Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2023 – 09:18 PM EDT

PDB ID	:	3ENE
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:

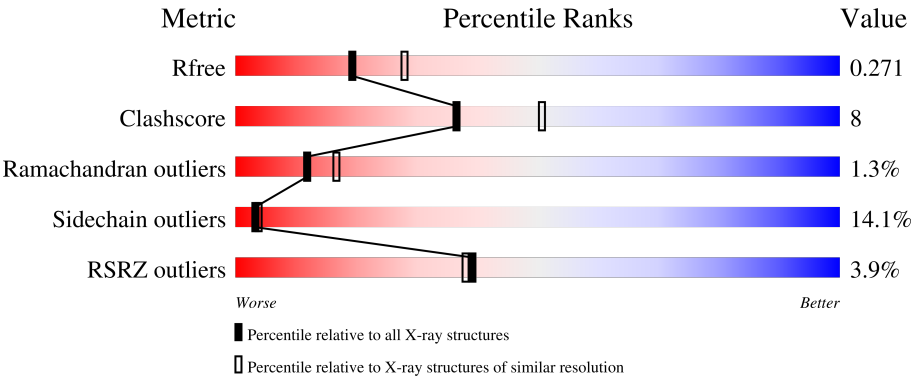
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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% 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	3% 63% 20% · 12%

2 Entry composition (i)

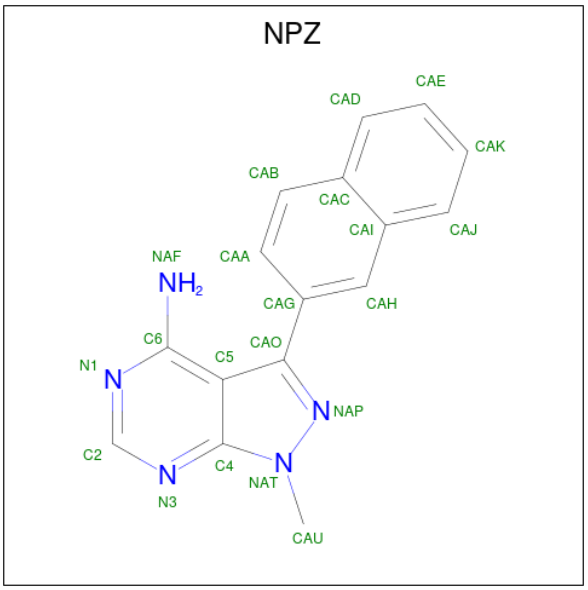
There are 3 unique types of molecules in this entry. The entry contains 6904 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 2 is 1-methyl-3-naphthalen-2-yl-1H-pyrazolo[3,4-d]pyrimidin-4-amine (three-letter code: NPZ) (formula: $C_{16}H_{13}N_5$).



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

- Molecule 3 is water.

