



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:24 AM UTC

PDB ID : 3ENE / pdb_00003ene
Title : Complex of PI3K gamma with an inhibitor
Authors : Apsel, B.; Blair, J.A.; Gonzalez, B.Z.; Nazif, T.M.; Feldman, M.E.; Williams, R.L.; Shokat, K.M.; Knight, Z.A.
Deposited on : 2008-09-25
Resolution : 2.40 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

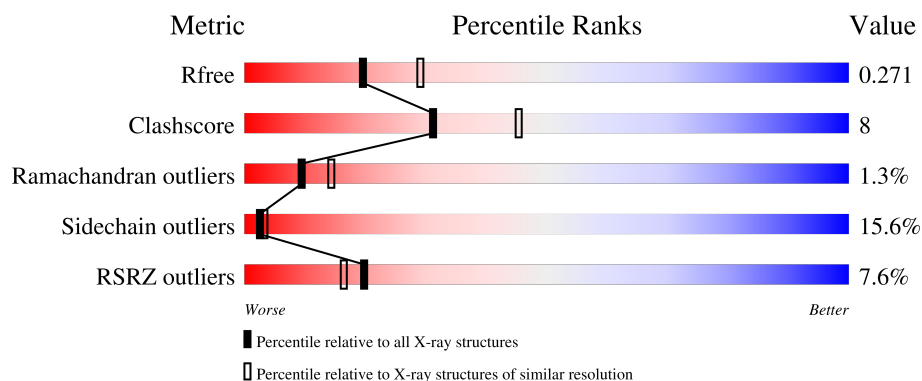
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 $\leq 5\%$. 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	959	7% 64% 19% 5% 12%

2 Entry composition [i](#)

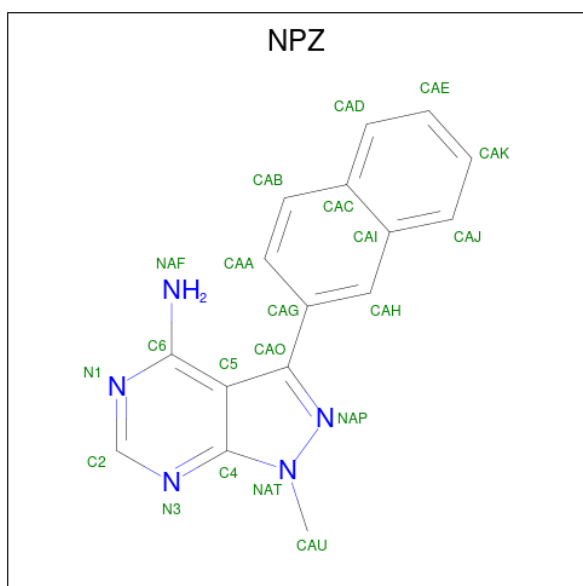
There are 3 unique types of molecules in this entry. The entry contains 6904 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	843	Total	C	N	O	S	0	0	0
			6845	4395	1171	1244	35			

- Molecule 2 is 1-methyl-3-naphthalen-2-yl-1H-pyrazolo[3,4-d]pyrimidin-4-amine (CCD ID: NPZ) (formula: C₁₆H₁₃N₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			21	16	5		

