



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:56 PM UTC

PDB ID : 6PYU / pdb_00006pyu
Title : Human PI3Kdelta in complex with Compound 4-2 ((3S)-1'-(cyclopropanecarbonyl)-5-(quinoxalin-6-yl)spiro[indole-3,2'-pyrrolidin]-2(1H)-one)
Authors : Lesburg, C.A.; Augustin, M.A.
Deposited on : 2019-07-30
Resolution : 2.54 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

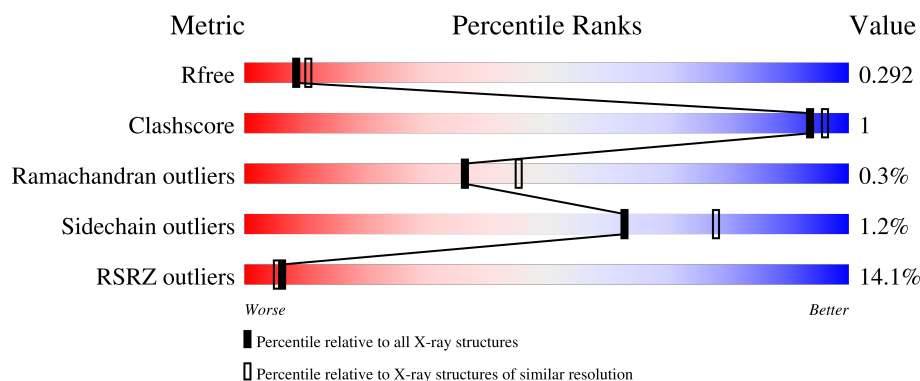
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

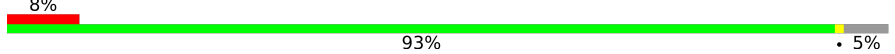
The reported resolution of this entry is 2.54 Å.

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	1018	
2	B	169	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8927 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 delta isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	930	7503	4802	1278	1370	53	323	0	0

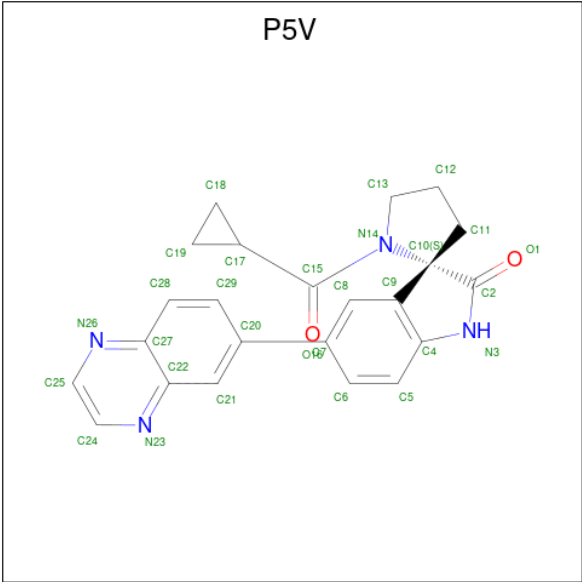
- Molecule 2 is a protein called Phosphatidylinositol 3-kinase regulatory subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	160	1383	859	250	269	5	73	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	469	ASP	GLU	conflict	UNP P27986
B	519	THR	LYS	conflict	UNP P27986
B	529	GLU	ASP	conflict	UNP P27986
B	539	VAL	ILE	conflict	UNP P27986

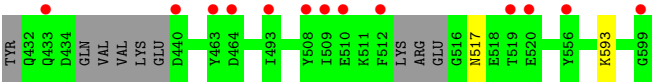
- Molecule 3 is (3S)-1'-(cyclopropanecarbonyl)-5-(quinoxalin-6-yl)spiro[indole-3,2'-pyrrolidin]-2(1H)-one (CCD ID: P5V) (formula: C₂₃H₂₀N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			29	23	4	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		
4	B	2	Total	O	0	0
			2	2		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.44Å 108.59Å 142.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.39 – 2.54 86.32 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.0 (86.39-2.54) 98.1 (86.32-2.54)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.240 , 0.292 0.238 , 0.292	Depositor DCC
R_{free} test set	948 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	68.8	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 66.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8927	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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: P5V

