



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:24 PM UTC

PDB ID : 6BMX / pdb_00006bmx
Title : Non-receptor Protein Tyrosine Phosphatase SHP2 in Complex with Allosteric Inhibitor SHP844
Authors : Stams, T.; Fodor, M.
Deposited on : 2017-11-15
Resolution : 2.42 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

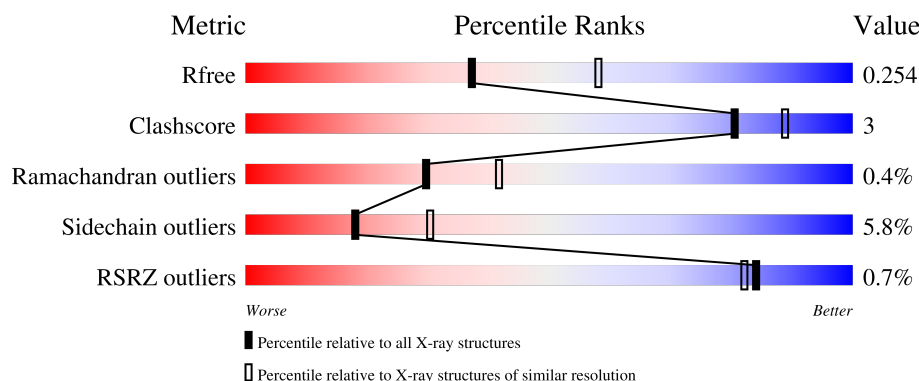
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	526	
1	B	526	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8582 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.

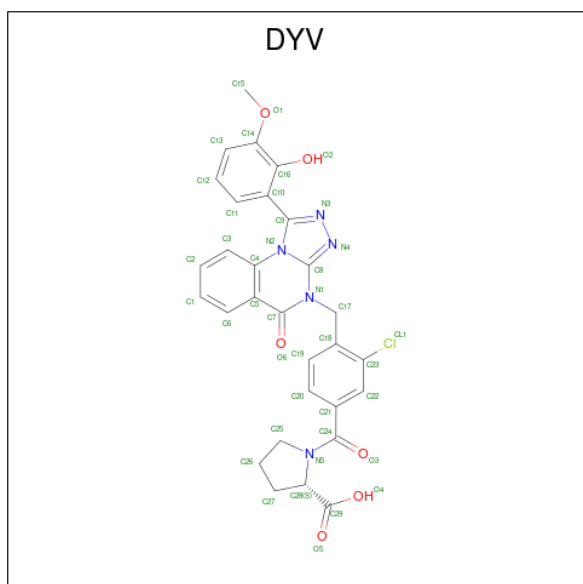
- Molecule 1 is a protein called Tyrosine-protein phosphatase non-receptor type 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	1	0
			3949	2489	700	741	19			
1	B	478	Total	C	N	O	S	0	3	0
			3886	2455	690	721	20			

There are 2 discrepancies between the modelled and reference sequences:

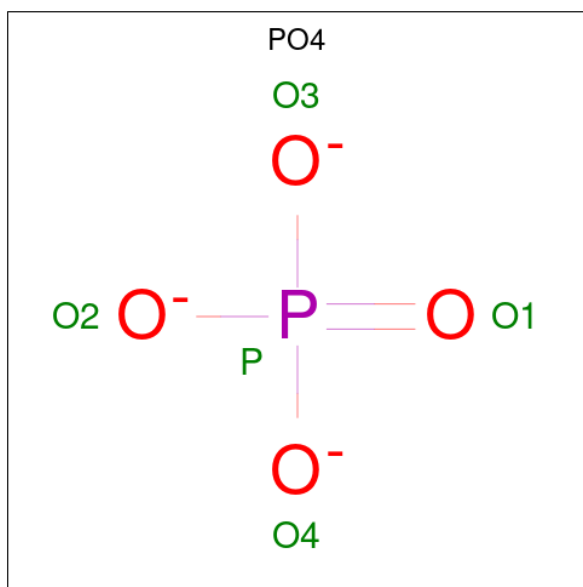
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q06124
B	0	SER	-	expression tag	UNP Q06124

- Molecule 2 is 1-(3-chloro-4-{[1-(2-hydroxy-3-methoxyphenyl)-5-oxo[1,2,4]triazolo[4,3-a]quinazolin-4(5H)-yl]methyl}benzene-1-carbonyl)-L-proline (CCD ID: DYV) (formula: C₂₉H₂₄ClN₅O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			41	29	1	5	6		
2	B	1	Total	C	Cl	N	O	0	0
			41	29	1	5	6		

- 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	A	1	Total	O	P	0	0
			5	4	1		
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 GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

