



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:44 PM UTC

PDB ID : 3APD / pdb_00003apd
Title : Crystal structure of human PI3K-gamma in complex with CH5108134
Authors : Nakamura, M.; Fukami, T.A.; Miyazaki, T.; Yoshida, M.
Deposited on : 2010-10-14
Resolution : 2.55 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

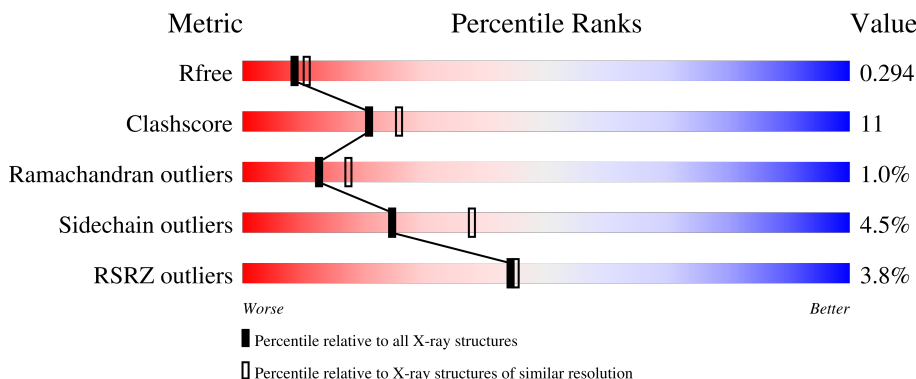
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	966	3% 65% 20% • 13%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6615 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.

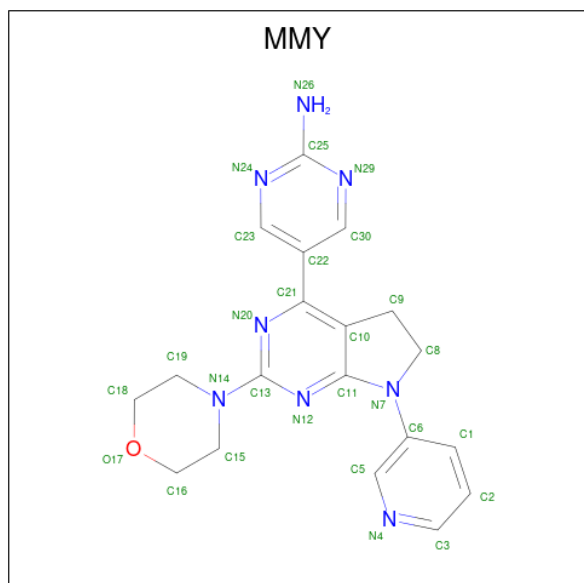
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	839	Total	C	N	O	S	0	0	0
			6562	4214	1109	1205	34			

There are 7 discrepancies between the modelled and reference sequences:

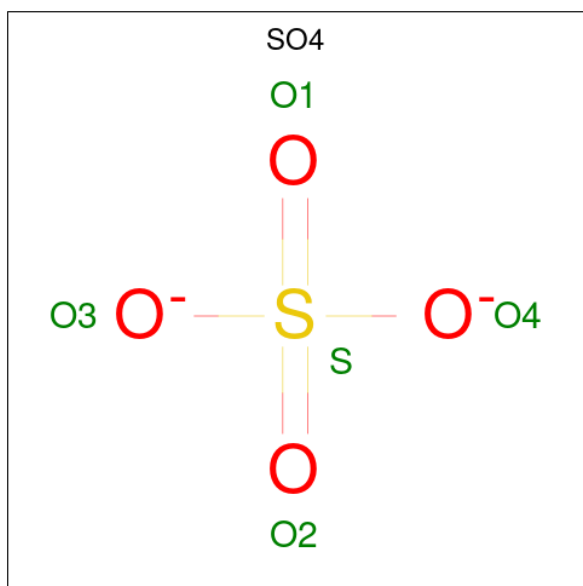
Chain	Residue	Modelled	Actual	Comment	Reference
A	137	GLY	-	expression tag	UNP P48736
A	138	PRO	-	expression tag	UNP P48736
A	139	LEU	-	expression tag	UNP P48736
A	140	HIS	-	expression tag	UNP P48736
A	141	MET	-	expression tag	UNP P48736
A	142	GLY	-	expression tag	UNP P48736
A	143	SER	-	expression tag	UNP P48736

