



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:10 PM UTC

PDB ID : 3VS5 / pdb_00003vs5
Title : Crystal structure of HCK complexed with a pyrrolo-pyrimidine inhibitor 7-(1-methylpiperidin-4-yl)-5-(4-phenoxyphenyl)-7H-pyrrolo[2,3-d]pyrimidin-4-amine
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Deposited on : 2012-04-21
Resolution : 2.85 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

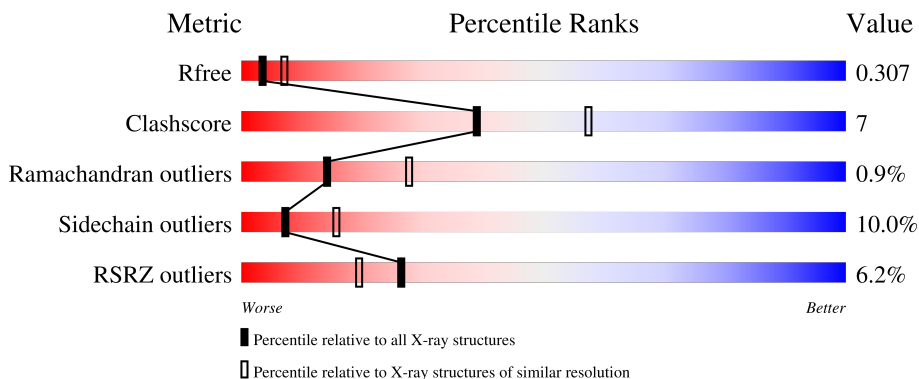
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	 4% 74% 18% • 5%
1	B	454	 8% 70% 21% • 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7027 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	430	3468	2217	583	647	1	20	0	0	0
1	B	428	3459	2213	581	644	1	20	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

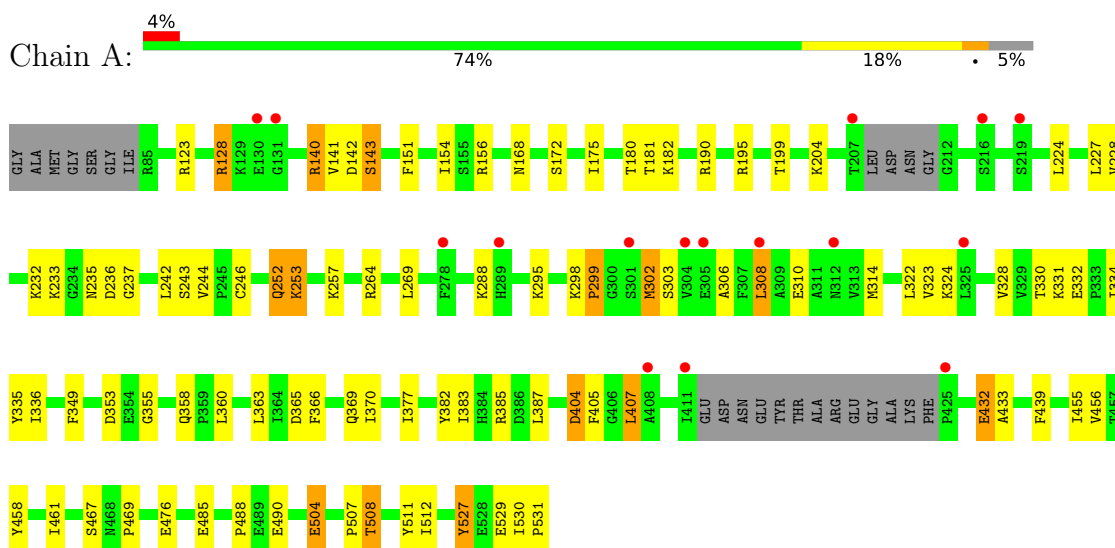
Chain	Residue	Modelled	Actual	Comment	Reference
A	78	GLY	-	expression tag	UNP P08631
A	79	ALA	-	expression tag	UNP P08631
A	80	MET	-	expression tag	UNP P08631
A	81	GLY	-	expression tag	UNP P08631
A	82	SER	-	expression tag	UNP P08631
A	83	GLY	-	expression tag	UNP P08631
A	84	ILE	-	expression tag	UNP P08631
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-(1-methylpiperidin-4-yl)-5-(4-phenoxyphenyl)-7H-pyrrolo[2,3-d]pyrimidin-4-amine (CCD ID: VSG) (formula: C₂₄H₂₅N₅O).