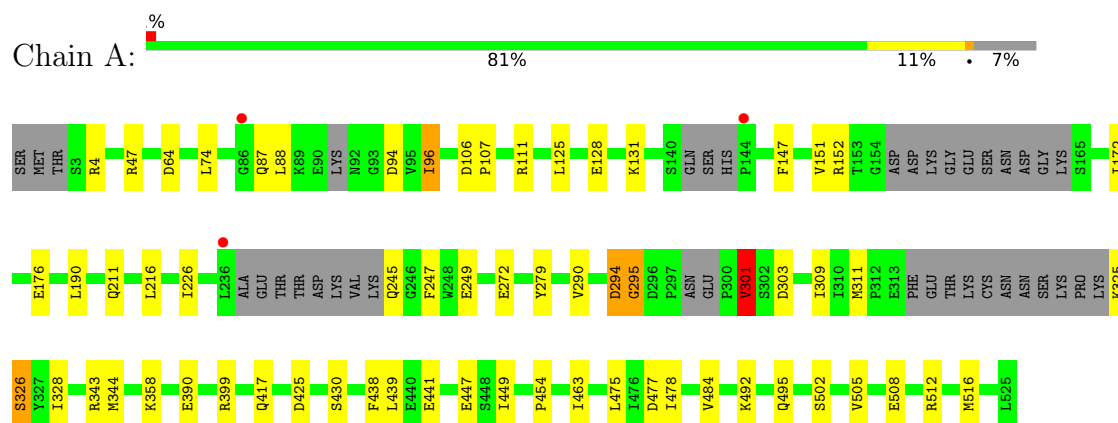
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	332	Total	O	0	0
			332	332		
5	B	307	Total	O	0	0
			307	307		

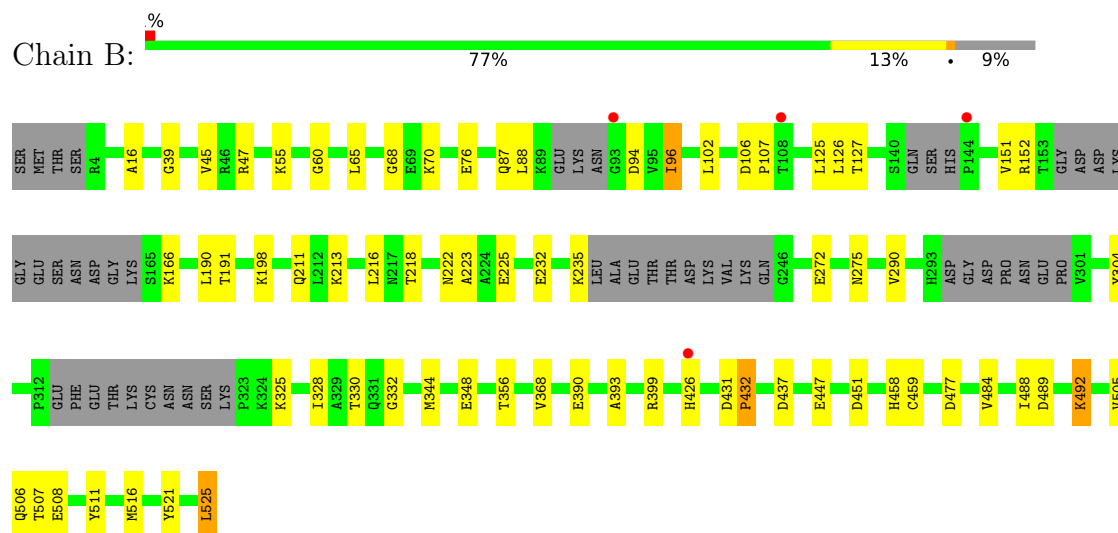
3 Residue-property plots [i](#)

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: Tyrosine-protein phosphatase non-receptor type 11



- Molecule 1: Tyrosine-protein phosphatase non-receptor type 11



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.13Å 215.00Å 56.04Å 90.00° 96.59° 90.00°	Depositor
Resolution (Å)	55.67 – 2.42 55.67 – 2.42	Depositor EDS
% Data completeness (in resolution range)	99.1 (55.67-2.42) 99.6 (55.67-2.42)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.42Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.167 , 0.252 0.169 , 0.254	Depositor DCC
R_{free} test set	1936 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 65.8	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	0.96	EDS
Total number of atoms	8582	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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: DYV, PO4, GOL

