



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:30 PM UTC

PDB ID : 6YM3 / pdb_00006ym3
Title : Crystal structure of Compound 1 with PIP4K2A
Authors : Holton, S.J.; Wortmann, L.; Braeuer, N.; Irlbacher, H.; Weiske, J.; Lechner, C.; Meier, R.; Puetter, V.; Christ, C.; ter Laak, T.; Lienau, P.; Lesche, R.; Nicke, B.; Bauser, M.; Haegebarth, A.; von Nussbaum, F.; Mumberg, D.; Lemos, C.
Deposited on : 2020-04-07
Resolution : 2.05 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](#) ①) 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

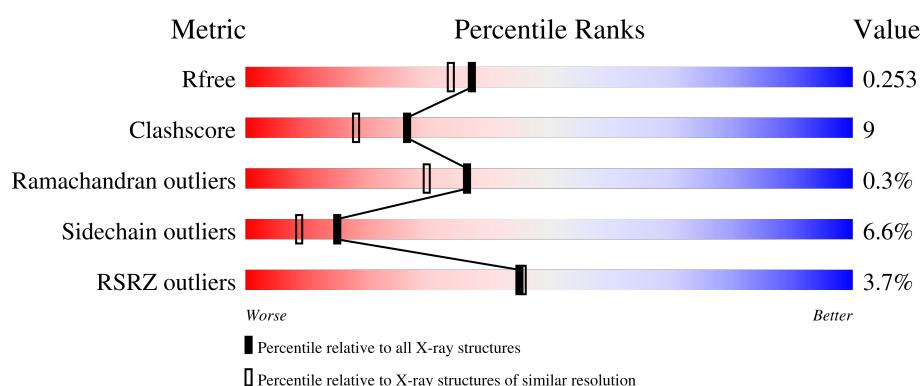
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	394	3% 63% 14% • 19%
1	B	394	3% 57% 19% • 22%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5415 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 5-phosphate 4-kinase type-2 alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	P	S	0	2	0
			2656	1702	445	494	1	14			
1	B	307	Total	C	N	O	P	S	0	1	0
			2537	1633	424	466	1	13			

There are 46 discrepancies between the modelled and reference sequences:

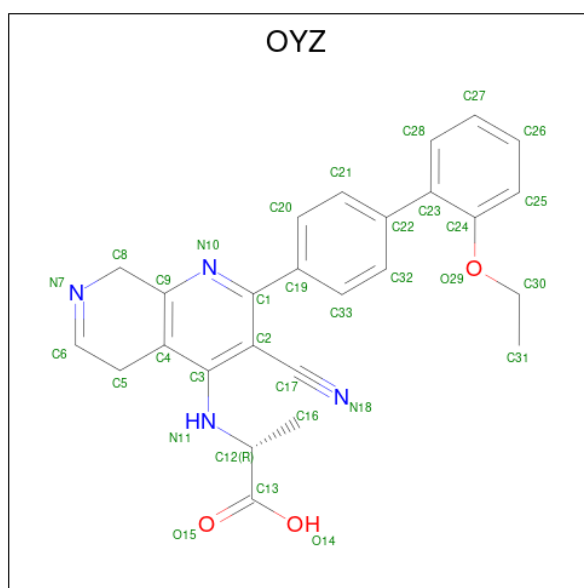
Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	initiating methionine	UNP P48426
A	13	HIS	-	expression tag	UNP P48426
A	14	HIS	-	expression tag	UNP P48426
A	15	HIS	-	expression tag	UNP P48426
A	16	HIS	-	expression tag	UNP P48426
A	17	HIS	-	expression tag	UNP P48426
A	18	HIS	-	expression tag	UNP P48426
A	19	SER	-	expression tag	UNP P48426
A	20	SER	-	expression tag	UNP P48426
A	21	GLY	-	expression tag	UNP P48426
A	22	VAL	-	expression tag	UNP P48426
A	23	ASP	-	expression tag	UNP P48426
A	24	LEU	-	expression tag	UNP P48426
A	25	GLY	-	expression tag	UNP P48426
A	26	THR	-	expression tag	UNP P48426
A	27	GLU	-	expression tag	UNP P48426
A	28	ASN	-	expression tag	UNP P48426
A	29	LEU	-	expression tag	UNP P48426
A	30	TYR	-	expression tag	UNP P48426
A	31	PHE	-	expression tag	UNP P48426
A	32	GLN	-	expression tag	UNP P48426
A	33	SER	-	expression tag	UNP P48426
A	34	MET	-	expression tag	UNP P48426
B	12	MET	-	initiating methionine	UNP P48426
B	13	HIS	-	expression tag	UNP P48426