- Molecule 2 is 5-(2-Morpholin-4-yl-7-pyridin-3-yl-6,7-dihydro-5H-pyrrolo[2,3-d]pyrimidin-4-yl)-pyrimidin-2-ylamine (CCD ID: MMY) (formula: C₁₉H₂₀N₈O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			28	19	8	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

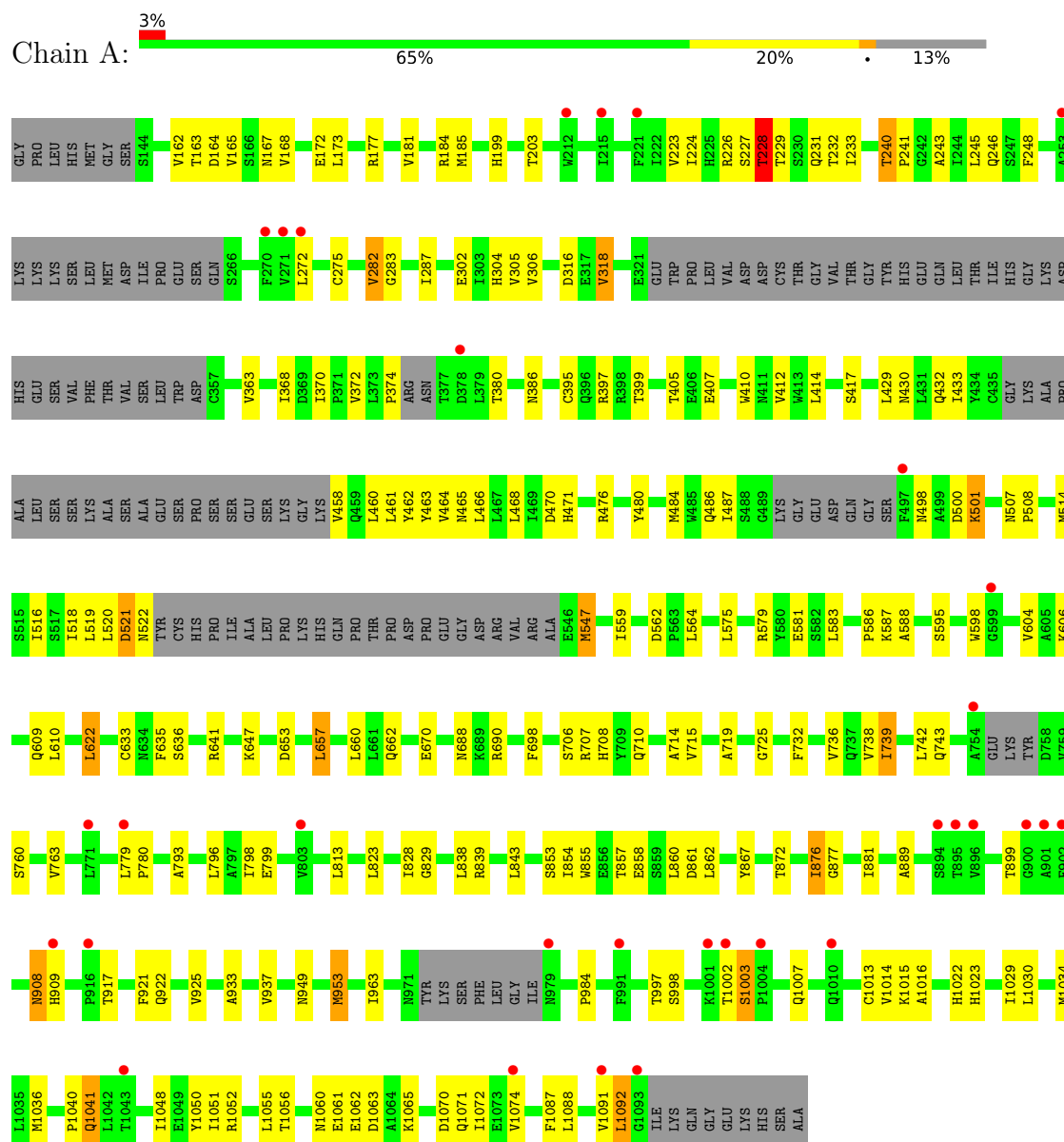
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total	O	0	0
			15	15		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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	142.95Å 67.46Å 106.28Å 90.00° 95.68° 90.00°	Depositor
Resolution (Å)	60.95 – 2.55 60.95 – 2.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (60.95-2.55) 99.6 (60.95-2.55)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.55Å)	Xtriage
Refinement program	REFMAC refmac_5.5.0109	Depositor
R, R_{free}	0.250 , 0.316 0.239 , 0.294	Depositor DCC
R_{free} test set	1675 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	63.7	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.9	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	0.94	EDS
Total number of atoms	6615	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, MMY