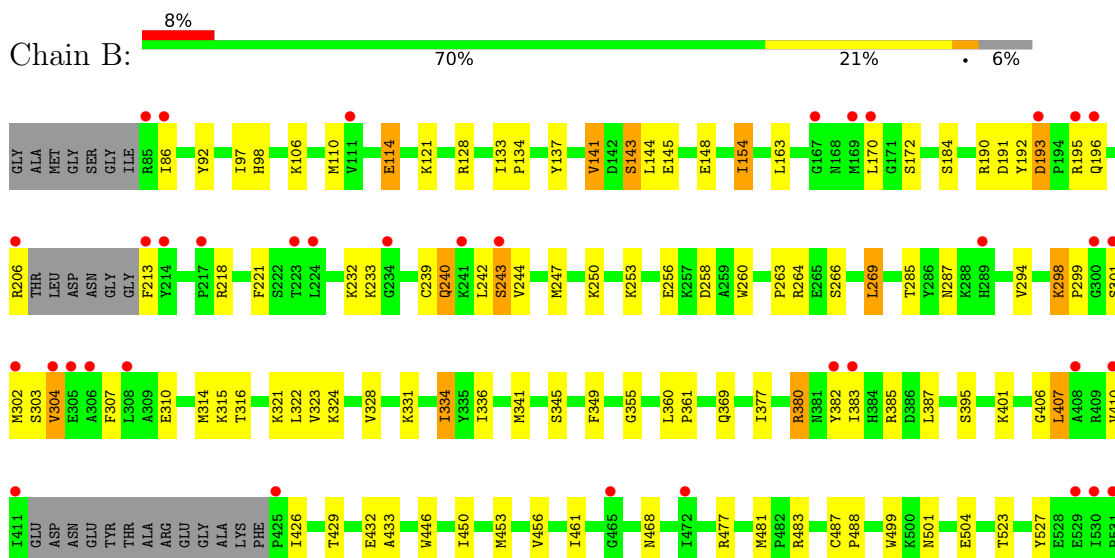
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Tyrosine-protein kinase HCK



- Molecule 1: Tyrosine-protein kinase HCK



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.49Å 94.83Å 179.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.80 – 2.85 48.80 – 2.85	Depositor EDS
% Data completeness (in resolution range)	88.9 (48.80-2.85) 89.0 (48.80-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.86Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.255 , 0.309 0.252 , 0.307	Depositor DCC
R_{free} test set	2000 reflections (7.46%)	wwPDB-VP
Wilson B-factor (Å ²)	48.6	Xtrriage
Anisotropy	0.796	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 24.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7027	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.36 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7682e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: VSG, CA, PTR

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	0.49	0/3533	0.81	2/4767 (0.0%)
1	B	0.48	0/3524	0.83	2/4755 (0.0%)
All	All	0.48	0/7057	0.82	4/9522 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	193	ASP	CA-C-N	5.35	125.67	119.47
1	B	193	ASP	C-N-CA	5.35	125.67	119.47
1	A	358	GLN	CA-C-N	-5.03	115.05	120.03
1	A	358	GLN	C-N-CA	-5.03	115.05	120.03

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	3468	0	3430	42	0
1	B	3459	0	3427	49	0
2	A	30	0	25	6	0
2	B	30	0	25	6	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	18	0	0	1	0
4	B	20	0	0	1	0
All	All	7027	0	6907	94	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 7.