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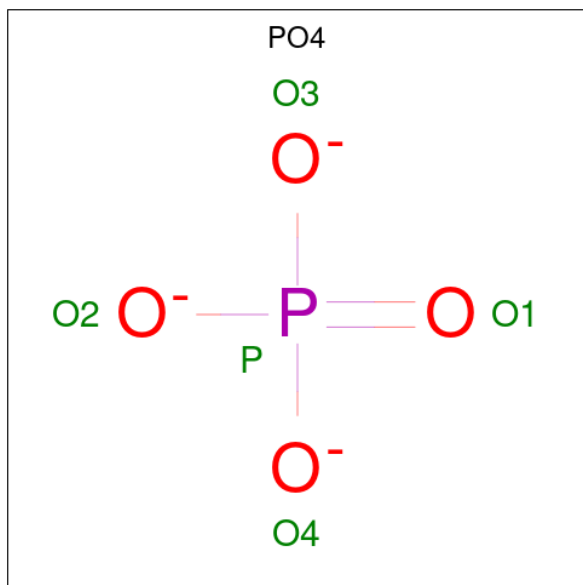
Chain	Residue	Modelled	Actual	Comment	Reference
B	14	HIS	-	expression tag	UNP P48426
B	15	HIS	-	expression tag	UNP P48426
B	16	HIS	-	expression tag	UNP P48426
B	17	HIS	-	expression tag	UNP P48426
B	18	HIS	-	expression tag	UNP P48426
B	19	SER	-	expression tag	UNP P48426
B	20	SER	-	expression tag	UNP P48426
B	21	GLY	-	expression tag	UNP P48426
B	22	VAL	-	expression tag	UNP P48426
B	23	ASP	-	expression tag	UNP P48426
B	24	LEU	-	expression tag	UNP P48426
B	25	GLY	-	expression tag	UNP P48426
B	26	THR	-	expression tag	UNP P48426
B	27	GLU	-	expression tag	UNP P48426
B	28	ASN	-	expression tag	UNP P48426
B	29	LEU	-	expression tag	UNP P48426
B	30	TYR	-	expression tag	UNP P48426
B	31	PHE	-	expression tag	UNP P48426
B	32	GLN	-	expression tag	UNP P48426
B	33	SER	-	expression tag	UNP P48426
B	34	MET	-	expression tag	UNP P48426

- Molecule 2 is (2 {R})-2-[[3-cyano-2-[4-(2-ethoxyphenyl)phenyl]-5,8-dihydro-1,7-naphthyridi n-4-yl]amino]propanoic acid (CCD ID: OYZ) (formula: C₂₆H₂₄N₄O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			33	26	4	3		
2	B	1	Total	C	N	O	0	0
			33	26	4	3		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

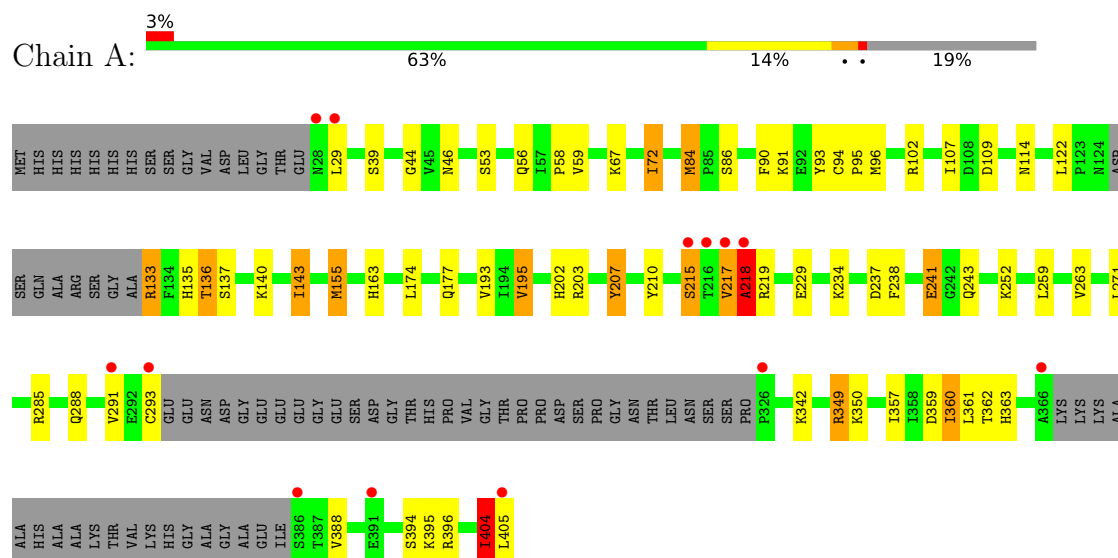
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	81	Total	O	0	0
			81	81		
4	B	65	Total	O	0	0
			65	65		