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	0.56	0/6703	0.81	2/9106 (0.0%)

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	547	MET	N-CA-C	5.53	113.20	108.22
1	A	839	ARG	N-CA-C	-5.10	105.42	111.69

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	521	ASP	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	6562	0	6360	141	0
2	A	28	0	20	6	0
3	A	10	0	0	0	0
4	A	15	0	0	0	0
All	All	6615	0	6380	144	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 11.

All (144) 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:433:ILE:HD13	1:A:484:MET:HE1	1.37	1.06
1:A:953:MET:HE2	1:A:963:ILE:HD13	1.47	0.95
1:A:165:VAL:HG12	1:A:165:VAL:O	1.73	0.88
1:A:559:ILE:HG23	1:A:588:ALA:HB2	1.55	0.86
1:A:953:MET:HE1	2:A:1:MMY:C13	2.11	0.80
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.64	0.80
1:A:953:MET:HE1	2:A:1:MMY:N12	2.01	0.74
1:A:363:VAL:HG23	1:A:520:LEU:CD2	2.19	0.72
1:A:227:SER:O	1:A:228:THR:HG22	1.91	0.70
1:A:275:CYS:SG	1:A:306:VAL:HG23	2.34	0.68
2:A:1:MMY:C9	2:A:1:MMY:H30	2.24	0.67
1:A:240:THR:HG22	1:A:243:ALA:H	1.60	0.67
1:A:953:MET:HE3	1:A:963:ILE:HG21	1.76	0.66
1:A:583:LEU:HD22	1:A:610:LEU:HD12	1.77	0.66
1:A:363:VAL:HG23	1:A:520:LEU:HD23	1.78	0.65
1:A:559:ILE:CG2	1:A:588:ALA:HB2	2.26	0.65
2:A:1:MMY:H30	2:A:1:MMY:H9A	1.78	0.65
1:A:165:VAL:O	1:A:165:VAL:CG1	2.45	0.64
1:A:272:LEU:HD22	1:A:305:VAL:HG21	1.81	0.63
1:A:163:THR:O	1:A:165:VAL:HG23	1.99	0.62
1:A:862:LEU:HD11	1:A:1016:ALA:HB2	1.81	0.61
1:A:430:ASN:ND2	1:A:465:ASN:OD1	2.19	0.61
1:A:899:THR:HG23	1:A:1087:PHE:CZ	2.37	0.60
1:A:368:ILE:HG22	1:A:516:ILE:HD12	1.84	0.58
1:A:231:GLN:O	1:A:233:ILE:HD12	2.03	0.58
1:A:466:LEU:HD11	1:A:476:ARG:HD3	1.85	0.58
1:A:908:ASN:C	1:A:908:ASN:HD22	2.12	0.58
1:A:370:ILE:O	1:A:370:ILE:HG23	2.04	0.57
1:A:899:THR:HG23	1:A:1087:PHE:CE1	2.39	0.57
1:A:732:PHE:O	1:A:736:VAL:HG23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ASN:ND2	1:A:432:GLN:HE21	2.02	0.56
1:A:397:ARG:HB3	1:A:414:LEU:HD22	1.87	0.55
1:A:583:LEU:HD22	1:A:610:LEU:CD1	2.36	0.55
1:A:363:VAL:HG23	1:A:520:LEU:HD21	1.88	0.55
1:A:386:ASN:HD21	1:A:432:GLN:HE21	1.54	0.55
1:A:1070:ASP:O	1:A:1074:VAL:HG23	2.06	0.54
1:A:240:THR:HG23	1:A:241:PRO:HD2	1.90	0.54
1:A:318:VAL:HG22	1:A:725:GLY:HA2	1.88	0.54
1:A:463:TYR:CD1	1:A:487:ILE:HD11	2.42	0.54
1:A:997:THR:HG22	1:A:998:SER:N	2.22	0.53
