



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:30 PM UTC

PDB ID : 3NZU / pdb_00003nzu
Title : Structure-based Optimization of Pyrazolo -Pyrimidine and -Pyridine Inhibitors of PI3-Kinase
Authors : Murray, J.M.; Wiesmann, C.
Deposited on : 2010-07-16
Resolution : 2.60 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

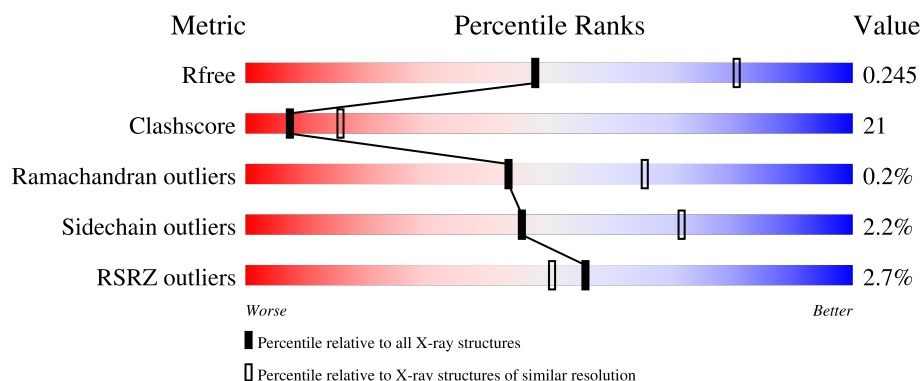
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

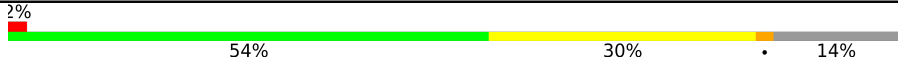
The reported resolution of this entry is 2.60 Å.

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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	954	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6697 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.

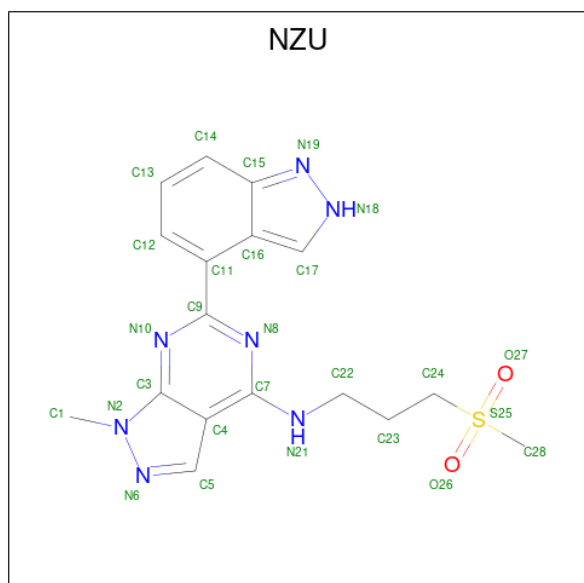
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	822	Total	C	N	O	S	37	0	0
			6670	4292	1137	1207	34			

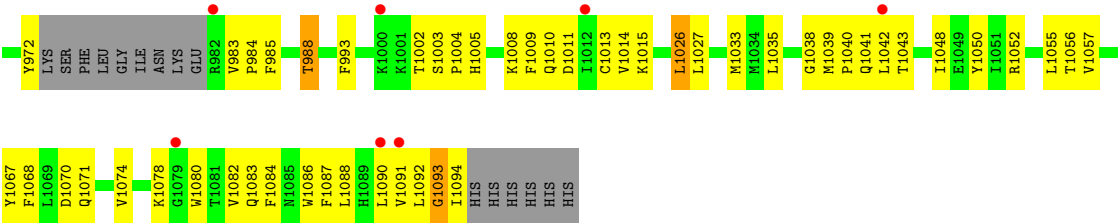
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1095	HIS	-	expression tag	UNP P48736
A	1096	HIS	-	expression tag	UNP P48736
A	1097	HIS	-	expression tag	UNP P48736
A	1098	HIS	-	expression tag	UNP P48736
A	1099	HIS	-	expression tag	UNP P48736
A	1100	HIS	-	expression tag	UNP P48736

- Molecule 2 is 6-(2H-indazol-4-yl)-1-methyl-N-[3-(methylsulfonyl)propyl]-1H-pyrazolo[3,4-d]pyrimidin-4-amine (CCD ID: NZU) (formula: C₁₇H₁₉N₇O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			27	17	7	2	1		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.00Å 67.68Å 106.36Å 90.00° 95.52° 90.00°	Depositor
Resolution (Å)	19.88 – 2.60 19.88 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.88-2.60) 99.6 (19.88-2.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 2.59Å)	Xtriage
Refinement program	PHENIX dev_392	Depositor
R, R_{free}	0.213 , 0.240 0.234 , 0.245	Depositor DCC
R_{free} test set	1588 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	70.7	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 60.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6697	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% 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: NZU

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	0.28	0/6814	0.72	8/9221 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	GLY	N-CA-C	-12.46	83.66	113.18
1	A	391	GLN	N-CA-C	-7.95	102.89	112.59
1	A	757	TYR	N-CA-C	5.56	126.56	111.00
1	A	788	ASP	CA-C-N	5.44	125.52	119.32
1	A	788	ASP	C-N-CA	5.44	125.52	119.32
1	A	988	THR	CA-C-N	5.19	125.49	119.47
1	A	988	THR	C-N-CA	5.19	125.49	119.47
1	A	916	PRO	CB-CA-C	-5.08	103.19	111.56

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	6670	0	6728	274	0
2	A	27	0	19	4	0
All	All	6697	0	6747	276	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 21.