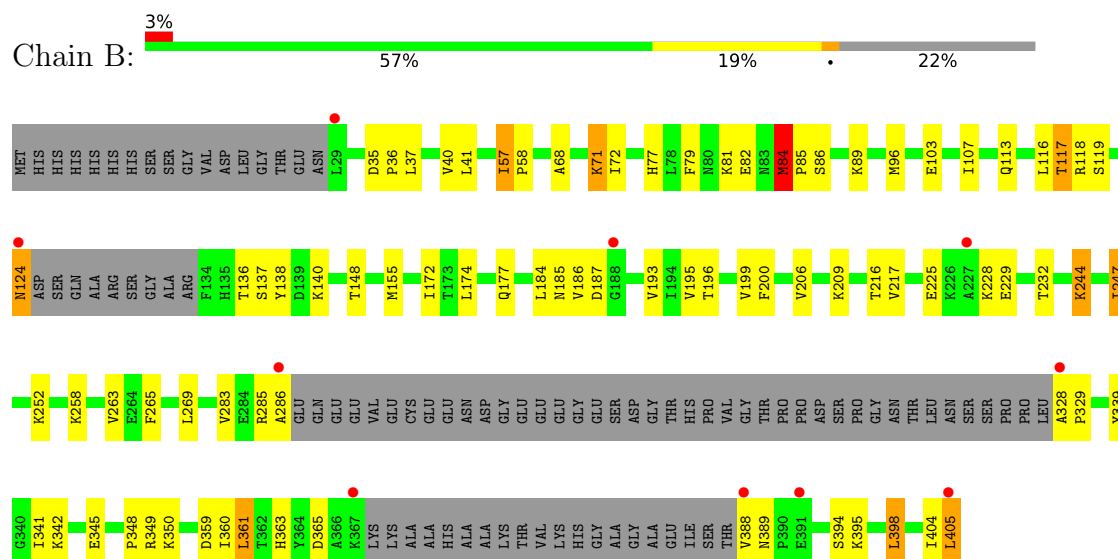
3 Residue-property plots [i](#)

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 5-phosphate 4-kinase type-2 alpha



- Molecule 1: Phosphatidylinositol 5-phosphate 4-kinase type-2 alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.93Å 98.13Å 104.26Å 90.00° 92.96° 90.00°	Depositor
Resolution (Å)	45.99 – 2.05 45.99 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.4 (45.99-2.05) 99.7 (45.99-2.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.202 , 0.250 0.215 , 0.253	Depositor DCC
R_{free} test set	2100 reflections (3.79%)	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5415	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.43% 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: PHD, PO4, OYZ

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	1.34	10/2702 (0.4%)	1.39	14/3640 (0.4%)
1	B	1.29	5/2583 (0.2%)	1.50	23/3483 (0.7%)
All	All	1.32	15/5285 (0.3%)	1.44	37/7123 (0.5%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	113	GLN	C-O	-8.49	1.14	1.24
1	A	215	SER	C-O	-7.45	1.17	1.24
1	B	195	VAL	C-O	6.76	1.31	1.24
1	A	136	THR	C-O	6.34	1.31	1.23
1	A	46	ASN	C-O	-6.18	1.17	1.24
1	B	79	PHE	C-O	6.14	1.30	1.23
1	A	163	HIS	CE1-NE2	6.09	1.38	1.32
1	A	195	VAL	C-O	6.02	1.30	1.24
1	A	53	SER	C-O	-5.79	1.16	1.24
1	B	84	MET	CA-C	-5.56	1.47	1.52
1	B	71	LYS	C-O	5.48	1.31	1.23
1	A	177	GLN	C-O	5.34	1.30	1.24
1	A	143	ILE	C-O	5.27	1.30	1.24
1	A	218	ALA	CA-C	5.23	1.59	1.52
1	A	39	SER	C-O	-5.12	1.18	1.24

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	VAL	N-CA-C	8.33	126.66	109.34
1	B	187	ASP	CA-CB-CG	7.31	119.91	112.60
1	B	148	THR	CA-CB-OG1	-6.99	99.11	109.60
1	A	217	VAL	CA-C-N	6.98	134.87	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	VAL	C-N-CA	6.98	134.87	121.54
1	B	345	GLU	CB-CG-CD	6.94	124.39	112.60
1	B	107	ILE	N-CA-C	6.60	117.62	107.99
1	B	229	GLU	N-CA-C	-6.38	103.62	111.40
1	B	57	ILE	CB-CA-C	-6.37	103.89	110.71
1	A	218	ALA	CA-C-N	6.23	132.66	122.07
1	A	218	ALA	C-N-CA	6.23	132.66	122.07
1	B	216	THR	N-CA-C	-6.08	104.58	111.14
1	B	200	PHE	CA-C-N	5.94	129.15	120.71
1	B	200	PHE	C-N-CA	5.94	129.15	120.71
1	B	404	ILE	CA-C-N	5.86	132.24	121.70
1	B	404	ILE	C-N-CA	5.86	132.24	121.70
1	B	68	ALA	N-CA-C	5.82	118.41	110.55
1	B	395	LYS	N-CA-C	-5.78	104.90	111.14
1	B	86	SER	N-CA-C	5.75	117.63	111.36
1	A	174	LEU	N-CA-C	-5.75	105.93	113.17
1	B	84	MET	N-CA-C	5.70	117.45	108.55
1	A	86	SER	N-CA-C	5.61	117.48	111.36
1	A	404	ILE	CA-C-N	5.61	131.80	121.70
1	A	404	ILE	C-N-CA	5.61	131.80	121.70
1	B	174	LEU	N-CA-C	-5.59	105.81	113.30
1	B	117	THR	N-CA-C	5.57	121.63	114.56
1	A	84	MET	N-CA-C	5.54	117.19	108.55
1	A	363	HIS	CA-CB-CG	-5.43	108.36	113.80
1	B	117	THR	N-CA-CB	-5.35	103.89	111.00
1	A	114	ASN	CA-C-N	5.29	127.36	120.28
1	A	114	ASN	C-N-CA	5.29	127.36	120.28
1	B	187	ASP	N-CA-C	-5.26	105.51	112.24
1	B	348	PRO	CA-C-N	5.18	130.71	122.74
1	B	348	PRO	C-N-CA	5.18	130.71	122.74
1	B	82	GLU	CA-C-N	5.13	127.57	120.29
1	B	82	GLU	C-N-CA	5.13	127.57	120.29
1	A	107	ILE	N-CA-C	5.03	115.33	107.99

There are no chirality outliers.