1:A:162:VAL:HG12	1:A:714:ALA:HB1	1.91	0.53
1:A:518:ILE:HD12	1:A:518:ILE:C	2.34	0.53
1:A:796:LEU:O	1:A:798:ILE:HD12	2.09	0.52
1:A:172:GLU:HG3	1:A:471:HIS:CD2	2.45	0.52
1:A:1062:GLU:O	1:A:1065:LYS:HB3	2.09	0.52
1:A:598:TRP:CE3	1:A:604:VAL:HG22	2.45	0.52
1:A:855:TRP:CH2	1:A:862:LEU:HD12	2.46	0.51
1:A:867:TYR:CE2	1:A:963:ILE:HG22	2.45	0.51
1:A:519:LEU:HD12	1:A:520:LEU:H	1.76	0.51
1:A:405:THR:OG1	1:A:407:GLU:O	2.28	0.51
1:A:410:TRP:HB3	1:A:412:VAL:HG22	1.92	0.51
1:A:547:MET:CE	1:A:581:GLU:HG3	2.41	0.51
1:A:562:ASP:OD1	1:A:1052:ARG:NH1	2.44	0.51
1:A:223:VAL:HG11	1:A:304:HIS:CE1	2.46	0.51
1:A:224:ILE:HD12	1:A:248:PHE:CD2	2.46	0.51
1:A:461:LEU:HB3	1:A:462:TYR:CD1	2.46	0.51
1:A:167:ASN:HD22	1:A:508:PRO:HB3	1.76	0.50
1:A:738:VAL:HG12	1:A:742:LEU:HD12	1.92	0.50
1:A:181:VAL:HG13	1:A:185:MET:HE3	1.93	0.50
1:A:861:ASP:OD1	1:A:861:ASP:C	2.55	0.50
1:A:1040:PRO:O	1:A:1041:GLN:CB	2.59	0.50
1:A:829:GLY:CA	1:A:881:ILE:HD12	2.42	0.50
1:A:240:THR:HG23	1:A:241:PRO:CD	2.42	0.49
1:A:1048:ILE:O	1:A:1051:ILE:HG22	2.11	0.49
1:A:372:VAL:HG12	1:A:374:PRO:HD3	1.93	0.49
2:A:1:MMY:C9	2:A:1:MMY:C30	2.90	0.49
1:A:586:PRO:O	1:A:588:ALA:N	2.45	0.49
1:A:739:ILE:HD12	1:A:739:ILE:C	2.38	0.48
1:A:432:GLN:HB3	1:A:460:LEU:CD1	2.44	0.48
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.14	0.48
1:A:641:ARG:NH1	1:A:670:GLU:OE2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:860:LEU:HD21	1:A:1015:LYS:HB3	1.96	0.48
1:A:586:PRO:C	1:A:588:ALA:H	2.23	0.47
1:A:1014:VAL:HG11	1:A:1065:LYS:HG3	1.96	0.47
1:A:889:ALA:HB2	1:A:949:ASN:OD1	2.15	0.47
1:A:1002:THR:HG22	1:A:1003:SER:N	2.29	0.47
1:A:579:ARG:CD	1:A:610:LEU:HD22	2.44	0.47
1:A:653:ASP:OD2	1:A:688:ASN:ND2	2.48	0.47
1:A:793:ALA:HA	1:A:828:ILE:HD12	1.96	0.46
1:A:760:SER:HB2	1:A:763:VAL:HG23	1.98	0.46
1:A:633:CYS:SG	1:A:1036:MET:HE1	2.56	0.46
1:A:953:MET:CE	1:A:963:ILE:HD13	2.31	0.46
1:A:1013:CYS:O	1:A:1016:ALA:HB3	2.16	0.46
1:A:854:ILE:HG23	1:A:1023:HIS:CD2	2.51	0.46
1:A:162:VAL:CG1	1:A:714:ALA:HB1	2.47	0.45
1:A:575:LEU:HD12	1:A:595:SER:OG	2.17	0.45
1:A:657:LEU:HD11	1:A:690:ARG:HG2	1.98	0.45
1:A:227:SER:O	1:A:228:THR:CG2	2.64	0.45
1:A:168:VAL:HG11	1:A:173:LEU:HD12	1.98	0.44
1:A:282:VAL:HG12	1:A:283:GLY:H	1.82	0.44
1:A:463:TYR:CE2	1:A:501:LYS:HA	2.52	0.44
1:A:480:TYR:HB2	1:A:518:ILE:HD11	1.97	0.44
1:A:165:VAL:HG13	1:A:168:VAL:HG22	1.99	0.44