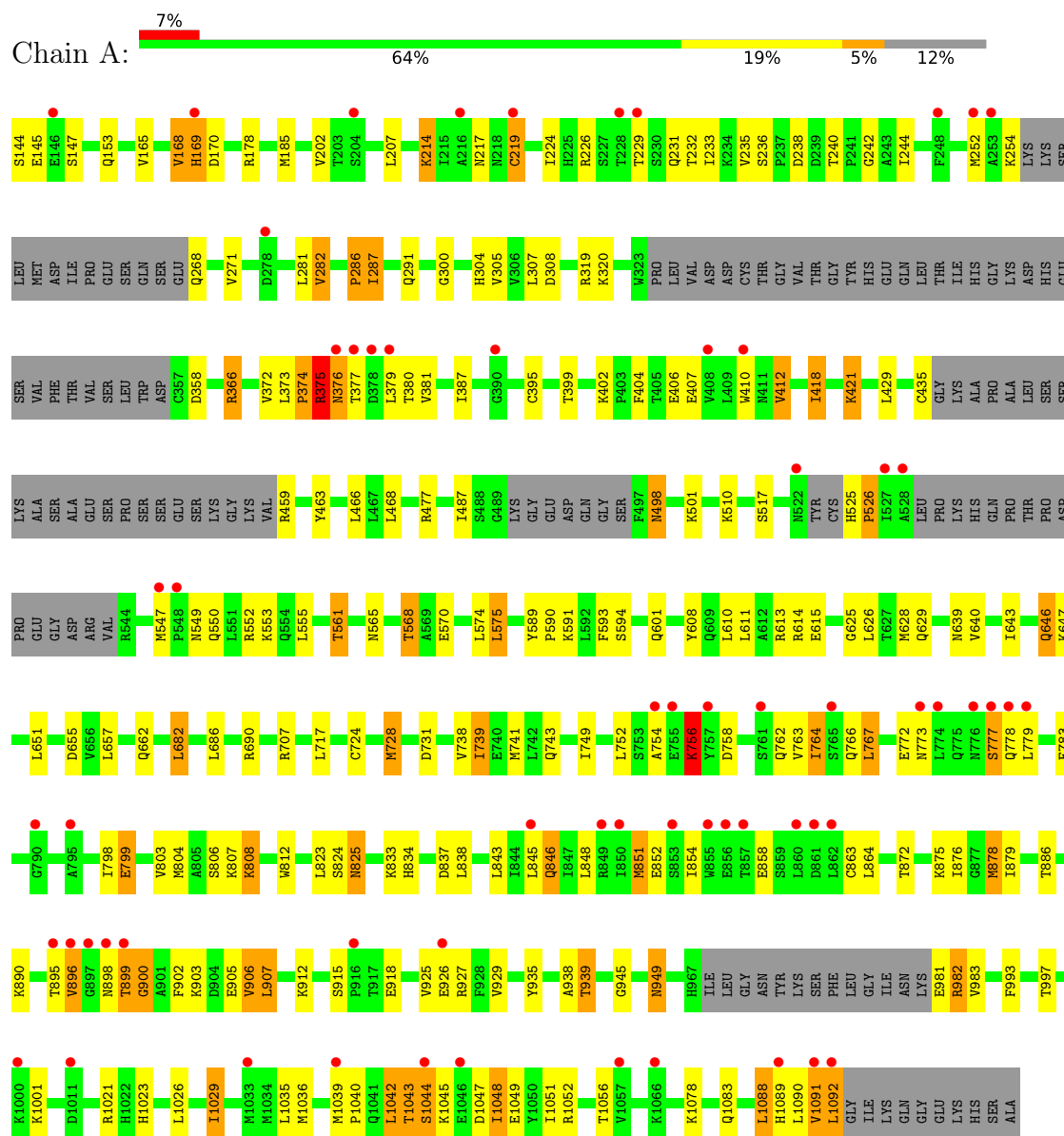
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total	O	0	0
			38	38		

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: Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.30Å 68.24Å 106.07Å 90.00° 95.19° 90.00°	Depositor
Resolution (Å)	57.07 – 2.40 57.07 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (57.07-2.40) 99.3 (57.07-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.227 , 0.276 0.228 , 0.271	Depositor DCC
R_{free} test set	1636 reflections (4.07%)	wwPDB-VP
Wilson B-factor (Å ²)	46.3	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.6	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	0.91	EDS
Total number of atoms	6904	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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: NPZ

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	0.94	9/6993 (0.1%)	1.01	7/9459 (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	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	851	MET	SD-CE	-15.96	1.39	1.79
1	A	728	MET	SD-CE	-8.44	1.58	1.79
1	A	762	GLN	CG-CD	8.09	1.72	1.52
1	A	900	GLY	C-N	7.84	1.44	1.33
1	A	547	MET	CG-SD	7.49	1.99	1.80
1	A	878	MET	SD-CE	7.28	1.97	1.79
1	A	169	HIS	CA-CB	6.59	1.65	1.53
1	A	739	ILE	CA-CB	6.01	1.61	1.54
1	A	185	MET	SD-CE	-5.32	1.66	1.79

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	808	LYS	N-CA-C	-7.46	100.91	110.53
1	A	906	VAL	CB-CA-C	-5.96	102.92	112.16
1	A	286	PRO	CA-C-O	-5.64	115.02	121.56
1	A	907	LEU	N-CA-C	-5.57	105.12	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	HIS	N-CA-C	-5.47	106.66	113.38
1	A	899	THR	N-CA-C	5.39	117.93	108.56
1	A	762	GLN	OE1-CD-NE2	-5.30	117.30	122.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	526	PRO	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	6845	0	6887	110	0
2	A	21	0	13	3	0
3	A	38	0	0	3	0
All	All	6904	0	6900	113	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 8.

