



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:08 PM UTC

PDB ID : 3VS2 / pdb_00003vs2
Title : Crystal structure of HCK complexed with a pyrrolo-pyrimidine inhibitor 7-[cis-4-(4-methylpiperazin-1-yl)cyclohexyl]-5-(4-phenoxyphenyl)-7H-pyrrolo[2,3-d]pyrimidin-4-amine
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Deposited on : 2012-04-21
Resolution : 2.61 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)
Xtrriage (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

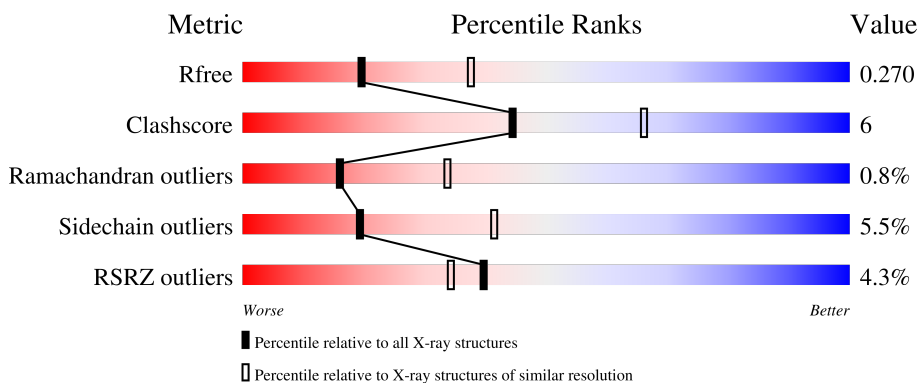
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	454	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">4% 80% 13% • 5%</p>
1	B	454	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 77%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">5% 77% 17% • •</p>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7189 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 kinase HCK.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	431	3487	2231	587	648	1	20	0	0	0
1	B	434	3504	2238	591	654	1	20	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	GLY	-	expression tag	UNP P08631
A	79	ALA	-	expression tag	UNP P08631
A	80	MET	-	expression tag	UNP P08631
A	81	GLY	-	expression tag	UNP P08631
A	82	SER	-	expression tag	UNP P08631
A	83	GLY	-	expression tag	UNP P08631
A	84	ILE	-	expression tag	UNP P08631
A	85	ARG	-	expression tag	UNP P08631
A	528	GLU	GLN	engineered mutation	UNP P08631
A	529	GLU	GLN	engineered mutation	UNP P08631
A	530	ILE	GLN	engineered mutation	UNP P08631
B	78	GLY	-	expression tag	UNP P08631
B	79	ALA	-	expression tag	UNP P08631
B	80	MET	-	expression tag	UNP P08631
B	81	GLY	-	expression tag	UNP P08631
B	82	SER	-	expression tag	UNP P08631
B	83	GLY	-	expression tag	UNP P08631
B	84	ILE	-	expression tag	UNP P08631
B	85	ARG	-	expression tag	UNP P08631
B	528	GLU	GLN	engineered mutation	UNP P08631
B	529	GLU	GLN	engineered mutation	UNP P08631
B	530	ILE	GLN	engineered mutation	UNP P08631

- Molecule 2 is 7-[cis-4-(4-methylpiperazin-1-yl)cyclohexyl]-5-(4-phenoxyphenyl)-7H-pyrrolo[2,3-d]pyrimidin-4-amine (CCD ID: VSB) (formula: C₂₉H₃₄N₆O).

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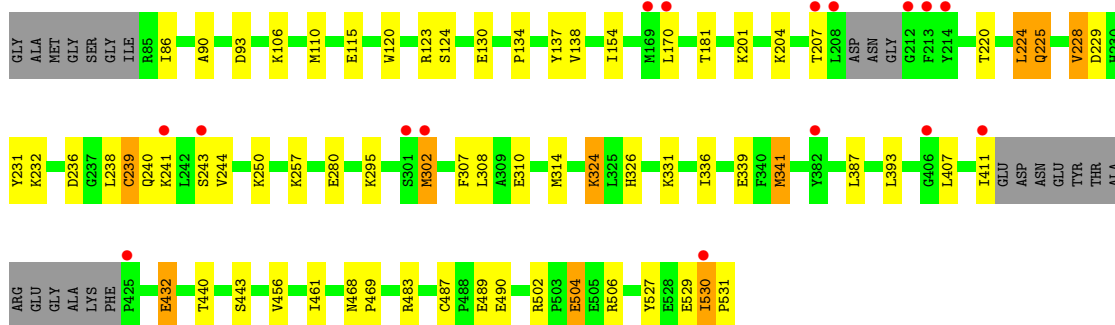
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	55	Total	O	0	0
			55	55		

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.