1:A:370:ILE:HB	1:A:514:MET:HE2	1.98	0.44
1:A:547:MET:HE1	1:A:581:GLU:HG3	2.00	0.44
1:A:583:LEU:HD13	1:A:610:LEU:HD11	2.00	0.44
1:A:199:HIS:ND1	1:A:199:HIS:O	2.50	0.44
1:A:519:LEU:HD12	1:A:520:LEU:N	2.32	0.44
1:A:395:CYS:HG	1:A:417:SER:HG	1.59	0.43
1:A:706:SER:O	1:A:710:GLN:HB3	2.18	0.43
1:A:167:ASN:O	1:A:167:ASN:OD1	2.35	0.43
1:A:823:LEU:HD12	1:A:823:LEU:O	2.18	0.43
1:A:838:LEU:HD12	1:A:877:GLY:HA3	1.99	0.43
1:A:876:ILE:HD13	1:A:877:GLY:N	2.33	0.43
1:A:984:PRO:HG3	1:A:1071:GLN:HE21	1.84	0.43
1:A:464:VAL:HG22	1:A:465:ASN:N	2.33	0.43
1:A:843:LEU:HD13	1:A:1034:MET:HG3	2.00	0.43
1:A:232:THR:C	1:A:233:ILE:HD12	2.43	0.43
1:A:363:VAL:CG2	1:A:520:LEU:HD21	2.49	0.43
1:A:429:LEU:HB2	1:A:468:LEU:HD21	2.00	0.43
1:A:462:TYR:CE2	1:A:486:GLN:HG3	2.54	0.43
1:A:463:TYR:HD1	1:A:487:ILE:HD11	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ARG:HG2	1:A:715:VAL:HG13	2.01	0.42
1:A:368:ILE:CG2	1:A:516:ILE:HD12	2.49	0.42
1:A:933:ALA:O	1:A:937:VAL:HG23	2.19	0.42
1:A:500:ASP:HB3	1:A:708:HIS:CD2	2.55	0.42
1:A:858:GLU:OE2	1:A:1022:HIS:ND1	2.53	0.42
1:A:908:ASN:C	1:A:908:ASN:ND2	2.77	0.42
1:A:1050:TYR:CD1	1:A:1050:TYR:C	2.97	0.42
1:A:461:LEU:HB3	1:A:462:TYR:CE1	2.54	0.42
1:A:1088:LEU:O	1:A:1092:LEU:N	2.43	0.42
1:A:1092:LEU:HD23	1:A:1092:LEU:O	2.19	0.42
1:A:853:SER:O	1:A:857:THR:HG23	2.20	0.41
1:A:660:LEU:HD23	1:A:698:PHE:CE2	2.55	0.41
1:A:829:GLY:C	1:A:881:ILE:HD12	2.45	0.41
1:A:586:PRO:C	1:A:588:ALA:N	2.78	0.41
1:A:921:PHE:O	1:A:925:VAL:HG23	2.19	0.41
1:A:399:THR:HG22	1:A:412:VAL:HG21	2.02	0.41
1:A:470:ASP:OD1	1:A:470:ASP:C	2.64	0.41
1:A:507:ASN:OD1	1:A:507:ASN:C	2.64	0.41
1:A:606:LYS:HA	1:A:609:GLN:HG2	2.02	0.41
1:A:742:LEU:HD22	1:A:813:LEU:CD1	2.51	0.41
1:A:953:MET:CE	2:A:1:MMY:C13	2.92	0.41
1:A:622:LEU:HG	1:A:647:LYS:HB3	2.03	0.40
1:A:1055:LEU:O	1:A:1056:THR:C	2.63	0.40
1:A:245:LEU:HD21	1:A:272:LEU:HG	2.03	0.40
1:A:662:GLN:NE2	1:A:1030:LEU:HD22	2.36	0.40
1:A:184:ARG:HD3	1:A:719:ALA:O	2.21	0.40
1:A:635:PHE:O	1:A:641:ARG:HD2	2.22	0.40
1:A:521:ASP:O	1:A:522:ASN:HB2	2.22	0.40
1:A:738:VAL:HG22	1:A:780:PRO:HD2	2.02	0.40
1:A:1029:ILE:HG22	1:A:1030:LEU:N	2.36	0.40
1:A:1060:ASN:HD21	1:A:1063:ASP:HB2	1.85	0.40
1:A:855:TRP:CZ3	1:A:862:LEU:HD12	2.57	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	821/966 (85%)	750 (91%)	63 (8%)	8 (1%)	12 17