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	0.88	0/4032	1.33	14/5434 (0.3%)
1	B	0.87	0/3974	1.36	24/5354 (0.4%)
All	All	0.88	0/8006	1.35	38/10788 (0.4%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	431	ASP	CA-CB-CG	7.26	119.86	112.60
1	B	106	ASP	CA-CB-CG	6.87	119.47	112.60
1	A	106	ASP	CA-CB-CG	6.63	119.23	112.60
1	A	64	ASP	CA-CB-CG	6.56	119.16	112.60
1	A	438	PHE	CA-CB-CG	6.53	120.33	113.80
1	B	506	GLN	N-CA-C	6.18	118.94	111.40
1	A	303	ASP	CA-CB-CG	6.07	118.67	112.60
1	B	511	TYR	CA-C-N	5.81	128.06	120.28
1	B	511	TYR	C-N-CA	5.81	128.06	120.28
1	B	521	TYR	CA-C-N	5.79	128.64	120.42
1	B	521	TYR	C-N-CA	5.79	128.64	120.42
1	B	76	GLU	CA-C-N	5.69	128.16	120.65
1	B	76	GLU	C-N-CA	5.69	128.16	120.65
1	A	495	GLN	CA-C-N	5.66	127.86	120.28
1	A	495	GLN	C-N-CA	5.66	127.86	120.28
1	B	304	TYR	N-CA-C	5.59	118.59	109.59
1	B	432	PRO	CA-C-N	5.55	126.27	119.99
1	B	432	PRO	C-N-CA	5.55	126.27	119.99
1	A	279	TYR	CA-C-N	5.54	129.13	120.82
1	A	279	TYR	C-N-CA	5.54	129.13	120.82
1	B	393	ALA	N-CA-C	-5.53	101.72	109.69
1	B	39	GLY	N-CA-C	-5.48	107.46	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	437	ASP	CA-CB-CG	5.46	118.06	112.60
1	B	191	THR	CA-C-N	5.35	127.40	120.44
1	B	191	THR	C-N-CA	5.35	127.40	120.44
1	B	16	ALA	CA-C-N	5.31	127.70	120.54
1	B	16	ALA	C-N-CA	5.31	127.70	120.54
1	B	127	THR	CA-C-N	5.21	127.22	120.44
1	B	127	THR	C-N-CA	5.21	127.22	120.44
1	B	198	LYS	N-CA-C	-5.19	105.71	111.36
1	B	332	GLY	CA-C-N	5.14	128.96	121.31
1	B	332	GLY	C-N-CA	5.14	128.96	121.31
1	A	358	LYS	N-CA-C	-5.11	102.96	110.52
1	A	247	PHE	CA-C-N	5.04	126.99	120.44
1	A	247	PHE	C-N-CA	5.04	126.99	120.44
1	A	425	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	449	ILE	CA-C-N	5.03	128.00	120.95
1	A	449	ILE	C-N-CA	5.03	128.00	120.95

There are no chirality outliers.

There are no planarity outliers.

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	3949	0	3889	20	0
1	B	3886	0	3850	20	0
2	A	41	0	0	0	0
2	B	41	0	0	0	0
3	A	15	0	0	0	0
3	B	5	0	0	0	0
4	B	6	0	8	0	0
5	A	332	0	0	1	0
5	B	307	0	0	0	0
All	All	8582	0	7747	40	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 3.