All (276) 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:969:LEU:HD13	1:A:1039:MET:HE1	1.39	1.04
1:A:798:ILE:HD12	1:A:798:ILE:H	1.26	1.00
1:A:1092:LEU:HD11	1:A:1094:ILE:HG13	1.48	0.95
1:A:1041:GLN:HG2	1:A:1042:LEU:CD1	2.01	0.90
1:A:216:ALA:O	1:A:217:ASN:HB2	1.72	0.87
1:A:1041:GLN:HG2	1:A:1042:LEU:HD13	1.55	0.87
1:A:1092:LEU:CD1	1:A:1094:ILE:HG13	2.05	0.87
1:A:887:THR:HG22	1:A:889:ALA:H	1.40	0.86
1:A:955:THR:HG22	1:A:957:THR:H	1.40	0.84
1:A:905:GLU:HG2	1:A:993:PHE:CE1	2.15	0.81
1:A:969:LEU:CD1	1:A:1039:MET:HE1	2.11	0.80
1:A:182:THR:HB	1:A:183:PRO:HD3	1.63	0.79
1:A:776:ASN:O	1:A:777:SER:OG	2.01	0.79
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.65	0.79
1:A:278:ASP:HB2	1:A:792:LYS:HE3	1.64	0.78
1:A:774:LEU:O	1:A:778:GLN:HB2	1.88	0.73
1:A:809:LYS:N	1:A:810:PRO:HD3	2.04	0.73
1:A:905:GLU:HG2	1:A:993:PHE:CZ	2.24	0.72
1:A:579:ARG:HB2	1:A:610:LEU:HD11	1.72	0.72
1:A:798:ILE:H	1:A:798:ILE:CD1	2.02	0.72
1:A:697:TRP:CH2	1:A:739:ILE:HD13	2.26	0.71
1:A:887:THR:HG22	1:A:889:ALA:N	2.06	0.71
1:A:947:ARG:HD2	1:A:968:ILE:HD12	1.71	0.70
1:A:625:GLY:O	1:A:629:GLN:HG3	1.92	0.70
1:A:983:VAL:HG23	1:A:984:PRO:HD2	1.74	0.70
1:A:775:GLN:HA	1:A:779:LEU:CD2	2.22	0.69
1:A:919:GLU:HG3	1:A:920:LYS:N	2.06	0.69
1:A:935:TYR:O	1:A:939:THR:HB	1.93	0.69
1:A:969:LEU:HD13	1:A:1039:MET:CE	2.20	0.69
1:A:896:VAL:HG11	1:A:901:ALA:HB3	1.75	0.68
1:A:768:LYS:O	1:A:772:GLU:HG3	1.94	0.67
1:A:735:GLN:O	1:A:739:ILE:HD12	1.95	0.67
1:A:693:HIS:CD2	1:A:789:PRO:HG3	2.30	0.67
1:A:271:VAL:CG2	1:A:282:VAL:HG22	2.25	0.67
1:A:969:LEU:HD22	1:A:1039:MET:HE1	1.76	0.66
1:A:1092:LEU:HD11	1:A:1094:ILE:CG1	2.25	0.66
1:A:741:MET:HE1	1:A:779:LEU:CB	2.25	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1041:GLN:HE21	1:A:1042:LEU:HD13	1.62	0.65
1:A:219:CYS:SG	1:A:234:LYS:HG3	2.37	0.65
1:A:1092:LEU:HD12	1:A:1093:GLY:N	2.11	0.64
1:A:969:LEU:HD22	1:A:1039:MET:CE	2.27	0.64
1:A:799:GLU:CD	1:A:799:GLU:H	2.05	0.64
1:A:843:LEU:O	1:A:847:ILE:HG12	1.97	0.64
1:A:775:GLN:HA	1:A:779:LEU:HD21	1.80	0.63
1:A:232:THR:HG22	1:A:233:ILE:N	2.14	0.62
1:A:947:ARG:CD	1:A:968:ILE:HD12	2.29	0.62
1:A:425:LYS:HD2	1:A:672:TYR:OH	1.99	0.61
1:A:889:ALA:O	1:A:893:GLN:HG3	2.00	0.61
1:A:181:VAL:O	1:A:185:MET:HG3	2.01	0.61
1:A:951:ASN:HA	1:A:963:ILE:HD11	1.83	0.61
1:A:1087:PHE:CD2	1:A:1091:VAL:HG21	2.36	0.61
1:A:919:GLU:HG3	1:A:920:LYS:H	1.66	0.60
1:A:583:LEU:HD22	1:A:610:LEU:CD2	2.31	0.60
1:A:1010:GLN:O	1:A:1014:VAL:HG23	2.02	0.60