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1041	GLN
1	A	229	THR
1	A	498	ASN
1	A	587	LYS
1	A	164	ASP
1	A	228	THR
1	A	226	ARG
1	A	287	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	693/862 (80%)	662 (96%)	31 (4%)	24 38

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	THR
1	A	228	THR
1	A	240	THR
1	A	246	GLN
1	A	282	VAL
1	A	302	GLU
1	A	316	ASP
1	A	318	VAL
1	A	380	THR

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Mol	Chain	Res	Type
1	A	458	VAL
1	A	501	LYS
1	A	622	LEU
1	A	636	SER
1	A	657	LEU
1	A	707	ARG
1	A	739	ILE
1	A	743	GLN
1	A	779	LEU
1	A	799	GLU
1	A	876	ILE
1	A	908	ASN
1	A	909	HIS
1	A	917	THR
1	A	922	GLN
1	A	953	MET
1	A	1003	SER
1	A	1007	GLN
1	A	1061	GLU
1	A	1072	ILE
1	A	1091	VAL
1	A	1092	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	HIS
1	A	432	GLN
1	A	471	HIS
1	A	522	ASN
1	A	565	ASN
1	A	662	GLN
1	A	711	GLN
1	A	737	GLN
1	A	769	GLN
1	A	893	GLN
1	A	908	ASN
1	A	922	GLN
1	A	967	HIS
1	A	1023	HIS
1	A	1071	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](#)

3 ligands are 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	$\# Z > 2$
3	SO4	A	1103	-	4,4,4	0.21	0	6,6,6	0.26	0
2	MMY	A	1	-	31,32,32	1.69	4 (12%)	42,45,45	2.20	18 (42%)
3	SO4	A	2	-	4,4,4	0.22	0	6,6,6	0.20	0

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	MMY	A	1	-	-	2/12/29/29	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	MMY	C22-C21	-7.53	1.40	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	MMY	C11-N7	-3.11	1.34	1.38
2	A	1	MMY	C6-N7	-2.88	1.34	1.41
2	A	1	MMY	C13-N14	2.24	1.40	1.35