There are no planarity outliers.

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	2656	0	2611	46	0
1	B	2537	0	2488	47	0
2	A	33	0	0	3	0
2	B	33	0	0	2	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	81	0	0	0	0
4	B	65	0	0	3	0
All	All	5415	0	5099	96	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 9.

All (96) 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:B:155:MET:HE2	1:B:361:LEU:HD21	1.33	1.06
1:B:155:MET:CE	1:B:361:LEU:HD21	1.95	0.96
1:B:118:ARG:HH11	1:B:118:ARG:HG3	1.35	0.90
1:B:252:LYS:HD2	1:B:405:LEU:HD13	1.61	0.80
1:A:217:VAL:HG12	1:A:219:ARG:HB3	1.63	0.78
1:A:155:MET:O	1:A:155:MET:HE2	1.91	0.69
1:B:40:VAL:HG21	1:B:186:VAL:HG22	1.73	0.69
1:A:357:ILE:CG2	1:A:360[A]:ILE:HD11	2.23	0.69
1:A:136:THR:CG2	1:A:140:LYS:HA	2.22	0.69
1:B:118:ARG:HG3	1:B:118:ARG:NH1	2.05	0.69
1:A:349:ARG:HH21	1:A:349:ARG:HB3	1.60	0.67
1:B:405:LEU:HD23	1:B:405:LEU:N	2.10	0.67
1:B:209:LYS:HE3	1:B:232:THR:OG1	1.96	0.66
1:B:252:LYS:HE3	1:B:405:LEU:HD22	1.77	0.66
1:B:252:LYS:CD	1:B:405:LEU:HD13	2.26	0.65
1:B:84:MET:HE3	1:B:85:PRO:HD2	1.79	0.64
1:B:84:MET:HB3	1:B:85:PRO:HD2	1.80	0.64
1:A:357:ILE:HG22	1:A:360[A]:ILE:CD1	2.27	0.63
1:B:71:LYS:C	1:B:72:ILE:HD12	2.25	0.62
1:A:357:ILE:HG21	1:A:360[A]:ILE:HD11	1.81	0.62
1:B:136:THR:HG22	1:B:137:SER:O	2.00	0.62
1:B:77:HIS:HE1	4:B:661:HOH:O	1.85	0.60
1:A:155:MET:HG2	1:A:361:LEU:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:LYS:CE	1:B:405:LEU:HD13	2.32	0.59
1:A:136:THR:HG22	1:A:140:LYS:HA	1.84	0.58
2:A:501:OYZ:C12	2:A:501:OYZ:C17	2.82	0.58
1:A:207:TYR:HD2	1:A:285:ARG:NH1	2.02	0.58
1:A:102:ARG:NH1	1:A:109:ASP:OD2	2.38	0.56
1:B:394:SER:O	1:B:398:LEU:HB2	2.05	0.56
1:B:71:LYS:O	1:B:72:ILE:HD12	2.06	0.55
1:B:136:THR:CG2	1:B:140:LYS:HA	2.38	0.54
1:A:237:ASP:O	1:A:241:GLU:HB2	2.10	0.52
1:A:263:VAL:HG12	1:A:394:SER:HB2	1.91	0.52
1:B:155:MET:CE	1:B:361:LEU:CD2	2.80	0.52
1:A:91:LYS:HE2	1:A:93:TYR:CE1	2.45	0.52
1:B:263:VAL:HG13	1:B:394:SER:HB2	1.91	0.51
1:B:172:ILE:HG22	1:B:258:LYS:HD3	1.91	0.51
1:A:349:ARG:HB3	1:A:349:ARG:NH2	2.26	0.51
1:B:89:LYS:HB2	1:B:185[B]:ASN:HB2	1.91	0.51
1:A:133:ARG:HB2	1:A:133:ARG:CZ	2.41	0.51
1:A:259:LEU:HD12	1:A:357:ILE:HD11	1.94	0.50
1:B:225:GLU:O	1:B:228:LYS:HG3	2.11	0.50
2:B:501:OYZ:C17	2:B:501:OYZ:C12	2.89	0.50
1:B:124:ASN:H	1:B:124:ASN:HD22	1.60	0.49
1:B:58:PRO:HD3	1:B:96:MET:HE1	1.94	0.49
1:B:363:HIS:HD2	1:B:365:ASP:H	1.59	0.49
1:A:357:ILE:CG2	1:A:360[A]:ILE:CD1	2.89	0.49
1:A:217:VAL:HB	1:A:218:ALA:H	1.36	0.48
1:B:252:LYS:HE3	1:B:405:LEU:HD13	1.94	0.48
1:A:67:LYS:HE2	4:B:661:HOH:O	2.13	0.48