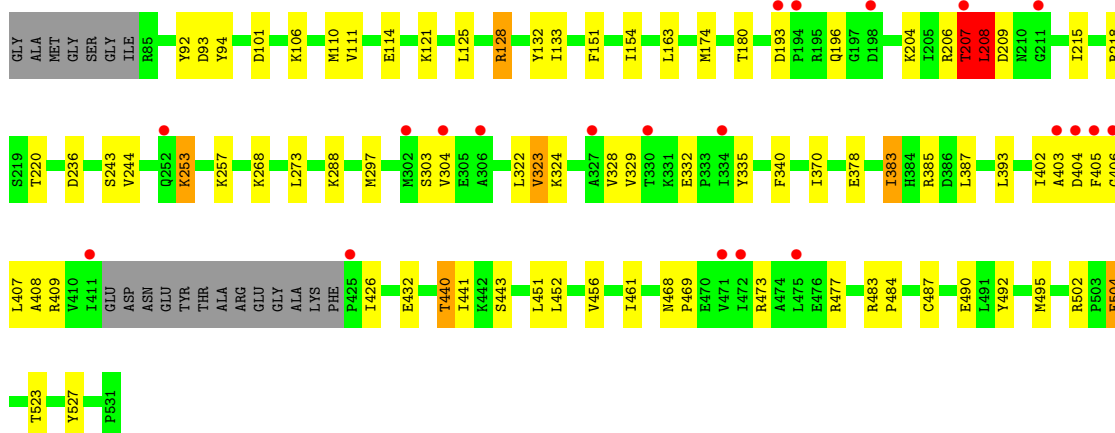
- Molecule 1: Tyrosine-protein kinase HCK

Chain A: 



- Molecule 1: Tyrosine-protein kinase HCK

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.51Å 73.09Å 180.96Å 90.00° 96.26° 90.00°	Depositor
Resolution (Å)	40.69 – 2.61 40.69 – 2.61	Depositor EDS
% Data completeness (in resolution range)	98.4 (40.69-2.61) 98.5 (40.69-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.61Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.226 , 0.279 0.222 , 0.270	Depositor DCC
R_{free} test set	1903 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	62.8	Xtrriage
Anisotropy	0.585	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.039 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7189	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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: CL, PTR, CA, VSB

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	0.27	0/3552	0.69	0/4792
1	B	0.27	0/3570	0.72	1/4818 (0.0%)
All	All	0.27	0/7122	0.71	1/9610 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	215	ILE	N-CA-C	-5.59	107.37	111.90

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	3487	0	3468	35	0
1	B	3504	0	3473	46	0
2	A	36	0	31	3	0
2	B	36	0	32	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	67	0	0	1	0
5	B	55	0	0	3	0
All	All	7189	0	7004	84	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 6.