1:A:583:LEU:HD22	1:A:610:LEU:HD22	1.84	0.60
1:A:862:LEU:N	1:A:862:LEU:HD22	2.17	0.59
1:A:410:TRP:HB3	1:A:412:VAL:HG23	1.84	0.59
1:A:1087:PHE:O	1:A:1091:VAL:HB	2.01	0.59
1:A:925:VAL:O	1:A:929:VAL:HG23	2.03	0.59
1:A:864:LEU:C	1:A:866:PRO:HD3	2.28	0.59
1:A:905:GLU:HA	1:A:993:PHE:CD2	2.38	0.59
1:A:838:LEU:HD12	1:A:877:GLY:HA3	1.85	0.59
1:A:640:VAL:O	1:A:643:ILE:HG12	2.02	0.58
1:A:433:ILE:HG13	1:A:484:MET:HE1	1.86	0.58
1:A:784:ARG:HH12	1:A:792:LYS:HE3	1.68	0.58
1:A:953:MET:O	1:A:960:LEU:HD12	2.04	0.58
1:A:466:LEU:HD11	1:A:476:ARG:HD3	1.85	0.58
1:A:806:SER:HB3	1:A:810:PRO:CD	2.33	0.58
1:A:733:THR:O	1:A:737:GLN:HG3	2.02	0.58
1:A:622:LEU:HD13	1:A:647:LYS:HB3	1.85	0.58
1:A:1041:GLN:HG2	1:A:1042:LEU:HD12	1.84	0.58
1:A:154:LEU:O	1:A:158:ILE:HG13	2.04	0.57
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.85	0.57
1:A:939:THR:HG23	1:A:945:GLY:HA3	1.87	0.57
1:A:838:LEU:HD12	1:A:877:GLY:CA	2.34	0.57
1:A:207:LEU:HD12	1:A:208:PRO:HD2	1.87	0.57
1:A:775:GLN:NE2	1:A:795:ALA:HB1	2.19	0.57
1:A:798:ILE:HD12	1:A:798:ILE:N	2.07	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:THR:HG22	1:A:233:ILE:H	1.69	0.56
1:A:555:LEU:O	1:A:559:ILE:HG13	2.05	0.56
1:A:697:TRP:HH2	1:A:739:ILE:HD13	1.67	0.56
1:A:969:LEU:CG	1:A:1039:MET:HE1	2.35	0.56
1:A:1041:GLN:CG	1:A:1042:LEU:HD13	2.33	0.56
1:A:625:GLY:HA2	1:A:1026:LEU:HD23	1.86	0.56
1:A:1092:LEU:HD12	1:A:1093:GLY:H	1.70	0.56
1:A:402:LYS:HG3	1:A:403:PRO:HD2	1.87	0.56
1:A:1088:LEU:HB3	1:A:1094:ILE:HB	1.87	0.56
1:A:274:VAL:HG21	1:A:292:TRP:CD1	2.41	0.56
1:A:914:LYS:O	1:A:916:PRO:HD3	2.06	0.56
1:A:988:THR:HG21	1:A:1083:GLN:HG3	1.88	0.56
1:A:483:HIS:CD2	1:A:510:LYS:HG2	2.41	0.56
1:A:271:VAL:HG21	1:A:282:VAL:CG2	2.36	0.55
1:A:760:SER:OG	1:A:763:VAL:HG12	2.06	0.55
1:A:969:LEU:CD2	1:A:1039:MET:HE1	2.36	0.55
1:A:461:LEU:HD22	1:A:461:LEU:N	2.22	0.55
1:A:767:LEU:HD22	1:A:803:VAL:HG23	1.88	0.55
1:A:796:LEU:HD21	1:A:815:PHE:CZ	2.41	0.55
1:A:779:LEU:HD12	1:A:779:LEU:O	2.07	0.55
1:A:757:TYR:N	1:A:757:TYR:CD2	2.72	0.55
1:A:1074:VAL:O	1:A:1078:LYS:HG2	2.06	0.55
1:A:743:GLN:O	1:A:747:LEU:HG	2.06	0.54
1:A:702:GLU:O	1:A:706:SER:HB3	2.07	0.54
1:A:731:ASP:O	1:A:735:GLN:HG3	2.08	0.54
1:A:477:ARG:HG2	1:A:478:GLY:N	2.22	0.54
1:A:983:VAL:CG2	1:A:984:PRO:HD2	2.38	0.54
1:A:955:THR:HG22	1:A:956:GLU:N	2.22	0.54
1:A:775:GLN:HA	1:A:779:LEU:HG	1.89	0.54
1:A:1082:VAL:HG12	1:A:1086:TRP:CD1	2.43	0.54
1:A:738:VAL:HA	1:A:741:MET:HE2	1.88	0.53
1:A:270:PHE:CG	1:A:307:LEU:HD21	2.44	0.53