All (113) 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:525:HIS:HB3	1:A:526:PRO:HD3	1.26	1.16
1:A:561:THR:HG21	1:A:565:ASN:HD22	1.33	0.92
1:A:614:ARG:HD2	3:A:99:HOH:O	1.78	0.84
1:A:851:MET:HE1	1:A:938:ALA:CB	2.07	0.83
1:A:935:TYR:O	1:A:939:THR:HB	1.79	0.83
1:A:851:MET:HE1	1:A:938:ALA:HB1	1.62	0.81
1:A:825:ASN:HD22	1:A:825:ASN:N	1.78	0.81
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.28	0.81
1:A:525:HIS:HB3	1:A:526:PRO:CD	2.08	0.80
1:A:1088:LEU:O	1:A:1091:VAL:HG22	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:GLN:NE2	3:A:99:HOH:O	2.18	0.76
2:A:1:NPZ:H1AF	2:A:1:NPZ:CAA	2.01	0.74
1:A:410:TRP:HB3	1:A:412:VAL:HG22	1.69	0.74
1:A:550:GLN:HE22	1:A:553:LYS:CE	2.01	0.73
1:A:743:GLN:NE2	1:A:872:THR:OG1	2.21	0.72
1:A:767:LEU:HD12	1:A:803:VAL:HG23	1.75	0.69
1:A:380:THR:O	1:A:435:CYS:HB3	1.93	0.69
1:A:214:LYS:NZ	1:A:300:GLY:HA2	2.12	0.65
1:A:271:VAL:HG23	1:A:282:VAL:HG13	1.79	0.65
1:A:568:THR:HG22	1:A:570:GLU:H	1.62	0.64
1:A:834:HIS:HB2	1:A:876:ILE:HD12	1.80	0.64
1:A:899:THR:HG23	1:A:899:THR:O	1.97	0.63
1:A:165:VAL:HG12	1:A:165:VAL:O	2.01	0.61
1:A:728:MET:HE1	3:A:39:HOH:O	2.00	0.60
1:A:738:VAL:HG21	1:A:783:PHE:CD1	2.38	0.59
1:A:1036:MET:HA	1:A:1042:LEU:HD11	1.86	0.57
1:A:1089:HIS:O	1:A:1092:LEU:N	2.37	0.57
1:A:804:MET:HE2	1:A:812:TRP:HB2	1.87	0.57
1:A:231:GLN:HE21	1:A:232:THR:H	1.53	0.56
1:A:825:ASN:N	1:A:825:ASN:ND2	2.50	0.56
1:A:939:THR:HG23	1:A:945:GLY:HA2	1.88	0.56
1:A:375:ARG:O	1:A:376:ASN:ND2	2.38	0.56
1:A:561:THR:HG21	1:A:565:ASN:ND2	2.14	0.55
2:A:1:NPZ:CAA	2:A:1:NPZ:NAF	2.70	0.55
1:A:593:PHE:CZ	1:A:611:LEU:HD21	2.41	0.55
1:A:799:GLU:H	1:A:799:GLU:CD	2.14	0.55
1:A:550:GLN:HE22	1:A:553:LYS:HE3	1.71	0.55
1:A:550:GLN:HE22	1:A:553:LYS:NZ	2.05	0.53
1:A:949:ASN:H	1:A:1083:GLN:NE2	2.03	0.53
1:A:756:LYS:HA	1:A:756:LYS:NZ	2.24	0.53
1:A:608:TYR:CZ	1:A:639:ASN:ND2	2.76	0.52
1:A:395:CYS:HB3	1:A:418:ILE:HD11	1.92	0.51
1:A:741:MET:HE1	1:A:778:GLN:O	2.11	0.51
1:A:1039:MET:HB3	1:A:1040:PRO:CD	2.40	0.51
1:A:308:ASP:N	1:A:308:ASP:OD1	2.39	0.51
1:A:900:GLY:O	1:A:902:PHE:CD1	2.64	0.51
1:A:981:GLU:N	1:A:982:ARG:CZ	2.73	0.51
1:A:380:THR:O	1:A:435:CYS:CB	2.59	0.50
1:A:498:ASN:OD1	1:A:498:ASN:C	2.55	0.50
1:A:905:GLU:HG2	1:A:993:PHE:CE2	2.47	0.50
1:A:410:TRP:HB3	1:A:412:VAL:CG2	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.95	0.49
2:A:1:NPZ:NAF	2:A:1:NPZ:HAA	2.27	0.49
1:A:217:ASN:HD22	1:A:219:CYS:HB3	1.78	0.48
1:A:935:TYR:O	1:A:939:THR:CB	2.56	0.48
1:A:640:VAL:O	1:A:643:ILE:HG12	2.14	0.48
1:A:808:LYS:HG3	1:A:833:LYS:NZ	2.29	0.48