All (84) 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:128:ARG:NH2	4:B:603:CL:CL	2.42	0.88
1:B:323:VAL:HB	1:B:403:ALA:HB2	1.80	0.64
1:B:483:ARG:NH1	1:B:487:CYS:O	2.30	0.63
1:B:180:THR:OG1	1:B:204:LYS:NZ	2.30	0.62
1:B:406:GLY:O	1:B:408:ALA:N	2.33	0.61
1:B:114:GLU:HB3	1:B:121:LYS:HB3	1.81	0.61
1:A:225:GLN:NE2	1:A:229:ASP:OD2	2.33	0.60
1:B:404:ASP:HA	1:B:405:PHE:HB3	1.82	0.60
1:A:530:ILE:HG12	1:A:531:PRO:HD2	1.82	0.60
1:A:502:ARG:HB3	1:A:504:GLU:HG2	1.83	0.59
1:B:385:ARG:NH1	1:B:408:ALA:O	2.35	0.59
2:B:601:VSB:H24	2:B:601:VSB:CAL	2.15	0.59
1:A:302:MET:SD	1:A:302:MET:N	2.75	0.56
2:A:601:VSB:H24	2:A:601:VSB:CAL	2.17	0.56
1:A:432:GLU:OE2	1:A:506:ARG:NH2	2.28	0.56
1:B:440:THR:O	1:B:443:SER:OG	2.21	0.56
1:B:502:ARG:HG2	1:B:504:GLU:HG2	1.87	0.55
1:A:93:ASP:O	1:A:250:LYS:NZ	2.40	0.55
1:B:236:ASP:OD2	5:B:747:HOH:O	2.17	0.54
1:B:151:PHE:HB3	1:B:154:ILE:HG13	1.90	0.53
1:B:492:TYR:HA	1:B:495:MET:HE3	1.92	0.52
1:B:383:ILE:HD11	1:B:409:ARG:HD2	1.92	0.51
1:B:110:MET:HA	1:B:125:LEU:HG	1.92	0.51
1:A:181:THR:OG1	1:A:204:LYS:NZ	2.40	0.50
1:A:483:ARG:NH1	1:A:487:CYS:O	2.43	0.48
1:A:489:GLU:CD	1:B:206:ARG:HH12	2.22	0.48
1:A:243:SER:OG	1:A:244:VAL:N	2.47	0.48
1:B:268:LYS:HE3	1:B:288:LYS:HE3	1.96	0.48
2:B:601:VSB:H24	2:B:601:VSB:H28	1.78	0.48
1:B:207:THR:O	1:B:208:LEU:HB2	2.14	0.47
1:A:490:GLU:HG2	1:B:523:THR:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LEU:O	1:A:228:VAL:HG12	2.15	0.47
1:B:111:VAL:HG23	1:B:125:LEU:HD21	1.97	0.47
1:B:403:ALA:HA	1:B:405:PHE:HB3	1.96	0.47
1:A:110:MET:HE3	1:A:110:MET:HB2	1.85	0.46
1:B:370:ILE:HD13	1:B:451:LEU:HD21	1.97	0.46
1:B:253:LYS:HE2	1:B:253:LYS:HB3	1.70	0.46
1:B:323:VAL:HG21	1:B:393:LEU:HD12	1.96	0.46
1:B:461:ILE:HD12	1:B:461:ILE:H	1.80	0.46
1:B:473:ARG:O	1:B:477:ARG:HG3	2.15	0.46
1:B:93:ASP:OD1	1:B:106:LYS:N	2.42	0.46
1:B:452:LEU:HD23	1:B:495:MET:HG3	1.98	0.46
1:A:231:TYR:HE1	1:A:236:ASP:HB2	1.81	0.46
1:B:378:GLU:HG3	1:B:441:ILE:HG12	1.97	0.46
1:A:90:ALA:HA	1:A:138:VAL:HG12	1.98	0.45
1:A:123:ARG:NH1	1:A:130:GLU:OE2	2.50	0.45
1:B:236:ASP:O	5:B:747:HOH:O	2.21	0.45
1:A:123:ARG:HB2	1:A:130:GLU:HG2	1.98	0.45
1:A:93:ASP:OD1	1:A:106:LYS:N	2.42	0.44
1:B:163:LEU:HG	1:B:174:MET:HE3	1.99	0.44
1:B:322:LEU:HD22	1:B:402:ILE:HB	1.98	0.44
1:A:110:MET:HG3	1:A:124:SER:HA	1.99	0.44
1:A:201:LYS:HG3	1:A:239:CYS:SG	2.58	0.44
1:B:273:LEU:HD11	1:B:340:PHE:HE1	1.83	0.44
1:B:426:ILE:HD11	1:B:468:ASN:HB3	1.99	0.44
1:B:110:MET:SD	1:B:133:ILE:HD13	2.58	0.43
1:B:180:THR:HG1	1:B:204:LYS:HZ1	1.63	0.43
1:A:232:LYS:HE2	1:A:232:LYS:HB3	1.84	0.43
1:B:94:TYR:HE1	1:B:253:LYS:HD2	1.83	0.43
1:A:170:LEU:HD12	1:A:240:GLN:HG3	2.01	0.42
1:B:393:LEU:HG	5:B:731:HOH:O	2.19	0.42
1:B:490:GLU:H	1:B:490:GLU:CD	2.17	0.42
1:A:339:GLU:OE1	1:A:341:MET:HE1	2.20	0.42
2:B:601:VSB:H10	2:B:601:VSB:H36	1.71	0.42
1:A:307:PHE:CZ	1:A:336:ILE:HD11	2.55	0.42
1:B:101:ASP:HA	1:B:132:TYR:H	1.85	0.41
1:B:243:SER:OG	1:B:244:VAL:N	2.52	0.41
1:A:341:MET:O	2:A:601:VSB:H22	2.20	0.41
2:A:601:VSB:H24	2:A:601:VSB:H28	1.82	0.41
1:A:341:MET:HG2	1:A:393:LEU:HB3	2.02	0.41
1:B:468:ASN:HB2	1:B:469:PRO:HD3	2.02	0.41
1:A:295:LYS:NZ	5:A:712:HOH:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:ILE:HD12	1:A:461:ILE:H	1.85	0.41
1:A:115:GLU:HA	1:A:120:TRP:CD1	2.56	0.41
1:B:324:LYS:HE3	1:B:324:LYS:HB3	1.86	0.41
1:B:483:ARG:HA	1:B:484:PRO:HD2	1.92	0.41
1:A:310:GLU:O	1:A:314:MET:HG3	2.21	0.40
1:A:324:LYS:HD2	1:A:326:HIS:CE1	2.55	0.40
1:A:468:ASN:HB2	1:A:469:PRO:HD3	2.03	0.40
1:B:329:VAL:HB	1:B:335:TYR:HB2	2.03	0.40
1:A:134:PRO:HG2	1:A:137:TYR:HB2	2.03	0.40
1:A:440:THR:O	1:A:443:SER:OG	2.37	0.40
1:B:297:MET:HA	1:B:297:MET:HE2	2.03	0.40
1:A:411:ILE:H	1:A:411:ILE:HG13	1.67	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	424/454 (93%)	398 (94%)	24 (6%)	2 (0%)	24	46
1	B	429/454 (94%)	398 (93%)	26 (6%)	5 (1%)	10	23
All	All	853/908 (94%)	796 (93%)	50 (6%)	7 (1%)	16	34