1:B:103:GLU:OE2	4:B:601:HOH:O	2.20	0.48
1:A:207:TYR:CD2	1:A:285:ARG:NH1	2.82	0.48
1:B:263:VAL:CG1	1:B:394:SER:HB2	2.43	0.48
1:B:118:ARG:NH1	1:B:118:ARG:CG	2.73	0.48
1:A:404:ILE:O	1:A:405:LEU:HB2	2.13	0.47
1:A:252:LYS:HD2	1:A:405:LEU:HG	1.95	0.47
1:B:265:PHE:CZ	1:B:269:LEU:HD11	2.49	0.47
1:A:219:ARG:HG3	1:A:234:LYS:HD3	1.96	0.47
1:A:271:LEU:HA	1:A:362:THR:O	2.14	0.47
1:B:119:SER:HB3	1:B:138:TYR:CG	2.50	0.47
1:A:210:TYR:CE2	1:A:243:GLN:HG2	2.50	0.47
1:B:37:LEU:HD23	1:B:186:VAL:HG23	1.96	0.46
2:B:501:OYZ:C17	2:B:501:OYZ:C33	2.93	0.46
1:A:56:GLN:OE1	1:A:56:GLN:N	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:501:OYZ:C17	2:A:501:OYZ:C16	2.93	0.46
1:A:44:GLY:HA3	1:A:90:PHE:CE2	2.50	0.46
1:A:155:MET:O	1:A:155:MET:CE	2.61	0.46
1:A:102:ARG:NH1	1:A:109:ASP:CG	2.74	0.46
1:B:360:ILE:HG13	1:B:361:LEU:HD13	1.96	0.46
1:A:102:ARG:HH11	1:A:109:ASP:CG	2.23	0.46
1:A:238:PHE:CE1	1:A:404:ILE:HB	2.51	0.45
1:A:136:THR:HG22	1:A:137:SER:O	2.17	0.45
1:B:199:VAL:HA	1:B:339:TYR:CD2	2.51	0.45
1:B:405:LEU:N	1:B:405:LEU:CD2	2.79	0.45
1:A:58:PRO:HD3	1:A:96:MET:CE	2.47	0.44
1:B:35:ASP:HA	1:B:36:PRO:HD2	1.88	0.44
1:A:72:ILE:HD11	1:B:72:ILE:HG23	1.99	0.44
1:B:244:LYS:HB2	1:B:244:LYS:HE3	1.40	0.44
1:A:285:ARG:HE	1:A:285:ARG:HB3	1.49	0.43
1:B:177:GLN:O	1:B:196:THR:HA	2.18	0.43
1:A:155:MET:HG2	1:A:361:LEU:CD1	2.48	0.43
1:A:217:VAL:HG12	1:A:219:ARG:CB	2.43	0.43
1:B:247:ILE:HG21	1:B:341:ILE:HG21	2.00	0.43
1:B:41:LEU:HB2	1:B:184:LEU:HD21	2.00	0.42
1:B:328:ALA:HB1	1:B:329:PRO:HD2	2.00	0.42
1:A:202:HIS:NE2	1:A:203:ARG:HG3	2.33	0.42
1:A:72:ILE:CD1	1:B:72:ILE:HG23	2.49	0.42
1:A:263:VAL:CG1	1:A:394:SER:HB2	2.49	0.42
1:A:143:ILE:O	1:A:195:VAL:HA	2.19	0.41
1:B:389:ASN:C	1:B:389:ASN:OD1	2.63	0.41
1:A:252:LYS:HD2	1:A:405:LEU:CD2	2.51	0.41
2:A:501:OYZ:C17	2:A:501:OYZ:C33	2.98	0.41
1:B:283:VAL:O	1:B:286:ALA:HB3	2.21	0.41
1:A:122:LEU:O	1:A:135:HIS:HA	2.21	0.40
1:A:94:CYS:N	1:A:95:PRO:HD3	2.37	0.40
1:A:215:SER:CB	1:A:396:ARG:HD3	2.52	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	311/394 (79%)	302 (97%)	7 (2%)	2 (1%)	21	13
1	B	299/394 (76%)	294 (98%)	5 (2%)	0	100	100
All	All	610/788 (77%)	596 (98%)	12 (2%)	2 (0%)	36	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	ALA
1	A	291	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	297/353 (84%)	277 (93%)	20 (7%)	15	8
1	B	280/353 (79%)	261 (93%)	19 (7%)	14	8
All	All	577/706 (82%)	538 (93%)	39 (7%)	15	8

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	59	VAL
1	A	72	ILE
1	A	84	MET
1	A	133	ARG
1	A	155	MET
1	A	193	VAL
1	A	207	TYR
1	A	229	GLU
1	A	241	GLU