1:A:1088:LEU:O	1:A:1092:LEU:HG	2.08	0.53
1:A:187:GLU:OE2	1:A:683:LYS:HG3	2.08	0.53
1:A:463:TYR:CE1	1:A:501:LYS:HA	2.44	0.53
1:A:779:LEU:HD12	1:A:779:LEU:C	2.34	0.53
1:A:939:THR:HG23	1:A:945:GLY:CA	2.39	0.53
1:A:364:LYS:HE3	1:A:413:TRP:CE2	2.44	0.53
1:A:202:VAL:HG12	1:A:290:PHE:CD2	2.44	0.52
1:A:918:GLU:O	1:A:921:PHE:HB3	2.09	0.52
1:A:775:GLN:OE1	1:A:798:ILE:HD11	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:806:SER:HB3	1:A:810:PRO:HD2	1.91	0.52
1:A:957:THR:HG22	1:A:957:THR:O	2.10	0.52
1:A:775:GLN:HA	1:A:779:LEU:CG	2.40	0.52
1:A:466:LEU:HD11	1:A:476:ARG:CD	2.40	0.52
1:A:963:ILE:C	1:A:963:ILE:HD12	2.35	0.51
1:A:216:ALA:O	1:A:217:ASN:CB	2.48	0.51
1:A:271:VAL:HG22	1:A:272:LEU:N	2.25	0.51
1:A:917:THR:OG1	1:A:920:LYS:HG3	2.10	0.51
1:A:422:ASP:HB3	1:A:599:GLY:O	2.11	0.50
1:A:429:LEU:HB2	1:A:468:LEU:CD2	2.40	0.50
1:A:182:THR:CB	1:A:183:PRO:HD3	2.39	0.50
1:A:373:LEU:C	1:A:373:LEU:HD12	2.37	0.50
1:A:1041:GLN:NE2	1:A:1042:LEU:HD13	2.26	0.50
1:A:500:ASP:HB3	1:A:708:HIS:CD2	2.47	0.50
1:A:852:GLU:OE2	1:A:864:LEU:HB2	2.11	0.50
1:A:895:THR:HG22	1:A:896:VAL:HG23	1.94	0.50
1:A:959:ASN:C	1:A:959:ASN:HD22	2.20	0.50
1:A:472:ARG:O	1:A:473:PHE:HB2	2.12	0.49
1:A:831:ILE:HG13	1:A:881:ILE:CG1	2.42	0.49
1:A:844:ILE:O	1:A:848:LEU:HG	2.12	0.49
1:A:852:GLU:HG3	1:A:864:LEU:HD12	1.94	0.49
2:A:1:NZU:H17	2:A:1:NZU:N10	2.28	0.49
2:A:1:NZU:N10	2:A:1:NZU:C17	2.76	0.49
1:A:301:GLU:HG2	1:A:302:GLU:N	2.28	0.49
1:A:271:VAL:HG21	1:A:282:VAL:HG21	1.95	0.48
1:A:786:PRO:HG2	1:A:878:MET:SD	2.53	0.48
1:A:554:GLN:O	1:A:558:ILE:HG13	2.12	0.48
1:A:608:TYR:CZ	1:A:639:ASN:ND2	2.80	0.48
1:A:886:THR:HG21	1:A:910:TRP:CZ2	2.48	0.48
1:A:886:THR:CG2	1:A:910:TRP:CZ2	2.96	0.48
1:A:898:ASN:O	1:A:1087:PHE:HZ	1.97	0.48
1:A:307:LEU:C	1:A:307:LEU:HD23	2.39	0.48
1:A:234:LYS:HB2	1:A:234:LYS:NZ	2.29	0.47
1:A:1041:GLN:CD	1:A:1041:GLN:H	2.22	0.47
1:A:734:GLN:O	1:A:738:VAL:HG23	2.13	0.47
1:A:589:TYR:HB2	1:A:590:PRO:HD3	1.95	0.47
1:A:741:MET:HE1	1:A:779:LEU:HA	1.94	0.47
1:A:887:THR:O	1:A:891:ILE:HG13	2.14	0.47
1:A:605:ALA:O	1:A:609:GLN:HG3	2.14	0.47
1:A:750:LYS:NZ	1:A:834:HIS:HD2	2.12	0.47
1:A:1005:HIS:O	1:A:1008:LYS:HB3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:LEU:HD12	1:A:373:LEU:O	2.15	0.47
1:A:840:GLN:O	1:A:844:ILE:HG12	2.14	0.47
1:A:760:SER:O	1:A:763:VAL:HG13	2.13	0.47
1:A:706:SER:O	1:A:710:GLN:HB3	2.15	0.47
1:A:1086:TRP:HE3	1:A:1090:LEU:HD13	1.80	0.46
1:A:181:VAL:HG22	1:A:184:ARG:HH22	1.81	0.46