All (40) 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:294:ASP:HB2	1:A:343:ARG:HE	1.39	0.88
1:B:232:GLU:HA	1:B:235:LYS:HE2	1.72	0.70
1:B:88:LEU:HG	1:B:96:ILE:HG23	1.75	0.67
1:A:294:ASP:CB	1:A:343:ARG:HE	2.11	0.64
1:A:272:GLU:HB3	1:A:301:VAL:HG11	1.80	0.63
1:B:222:ASN:O	1:B:225:GLU:HG2	2.01	0.60
1:A:272:GLU:CB	1:A:301:VAL:HG11	2.35	0.57
1:B:356:THR:OG1	1:B:459:CYS:HB3	2.04	0.57
1:B:65:LEU:HD23	1:B:68:GLY:HA3	1.92	0.52
1:A:47:ARG:HH21	1:A:94:ASP:HB3	1.75	0.51
1:A:294:ASP:HB2	1:A:343:ARG:NE	2.16	0.51
1:B:126:LEU:HD22	1:B:152:ARG:HB2	1.94	0.50
1:A:390:GLU:HG2	1:A:399:ARG:HG2	1.93	0.50
1:A:125:LEU:HB3	1:A:216:LEU:HD21	1.93	0.49
1:A:290:VAL:HG11	1:A:344:MET:HG3	1.94	0.49
1:B:390:GLU:HG2	1:B:399:ARG:HG2	1.96	0.47
1:B:330:THR:HG23	1:B:458:HIS:HB3	1.96	0.47
1:A:295:GLY:H	1:A:343:ARG:NH2	2.13	0.46
1:B:432:PRO:HG3	1:B:516[A]:MET:HG2	1.97	0.46
1:A:399:ARG:HD2	1:A:417:GLN:OE1	2.15	0.46
1:A:309:ILE:HD13	1:A:328:ILE:HG12	1.97	0.46
1:A:294:ASP:HB2	1:A:343:ARG:HH21	1.82	0.45
1:A:326:SER:HB3	1:A:454:PRO:HB3	1.98	0.45
1:A:147:PHE:HB2	1:A:172:ILE:HB	2.00	0.44
1:B:125:LEU:HB3	1:B:216:LEU:HD21	1.99	0.44
1:A:475:LEU:HA	1:A:478:ILE:HD12	1.99	0.43
1:B:328:ILE:HD11	1:B:348:GLU:HG3	2.01	0.43
1:A:4:ARG:HH21	1:A:74:LEU:HB2	1.83	0.43
1:B:489:ASP:CG	1:B:492:LYS:HB2	2.44	0.42
1:B:525:LEU:HD12	1:B:525:LEU:HA	1.95	0.42
1:A:107:PRO:HG3	1:A:190:LEU:HD12	2.02	0.42
1:A:463:ILE:HG12	5:A:805:HOH:O	2.20	0.42
1:A:88:LEU:HG	1:A:96:ILE:HD12	2.02	0.42
1:B:223:ALA:HB3	1:B:484:VAL:O	2.19	0.41
1:B:65:LEU:HD21	1:B:88:LEU:HD13	2.00	0.41
1:B:45:VAL:HB	1:B:96:ILE:HD11	2.03	0.41
1:B:107:PRO:HG3	1:B:190:LEU:HD12	2.03	0.41
1:B:211:GLN:HB3	1:B:213:LYS:HG3	2.03	0.41
1:B:290:VAL:HG11	1:B:344:MET:HG3	2.02	0.41
1:B:60:GLY:HA2	1:B:507:THR:HG23	2.03	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	475/526 (90%)	456 (96%)	16 (3%)	3 (1%)	21	30
1	B	467/526 (89%)	453 (97%)	13 (3%)	1 (0%)	43	57
All	All	942/1052 (90%)	909 (96%)	29 (3%)	4 (0%)	30	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	301	VAL
1	A	295	GLY
1	A	505	VAL
1	B	505	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	434/468 (93%)	405 (93%)	29 (7%)	15	24
1	B	428/468 (92%)	406 (95%)	22 (5%)	21	35
All	All	862/936 (92%)	811 (94%)	51 (6%)	18	30

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	96	ILE
1	A	111	ARG
1	A	128	GLU
1	A	131	LYS
1	A	151	VAL
1	A	152	ARG
1	A	176	GLU
1	A	211	GLN
1	A	226	ILE
1	A	245	GLN
1	A	249	GLU
1	A	294	ASP
1	A	301	VAL
1	A	311	MET
1	A	325	LYS
1	A	326	SER
1	A	430	SER
1	A	439	LEU
1	A	441	GLU
1	A	447	GLU
1	A	477	ASP
1	A	484	VAL
1	A	492	LYS
1	A	502	SER
1	A	508	GLU
1	A	512	ARG
1	A	516[A]	MET
1	A	516[B]	MET
1	B	47	ARG
1	B	55	LYS
1	B	70	LYS
1	B	87	GLN
1	B	94	ASP
1	B	96	ILE
1	B	102	LEU
1	B	151	VAL
1	B	166	LYS
1	B	218	THR
1	B	272	GLU
1	B	275	ASN
1	B	325	LYS
1	B	368	VAL

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Mol	Chain	Res	Type
1	B	426	HIS
1	B	447	GLU
1	B	451	ASP
1	B	477	ASP
1	B	488	ILE
1	B	492	LYS
1	B	508	GLU
1	B	525	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	85	HIS
1	A	256	GLN
1	A	339	ASN
1	A	408	GLN
1	B	87	GLN
1	B	103	ASN
1	B	281	ASN
1	B	446	GLN
1	B	519	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 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	603	-	4,4,4	2.57	3 (75%)	6,6,6	0.51	0
3	PO4	B	602	-	4,4,4	2.53	2 (50%)	6,6,6	0.91	0
2	DYV	B	601	-	46,46,46	1.76	10 (21%)	64,68,68	1.37	8 (12%)
4	GOL	B	603	-	5,5,5	0.14	0	5,5,5	0.27	0
3	PO4	A	604	-	4,4,4	2.16	3 (75%)	6,6,6	0.53	0
2	DYV	A	601	-	46,46,46	1.64	10 (21%)	64,68,68	1.37	10 (15%)
3	PO4	A	602	-	4,4,4	2.55	2 (50%)	6,6,6	0.61	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
4	GOL	B	603	-	-	2/4/4/4	-
2	DYV	A	601	-	-	10/22/32/32	0/6/6/6
2	DYV	B	601	-	-	11/22/32/32	0/6/6/6