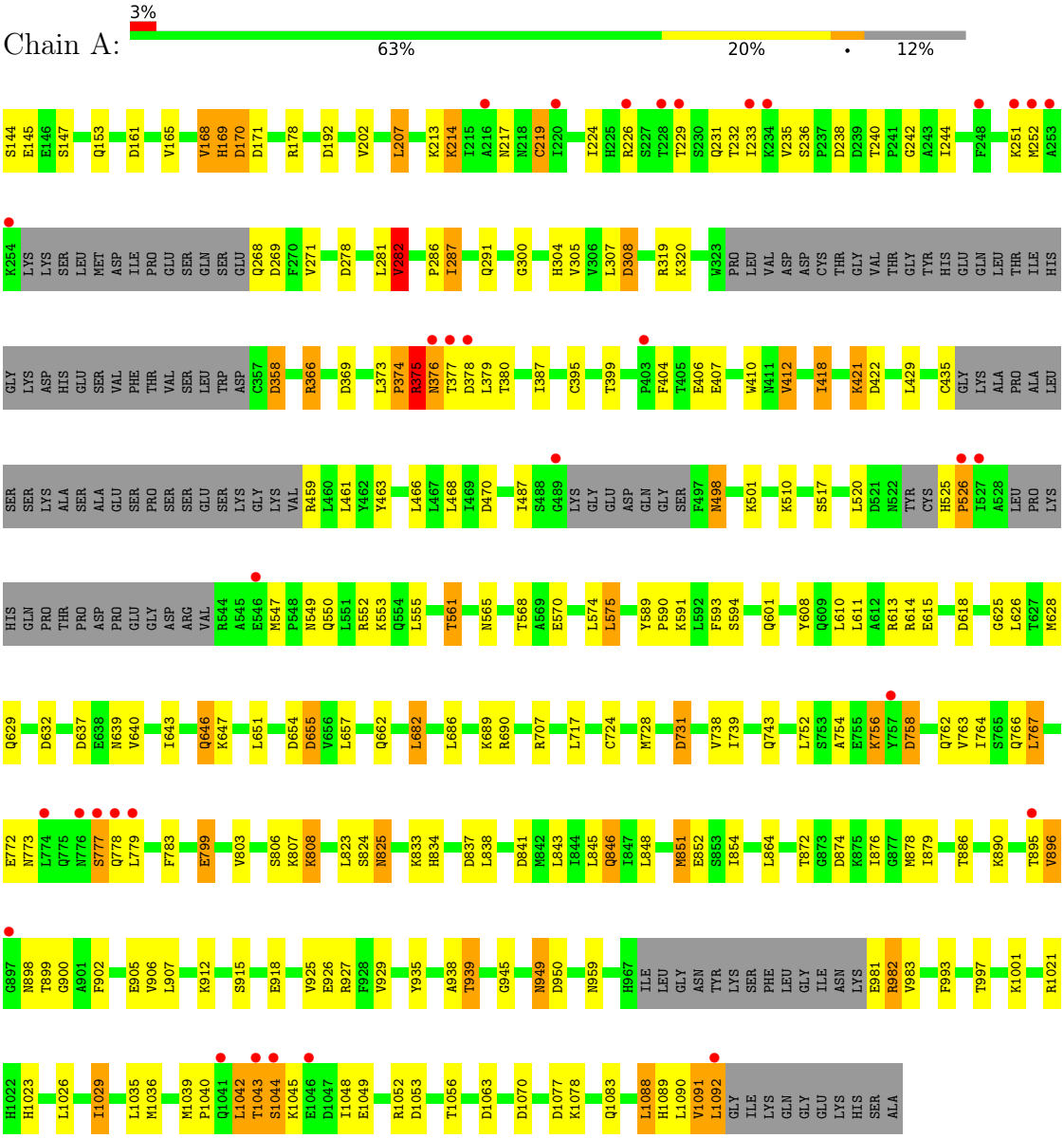
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O			
3	A	38	38	38		0	0

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

Chain A:



4 Data and refinement statistics (i)

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 57.06 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (57.07-2.40) 99.3 (57.06-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 , 36.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	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.*

[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: 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	0.72	4/6993 (0.1%)	0.87	29/9459 (0.3%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	762	GLN	CG-CD	9.23	1.72	1.51
1	A	547	MET	CG-SD	7.05	1.99	1.81
1	A	851	MET	SD-CE	-6.82	1.39	1.77
1	A	169	HIS	CA-CB	5.07	1.65	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	655	ASP	CB-CG-OD2	7.46	125.01	118.30
1	A	1070	ASP	CB-CG-OD2	7.09	124.68	118.30
1	A	171	ASP	CB-CG-OD2	6.68	124.31	118.30
1	A	632	ASP	CB-CG-OD1	6.61	124.25	118.30
1	A	950	ASP	CB-CG-OD2	6.42	124.08	118.30
1	A	618	ASP	CB-CG-OD2	6.32	123.99	118.30
1	A	170	ASP	CB-CG-OD1	6.30	123.97	118.30
1	A	161	ASP	CB-CG-OD2	6.13	123.82	118.30
1	A	269	ASP	CB-CG-OD2	6.09	123.79	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	731	ASP	CB-CG-OD2	6.08	123.78	118.30
1	A	470	ASP	CB-CG-OD1	6.03	123.73	118.30
1	A	369	ASP	CB-CG-OD2	5.99	123.69	118.30
1	A	192	ASP	CB-CG-OD2	5.98	123.69	118.30
1	A	654	ASP	CB-CG-OD1	-5.81	113.07	118.30
1	A	1053	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	637	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	874	ASP	CB-CG-OD2	5.55	123.29	118.30
1	A	758	ASP	CB-CG-OD2	5.54	123.28	118.30
1	A	422	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	1063	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	358	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	378	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	1077	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	841	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	278	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	308	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	207	LEU	CA-CB-CG	5.18	127.21	115.30
1	A	520	LEU	CA-CB-CG	5.12	127.08	115.30
1	A	282	VAL	CB-CA-C	-5.11	101.69	111.40