1:A:399:THR:HB	1:A:410:TRP:CD1	2.49	0.48
1:A:568:THR:HG22	1:A:570:GLU:N	2.28	0.48
1:A:463:TYR:CE1	1:A:501:LYS:HA	2.49	0.47
1:A:949:ASN:N	1:A:1083:GLN:HE22	2.05	0.47
1:A:1036:MET:HG2	1:A:1042:LEU:HD21	1.96	0.47
1:A:682:LEU:HD22	1:A:686:LEU:CD1	2.45	0.46
1:A:925:VAL:O	1:A:929:VAL:HG23	2.15	0.46
1:A:878:MET:C	1:A:879:ILE:HG13	2.41	0.46
1:A:777:SER:HB3	1:A:778:GLN:NE2	2.30	0.46
1:A:240:THR:HG22	1:A:242:GLY:H	1.81	0.46
1:A:550:GLN:NE2	1:A:553:LYS:HE3	2.31	0.46
1:A:165:VAL:O	1:A:165:VAL:CG1	2.64	0.45
1:A:399:THR:HB	1:A:410:TRP:NE1	2.31	0.45
1:A:662:GLN:HE22	1:A:846:GLN:HB3	1.81	0.45
1:A:651:LEU:HD22	1:A:655:ASP:HB3	1.98	0.45
1:A:852:GLU:HG3	1:A:864:LEU:HD12	1.98	0.45
1:A:168:VAL:HG13	1:A:170:ASP:O	2.17	0.45
1:A:366:ARG:HB2	1:A:517:SER:HB2	1.98	0.45
1:A:550:GLN:NE2	1:A:553:LYS:CE	2.75	0.45
1:A:1043:THR:C	1:A:1045:LYS:N	2.75	0.45
1:A:561:THR:HG22	1:A:591:LYS:NZ	2.32	0.44
1:A:1043:THR:OG1	1:A:1047:ASP:CG	2.61	0.44
1:A:806:SER:O	1:A:808:LYS:O	2.36	0.43
1:A:1043:THR:C	1:A:1045:LYS:H	2.26	0.43
1:A:555:LEU:HD11	1:A:575:LEU:HD12	1.99	0.43
1:A:421:LYS:HD2	1:A:421:LYS:HA	1.92	0.43
1:A:1042:LEU:HD23	1:A:1048:ILE:HD11	2.00	0.43
1:A:629:GLN:HG2	1:A:1029:ILE:HG13	1.99	0.43
1:A:854:ILE:HG23	1:A:1023:HIS:CD2	2.54	0.43
1:A:238:ASP:HA	1:A:286:PRO:HB3	2.01	0.43
1:A:271:VAL:CG2	1:A:282:VAL:HG13	2.46	0.43
1:A:900:GLY:O	1:A:902:PHE:CE1	2.72	0.43
1:A:764:ILE:HG22	1:A:764:ILE:O	2.19	0.43
1:A:825:ASN:HD22	1:A:825:ASN:H	1.65	0.43
1:A:525:HIS:CB	1:A:526:PRO:CD	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:LYS:HA	1:A:756:LYS:HZ3	1.84	0.42
1:A:374:PRO:O	1:A:376:ASN:N	2.53	0.42
1:A:1089:HIS:O	1:A:1091:VAL:N	2.52	0.42
1:A:777:SER:HB3	1:A:778:GLN:HE21	1.85	0.42
1:A:589:TYR:N	1:A:590:PRO:HD2	2.35	0.42
1:A:608:TYR:CE1	1:A:639:ASN:ND2	2.88	0.42
1:A:657:LEU:HD11	1:A:690:ARG:HD3	2.02	0.42
1:A:1021:ARG:HE	1:A:1056:THR:HG23	1.84	0.42
1:A:682:LEU:HD22	1:A:686:LEU:HD11	2.01	0.41
1:A:224:ILE:CD1	1:A:233:ILE:HD13	2.51	0.41
1:A:287:ILE:HD12	1:A:287:ILE:N	2.35	0.41
1:A:291:GLN:HE21	1:A:291:GLN:HB3	1.73	0.41
1:A:724:CYS:HB2	1:A:728:MET:HE3	2.03	0.41
1:A:1035:LEU:HB3	1:A:1042:LEU:HG	2.02	0.41
1:A:387:ILE:HG13	1:A:418:ILE:CD1	2.51	0.41
1:A:628:MET:HB2	1:A:1029:ILE:HG21	2.03	0.41
1:A:939:THR:HG23	1:A:945:GLY:CA	2.50	0.41
1:A:304:HIS:CG	1:A:823:LEU:HD21	2.56	0.40
1:A:625:GLY:O	1:A:629:GLN:HG3	2.20	0.40
1:A:169:HIS:CE1	1:A:466:LEU:CD1	3.05	0.40
1:A:240:THR:O	1:A:244:ILE:HG13	2.22	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	827/959 (86%)	783 (95%)	33 (4%)	11 (1%)	9 14