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	DYV	O5-C29	4.90	1.36	1.22
2	B	601	DYV	O5-C29	4.87	1.36	1.22
3	A	602	PO4	P-O1	4.25	1.60	1.50
3	A	603	PO4	P-O1	4.24	1.60	1.50
3	B	602	PO4	P-O1	4.16	1.60	1.50
2	B	601	DYV	C8-N1	3.77	1.45	1.38
2	A	601	DYV	C8-N2	-2.77	1.33	1.39
2	A	601	DYV	C8-N1	2.75	1.43	1.38
2	B	601	DYV	C5-C7	2.68	1.52	1.47
3	A	604	PO4	P-O1	2.54	1.56	1.50
2	B	601	DYV	C3-C4	2.49	1.43	1.39
2	A	601	DYV	C5-C4	2.37	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	DYV	C20-C21	2.37	1.43	1.39
2	A	601	DYV	C20-C21	2.37	1.43	1.39
2	B	601	DYV	O4-C29	-2.33	1.23	1.30
2	A	601	DYV	C3-C4	2.33	1.43	1.39
2	A	601	DYV	O4-C29	-2.29	1.23	1.30
2	B	601	DYV	C8-N2	-2.25	1.34	1.39
2	A	601	DYV	C22-C21	2.21	1.42	1.39
2	B	601	DYV	C5-C4	2.18	1.44	1.41
2	A	601	DYV	C11-C10	2.11	1.43	1.39
2	B	601	DYV	C23-C18	2.05	1.42	1.39
3	A	604	PO4	P-O4	2.04	1.60	1.54
2	B	601	DYV	C14-C16	2.04	1.43	1.40
3	A	603	PO4	P-O3	2.02	1.60	1.54
2	A	601	DYV	C5-C7	2.02	1.51	1.47
3	B	602	PO4	P-O2	2.02	1.60	1.54
3	A	604	PO4	P-O2	2.01	1.60	1.54
3	A	602	PO4	P-O4	2.01	1.60	1.54
3	A	603	PO4	P-O4	2.01	1.60	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	DYV	C18-C17-N1	4.68	118.79	113.14
2	A	601	DYV	C25-N5-C28	-4.12	105.55	112.01
2	B	601	DYV	C15-O1-C14	3.75	123.01	117.51
2	B	601	DYV	O4-C29-C28	3.14	123.58	113.34
2	A	601	DYV	C18-C17-N1	3.06	116.83	113.14
2	A	601	DYV	C15-O1-C14	3.04	121.97	117.51
2	A	601	DYV	O6-C7-N1	2.85	124.80	120.15
2	A	601	DYV	O4-C29-C28	2.81	122.53	113.34
2	B	601	DYV	O4-C29-O5	-2.62	118.14	124.08
2	A	601	DYV	C22-C23-C18	-2.52	120.21	122.41
2	B	601	DYV	O6-C7-N1	2.40	124.06	120.15
2	B	601	DYV	C10-C16-C14	2.35	121.48	119.56
2	A	601	DYV	C10-C16-C14	2.31	121.44	119.56
2	B	601	DYV	C29-C28-N5	2.27	117.10	112.54
2	B	601	DYV	C26-C25-N5	2.22	107.06	103.24
2	A	601	DYV	C13-C14-C16	-2.17	117.97	119.98
2	A	601	DYV	C19-C18-C23	2.14	120.28	116.91
2	A	601	DYV	C29-C28-N5	2.13	116.81	112.54

There are no chirality outliers.