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	1.09	4/7667 (0.1%)	1.48	16/10365 (0.2%)
2	B	1.03	0/1400	1.63	1/1865 (0.1%)
All	All	1.08	4/9067 (0.0%)	1.50	17/12230 (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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	821	ARG	NE-CZ	8.61	1.42	1.33
1	A	955	ARG	CD-NE	-7.57	1.35	1.46
1	A	191	LEU	CB-CG	-5.64	1.42	1.53
1	A	195	LYS	CD-CE	-5.12	1.37	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	991	CYS	CA-C-N	6.18	128.85	120.38
1	A	991	CYS	C-N-CA	6.18	128.85	120.38
1	A	853	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	605	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	82	LEU	CA-C-N	5.39	127.50	120.28
1	A	82	LEU	C-N-CA	5.39	127.50	120.28
1	A	352	GLU	CB-CG-CD	5.39	121.76	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	813	TYR	CA-C-N	5.36	125.77	120.31
1	A	813	TYR	C-N-CA	5.36	125.77	120.31
1	A	832	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	458	THR	CA-C-N	5.12	128.75	121.02
1	A	458	THR	C-N-CA	5.12	128.75	121.02
1	A	664	PHE	CA-C-O	-5.09	115.16	120.55
1	A	93	GLN	CB-CA-C	5.06	115.40	111.00
1	A	700	LYS	CA-C-N	5.06	127.33	120.65
1	A	700	LYS	C-N-CA	5.06	127.33	120.65
2	B	593	LYS	N-CA-C	-5.06	105.47	111.69

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	496	ARG	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	7503	0	7485	23	0
2	B	1383	0	1368	0	0
3	A	29	0	0	0	0
4	A	10	0	0	0	0
4	B	2	0	0	0	0
All	All	8927	0	8853	23	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 1.

All (23) 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:322:PRO:HA	1:A:380:ASN:HA	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:PHE:HB3	1:A:592:VAL:HG11	1.90	0.53
1:A:954:GLU:OE1	1:A:957:ARG:NH2	2.43	0.52
1:A:74:ASN:OD1	1:A:76:THR:HG22	2.14	0.48
1:A:167:PHE:CE1	1:A:247:HIS:HB3	2.49	0.47
1:A:247:HIS:CD2	1:A:732:GLN:HE21	2.33	0.46
1:A:1023:LEU:O	1:A:1026:SER:HB3	2.15	0.46
1:A:26:LEU:HB3	1:A:27:PRO:HD2	1.98	0.45
1:A:158:GLY:O	1:A:160:GLU:N	2.50	0.44
1:A:790:THR:HG21	1:A:912:PHE:CG	2.53	0.44
1:A:583:LEU:HD11	1:A:600:LEU:HD11	2.00	0.43
1:A:507:GLU:HB3	1:A:534:LEU:HD11	2.01	0.43
1:A:424:MET:HG2	1:A:459:VAL:HG11	2.01	0.43
1:A:757:LYS:N	1:A:758:PRO:CD	2.82	0.43
1:A:221:LEU:HD22	1:A:236:PRO:HB3	2.00	0.43
1:A:236:PRO:HD2	1:A:237:GLU:OE1	2.19	0.42
1:A:187:ASN:OD1	1:A:187:ASN:N	2.52	0.42
1:A:41:ASN:HA	1:A:87:ARG:O	2.20	0.42
1:A:383:ASP:HB3	1:A:556:ASN:O	2.20	0.42
1:A:158:GLY:O	1:A:161:ALA:N	2.51	0.41
1:A:750:THR:OG1	1:A:751:PHE:N	2.53	0.41
1:A:882:TYR:HB3	1:A:909:HIS:CD2	2.56	0.41
1:A:950:SER:O	1:A:954:GLU:HG2	2.21	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	912/1018 (90%)	872 (96%)	37 (4%)	3 (0%)	36	45
2	B	154/169 (91%)	150 (97%)	4 (3%)	0	100	100
All	All	1066/1187 (90%)	1022 (96%)	41 (4%)	3 (0%)	36	45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	TRP
1	A	754	SER
1	A	820	ASP