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	PRO
1	A	375	ARG
1	A	754	ALA
1	A	756	LYS
1	A	949	ASN
1	A	252	MET
1	A	1044	SER
1	A	404	PHE
1	A	1090	LEU
1	A	896	VAL
1	A	1091	VAL

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	758/857 (88%)	640 (84%)	118 (16%)	2 3

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	SER
1	A	145	GLU
1	A	147	SER
1	A	153	GLN
1	A	168	VAL
1	A	178	ARG
1	A	202	VAL
1	A	207	LEU
1	A	214	LYS
1	A	219	CYS
1	A	226	ARG
1	A	229	THR
1	A	235	VAL
1	A	236	SER
1	A	254	LYS
1	A	268	GLN

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Mol	Chain	Res	Type
1	A	281	LEU
1	A	282	VAL
1	A	287	ILE
1	A	305	VAL
1	A	307	LEU
1	A	319	ARG
1	A	320	LYS
1	A	358	ASP
1	A	366	ARG
1	A	372	VAL
1	A	373	LEU
1	A	375	ARG
1	A	376	ASN
1	A	377	THR
1	A	379	LEU
1	A	381	VAL
1	A	402	LYS
1	A	406	GLU
1	A	407	GLU
1	A	412	VAL
1	A	418	ILE
1	A	421	LYS
1	A	459	ARG
1	A	477	ARG
1	A	487	ILE
1	A	498	ASN
1	A	510	LYS
1	A	549	ASN
1	A	552	ARG
1	A	561	THR
1	A	568	THR
1	A	574	LEU
1	A	575	LEU
1	A	594	SER
1	A	601	GLN
1	A	610	LEU
1	A	613	ARG
1	A	615	GLU
1	A	626	LEU
1	A	646	GLN
1	A	647	LYS
1	A	682	LEU

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Mol	Chain	Res	Type
1	A	707	ARG
1	A	717	LEU
1	A	731	ASP
1	A	739	ILE
1	A	749	ILE
1	A	752	LEU
1	A	756	LYS
1	A	758	ASP
1	A	763	VAL
1	A	764	ILE
1	A	766	GLN
1	A	767	LEU
1	A	772	GLU
1	A	773	ASN
1	A	777	SER
1	A	779	LEU
1	A	798	ILE
1	A	799	GLU
1	A	807	LYS
1	A	824	SER
1	A	825	ASN
1	A	837	ASP
1	A	838	LEU
1	A	843	LEU
1	A	845	LEU
1	A	846	GLN
1	A	848	LEU
1	A	858	GLU
1	A	863	CYS
1	A	875	LYS
1	A	886	THR
1	A	890	LYS
1	A	895	THR
1	A	896	VAL
1	A	898	ASN
1	A	903	LYS
1	A	906	VAL
1	A	907	LEU
1	A	912	LYS
1	A	915	SER
1	A	918	GLU
1	A	926	GLU