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Mol	Chain	Res	Type
1	A	288	GLN
1	A	293	CYS
1	A	342	LYS
1	A	349	ARG
1	A	350	LYS
1	A	360[A]	ILE
1	A	360[B]	ILE
1	A	388	VAL
1	A	395	LYS
1	A	404	ILE
1	B	57	ILE
1	B	81	LYS
1	B	84	MET
1	B	116	LEU
1	B	117	THR
1	B	124	ASN
1	B	193	VAL
1	B	206	VAL
1	B	217	VAL
1	B	244	LYS
1	B	247	ILE
1	B	285	ARG
1	B	342	LYS
1	B	349	ARG
1	B	350	LYS
1	B	361	LEU
1	B	388	VAL
1	B	398	LEU
1	B	405	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	240	ASN
1	A	268	GLN
1	A	288	GLN
1	B	110	GLN
1	B	124	ASN
1	B	202	HIS
1	B	240	ASN
1	B	363	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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
1	PHD	A	359	1	9,11,12	2.78	2 (22%)	9,15,17	1.10	0
1	PHD	B	359	1	9,11,12	3.46	2 (22%)	9,15,17	2.32	3 (33%)

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
1	PHD	A	359	1	-	0/8/11/13	-
1	PHD	B	359	1	-	0/8/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	359	PHD	P-OD1	9.52	1.76	1.59
1	A	359	PHD	P-OD1	6.54	1.71	1.59
1	A	359	PHD	P-OP1	4.50	1.64	1.50
1	B	359	PHD	P-OP2	3.04	1.66	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	359	PHD	OD1-P-OP1	-5.66	91.34	109.47
1	B	359	PHD	OP2-P-OD1	2.92	113.84	105.32
1	B	359	PHD	OP3-P-OP1	2.02	118.71	110.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	PO4	A	502	-	4,4,4	0.56	0	6,6,6	0.60	0
2	OYZ	A	501	-	34,36,36	3.91	12 (35%)	42,50,50	2.08	15 (35%)
2	OYZ	B	501	-	34,36,36	3.74	11 (32%)	42,50,50	1.67	11 (26%)
3	PO4	B	502	-	4,4,4	0.67	0	6,6,6	0.65	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	OYZ	A	501	-	-	3/21/28/28	0/3/4/4
2	OYZ	B	501	-	-	3/21/28/28	0/3/4/4

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	OYZ	C8-N7	-13.80	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	OYZ	C8-N7	-13.70	1.33	1.46
2	A	501	OYZ	C8-C9	-11.17	1.33	1.50
2	B	501	OYZ	C8-C9	-9.80	1.35	1.50
2	A	501	OYZ	C19-C1	-8.60	1.39	1.49
2	B	501	OYZ	C5-C4	-7.06	1.36	1.51
2	B	501	OYZ	C19-C1	-6.65	1.41	1.49
2	A	501	OYZ	C5-C4	-6.29	1.38	1.51
2	B	501	OYZ	C23-C22	-5.05	1.40	1.49
2	A	501	OYZ	C23-C22	-4.84	1.40	1.49
2	B	501	OYZ	C2-C17	-3.41	1.38	1.44
2	A	501	OYZ	C1-N10	-3.09	1.29	1.34
2	B	501	OYZ	C12-C13	3.07	1.56	1.52
2	B	501	OYZ	C3-C4	-2.92	1.37	1.40
2	A	501	OYZ	C23-C24	-2.82	1.34	1.40
2	A	501	OYZ	O14-C13	-2.64	1.22	1.30
2	A	501	OYZ	C3-C2	-2.63	1.35	1.41
2	A	501	OYZ	C4-C9	-2.50	1.36	1.40
2	B	501	OYZ	C4-C9	-2.33	1.37	1.40
2	A	501	OYZ	C9-N10	-2.21	1.30	1.34
2	B	501	OYZ	O14-C13	-2.19	1.23	1.30
2	A	501	OYZ	C12-N11	2.17	1.53	1.45
2	B	501	OYZ	C23-C24	-2.09	1.35	1.40

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	OYZ	C30-O29-C24	-5.69	106.46	118.08
2	B	501	OYZ	C16-C12-N11	4.58	120.81	110.19
2	A	501	OYZ	O29-C30-C31	-4.16	95.07	108.04
2	A	501	OYZ	C16-C12-N11	4.02	119.51	110.19
2	B	501	OYZ	C8-C9-C4	-3.89	116.95	121.34
2	A	501	OYZ	C8-C9-C4	-3.63	117.24	121.34
2	B	501	OYZ	C2-C1-N10	-3.39	117.49	121.27
2	A	501	OYZ	C27-C26-C25	-3.31	116.16	120.24
2	A	501	OYZ	C2-C1-N10	-3.22	117.67	121.27
2	A	501	OYZ	C19-C1-N10	3.21	119.48	115.10
2	A	501	OYZ	C1-N10-C9	3.06	123.17	117.32
2	A	501	OYZ	C32-C33-C19	2.75	124.65	121.12
2	A	501	OYZ	C20-C21-C22	2.59	124.45	121.12
2	A	501	OYZ	C16-C12-C13	-2.52	104.70	110.23
2	B	501	OYZ	C27-C26-C25	-2.45	117.22	120.24
2	B	501	OYZ	C2-C17-N18	-2.36	172.24	177.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	OYZ	C2-C17-N18	-2.31	172.35	177.46
2	B	501	OYZ	C1-N10-C9	2.28	121.68	117.32
2	B	501	OYZ	C30-O29-C24	-2.26	113.46	118.08
2	B	501	OYZ	C1-C2-C17	-2.21	117.32	121.06
2	B	501	OYZ	O29-C30-C31	-2.21	101.14	108.04
2	B	501	OYZ	C32-C33-C19	2.17	123.91	121.12
2	B	501	OYZ	C19-C1-N10	2.09	117.95	115.10
2	A	501	OYZ	C32-C22-C23	2.09	124.36	120.91
2	A	501	OYZ	C4-C9-N10	-2.06	121.90	123.48
2	A	501	OYZ	C5-C4-C9	-2.03	119.18	121.63

There are no chirality outliers.