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 (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	6845	0	6887	106	0
2	A	21	0	13	3	0
3	A	38	0	0	2	0
All	All	6904	0	6900	109	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 (109) 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:935:TYR:O	1:A:939:THR:HB	1.79	0.83
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:851:MET:HE1	1:A:938:ALA:HB1	1.63	0.79
1:A:1088:LEU:O	1:A:1091:VAL:HG22	1.84	0.77
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:851:MET:HE1	1:A:938:ALA:CB	2.19	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: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: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:308:ASP:N	1:A:308:ASP:OD1	2.39	0.55
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1039:MET:HB3	1:A:1040:PRO:CD	2.40	0.51
1:A:900:GLY:O	1:A:902:PHE:CD1	2.64	0.51
1:A:799:GLU:H	1:A:799:GLU:CD	2.14	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:724:CYS:HB2	1:A:728:MET:HE3	1.93	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
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:689:LYS:HG2	1:A:728:MET:HE1	1.97	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:498:ASN:OD1	1:A:498:ASN:C	2.55	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:851:MET:CE	1:A:938:ALA:CB	2.93	0.45
1:A:561:THR:HG22	1:A:591:LYS:NZ	2.32	0.44
1:A:806:SER:O	1:A:808:LYS:O	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:878:MET:C	1:A:879:ILE:HG13	2.41	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: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:1043:THR:C	1:A:1045:LYS:N	2.75	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%)	12 17

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 (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	758/857 (88%)	651 (86%)	107 (14%)	3 4

All (107) 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

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Mol	Chain	Res	Type
1	A	213	LYS
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	251	LYS
1	A	268	GLN
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	373	LEU
1	A	375	ARG
1	A	376	ASN
1	A	377	THR
1	A	379	LEU
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	461	LEU
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	574	LEU
1	A	575	LEU
1	A	594	SER
1	A	601	GLN
1	A	610	LEU
1	A	613	ARG

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Mol	Chain	Res	Type
1	A	615	GLU
1	A	626	LEU
1	A	646	GLN
1	A	647	LYS
1	A	682	LEU
1	A	707	ARG
1	A	717	LEU
1	A	731	ASP
1	A	739	ILE
1	A	752	LEU
1	A	758	ASP
1	A	763	VAL
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	799	GLU
1	A	807	LYS
1	A	808	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	886	THR
1	A	890	LYS
1	A	895	THR
1	A	896	VAL
1	A	898	ASN
1	A	906	VAL
1	A	907	LEU
1	A	912	LYS
1	A	915	SER
1	A	918	GLU
1	A	926	GLU
1	A	927	ARG
1	A	939	THR

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Mol	Chain	Res	Type
1	A	959	ASN
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	1049	GLU
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 (28) 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	432	GLN
1	A	522	ASN
1	A	549	ASN
1	A	550	GLN
1	A	565	ASN
1	A	601	GLN
1	A	662	GLN
1	A	743	GLN
1	A	766	GLN
1	A	773	ASN
1	A	778	GLN
1	A	825	ASN
1	A	898	ASN
1	A	909	HIS
1	A	948	HIS

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Mol	Chain	Res	Type
1	A	959	ASN
1	A	1007	GLN
1	A	1023	HIS
1	A	1041	GLN
1	A	1083	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

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	-	19,24,24	1.15	0	20,35,35	1.86	5 (25%)

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	-	-	0/0/4/4	0/4/4/4

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	NPZ	N3-C2-N1	-4.49	121.67	128.68
2	A	1	NPZ	CAU-NAT-C4	4.17	133.19	124.18
2	A	1	NPZ	CAI-CAH-CAG	-2.84	117.81	121.92
2	A	1	NPZ	CAD-CAC-CAB	-2.76	116.74	123.19
2	A	1	NPZ	CAD-CAC-CAI	2.55	123.49	118.92

There are no chirality outliers.