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Mol	Chain	Res	Type
1	A	927	ARG
1	A	939	THR
1	A	982	ARG
1	A	983	VAL
1	A	997	THR
1	A	1001	LYS
1	A	1026	LEU
1	A	1029	ILE
1	A	1042	LEU
1	A	1043	THR
1	A	1044	SER
1	A	1048	ILE
1	A	1049	GLU
1	A	1051	ILE
1	A	1052	ARG
1	A	1078	LYS
1	A	1088	LEU
1	A	1092	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	169	HIS
1	A	217	ASN
1	A	231	GLN
1	A	268	GLN
1	A	291	GLN
1	A	304	HIS
1	A	376	ASN
1	A	386	ASN
1	A	389	HIS
1	A	391	GLN
1	A	396	GLN
1	A	432	GLN
1	A	549	ASN
1	A	550	GLN
1	A	565	ASN
1	A	600	GLN
1	A	601	GLN
1	A	634	ASN
1	A	662	GLN

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Mol	Chain	Res	Type
1	A	708	HIS
1	A	743	GLN
1	A	762	GLN
1	A	766	GLN
1	A	778	GLN
1	A	825	ASN
1	A	909	HIS
1	A	948	HIS
1	A	1010	GLN
1	A	1022	HIS
1	A	1041	GLN
1	A	1083	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	NPZ	A	1	-	24,24,24	1.98	7 (29%)	31,35,35	3.53	16 (51%)

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	NPZ	A	1	-	-	0/4/4/4	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	NPZ	CAG-CAO	-6.51	1.40	1.49
2	A	1	NPZ	NAT-NAP	2.94	1.40	1.36
2	A	1	NPZ	CAU-NAT	2.62	1.50	1.46
2	A	1	NPZ	C5-CAO	2.62	1.50	1.44
2	A	1	NPZ	CAO-NAP	2.20	1.35	1.33
2	A	1	NPZ	CAB-CAC	-2.17	1.37	1.42
2	A	1	NPZ	CAH-CAG	2.04	1.41	1.37

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	NPZ	CAA-CAG-CAO	-7.25	111.68	120.64
2	A	1	NPZ	CAG-CAO-NAP	7.19	128.25	118.91
2	A	1	NPZ	CAU-NAT-C4	6.96	133.19	128.30
2	A	1	NPZ	C5-C4-N3	-6.68	119.89	126.97
2	A	1	NPZ	C5-CAO-CAG	-5.37	124.91	131.28
2	A	1	NPZ	C5-CAO-NAP	-5.22	106.61	110.19
2	A	1	NPZ	CAU-NAT-NAP	-4.70	113.57	119.97
2	A	1	NPZ	N3-C2-N1	-4.57	121.67	128.58
2	A	1	NPZ	C6-C5-CAO	-4.07	134.95	139.07
2	A	1	NPZ	C4-NAT-NAP	3.60	113.13	110.98
2	A	1	NPZ	C6-C5-C4	3.46	118.33	115.74
2	A	1	NPZ	C2-N3-C4	3.36	120.04	111.83
2	A	1	NPZ	C4-C5-CAO	2.83	106.71	104.74
2	A	1	NPZ	CAD-CAC-CAB	-2.75	116.74	123.01
2	A	1	NPZ	CAD-CAC-CAI	2.67	123.49	118.91
2	A	1	NPZ	CAG-CAH-CAI	-2.19	117.81	121.19

There are no chirality outliers.