1:A:702:GLU:OE1	1:A:702:GLU:HA	2.15	0.46
1:A:815:PHE:O	1:A:827:THR:HB	2.16	0.46
1:A:917:THR:HB	1:A:919:GLU:HG2	1.97	0.46
1:A:180:LEU:C	1:A:183:PRO:HD2	2.41	0.46
1:A:280:TYR:HB3	1:A:282:VAL:HG23	1.97	0.46
1:A:661:LEU:O	1:A:665:GLN:HG2	2.16	0.46
1:A:1070:ASP:O	1:A:1074:VAL:HG23	2.16	0.46
1:A:912:LYS:HG3	1:A:921:PHE:CE1	2.51	0.46
1:A:235:VAL:HG12	1:A:236:SER:N	2.31	0.46
1:A:1052:ARG:O	1:A:1057:VAL:HG23	2.17	0.46
1:A:148:GLN:C	1:A:150:PHE:H	2.23	0.45
1:A:955:THR:CG2	1:A:956:GLU:N	2.78	0.45
1:A:651:LEU:HD22	1:A:655:ASP:HB3	1.97	0.45
1:A:363:VAL:HG12	1:A:416:PHE:HE1	1.81	0.45
1:A:589:TYR:CD2	1:A:593:PHE:HE1	2.34	0.45
1:A:804:MET:HE3	2:A:1:NZU:H22	1.98	0.45
1:A:274:VAL:HG11	1:A:292:TRP:CE2	2.52	0.45
1:A:689:LYS:HG2	1:A:728:MET:SD	2.56	0.45
1:A:760:SER:O	1:A:763:VAL:CG1	2.64	0.45
1:A:818:ALA:O	1:A:820:PRO:HD3	2.16	0.45
1:A:1055:LEU:O	1:A:1056:THR:C	2.59	0.45
1:A:555:LEU:HD11	1:A:575:LEU:HD23	1.98	0.45
1:A:302:GLU:HG3	1:A:304:HIS:NE2	2.32	0.44
1:A:1035:LEU:HD12	1:A:1039:MET:HG3	1.99	0.44
1:A:858:GLU:O	1:A:859:SER:HB2	2.17	0.44
1:A:721:LEU:O	1:A:729:LEU:HD21	2.17	0.44
1:A:187:GLU:OE1	1:A:687:ARG:HG3	2.17	0.44
1:A:201:TRP:CE2	1:A:291:GLN:HG3	2.53	0.44
1:A:1050:TYR:CD2	1:A:1050:TYR:C	2.94	0.44
1:A:1084:PHE:O	1:A:1087:PHE:HB3	2.18	0.44
1:A:275:CYS:HB3	1:A:823:LEU:HD13	1.99	0.44
1:A:687:ARG:HG3	1:A:687:ARG:HH11	1.82	0.44
1:A:184:ARG:HD3	1:A:719:ALA:O	2.17	0.43
1:A:562:ASP:HB2	1:A:563:PRO:HD2	1.99	0.43
1:A:741:MET:HE1	1:A:779:LEU:CA	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:775:GLN:NE2	1:A:796:LEU:H	2.16	0.43
1:A:796:LEU:CD2	1:A:815:PHE:CE2	3.01	0.43
1:A:423:LEU:HA	1:A:424:PRO:HD3	1.88	0.43
1:A:776:ASN:C	1:A:777:SER:HG	2.13	0.43
1:A:804:MET:CE	2:A:1:NZU:H22	2.47	0.43
1:A:889:ALA:HB2	1:A:949:ASN:OD1	2.18	0.43
1:A:565:ASN:HA	1:A:566:PRO:HD3	1.82	0.43
1:A:802:LYS:HG3	1:A:812:TRP:HB3	1.99	0.43
1:A:809:LYS:N	1:A:810:PRO:CD	2.76	0.43
1:A:418:ILE:HD13	1:A:423:LEU:HD23	1.99	0.43
1:A:435:CYS:SG	1:A:461:LEU:HD21	2.58	0.43
1:A:862:LEU:N	1:A:862:LEU:CD2	2.81	0.43
1:A:862:LEU:HD22	1:A:862:LEU:H	1.83	0.43
1:A:1038:GLY:C	1:A:1040:PRO:HD3	2.43	0.43
1:A:199:HIS:N	1:A:200:PRO:HD3	2.34	0.43
1:A:148:GLN:C	1:A:150:PHE:N	2.76	0.43
1:A:232:THR:CG2	1:A:233:ILE:N	2.82	0.43
1:A:234:LYS:NZ	1:A:234:LYS:CB	2.82	0.43
1:A:271:VAL:HG22	1:A:272:LEU:H	1.82	0.43
1:A:393:VAL:O	1:A:393:VAL:HG23	2.18	0.43
1:A:775:GLN:NE2	1:A:796:LEU:N	2.67	0.43
1:A:235:VAL:CG1	1:A:236:SER:N	2.82	0.42
1:A:282:VAL:HG12	1:A:283:GLY:N	2.34	0.42