There are no torsion outliers.

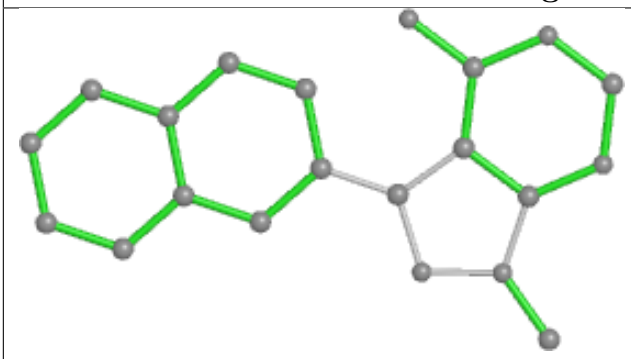
There are no ring outliers.

1 monomer is involved in 3 short contacts:

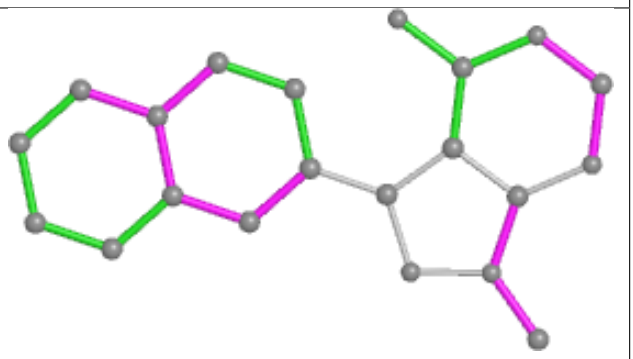
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	NPZ	3	0

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 then 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.

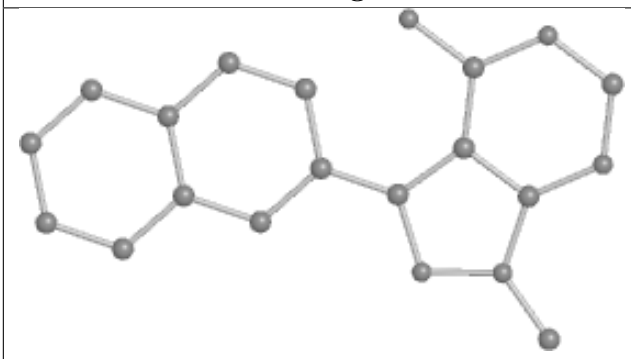
Ligand NPZ A 1



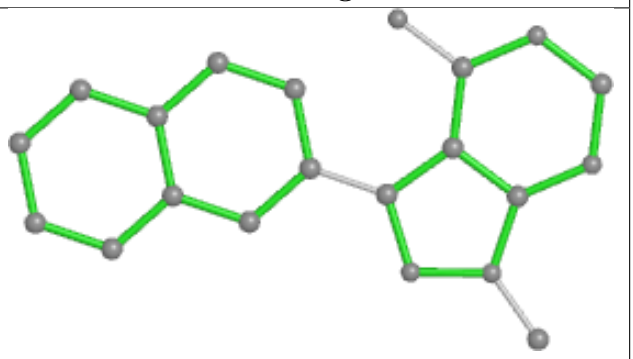
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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%)	0.18	33 (3%) 39 38	19, 26, 32, 51	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	376	ASN	7.0
1	A	1044	SER	6.9
1	A	216	ALA	6.4
1	A	1092	LEU	5.5
1	A	253	ALA	5.4
1	A	248	PHE	4.6
1	A	777	SER	4.4
1	A	252	MET	4.4
1	A	897	GLY	4.4
1	A	757	TYR	3.9
1	A	228	THR	3.7
1	A	254	LYS	3.6
1	A	378	ASP	3.6
1	A	774	LEU	3.5
1	A	778	GLN	3.4
1	A	776	ASN	3.4
1	A	234	LYS	3.4
1	A	489	GLY	3.2
1	A	403	PRO	3.1
1	A	251	LYS	3.0
1	A	226	ARG	3.0
1	A	1041	GLN	2.9
1	A	779	LEU	2.9
1	A	377	THR	2.8
1	A	229	THR	2.8
1	A	526	PRO	2.7
1	A	1043	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	233	ILE	2.3
1	A	546	GLU	2.2
1	A	895	THR	2.2
1	A	527	ILE	2.1
1	A	1046	GLU	2.1
1	A	220	ILE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