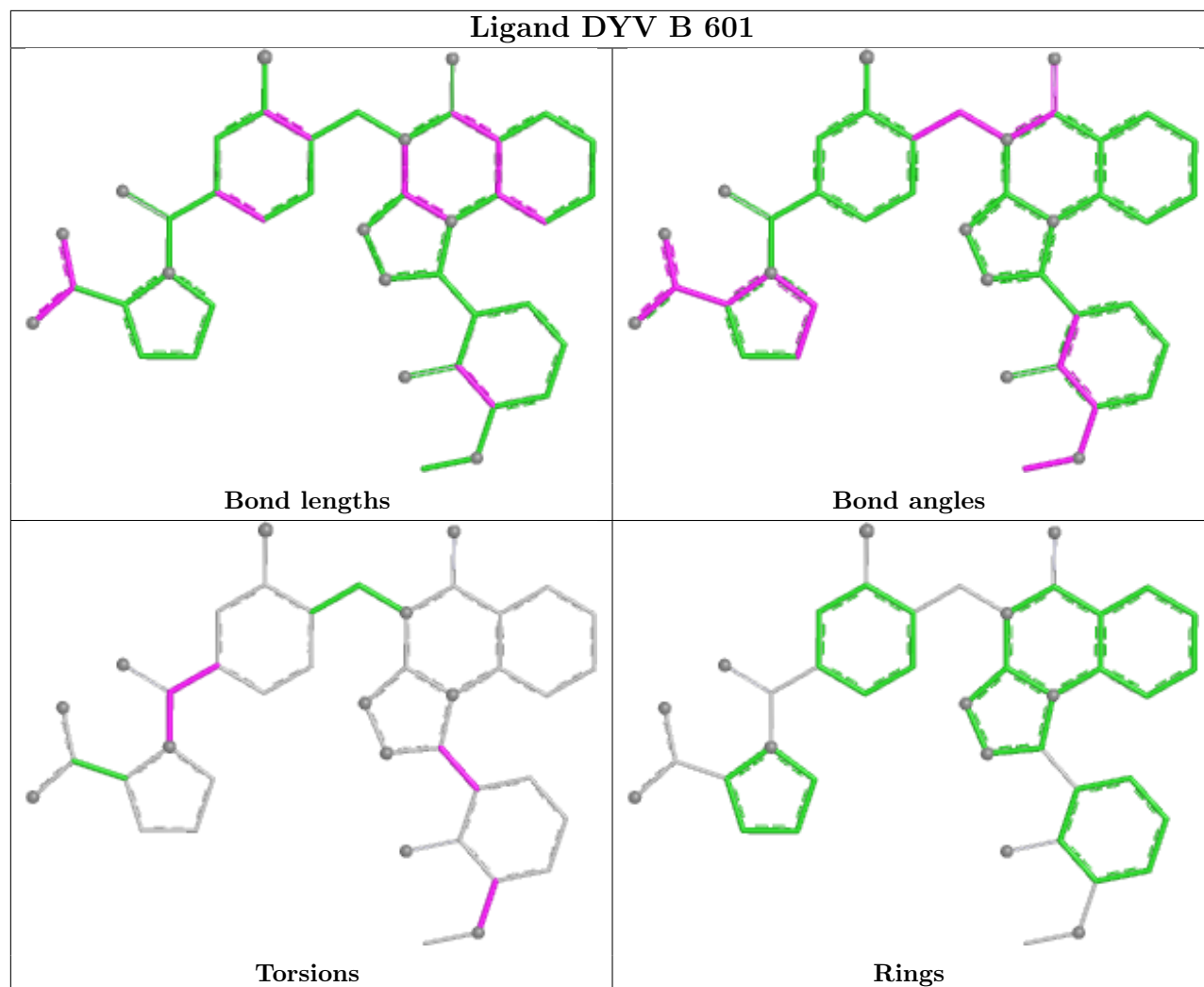
All (23) torsion outliers are listed below:

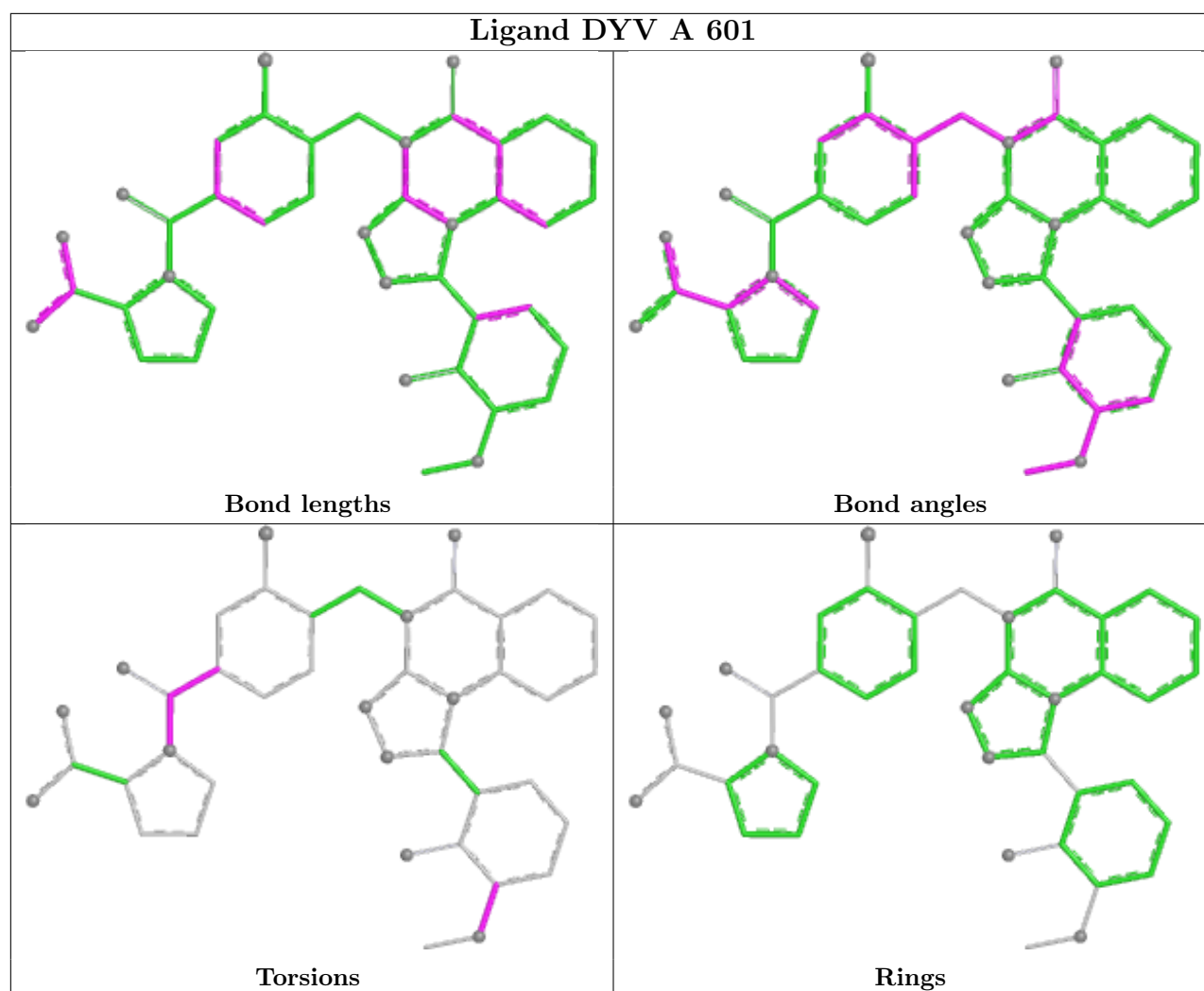
Mol	Chain	Res	Type	Atoms
2	A	601	DYV	C21-C24-N5-C25
2	A	601	DYV	C21-C24-N5-C28
2	A	601	DYV	O3-C24-N5-C25
2	A	601	DYV	O3-C24-N5-C28
2	B	601	DYV	C21-C24-N5-C25
2	B	601	DYV	C21-C24-N5-C28
2	B	601	DYV	O3-C24-N5-C25
2	B	601	DYV	O3-C24-N5-C28
4	B	603	GOL	O1-C1-C2-O2
2	A	601	DYV	C16-C14-O1-C15
4	B	603	GOL	O1-C1-C2-C3
2	A	601	DYV	C13-C14-O1-C15
2	A	601	DYV	C20-C21-C24-O3
2	A	601	DYV	C20-C21-C24-N5
2	B	601	DYV	C20-C21-C24-O3
2	B	601	DYV	C20-C21-C24-N5
2	B	601	DYV	C16-C14-O1-C15
2	A	601	DYV	C22-C21-C24-O3
2	B	601	DYV	C13-C14-O1-C15
2	A	601	DYV	C22-C21-C24-N5
2	B	601	DYV	C22-C21-C24-N5
2	B	601	DYV	C22-C21-C24-O3
2	B	601	DYV	C11-C10-C9-N3

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	488/526 (92%)	-0.18	3 (0%) 85 84	21, 42, 68, 93	1 (0%)
1	B	478/526 (90%)	-0.12	4 (0%) 82 80	22, 43, 68, 93	3 (0%)
All	All	966/1052 (91%)	-0.15	7 (0%) 84 82	21, 42, 68, 93	4 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	86	GLY	3.7
1	A	236	LEU	3.0
1	B	426	HIS	3.0
1	B	144	PRO	2.6
1	B	93	GLY	2.5
1	B	108	THR	2.3
1	A	144	PRO	2.2

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](#)