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	829/903 (92%)	818 (99%)	11 (1%)	61	76
2	B	151/160 (94%)	150 (99%)	1 (1%)	76	85
All	All	980/1063 (92%)	968 (99%)	12 (1%)	63	78

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	71	THR
1	A	240	THR
1	A	373	GLN
1	A	522	GLU
1	A	559	GLU
1	A	590	CYS
1	A	861	SER
1	A	915	PHE
1	A	990	SER
1	A	1032	ASN
2	B	517	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	47	GLN

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Mol	Chain	Res	Type
1	A	51	HIS
1	A	116	GLN
1	A	145	GLN
1	A	247	HIS
1	A	321	GLN
1	A	380	ASN
1	A	617	GLN
1	A	656	HIS
1	A	696	ASN
1	A	914	HIS

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 oligosaccharides 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	$\# Z > 2$
3	P5V	A	1101	-	34,34,34	1.15	2 (5%)	45,52,52	1.30	5 (11%)

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
3	P5V	A	1101	-	-	4/12/43/43	0/6/6/6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	P5V	C10-C2	-2.94	1.51	1.55
3	A	1101	P5V	C22-N23	-2.09	1.33	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	P5V	C12-C13-N14	5.12	109.01	103.32
3	A	1101	P5V	O16-C15-C17	-2.77	116.78	120.86
3	A	1101	P5V	C17-C15-N14	2.31	120.94	118.79
3	A	1101	P5V	C5-C4-C9	-2.22	119.85	121.92
3	A	1101	P5V	C10-C9-C4	-2.18	107.02	108.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

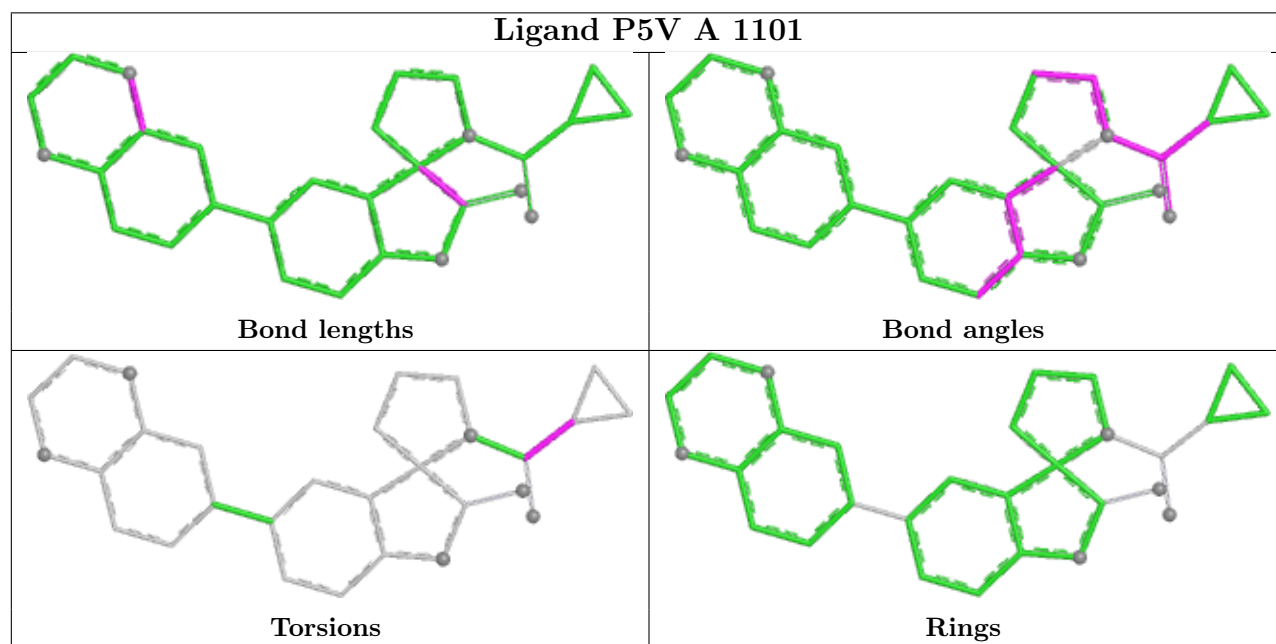
Mol	Chain	Res	Type	Atoms
3	A	1101	P5V	N14-C15-C17-C19
3	A	1101	P5V	O16-C15-C17-C19
3	A	1101	P5V	O16-C15-C17-C18
3	A	1101	P5V	N14-C15-C17-C18