All (94) 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:298:LYS:HD3	1:B:299:PRO:HD2	1.70	0.73
1:A:123:ARG:HH21	1:A:128:ARG:HH22	1.42	0.68
1:B:213:PHE:N	1:B:221:PHE:O	2.29	0.66
1:B:483:ARG:NH1	1:B:487:CYS:O	2.31	0.64
1:A:360:LEU:HD21	1:A:488:PRO:HD3	1.79	0.63
1:B:191:ASP:OD1	1:B:192:TYR:N	2.32	0.63
2:A:601:VSG:H18	2:A:601:VSG:H17	1.64	0.63
1:B:239:CYS:O	1:B:240:GLN:NE2	2.31	0.63
1:A:252:GLN:NE2	4:A:712:HOH:O	2.31	0.62
1:A:308:LEU:HD11	1:A:330:THR:HG22	1.82	0.62
1:B:264:ARG:NH2	1:B:331:LYS:O	2.28	0.61
2:A:601:VSG:H17	2:A:601:VSG:CAP	2.15	0.60
1:A:404:ASP:OD1	2:A:601:VSG:H21	2.01	0.60
1:A:508:THR:HG23	1:A:511:TYR:H	1.68	0.59
1:A:235:ASN:O	1:A:237:GLY:N	2.33	0.58
1:B:287:ASN:OD1	4:B:704:HOH:O	2.17	0.58
1:B:307:PHE:CZ	1:B:336:ILE:HD11	2.39	0.58
1:B:163:LEU:O	1:B:190:ARG:NH1	2.36	0.57
1:B:321:LYS:HD2	1:B:369:GLN:HB3	1.85	0.57
1:B:110:MET:HE1	1:B:133:ILE:HG21	1.87	0.56
1:A:377:ILE:HG23	1:A:382:TYR:HB3	1.87	0.55
1:A:383:ILE:HG22	1:A:385:ARG:HG3	1.89	0.54
1:A:180:THR:OG1	1:A:204:LYS:NZ	2.39	0.54
1:A:323:VAL:HG11	2:A:601:VSG:H26	1.89	0.53
1:B:377:ILE:HG23	1:B:382:TYR:HB3	1.89	0.53
2:B:601:VSG:CAP	2:B:601:VSG:H17	2.23	0.52
1:A:467:SER:OG	1:A:469:PRO:HD2	2.10	0.51
2:A:601:VSG:H18	2:A:601:VSG:NAK	2.27	0.50
1:A:141:VAL:C	1:A:143:SER:H	2.20	0.50
1:B:341:MET:O	2:B:601:VSG:H15	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:ILE:HD12	1:B:461:ILE:H	1.77	0.49
1:B:260:TRP:CZ3	1:B:315:LYS:HD3	2.47	0.49
1:A:123:ARG:HH21	1:A:128:ARG:NH2	2.10	0.49
1:B:97:ILE:HG13	1:B:98:HIS:ND1	2.27	0.49
1:B:232:LYS:HG2	1:B:242:LEU:HB2	1.93	0.49
1:A:175:ILE:HD13	1:A:224:LEU:HD22	1.94	0.49
1:B:114:GLU:HB2	1:B:121:LYS:HB3	1.95	0.49
1:B:310:GLU:HG3	1:B:314:MET:HE3	1.94	0.48
1:A:168:ASN:HB2	1:A:190:ARG:HH11	1.78	0.48
1:A:349:PHE:O	1:A:355:GLY:HA3	2.14	0.48
1:B:141:VAL:C	1:B:143:SER:H	2.21	0.48
1:A:507:PRO:HG2	1:A:512:ILE:HD11	1.95	0.47
1:B:106:LYS:NZ	1:B:148:GLU:OE2	2.33	0.47
1:A:404:ASP:OD1	1:A:404:ASP:N	2.46	0.47
1:B:323:VAL:HG11	2:B:601:VSG:H26	1.95	0.47
1:A:232:LYS:HA	1:A:242:LEU:HB2	1.97	0.47
1:B:154:ILE:HA	1:B:154:ILE:HD12	1.70	0.47
1:A:156:ARG:HD3	1:A:527:PTR:CE2	2.45	0.47
1:B:407:LEU:HD13	2:B:601:VSG:H23	1.95	0.47
1:A:407:LEU:HD13	2:A:601:VSG:H23	1.97	0.46
1:A:432:GLU:H	1:A:432:GLU:CD	2.23	0.46
1:A:530:ILE:HA	1:A:531:PRO:HD3	1.64	0.46
1:B:349:PHE:O	1:B:355:GLY:HA3	2.16	0.46
1:A:140:ARG:O	1:A:143:SER:HB3	2.15	0.46
1:A:303:SER:HB3	1:A:306:ALA:HB3	1.98	0.46
1:A:504:GLU:H	1:A:504:GLU:CD	2.24	0.46
1:A:172:SER:HA	1:A:244:VAL:O	2.16	0.46
1:B:360:LEU:HD21	1:B:488:PRO:HD3	1.98	0.45
1:B:170:LEU:O	1:B:243:SER:OG	2.32	0.45
1:B:345:SER:HB2	2:B:601:VSG:CAU	2.47	0.45
1:A:310:GLU:O	1:A:314:MET:HG3	2.17	0.45
1:A:168:ASN:HB2	1:A:190:ARG:NH1	2.32	0.44
1:B:110:MET:HB3	1:B:110:MET:HE2	1.79	0.44
1:B:301:SER:O	1:B:303:SER:N	2.50	0.44
1:B:263:PRO:O	1:B:266:SER:OG	2.34	0.44
1:B:446:TRP:CE3	1:B:499:TRP:HA	2.53	0.44
1:B:453:MET:HE3	1:B:481:MET:HB3	2.00	0.44
1:B:134:PRO:HB2	1:B:137:TYR:CD1	2.53	0.44
1:B:172:SER:HA	1:B:244:VAL:O	2.18	0.43
1:B:191:ASP:OD2	1:B:239:CYS:HB2	2.18	0.43
1:A:243:SER:OG	1:A:244:VAL:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ARG:HD3	1:A:335:TYR:CE2	2.54	0.43
1:A:299:PRO:HB3	1:A:332:GLU:HG2	2.00	0.43
1:A:365:ASP:O	1:A:369:GLN:HG3	2.18	0.43
1:A:295:LYS:HB3	1:A:336:ILE:HB	2.01	0.43
1:A:253:LYS:H	1:A:253:LYS:HG3	1.54	0.43
1:A:151:PHE:CZ	1:A:246:CYS:HB3	2.54	0.43
1:B:345:SER:HB2	2:B:601:VSG:H10	2.01	0.43
1:B:382:TYR:OH	1:B:406:GLY:HA3	2.19	0.43
1:B:304:VAL:HG13	1:B:334:ILE:HD11	2.00	0.43
1:B:383:ILE:HG22	1:B:385:ARG:HG3	2.00	0.42
1:B:426:ILE:HD11	1:B:468:ASN:HB3	2.01	0.42
1:B:316:THR:O	1:B:380:ARG:NH2	2.53	0.42
1:B:134:PRO:HB2	1:B:137:TYR:HD1	1.84	0.42
1:B:341:MET:HE2	1:B:401:LYS:HG3	2.00	0.42
1:A:433:ALA:HB1	1:A:439:PHE:CE2	2.54	0.41
1:B:429:THR:HG22	1:B:433:ALA:HB3	2.02	0.41
1:A:228:VAL:O	1:A:232:LYS:HB2	2.20	0.41
1:B:269:LEU:HD22	1:B:294:VAL:HG21	2.02	0.41
1:A:490:GLU:HG2	1:B:523:THR:O	2.19	0.41
1:B:360:LEU:HB3	1:B:361:PRO:HD3	2.03	0.41
1:B:341:MET:HE1	1:B:395:SER:HB3	2.03	0.40
1:A:363:LEU:HD11	1:A:458:TYR:CZ	2.56	0.40
1:A:366:PHE:O	1:A:370:ILE:HG13	2.21	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	423/454 (93%)	400 (95%)	19 (4%)	4 (1%)	14 28
1	B	421/454 (93%)	400 (95%)	17 (4%)	4 (1%)	12 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	844/908 (93%)	800 (95%)	36 (4%)	8 (1%)	14	28