All (6) torsion outliers are listed below:

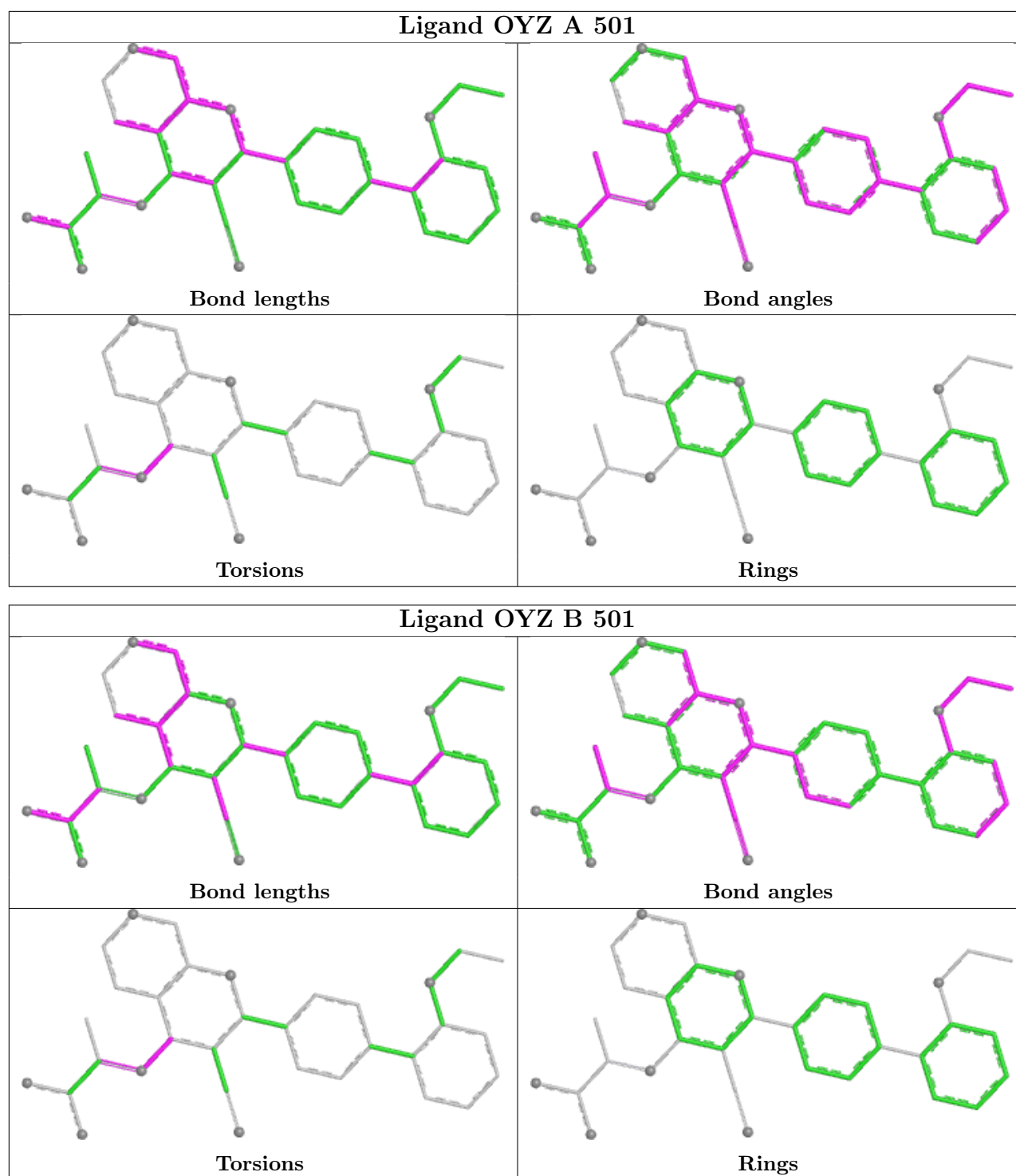
Mol	Chain	Res	Type	Atoms
2	A	501	OYZ	C16-C12-N11-C3
2	B	501	OYZ	C16-C12-N11-C3
2	A	501	OYZ	C4-C3-N11-C12
2	B	501	OYZ	C4-C3-N11-C12
2	A	501	OYZ	C2-C3-N11-C12
2	B	501	OYZ	C2-C3-N11-C12

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	OYZ	3	0
2	B	501	OYZ	2	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 ⓘ