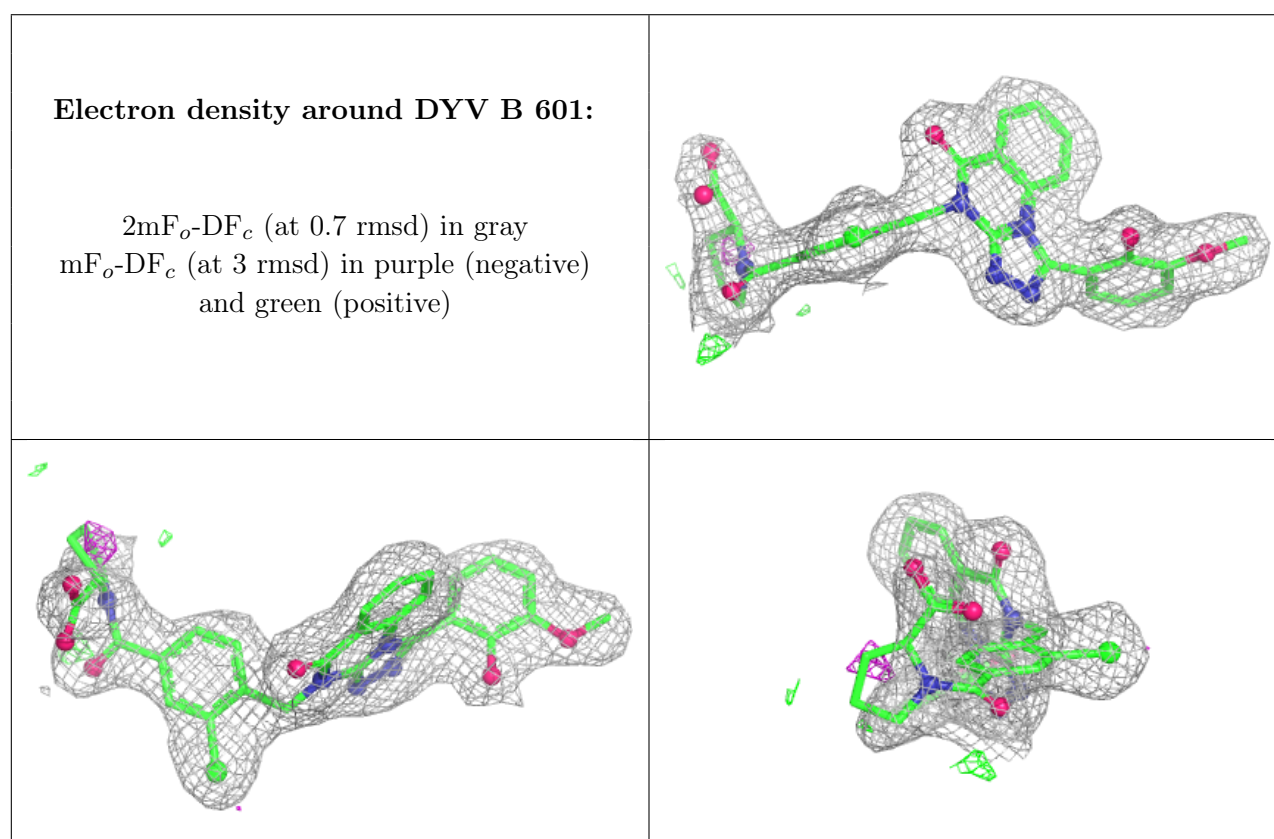
There are no oligosaccharides in this entry.

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.

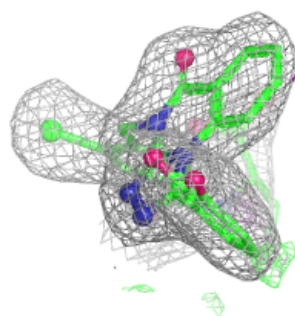
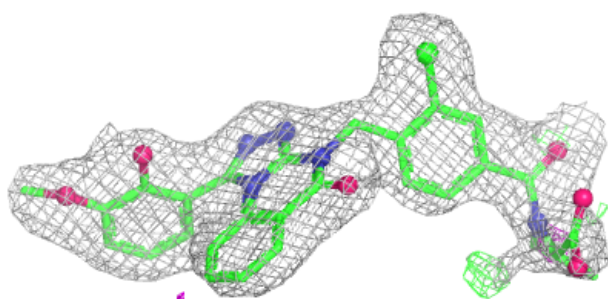
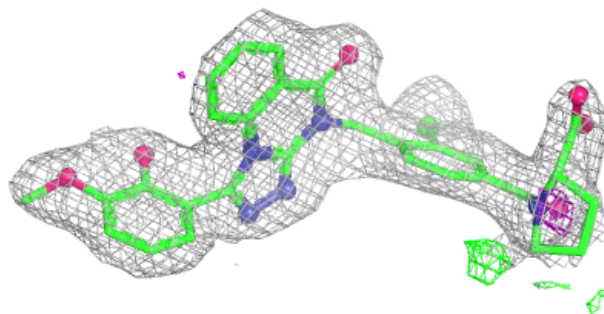
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PO4	A	604	5/5	0.81	0.13	108,109,109,110	0
4	GOL	B	603	6/6	0.86	0.11	57,69,70,72	0
3	PO4	A	603	5/5	0.89	0.09	90,90,91,93	0
3	PO4	A	602	5/5	0.90	0.11	79,80,81,81	0
3	PO4	B	602	5/5	0.93	0.09	52,53,55,57	0
2	DYV	B	601	41/41	0.94	0.08	27,37,81,84	0
2	DYV	A	601	41/41	0.94	0.09	34,40,69,71	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 DYV A 601:

$2mF_o-DF_c$ (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.