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	195	ARG
1	B	302	MET
1	A	236	ASP
1	A	302	MET
1	B	243	SER
1	A	142	ASP
1	B	256	GLU
1	A	299	PRO

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	374/393 (95%)	337 (90%)	37 (10%)	7	16
1	B	374/393 (95%)	336 (90%)	38 (10%)	7	15
All	All	748/786 (95%)	673 (90%)	75 (10%)	7	16

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	ARG
1	A	140	ARG
1	A	143	SER
1	A	154	ILE
1	A	181	THR
1	A	182	LYS
1	A	195	ARG
1	A	199	THR
1	A	227	LEU
1	A	233	LYS

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Mol	Chain	Res	Type
1	A	252	GLN
1	A	253	LYS
1	A	257	LYS
1	A	269	LEU
1	A	288	LYS
1	A	298	LYS
1	A	302	MET
1	A	308	LEU
1	A	322	LEU
1	A	324	LYS
1	A	328	VAL
1	A	331	LYS
1	A	334	ILE
1	A	353	ASP
1	A	387	LEU
1	A	404	ASP
1	A	405	PHE
1	A	407	LEU
1	A	432	GLU
1	A	455	ILE
1	A	456	VAL
1	A	461	ILE
1	A	476	GLU
1	A	485	GLU
1	A	504	GLU
1	A	508	THR
1	A	529	GLU
1	B	86	ILE
1	B	92	TYR
1	B	114	GLU
1	B	128	ARG
1	B	141	VAL
1	B	143	SER
1	B	144	LEU
1	B	145	GLU
1	B	154	ILE
1	B	184	SER
1	B	193	ASP
1	B	196	GLN
1	B	206	ARG
1	B	218	ARG
1	B	233	LYS