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	207	THR
1	B	208	LEU
1	B	407	LEU
1	A	239	CYS
1	B	303	SER
1	B	196	GLN

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Mol	Chain	Res	Type
1	A	207	THR

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	378/393 (96%)	356 (94%)	22 (6%)	18	39
1	B	379/393 (96%)	359 (95%)	20 (5%)	20	43
All	All	757/786 (96%)	715 (94%)	42 (6%)	19	41

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	ILE
1	A	154	ILE
1	A	220	THR
1	A	224	LEU
1	A	225	GLN
1	A	228	VAL
1	A	238	LEU
1	A	241	LYS
1	A	257	LYS
1	A	280	GLU
1	A	302	MET
1	A	308	LEU
1	A	324	LYS
1	A	331	LYS
1	A	341	MET
1	A	387	LEU
1	A	407	LEU
1	A	432	GLU
1	A	456	VAL
1	A	504	GLU
1	A	529	GLU
1	A	530	ILE

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Mol	Chain	Res	Type
1	B	92	TYR
1	B	128	ARG
1	B	193	ASP
1	B	207	THR
1	B	208	LEU
1	B	209	ASP
1	B	218	ARG
1	B	220	THR
1	B	253	LYS
1	B	257	LYS
1	B	304	VAL
1	B	323	VAL
1	B	328	VAL
1	B	332	GLU
1	B	383	ILE
1	B	387	LEU
1	B	432	GLU
1	B	440	THR
1	B	456	VAL
1	B	504	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	318	GLN
1	A	381	ASN
1	B	326	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	PTR	A	527	3,1	15,16,17	1.37	1 (6%)	17,22,24	0.51	0
1	PTR	B	527	3,1	15,16,17	1.22	1 (6%)	17,22,24	0.53	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
1	PTR	A	527	3,1	-	0/10/11/13	0/1/1/1
1	PTR	B	527	3,1	-	1/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	PTR	OH-CZ	-4.66	1.30	1.40
1	B	527	PTR	OH-CZ	-4.50	1.30	1.40

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	527	PTR	C-CA-CB-CG

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](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	VSB	B	601	-	41,41,41	2.80	14 (34%)	55,58,58	8.59	32 (58%)
2	VSB	A	601	-	41,41,41	3.18	15 (36%)	55,58,58	8.80	31 (56%)

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	VSB	B	601	-	-	3/16/36/36	0/6/6/6
2	VSB	A	601	-	-	0/16/36/36	0/6/6/6

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	VSB	CAR-CAS	-8.57	1.32	1.52
2	A	601	VSB	CAV-CAU	-7.75	1.34	1.52
2	B	601	VSB	CAV-CAU	-7.32	1.35	1.52
2	B	601	VSB	CBB-NAW	-6.54	1.35	1.47
2	A	601	VSB	CAX-NAW	-6.53	1.35	1.47
2	B	601	VSB	CAR-CAS	-6.11	1.38	1.52
2	A	601	VSB	CAU-CAT	6.03	1.67	1.52
2	A	601	VSB	CAS-CAT	5.94	1.67	1.52
2	A	601	VSB	CAR-CAQ	5.61	1.66	1.52
2	B	601	VSB	CBA-NAZ	5.36	1.59	1.46
2	B	601	VSB	CAX-NAW	5.34	1.57	1.47
2	A	601	VSB	CBB-NAW	5.08	1.56	1.47
2	A	601	VSB	CAJ-CAI	-4.74	1.42	1.49
2	B	601	VSB	CAJ-CAI	-4.69	1.42	1.49
2	A	601	VSB	CAV-CAQ	4.12	1.62	1.52
2	B	601	VSB	CAV-CAQ	4.00	1.62	1.52
2	B	601	VSB	CAR-CAQ	3.98	1.62	1.52
2	A	601	VSB	CBB-CBA	3.96	1.66	1.51
2	A	601	VSB	CAH-NAG	-3.57	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	VS	CAU-CAT	3.46	1.61	1.52
2	B	601	VS	CAY-CAX	3.45	1.64	1.51
2	B	601	VS	CAS-CAT	3.44	1.61	1.52
2	B	601	VS	CAH-NAG	-3.28	1.32	1.38
2	A	601	VS	CAQ-NAG	2.97	1.51	1.46
2	A	601	VS	CAH-CAI	-2.88	1.34	1.37
2	B	601	VS	CAH-CAI	-2.29	1.34	1.37
2	B	601	VS	C5-CAI	-2.29	1.40	1.46
2	A	601	VS	C5-CAI	-2.20	1.41	1.46
2	A	601	VS	CAY-CAX	-2.11	1.43	1.51