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	MMY	C21-N20-C13	5.93	122.04	116.27
2	A	1	MMY	N29-C25-N24	-4.04	120.41	124.54
2	A	1	MMY	C8-N7-C11	3.92	112.17	109.46
2	A	1	MMY	N12-C11-N7	3.46	131.66	125.27
2	A	1	MMY	C19-N14-C15	3.25	118.88	111.57
2	A	1	MMY	N20-C13-N12	-3.19	120.59	126.27
2	A	1	MMY	C22-C21-N20	3.18	119.43	115.10
2	A	1	MMY	C10-C21-N20	-3.17	117.78	122.75
2	A	1	MMY	C22-C30-N29	-3.09	119.37	124.28
2	A	1	MMY	C13-N12-C11	2.90	120.76	114.97
2	A	1	MMY	C30-N29-C25	2.79	121.21	116.29
2	A	1	MMY	C3-N4-C5	2.77	121.70	116.85
2	A	1	MMY	N12-C13-N14	2.53	120.71	117.12
2	A	1	MMY	C22-C23-N24	-2.50	120.31	124.28
2	A	1	MMY	C23-N24-C25	2.48	120.65	116.29
2	A	1	MMY	N26-C25-N29	2.35	119.83	117.40
2	A	1	MMY	N26-C25-N24	2.28	119.76	117.40
2	A	1	MMY	C30-C22-C23	2.17	118.04	114.73

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	MMY	N20-C21-C22-C30
2	A	1	MMY	C10-C21-C22-C30

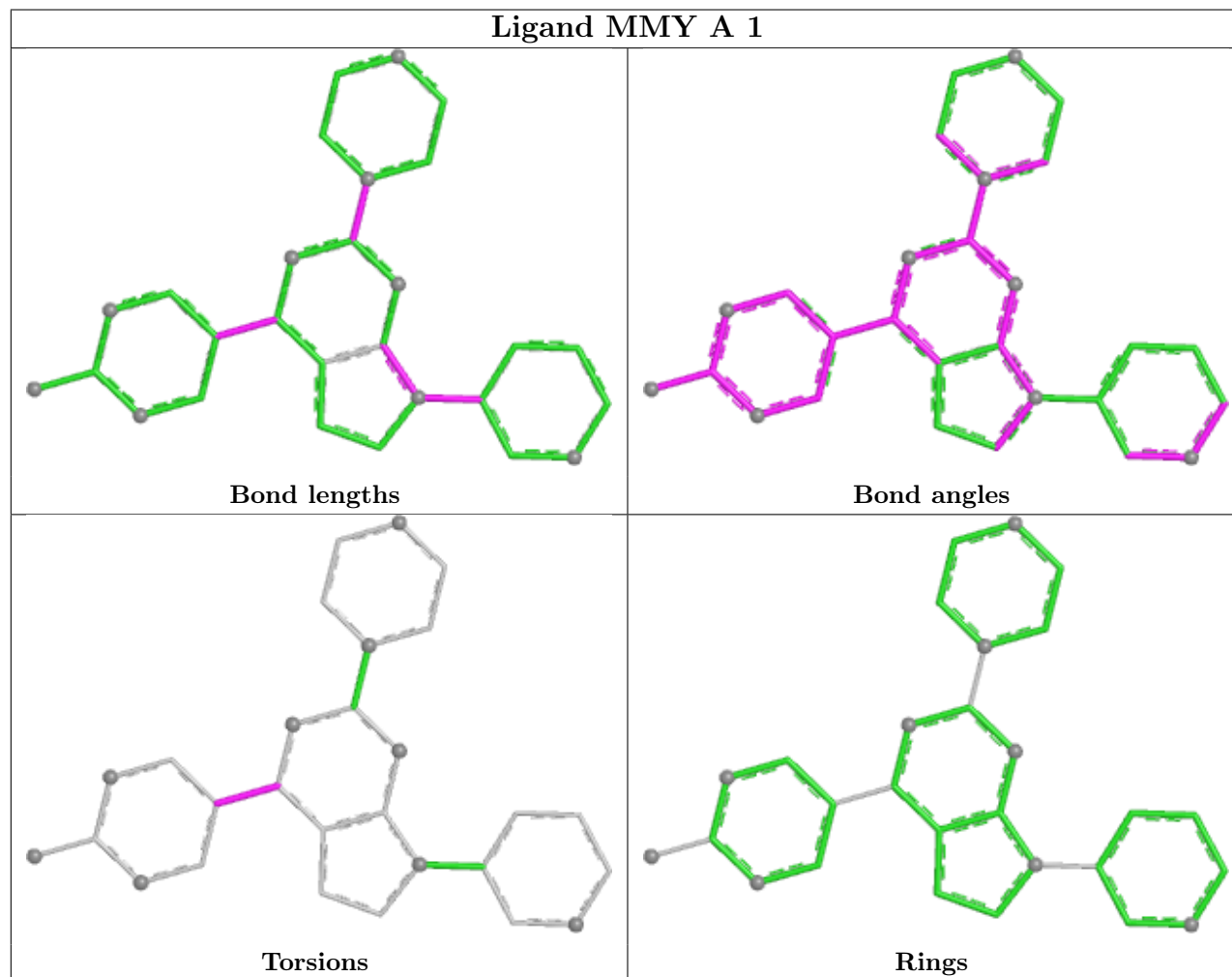
There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	MMY	6	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