There are no ring outliers.

No monomer is involved in short contacts.

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	930/1018 (91%)	1.06	141 (15%) 5 5	42, 97, 160, 212	99 (10%)
2	B	160/169 (94%)	0.63	13 (8%) 18 17	54, 91, 128, 152	24 (15%)
All	All	1090/1187 (91%)	1.00	154 (14%) 6 5	42, 95, 156, 212	123 (11%)

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	60	HIS	7.7
1	A	471	LEU	6.5
1	A	938	PHE	5.1
1	A	806	LEU	4.9
2	B	556	TYR	4.8
1	A	216	LEU	4.8
1	A	507	GLU	4.4
1	A	591	HIS	4.3
1	A	875	PHE	4.2
1	A	671	TYR	4.2
1	A	867	ALA	4.2
1	A	588	PRO	4.1
2	B	433	GLN	4.1
1	A	1034	LEU	4.1
1	A	392	PHE	4.1
1	A	948	ASN	4.0
1	A	441	MET	4.0
1	A	960	CYS	4.0
1	A	594	SER	3.9
1	A	186	PRO	3.9
1	A	243	VAL	3.9
1	A	328	ILE	3.9
1	A	638	LEU	3.8
1	A	534	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	864	PRO	3.8
1	A	259	PHE	3.8
1	A	220	ALA	3.7
1	A	327	LEU	3.6
1	A	1031	VAL	3.6
1	A	565	LEU	3.6
1	A	123	LYS	3.5
1	A	219	CYS	3.5
1	A	1023	LEU	3.5
2	B	512	PHE	3.5
1	A	786	GLN	3.4
1	A	58	LEU	3.4
1	A	282	ILE	3.4
1	A	144	CYS	3.4
1	A	506	GLU	3.4
2	B	520	GLU	3.4
2	B	508	TYR	3.3
1	A	314	VAL	3.3
1	A	254	TYR	3.3
1	A	569	CYS	3.3
1	A	347	LEU	3.3
1	A	740	LEU	3.3
2	B	440	ASP	3.3
1	A	590	CYS	3.3
1	A	805	GLY	3.3
1	A	250	LEU	3.2
1	A	855	LEU	3.2
1	A	856	LEU	3.2
1	A	122	GLY	3.2
1	A	510	GLN	3.1
1	A	128	PHE	3.1
1	A	511	LEU	3.1
1	A	488	LEU	3.0
1	A	335	ALA	3.0
1	A	212	VAL	3.0
1	A	71	THR	3.0
2	B	519	THR	2.9
1	A	1033	TRP	2.9
1	A	1015	PHE	2.9
1	A	985	GLY	2.9
1	A	273	HIS	2.9
1	A	119	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	235	GLN	2.9
1	A	241	LEU	2.9
1	A	893	ASP	2.9
1	A	761	ILE	2.9
1	A	61	MET	2.8
1	A	369	PRO	2.8
1	A	274	LEU	2.8
1	A	838	GLN	2.8
1	A	70	PHE	2.8
1	A	491	ILE	2.8
2	B	509	ILE	2.8
1	A	256	LEU	2.8
1	A	139	PHE	2.8
1	A	213	PRO	2.7
1	A	164	GLN	2.7
2	B	493	ILE	2.7
1	A	125	LEU	2.7
1	A	475	LEU	2.7
1	A	928	GLU	2.7
1	A	72	CYS	2.6
1	A	343	VAL	2.6
1	A	1026	SER	2.6
1	A	283	LEU	2.6
1	A	936	TYR	2.6
1	A	379	ILE	2.6
1	A	342	VAL	2.6
1	A	827	VAL	2.6
1	A	735	LEU	2.5
1	A	530	LEU	2.5
1	A	432	LEU	2.5
1	A	156	GLN	2.5
1	A	118	SER	2.5
1	A	466	ASP	2.5
2	B	463	TYR	2.5
1	A	425	LEU	2.5
1	A	717	LEU	2.5
1	A	865	GLY	2.4
2	B	599	GLY	2.4
1	A	815	CYS	2.4
1	A	760	TRP	2.4
1	A	852	LYS	2.4
1	A	508	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	956	PHE	2.4
1	A	152	ALA	2.4
2	B	464	ASP	2.3
1	A	828	VAL	2.3
1	A	359	SER	2.3
1	A	239	TYR	2.3
1	A	370	VAL	2.3
1	A	505	GLU	2.3
1	A	1012	LEU	2.3
1	A	1013	LYS	2.3
1	A	932	PHE	2.3
1	A	175	ALA	2.3
1	A	868	LEU	2.3
1	A	148	GLU	2.3
1	A	939	VAL	2.3
1	A	472	LEU	2.2
1	A	759	LEU	2.2
1	A	489	GLU	2.2
1	A	146	PHE	2.2
1	A	205	PHE	2.2
1	A	187	ASN	2.2
1	A	394	LEU	2.2
1	A	834	ILE	2.2
1	A	83	GLU	2.2
1	A	388	ALA	2.2
1	A	870	ARG	2.2
1	A	207	VAL	2.2
1	A	526	HIS	2.2
1	A	158	GLY	2.2
1	A	1005	GLY	2.2
1	A	197	GLU	2.2
1	A	521	GLY	2.1
1	A	998	LEU	2.1
1	A	221	LEU	2.1
1	A	350	GLY	2.1
1	A	744	VAL	2.1
1	A	858	TRP	2.1
1	A	193	ASN	2.1
1	A	512	ARG	2.1
1	A	634	LEU	2.1
1	A	915	PHE	2.0
2	B	510	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	339	MET	2.0
1	A	585	PHE	2.0
1	A	40	ALA	2.0
1	A	226	THR	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](#)