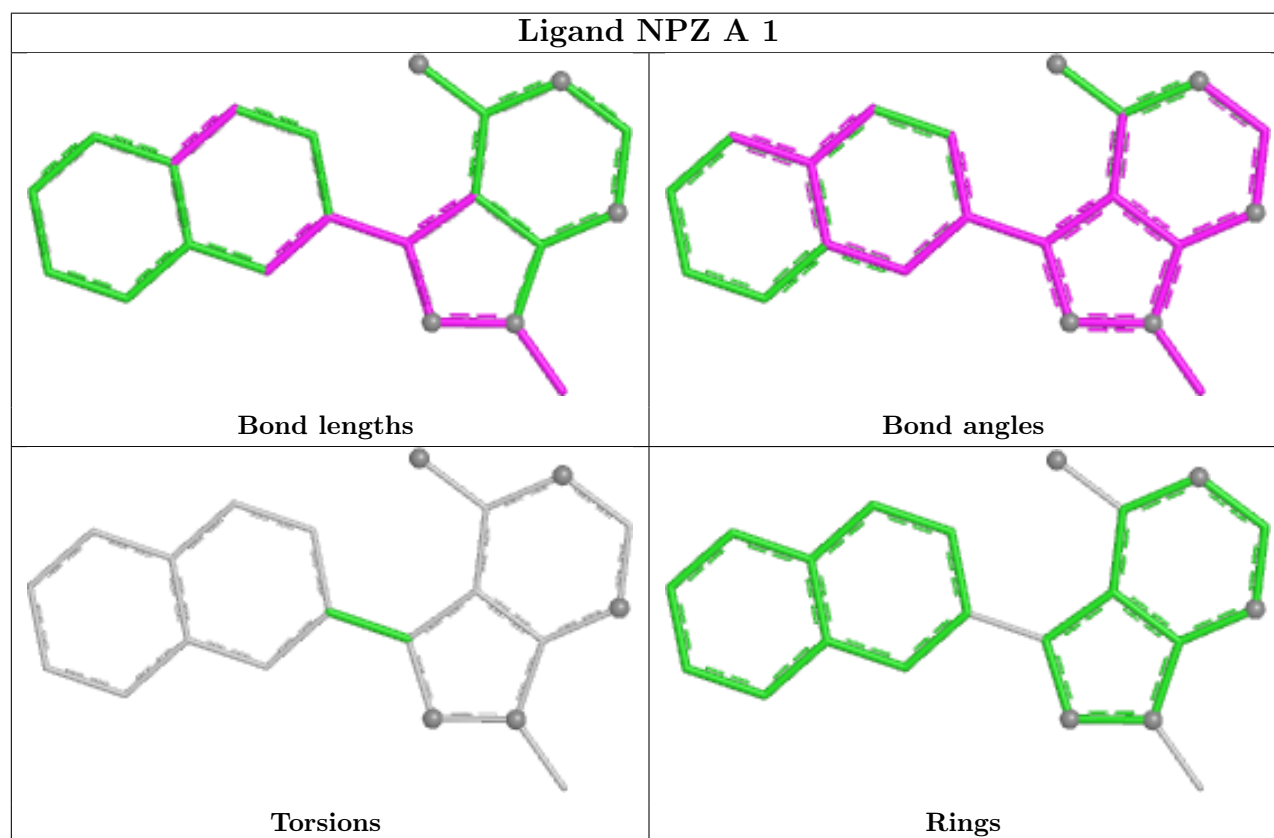
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	NPZ	3	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 ⓘ

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	843/959 (87%)	0.53	64 (7%) 20 16	19, 26, 32, 51	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1044	SER	8.8
1	A	897	GLY	6.3
1	A	1092	LEU	5.4
1	A	216	ALA	4.1
1	A	376	ASN	3.9
1	A	855	TRP	3.8
1	A	757	TYR	3.5
1	A	895	THR	3.3
1	A	860	LEU	3.3
1	A	773	ASN	3.1
1	A	754	ALA	3.1
1	A	548	PRO	3.0
1	A	774	LEU	3.0
1	A	527	ILE	2.9
1	A	379	LEU	2.8
1	A	896	VAL	2.8
1	A	778	GLN	2.7
1	A	850	ILE	2.7
1	A	253	ALA	2.7
1	A	853	SER	2.7
1	A	849	ARG	2.6
1	A	1091	VAL	2.6
1	A	252	MET	2.6
1	A	765	SER	2.6
1	A	926	GLU	2.5
1	A	862	LEU	2.5
1	A	776	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	278	ASP	2.5
1	A	219	CYS	2.4
1	A	1066	LYS	2.4
1	A	377	THR	2.4
1	A	248	PHE	2.4
1	A	547	MET	2.4
1	A	228	THR	2.4
1	A	777	SER	2.4
1	A	898	ASN	2.4
1	A	1046	GLU	2.3
1	A	410	TRP	2.3
1	A	390	GLY	2.3
1	A	378	ASP	2.3
1	A	528	ALA	2.3
1	A	1057	VAL	2.3
1	A	916	PRO	2.3
1	A	761	SER	2.2
1	A	857	THR	2.2
1	A	408	VAL	2.2
1	A	522	ASN	2.2
1	A	146	GLU	2.2
1	A	1089	HIS	2.2
1	A	899	THR	2.1
1	A	1039	MET	2.1
1	A	1011	ASP	2.1
1	A	1033	MET	2.1
1	A	229	THR	2.1
1	A	204	SER	2.1
1	A	779	LEU	2.1
1	A	1000	LYS	2.1
1	A	861	ASP	2.1
1	A	169	HIS	2.1
1	A	795	ALA	2.0
1	A	755	GLU	2.0
1	A	856	GLU	2.0
1	A	845	LEU	2.0
1	A	790	GLY	2.0