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	839/966 (86%)	0.39	32 (3%) 44 45	23, 57, 90, 101	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	901	ALA	4.3
1	A	902	PHE	3.6
1	A	754	ALA	3.3
1	A	497	PHE	3.2
1	A	1093	GLY	3.0
1	A	599	GLY	2.8
1	A	979	ASN	2.7
1	A	1004	PRO	2.7
1	A	900	GLY	2.6
1	A	895	THR	2.6
1	A	1074	VAL	2.5
1	A	894	SER	2.5
1	A	1001	LYS	2.5
1	A	378	ASP	2.5
1	A	253	ALA	2.5
1	A	212	TRP	2.4
1	A	896	VAL	2.4
1	A	271	VAL	2.4
1	A	215	ILE	2.3
1	A	909	HIS	2.3
1	A	779	LEU	2.3
1	A	1091	VAL	2.3
1	A	916	PRO	2.3
1	A	270	PHE	2.2
1	A	803	VAL	2.2
1	A	1043	THR	2.1
1	A	771	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	991	PHE	2.1
1	A	272	LEU	2.1
1	A	221	PHE	2.1
1	A	1002	THR	2.0
1	A	1010	GLN	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](#)

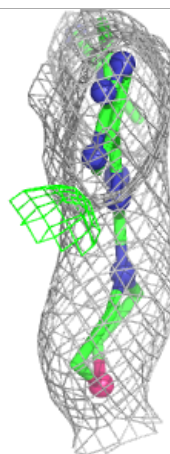
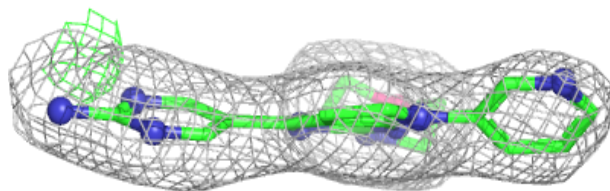
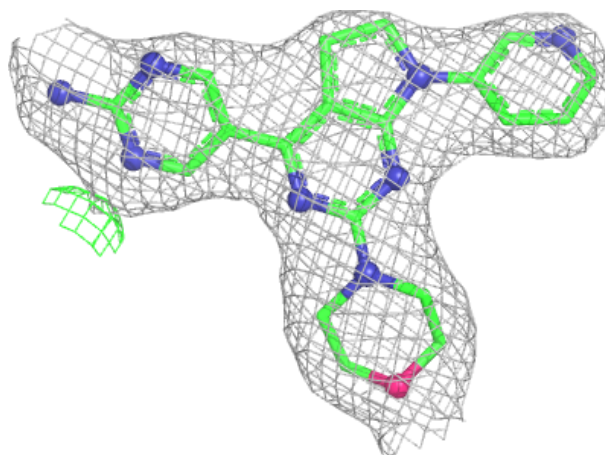
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	SO4	A	1103	5/5	0.85	0.12	80,80,82,85	0
3	SO4	A	2	5/5	0.89	0.09	97,99,101,103	0
2	MMY	A	1	28/28	0.91	0.10	36,48,56,60	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 MMY 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.