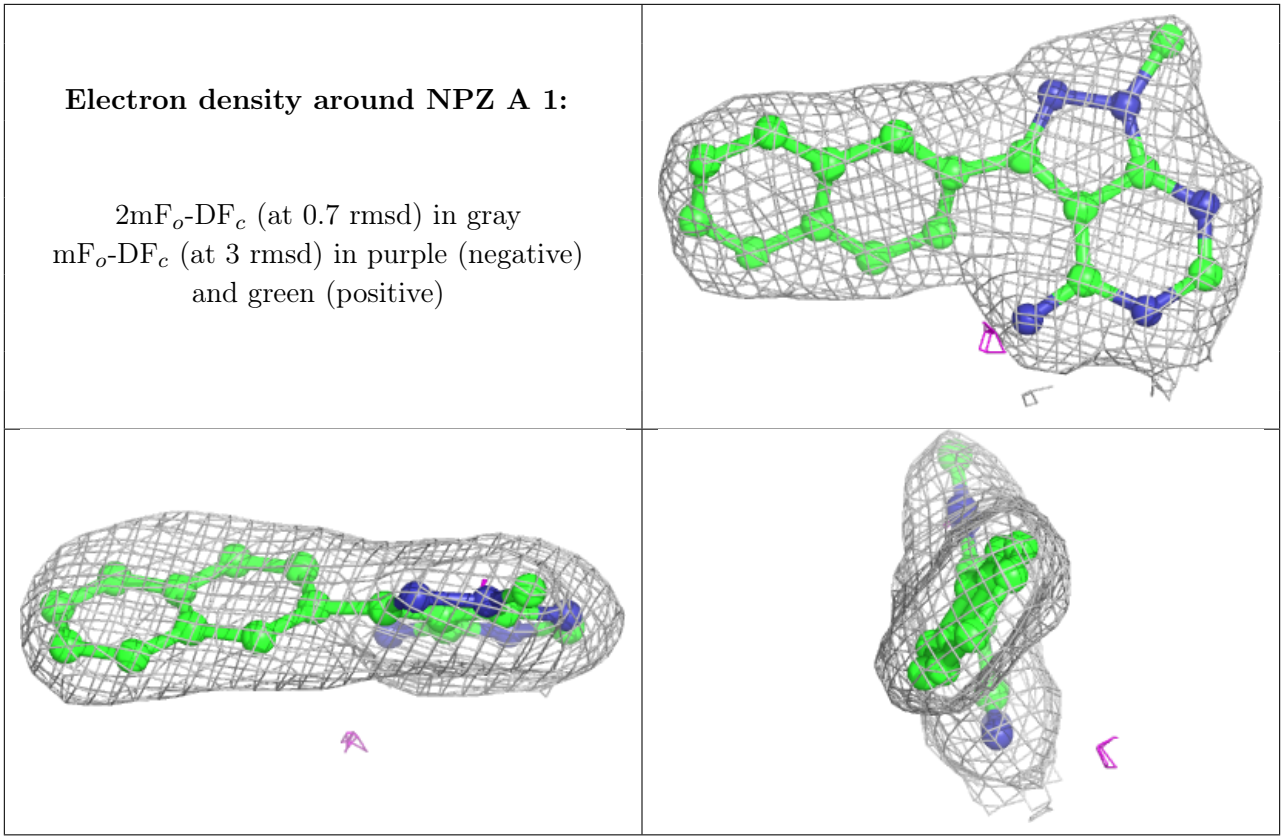
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	NPZ	A	1	21/21	0.97	0.10	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.

Electron density around NPZ A 1:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.