1:A:931:SER:O	1:A:935:TYR:HD1	2.02	0.42
1:A:182:THR:HB	1:A:183:PRO:CD	2.43	0.42
1:A:1011:ASP:O	1:A:1015:LYS:HG3	2.20	0.42
1:A:1039:MET:O	1:A:1043:THR:HG23	2.19	0.42
1:A:382:PHE:C	1:A:382:PHE:CD2	2.96	0.42
1:A:741:MET:HE1	1:A:779:LEU:HB3	1.99	0.42
1:A:891:ILE:O	1:A:891:ILE:HG22	2.19	0.42
1:A:624:VAL:O	1:A:628:MET:HG2	2.19	0.42
1:A:234:LYS:HB2	1:A:234:LYS:HZ2	1.84	0.42
1:A:939:THR:CG2	1:A:945:GLY:CA	2.98	0.42
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.54	0.42
1:A:564:LEU:CD1	1:A:1048:ILE:HG22	2.47	0.42
1:A:968:ILE:HG12	1:A:968:ILE:O	2.19	0.42
1:A:972:TYR:HB3	1:A:1042:LEU:HD11	2.02	0.42
1:A:165:VAL:O	1:A:168:VAL:HG22	2.20	0.41
1:A:281:LEU:HD12	1:A:305:VAL:HG11	2.02	0.41
1:A:507:ASN:HA	1:A:508:PRO:HD3	1.85	0.41
1:A:1067:TYR:O	1:A:1071:GLN:HG2	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:832:PHE:CE2	1:A:878:MET:HE2	2.55	0.41
1:A:476:ARG:HG2	1:A:520:LEU:HD22	2.02	0.41
1:A:1092:LEU:CD1	1:A:1093:GLY:H	2.33	0.41
1:A:301:GLU:HG2	1:A:302:GLU:H	1.85	0.41
1:A:865:LEU:HA	1:A:865:LEU:HD12	1.80	0.41
1:A:1002:THR:O	1:A:1003:SER:HB3	2.21	0.41
1:A:240:THR:HB	1:A:241:PRO:HD2	2.02	0.41
1:A:371:PRO:HG2	1:A:511:GLU:O	2.21	0.41
1:A:892:GLN:HE22	1:A:1080:TRP:HH2	1.68	0.41
1:A:201:TRP:NE1	1:A:291:GLN:HG3	2.36	0.41
1:A:223:VAL:HG12	1:A:225:HIS:NE2	2.36	0.41
1:A:808:LYS:C	1:A:810:PRO:HD3	2.45	0.41
1:A:810:PRO:HB3	1:A:833:LYS:HB2	2.02	0.41
1:A:945:GLY:O	1:A:985:PHE:HA	2.20	0.41
1:A:424:PRO:HD2	1:A:427:ALA:HB2	2.02	0.41
1:A:699:LEU:O	1:A:703:ILE:HG13	2.21	0.41
1:A:775:GLN:CA	1:A:779:LEU:HD21	2.49	0.41
1:A:831:ILE:HG13	1:A:881:ILE:HG12	2.02	0.41
1:A:915:SER:OG	1:A:921:PHE:HB2	2.21	0.41
1:A:919:GLU:CG	1:A:920:LYS:N	2.81	0.41
1:A:703:ILE:CD1	1:A:714:ALA:HA	2.51	0.41
1:A:461:LEU:N	1:A:461:LEU:CD2	2.85	0.40
1:A:176:THR:O	1:A:180:LEU:HG	2.22	0.40
1:A:846:GLN:OE1	1:A:846:GLN:HA	2.22	0.40
1:A:929:VAL:HG13	1:A:1009:PHE:HB2	2.02	0.40
1:A:198:MET:SD	1:A:282:VAL:HG21	2.61	0.40
1:A:393:VAL:O	1:A:393:VAL:CG2	2.69	0.40
1:A:632:ASP:HB3	1:A:1033:MET:HE3	2.04	0.40
1:A:1003:SER:HA	1:A:1004:PRO:HD3	1.87	0.40
1:A:278:ASP:HB2	1:A:792:LYS:CE	2.44	0.40
1:A:364:LYS:HE3	1:A:413:TRP:NE1	2.37	0.40
1:A:380:THR:O	1:A:435:CYS:HA	2.22	0.40
1:A:593:PHE:CE2	1:A:611:LEU:HD21	2.56	0.40
1:A:633:CYS:HB3	1:A:669:PHE:CE2	2.57	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	806/954 (84%)	759 (94%)	45 (6%)	2 (0%)	43	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	ASN
1	A	1093	GLY