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Mol	Chain	Res	Type
1	B	240	GLN
1	B	247	MET
1	B	250	LYS
1	B	253	LYS
1	B	258	ASP
1	B	269	LEU
1	B	285	THR
1	B	298	LYS
1	B	304	VAL
1	B	322	LEU
1	B	324	LYS
1	B	328	VAL
1	B	334	ILE
1	B	380	ARG
1	B	387	LEU
1	B	407	LEU
1	B	410	VAL
1	B	432	GLU
1	B	450	ILE
1	B	456	VAL
1	B	477	ARG
1	B	501	ASN
1	B	504	GLU

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	136	ASN
1	A	230	HIS
1	A	240	GLN
1	A	277	GLN
1	A	318	GLN
1	A	513	GLN
1	B	252	GLN
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	1.27	1 (6%)	17,22,24	0.50	0
1	PTR	B	527	3,1	15,16,17	1.17	1 (6%)	17,22,24	0.43	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	-	1/10/11/13	0/1/1/1
1	PTR	B	527	3,1	-	0/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	527	PTR	OH-CZ	-4.34	1.30	1.40
1	A	527	PTR	OH-CZ	-4.24	1.31	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	A	527	PTR	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	527	PTR	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 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	VSG	B	601	-	34,34,34	0.96	3 (8%)	45,48,48	2.48	14 (31%)
2	VSG	A	601	-	34,34,34	0.94	2 (5%)	45,48,48	2.40	13 (28%)

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	VSG	B	601	-	-	0/12/22/22	0/5/5/5
2	VSG	A	601	-	-	0/12/22/22	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	VSG	C5-CAI	-2.49	1.40	1.46
2	A	601	VSG	CAH-CAI	2.48	1.39	1.37
2	B	601	VSG	CAH-CAI	2.41	1.39	1.37
2	A	601	VSG	C5-CAI	-2.20	1.41	1.46
2	B	601	VSG	CAH-NAG	-2.05	1.34	1.38

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	VSG	C5-C4-N3	-6.89	119.66	126.97
2	A	601	VSG	CAU-NAT-CAS	6.67	120.16	109.54
2	A	601	VSG	C5-C4-N3	-6.55	120.02	126.97
2	B	601	VSG	CAU-NAT-CAS	6.48	119.85	109.54
2	B	601	VSG	CAR-CAS-NAT	-5.29	104.38	111.20
2	B	601	VSG	CAW-NAT-CAS	5.10	120.36	110.63
2	A	601	VSG	CAW-NAT-CAU	4.94	120.05	110.63
2	A	601	VSG	N1-C2-N3	-4.83	121.27	128.58
2	B	601	VSG	CAW-NAT-CAU	4.80	119.79	110.63
2	A	601	VSG	CAW-NAT-CAS	4.79	119.77	110.63
2	B	601	VSG	N1-C2-N3	-4.54	121.71	128.58
2	A	601	VSG	CAR-CAS-NAT	-4.21	105.77	111.20
2	A	601	VSG	CAY-OAX-CAN	4.00	127.93	118.78
2	B	601	VSG	CAY-OAX-CAN	3.93	127.77	118.78
2	B	601	VSG	C6-C5-C4	3.66	118.48	115.74
2	A	601	VSG	C2-N3-C4	3.54	120.48	111.83
2	B	601	VSG	C2-N3-C4	3.40	120.13	111.83
2	B	601	VSG	CAR-CAQ-NAG	-2.91	108.17	111.40
2	A	601	VSG	C6-C5-C4	2.75	117.80	115.74
2	B	601	VSG	CAI-CAH-NAG	-2.49	109.50	110.54
2	B	601	VSG	N3-C4-NAG	2.44	131.32	127.17
2	A	601	VSG	CAI-CAH-NAG	-2.42	109.53	110.54
2	B	601	VSG	CAV-CAU-NAT	-2.35	108.16	111.20
2	A	601	VSG	CAV-CAQ-NAG	-2.33	108.82	111.40
2	A	601	VSG	CAV-CAU-NAT	-2.23	108.31	111.20
2	B	601	VSG	CAS-CAR-CAQ	2.12	114.66	110.78
2	A	601	VSG	N3-C4-NAG	2.06	130.66	127.17

There are no chirality outliers.