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	318/394 (80%)	0.24	13 (4%) 41 41	18, 43, 70, 111	2 (0%)
1	B	306/394 (77%)	0.27	10 (3%) 49 49	20, 43, 70, 86	1 (0%)
All	All	624/788 (79%)	0.25	23 (3%) 45 45	18, 43, 70, 111	3 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	286	ALA	5.6
1	A	217	VAL	4.9
1	A	216	THR	4.3
1	A	218	ALA	3.9
1	A	215	SER	3.7
1	B	388	VAL	3.6
1	A	366	ALA	3.6
1	B	328	ALA	3.5
1	B	391	GLU	3.3
1	B	367	LYS	3.2
1	A	405	LEU	3.2
1	A	291	VAL	3.1
1	A	326	PRO	2.9
1	A	28	ASN	2.8
1	B	405	LEU	2.7
1	B	29	LEU	2.6
1	B	188	GLY	2.5
1	A	293	CYS	2.4
1	B	124	ASN	2.3
1	A	391	GLU	2.2
1	A	29	LEU	2.2
1	A	386	SER	2.1
1	B	227	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	PHD	B	359	12/13	0.88	0.13	34,41,50,61	0
1	PHD	A	359	12/13	0.94	0.09	33,41,62,63	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

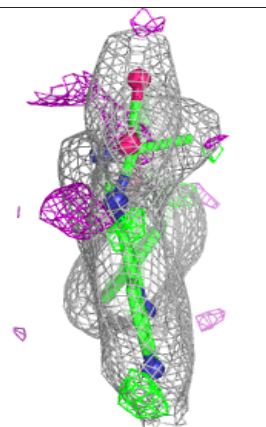
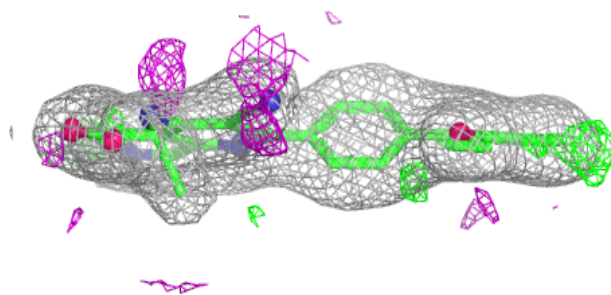
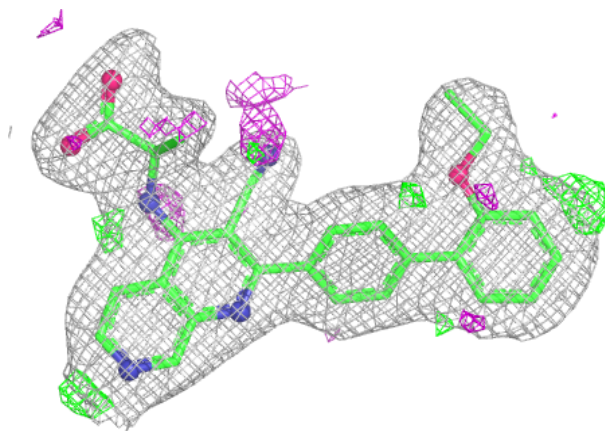
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PO4	B	502	5/5	0.66	0.15	67,69,76,90	0
3	PO4	A	502	5/5	0.87	0.09	59,64,77,84	0
2	OYZ	B	501	33/33	0.92	0.10	24,29,39,43	0
2	OYZ	A	501	33/33	0.94	0.09	18,24,37,42	0

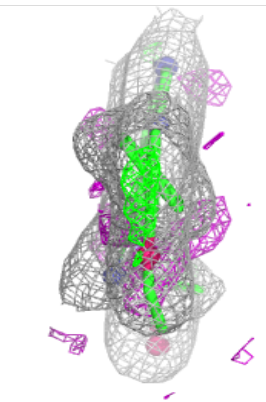
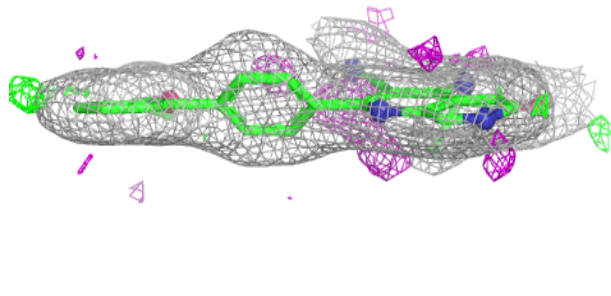
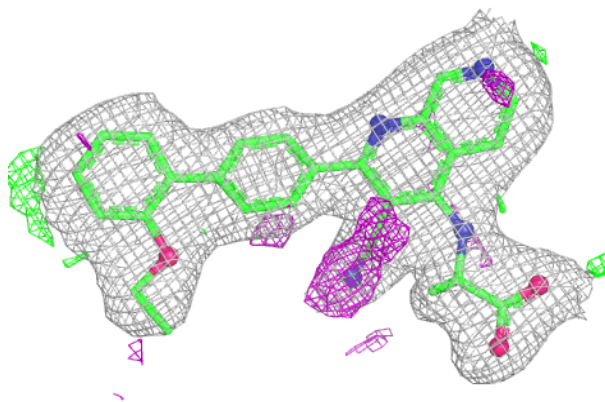
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around OYZ B 501:

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

**Electron density around OYZ A 501:**

$2mF_o-DF_c$ (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.