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	VS	CAR-CAQ-NAG	-32.73	75.15	111.40
2	A	601	VS	CAR-CAQ-NAG	-25.99	82.61	111.40
2	B	601	VS	CAX-CAY-NAZ	-22.03	75.46	110.86
2	A	601	VS	CBA-CBB-NAW	20.56	146.82	110.61
2	A	601	VS	CBB-CBA-NAZ	-20.40	78.07	110.86
2	A	601	VS	CAY-CAX-NAW	19.77	145.42	110.61
2	A	601	VS	CBB-NAW-CAX	-19.20	72.54	109.13
2	A	601	VS	CAX-NAW-CAT	19.01	161.16	112.79
2	B	601	VS	CAV-CAQ-NAG	18.31	131.69	111.40
2	B	601	VS	CBB-NAW-CAX	-17.83	75.14	109.13
2	B	601	VS	CAU-CAT-NAW	-17.79	67.06	112.66
2	B	601	VS	CAY-CAX-NAW	17.28	141.04	110.61
2	A	601	VS	CAV-CAU-CAT	-16.14	78.82	109.98
2	A	601	VS	CAU-CAT-NAW	-14.73	74.91	112.66
2	A	601	VS	CAS-CAR-CAQ	-13.74	83.46	109.98
2	A	601	VS	C5-C4-N3	-12.50	113.70	126.97
2	B	601	VS	CBC-NAZ-CAY	12.30	134.08	110.63
2	B	601	VS	CBB-NAW-CAT	12.26	143.98	112.79
2	B	601	VS	C4-NAG-CAH	-11.49	103.32	108.08
2	B	601	VS	CBC-NAZ-CBA	11.38	132.32	110.63
2	A	601	VS	CAV-CAQ-NAG	11.37	123.99	111.40
2	B	601	VS	C5-C4-N3	-10.29	116.06	126.97
2	A	601	VS	CAX-CAY-NAZ	-10.28	94.34	110.86
2	B	601	VS	CBA-NAZ-CAY	-10.22	93.27	109.54
2	B	601	VS	CAS-CAT-NAW	9.20	136.25	112.66
2	A	601	VS	C4-NAG-CAH	-8.75	104.45	108.08
2	A	601	VS	CAS-CAT-CAU	8.67	130.78	111.17
2	B	601	VS	CAI-CAH-NAG	8.44	114.07	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	VS	CBA-NAZ-CAY	8.37	122.86	109.54
2	B	601	VS	CAV-CAU-CAT	-7.63	95.25	109.98
2	A	601	VS	C6-C5-C4	6.99	120.98	115.74
2	A	601	VS	CAS-CAT-NAW	6.39	129.05	112.66
2	B	601	VS	CBA-CBB-NAW	-6.34	99.43	110.61
2	A	601	VS	CAR-CAQ-CAV	6.30	125.42	111.17
2	A	601	VS	CBC-NAZ-CAY	5.44	120.99	110.63
2	B	601	VS	CAS-CAR-CAQ	-5.39	99.57	109.98
2	A	601	VS	N3-C4-NAG	5.19	136.00	127.17
2	A	601	VS	CAR-CAS-CAT	-5.12	100.09	109.98
2	A	601	VS	CAI-CAH-NAG	5.07	112.66	110.54
2	A	601	VS	C2-N3-C4	5.07	124.21	111.83
2	B	601	VS	C2-N3-C4	4.73	123.39	111.83
2	B	601	VS	CAU-CAV-CAQ	4.35	118.37	109.98
2	B	601	VS	C6-C5-C4	4.25	118.92	115.74
2	B	601	VS	N1-C2-N3	-4.09	122.39	128.58
2	B	601	VS	C5-CAI-CAH	-3.92	103.74	106.03
2	B	601	VS	N3-C4-NAG	3.72	133.49	127.17
2	A	601	VS	N1-C2-N3	-3.62	123.10	128.58
2	B	601	VS	CAL-CAJ-CAP	-3.37	114.28	118.57
2	A	601	VS	CBE-OBD-CAN	3.11	125.90	118.78
2	B	601	VS	CBE-OBD-CAN	3.02	125.69	118.78
2	B	601	VS	CAS-CAT-CAU	2.77	117.42	111.17
2	A	601	VS	CAL-CAJ-CAP	-2.67	115.17	118.57
2	B	601	VS	CAM-CAL-CAJ	2.63	123.61	120.80
2	B	601	VS	C4-NAG-CAQ	-2.41	120.35	125.82
2	A	601	VS	CBC-NAZ-CBA	2.40	115.20	110.63
2	B	601	VS	C5-C4-NAG	2.29	110.35	108.67
2	B	601	VS	CBB-CBA-NAZ	2.24	114.45	110.86
2	A	601	VS	C5-C6-N1	2.22	120.63	118.64
2	A	601	VS	CBB-NAW-CAT	2.18	118.33	112.79
2	A	601	VS	OBD-CAN-CAO	2.15	126.83	119.36
2	A	601	VS	CAM-CAL-CAJ	2.13	123.08	120.80
2	B	601	VS	OBD-CAN-CAO	2.10	126.68	119.36
2	B	601	VS	C5-C6-N1	2.10	120.52	118.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	VS	CAS-CAT-NAW-CBB
2	B	601	VS	CAV-CAQ-NAG-CAH