5.3.2 Protein sidechains [i](#)

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	740/854 (87%)	724 (98%)	16 (2%)	45	72

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	234	LYS
1	A	393	VAL
1	A	610	LEU
1	A	739	ILE
1	A	757	TYR
1	A	763	VAL
1	A	764	ILE
1	A	798	ILE
1	A	832	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	862	LEU
1	A	865	LEU
1	A	886	THR
1	A	907	LEU
1	A	939	THR
1	A	1026	LEU
1	A	1027	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	396	GLN
1	A	634	ASN
1	A	705	GLN
1	A	708	HIS
1	A	730	HIS
1	A	743	GLN
1	A	834	HIS
1	A	840	GLN
1	A	959	ASN

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](#)

1 ligand is 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	NZU	A	1	-	29,30,30	2.24	15 (51%)	34,44,44	2.77	10 (29%)

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	NZU	A	1	-	-	5/12/12/12	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	NZU	C17-N18	-4.01	1.28	1.34
2	A	1	NZU	C5-N6	-3.91	1.27	1.32
2	A	1	NZU	C11-C16	-3.71	1.39	1.44
2	A	1	NZU	C3-N10	-3.46	1.29	1.34
2	A	1	NZU	O26-S25	-3.04	1.38	1.44
2	A	1	NZU	C7-N8	-2.85	1.29	1.34
2	A	1	NZU	C14-C15	-2.64	1.37	1.40
2	A	1	NZU	C4-C7	-2.55	1.39	1.42
2	A	1	NZU	C9-N10	-2.54	1.28	1.34
2	A	1	NZU	O27-S25	-2.54	1.39	1.44
2	A	1	NZU	C15-C16	-2.51	1.38	1.43
2	A	1	NZU	C24-S25	2.42	1.81	1.78
2	A	1	NZU	C4-C5	-2.28	1.39	1.42
2	A	1	NZU	C3-N2	-2.08	1.32	1.35
2	A	1	NZU	C9-N8	-2.01	1.29	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	NZU	C4-C3-N10	-11.86	119.03	126.56
2	A	1	NZU	C1-N2-N6	4.73	125.91	120.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	NZU	C1-N2-C3	-4.39	125.21	128.30
2	A	1	NZU	C5-N6-N2	3.59	108.90	106.36
2	A	1	NZU	C4-C5-N6	-3.04	109.07	111.38
2	A	1	NZU	C9-C11-C16	-2.49	120.41	123.35
2	A	1	NZU	C7-N8-C9	2.36	120.61	116.36
2	A	1	NZU	C3-N2-N6	-2.24	108.88	110.91
2	A	1	NZU	O27-S25-C24	2.10	109.84	108.33
2	A	1	NZU	C17-N18-N19	-2.03	109.48	112.59

There are no chirality outliers.

All (5) torsion outliers are listed below:

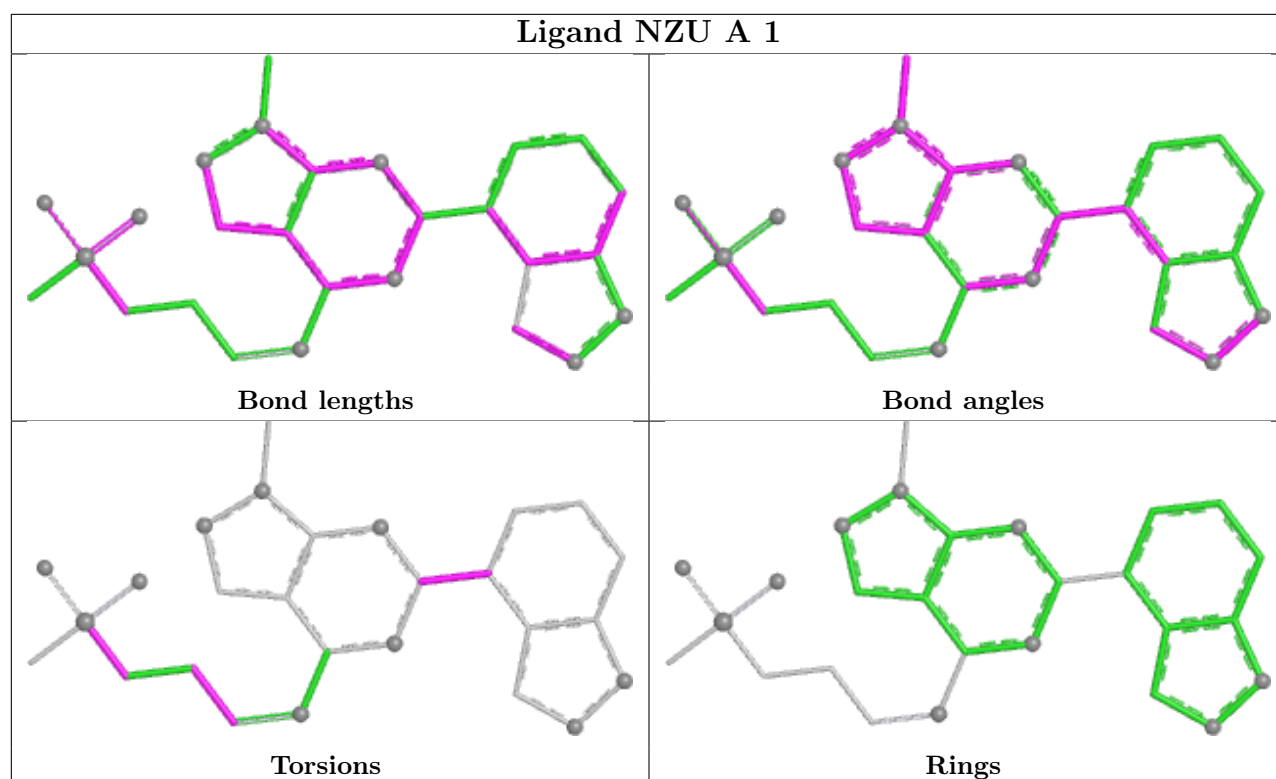
Mol	Chain	Res	Type	Atoms
2	A	1	NZU	C23-C24-S25-O26
2	A	1	NZU	C23-C24-S25-O27
2	A	1	NZU	C23-C24-S25-C28
2	A	1	NZU	N21-C22-C23-C24
2	A	1	NZU	C16-C11-C9-N10