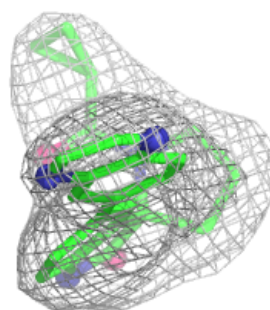
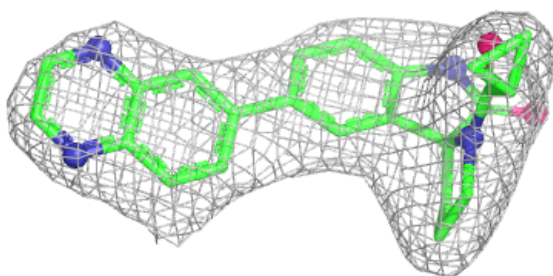
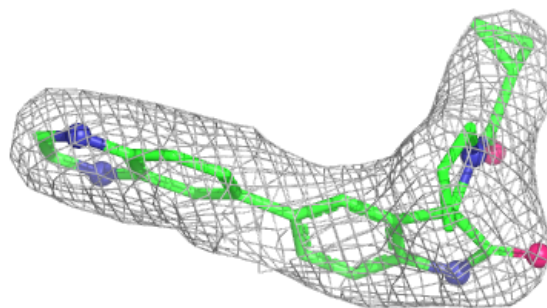
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	P5V	A	1101	29/29	0.91	0.09	46,74,92,105	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 P5V A 1101:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.