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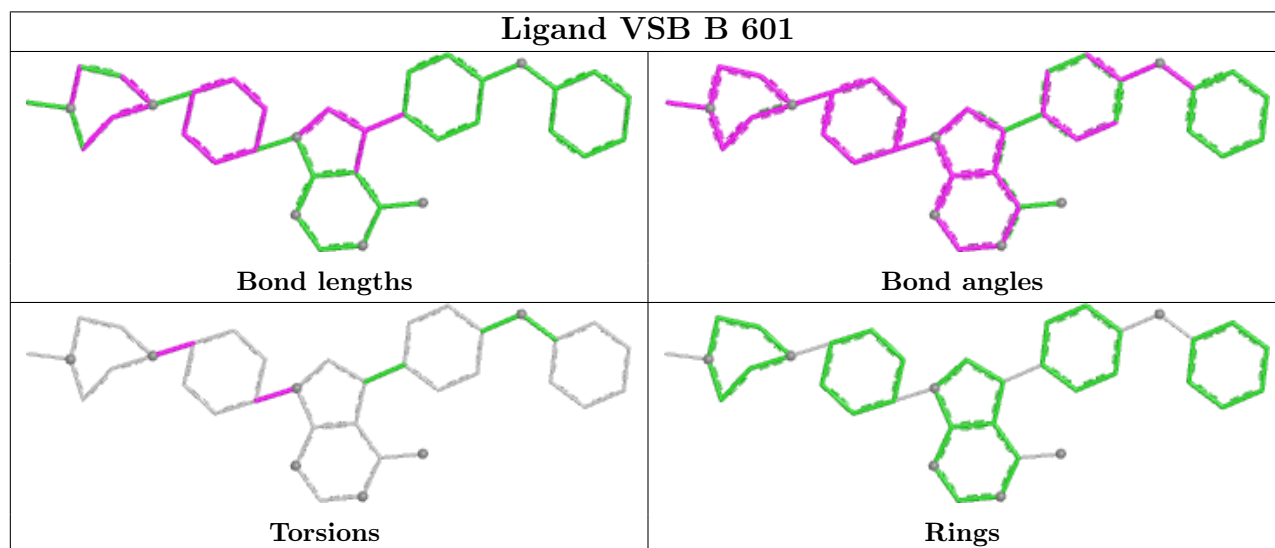
Mol	Chain	Res	Type	Atoms
2	B	601	VSB	CAU-CAT-NAW-CBB

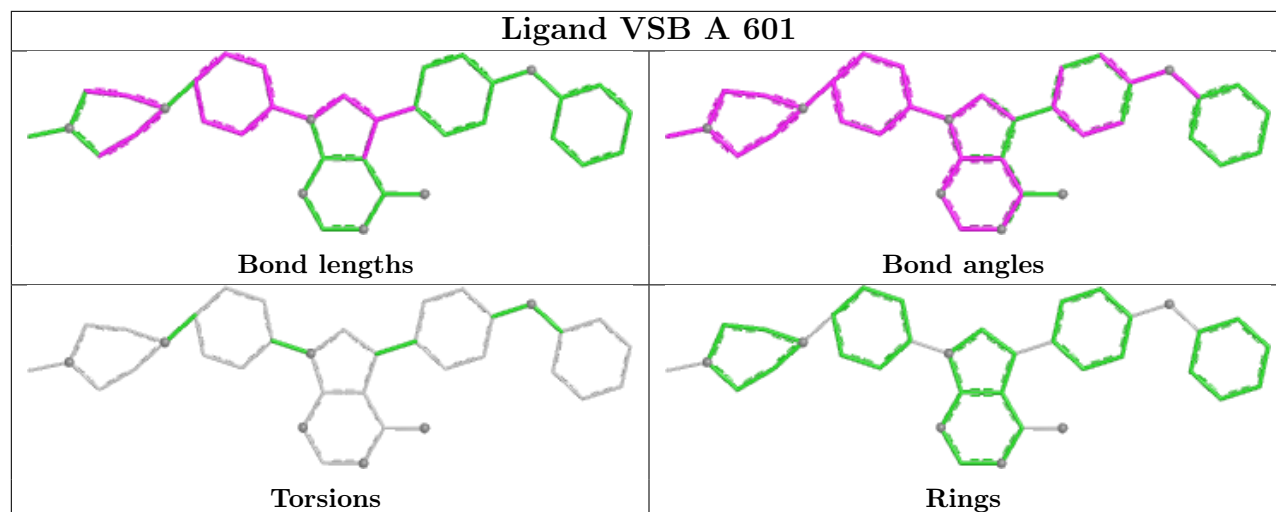
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	VSB	3	0
2	A	601	VSB	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	430/454 (94%)	0.49	16 (3%) 45 39	41, 70, 113, 134	0
1	B	433/454 (95%)	0.47	21 (4%) 35 30	46, 75, 114, 143	1 (0%)
All	All	863/908 (95%)	0.48	37 (4%) 40 34	41, 73, 114, 143	1 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	382	TYR	4.2
1	B	425	PRO	4.1
1	A	208	LEU	3.7
1	B	406	GLY	3.3
1	B	405	PHE	3.1
1	A	213	PHE	3.0
1	B	304	VAL	3.0
1	B	471	VAL	3.0
1	B	475	LEU	2.9
1	B	211	GLY	2.8
1	B	194	PRO	2.7
1	B	198	ASP	2.6
1	A	530	ILE	2.6
1	B	403	ALA	2.6
1	B	404	ASP	2.5
1	A	214	TYR	2.5
1	A	207	THR	2.5
1	A	170	LEU	2.4
1	B	207	THR	2.4
1	A	302	MET	2.4
1	B	193	ASP	2.3
1	A	212	GLY	2.3
1	A	406	GLY	2.3
1	B	327	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	411	ILE	2.2
1	B	330	THR	2.2
1	A	243	SER	2.2
1	B	411	ILE	2.2
1	B	302	MET	2.1
1	A	301	SER	2.1
1	B	334	ILE	2.1
1	B	472	ILE	2.1
1	A	425	PRO	2.1
1	A	169	MET	2.1
1	A	241	LYS	2.1
1	B	306	ALA	2.0
1	B	252	GLN	2.0