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	NZU	4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	818/954 (85%)	-0.00	22 (2%)	56 50	43, 91, 157, 208	1 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1000	LYS	4.9
1	A	778	GLN	4.4
1	A	777	SER	4.3
1	A	982	ARG	4.2
1	A	779	LEU	4.1
1	A	248	PHE	3.4
1	A	1012	ILE	3.1
1	A	1090	LEU	3.0
1	A	391	GLN	2.8
1	A	809	LYS	2.8
1	A	295	HIS	2.7
1	A	1042	LEU	2.7
1	A	907	LEU	2.4
1	A	435	CYS	2.4
1	A	521	ASP	2.3
1	A	307	LEU	2.2
1	A	278	ASP	2.2
1	A	379	LEU	2.2
1	A	758	ASP	2.1
1	A	357	CYS	2.1
1	A	1079	GLY	2.0
1	A	1091	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](#)

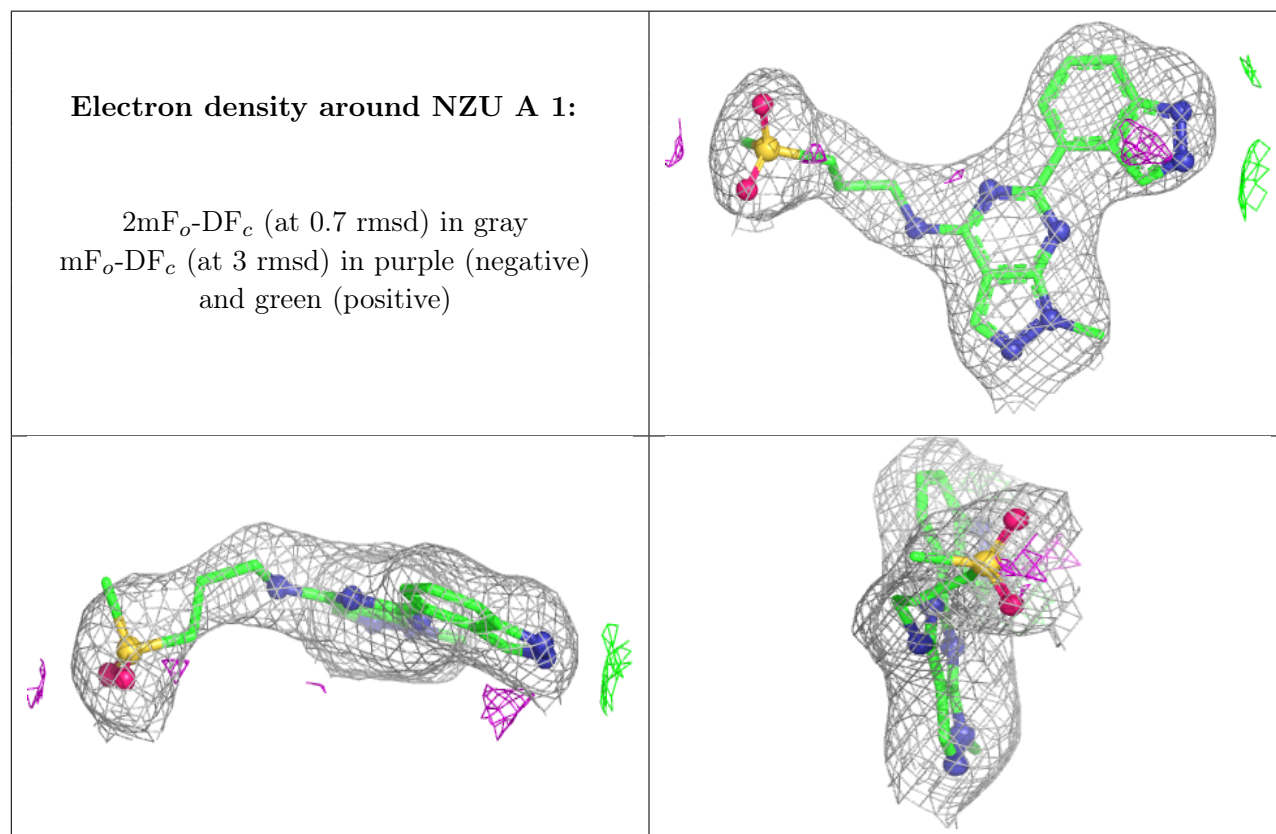
There are no oligosaccharides in this entry.

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	NZU	A	1	27/27	0.88	0.11	70,77,118,124	0

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.



6.5 Other polymers [i](#)

There are no such residues in this entry.