CZ3	1:A:440:SER:HB3	2.47	0.47
1:A:126:GLU:OE2	1:A:160:LYS:HG2	2.15	0.47
1:A:381:VAL:HG22	1:A:382:ARG:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:SER:HB2	4:A:468:RA2:H302	1.96	0.47
1:A:313:GLU:OE2	1:A:315:ARG:NE	2.37	0.47
1:A:202:VAL:O	1:A:213:THR:HA	2.15	0.47
1:A:300:ARG:O	1:A:317:MET:HG3	2.16	0.46
1:A:322:TYR:HB2	1:A:327:ARG:HD3	1.97	0.46
1:A:316:LEU:HD11	1:A:340:ASN:HD21	1.79	0.46
1:A:224:THR:OG1	1:A:238:LEU:HD11	2.16	0.45
1:A:252:ARG:HG2	1:A:266:LEU:HD23	1.99	0.45
1:A:396:LEU:HD12	1:A:397:SER:N	2.31	0.45
1:A:119:PHE:HA	1:A:411:PHE:CZ	2.52	0.45
1:A:263:LYS:HG2	1:A:264:GLU:N	2.32	0.44
1:A:369:MET:HB3	1:A:403:ILE:HG22	1.98	0.44
1:A:306:ASN:OD1	1:A:308:GLU:N	2.51	0.44
1:A:177:TRP:O	4:A:468:RA2:H421	2.18	0.43
1:A:227:SER:CB	1:A:349:LYS:HZ1	2.31	0.43
1:A:86:SER:HA	1:A:421:ASP:O	2.19	0.43
1:A:246:SER:HA	1:A:295:SER:CB	2.40	0.43
1:A:225:GLN:O	1:A:226:GLU:CB	2.66	0.42
1:A:181:ALA:O	1:A:228:ALA:HA	2.19	0.42
1:A:103:PHE:O	1:A:110:SER:HB2	2.19	0.42
1:A:176:ALA:HA	1:A:194:ASP:HB3	2.01	0.42
1:A:232:ILE:HG23	1:A:232:ILE:O	2.19	0.42
1:A:110:SER:HA	5:A:609:HOH:O	2.20	0.42
1:A:115:ILE:HG12	1:A:116:ARG:N	2.34	0.42
1:A:373:ASN:N	1:A:373:ASN:ND2	2.67	0.42
1:A:368:THR:HG22	1:A:377:MET:CE	2.50	0.42
1:A:143:TYR:CD1	1:A:438:TRP:HB3	2.54	0.42
1:A:353:VAL:HG22	1:A:354:HIS:N	2.35	0.41
1:A:256:ILE:HG22	5:A:758:HOH:O	2.20	0.41
1:A:305:LEU:HD23	1:A:305:LEU:C	2.41	0.41
1:A:327:ARG:HH12	1:A:371:LYS:HG2	1.83	0.41
1:A:130:PHE:CD2	1:A:158:SER:HB3	2.55	0.41
1:A:419:LYS:HB3	1:A:419:LYS:NZ	2.37	0.40
1:A:176:ALA:HB1	1:A:193:VAL:H	1.87	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%)	354 (91%)	31 (8%)	3 (1%)	22	24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	GLU
1	A	200	ALA
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%)	274 (84%)	52 (16%)	3	2

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	GLU
1	A	84	ARG
1	A	93	GLN
1	A	97	LEU
1	A	115	ILE
1	A	116	ARG
1	A	125	LYS
1	A	132	LEU

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Mol	Chain	Res	Type
1	A	135	TYR
1	A	148	LYS
1	A	153	LEU
1	A	160	LYS
1	A	168	GLU
1	A	171	ILE
1	A	201	LEU
1	A	204	ILE
1	A	225	GLN
1	A	229	CYS
1	A	238	LEU
1	A	258	GLU
1	A	260	ARG
1	A	268	THR
1	A	270	ARG
1	A	283	SER
1	A	285	LYS
1	A	292	ARG
1	A	315	ARG
1	A	320	LYS
1	A	327	ARG
1	A	329	ASP
1	A	338	GLU
1	A	339	SER
1	A	357	MET
1	A	359	SER
1	A	361	ILE
1	A	373	ASN
1	A	374	ARG
1	A	378	GLU
1	A	379	LEU
1	A	382	ARG
1	A	390	ASP
1	A	392	ASP
1	A	394	LEU
1	A	402	SER
1	A	403	ILE
1	A	404	GLU
1	A	419	LYS
1	A	435	LYS
1	A	453	GLN
1	A	454	LEU

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Mol	Chain	Res	Type
1	A	455	LEU
1	A	456	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	144	ASN
1	A	169	ASN
1	A	230	ASN
1	A	340	ASN
1	A	373	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 carbohydrates 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	#$\|Z\|>2$
2	NAG	A	467	-	14,14,15	1.31	2 (14%)	15,19,21	1.36	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|>2$	Counts	RMSZ	#$\|Z\|>2$
4	RA2	A	468	-	23,26,26	1.53	5 (21%)	25,37,37	1.35	4 (16%)

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	NAG	A	467	-	-	0/6/23/26	0/1/1/1
4	RA2	A	468	-	-	0/18/38/38	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	468	RA2	C2-N11	-2.24	1.40	1.43
4	A	468	RA2	C6-C1	2.24	1.42	1.38
2	A	467	NAG	C3-C2	2.30	1.57	1.52
4	A	468	RA2	C42-C29	2.87	1.56	1.53
4	A	468	RA2	C3-C2	3.02	1.44	1.40
4	A	468	RA2	C38-C29	3.45	1.57	1.53
2	A	467	NAG	C4-C3	3.98	1.62	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	468	RA2	C2-C3-N12	-3.30	118.48	123.10
4	A	468	RA2	C30-C31-C32	-3.09	101.22	104.63
2	A	467	NAG	O5-C1-C2	-2.70	107.72	111.47
2	A	467	NAG	C1-C2-N2	-2.64	105.98	110.49
4	A	468	RA2	O37-C32-N11	2.11	127.22	125.23
2	A	467	NAG	C6-C5-C4	2.19	118.13	113.00
4	A	468	RA2	C29-N11-C2	2.28	126.63	121.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	467	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	468	RA2	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 ⓘ

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	390/390 (100%)	-0.62	3 (0%)	86	92	2, 14, 31, 65	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	77	GLU	4.2
1	A	78	PRO	3.7
1	A	436	ASP	2.1

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å²)	Q<0.9
2	NAG	A	467	14/15	0.85	0.15	1.68	32,40,44,46	0
4	RA2	A	468	25/25	0.94	0.11	0.59	14,25,32,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	CA	A	500	1/1	0.99	0.06	-0.98	20,20,20,20	0
3	CA	A	501	1/1	0.95	0.12	-	40,40,40,40	0

6.5 Other polymers ⓘ

There are no such residues in this entry.