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(\AA^2)	Q<0.9
1	PTR	A	527	16/17	0.93	0.10	49,68,77,85	0
1	PTR	B	527	16/17	0.93	0.10	43,59,64,71	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.

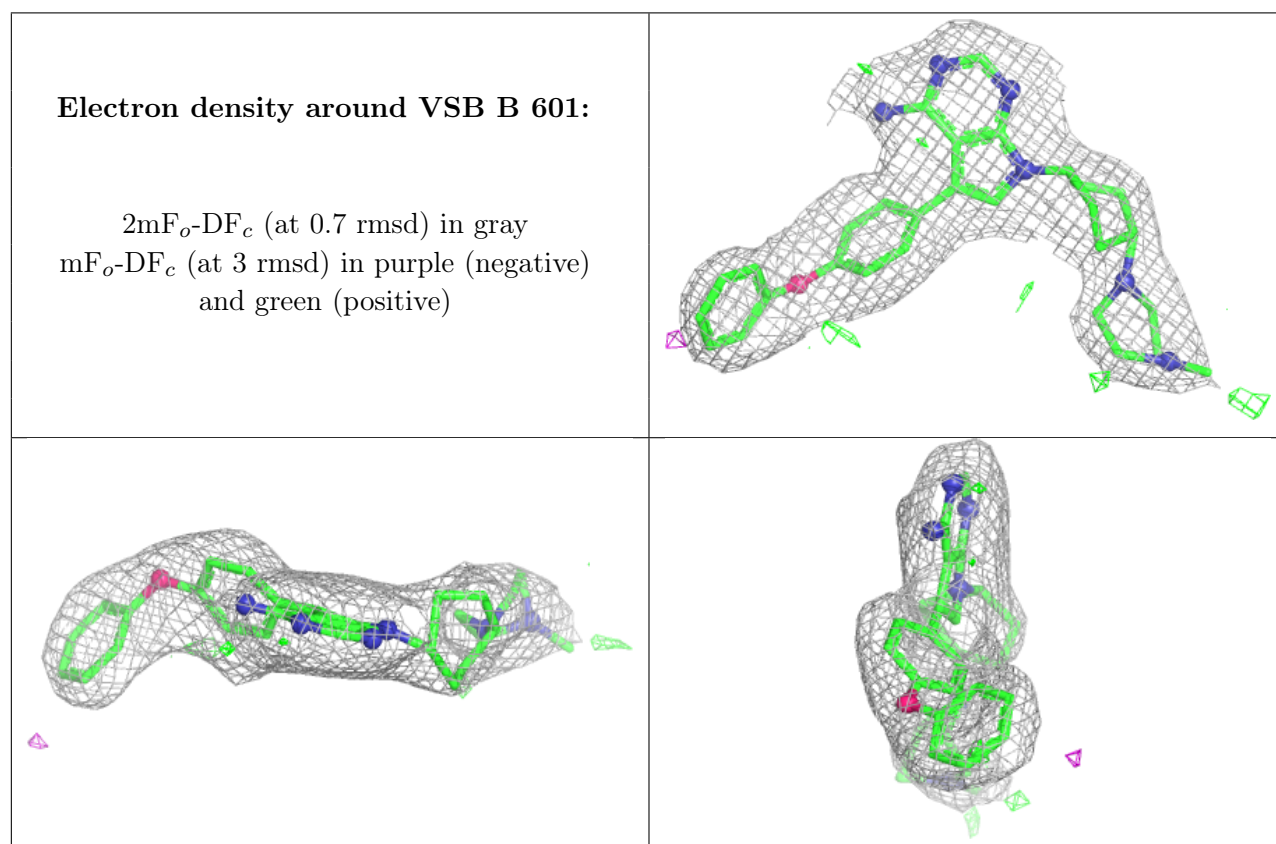
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CA	A	602	1/1	0.61	0.19	83,83,83,83	0
3	CA	B	602	1/1	0.77	0.25	89,89,89,89	0
2	VSB	B	601	36/36	0.92	0.13	42,63,110,114	0