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 [i](#)

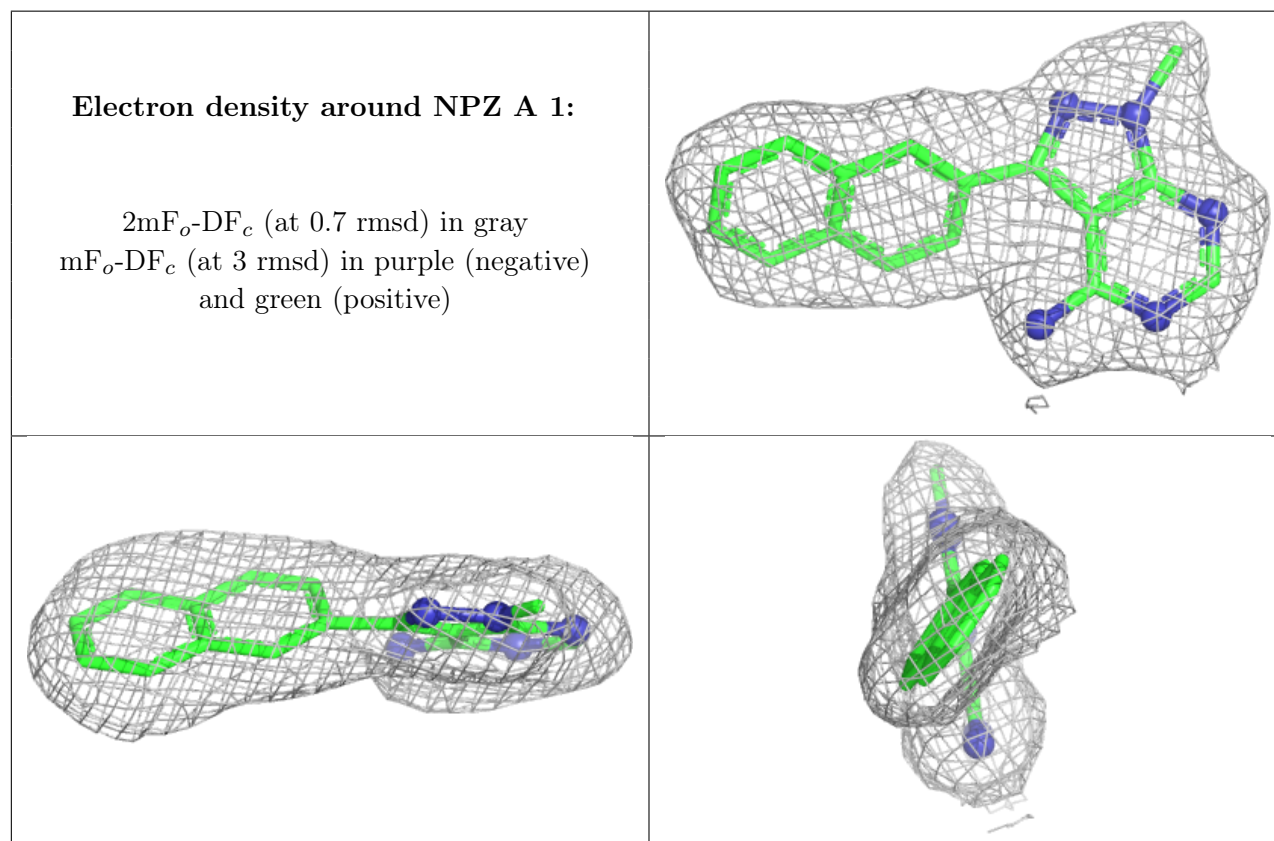
There are no oligosaccharides in this entry.

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	NPZ	A	1	21/21	0.92	0.08	33,38,40,42	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.