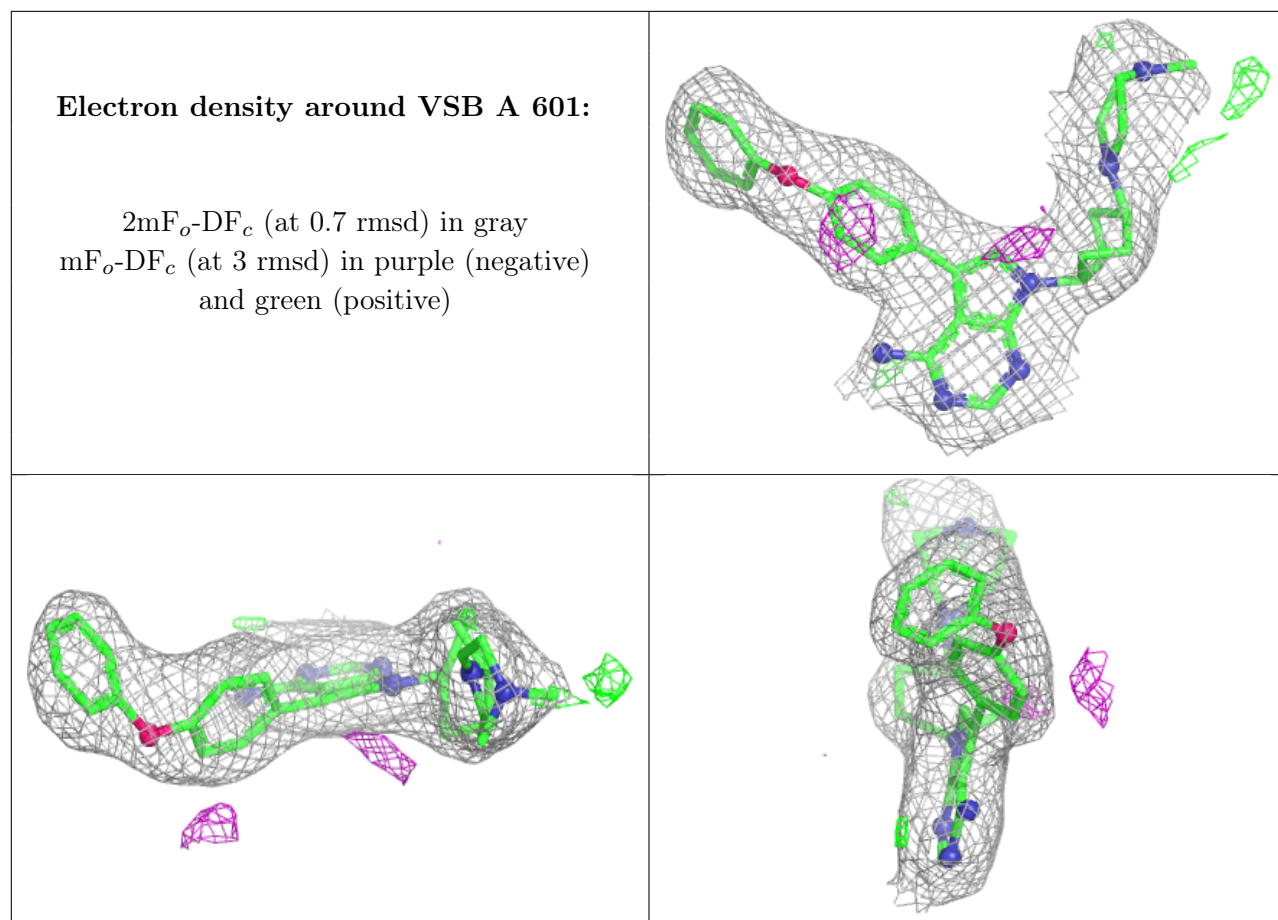
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	VSB	A	601	36/36	0.93	0.11	34,52,97,104	0
4	CL	A	603	1/1	0.96	0.25	73,73,73,73	0
4	CL	B	603	1/1	0.97	0.12	78,78,78,78	0

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.





6.5 Other polymers [i](#)

There are no such residues in this entry.