There are no torsion outliers.

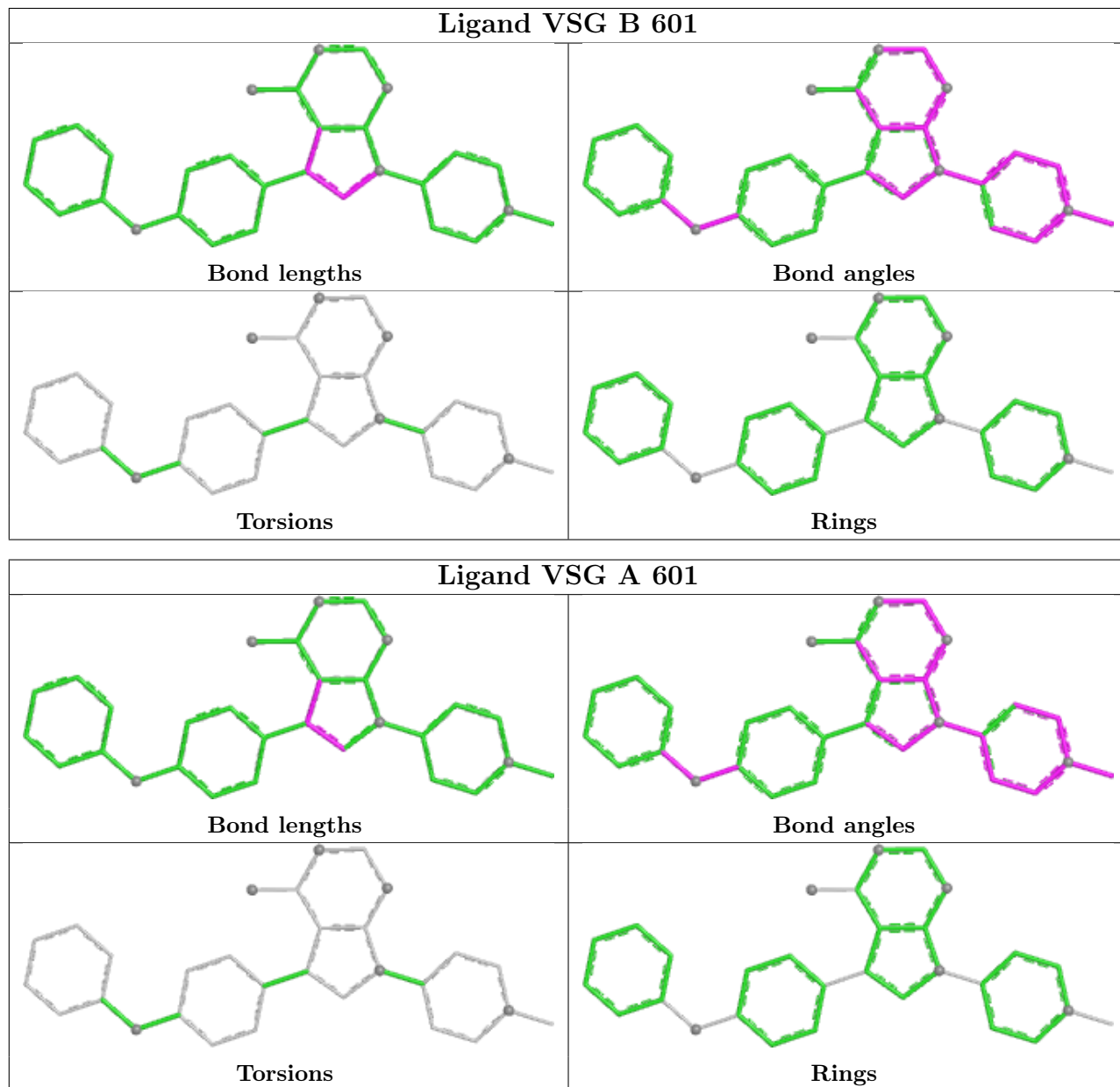
There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	VSG	6	0
2	A	601	VSG	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	429/454 (94%)	0.53	16 (3%) 45 35	28, 49, 72, 89	1 (0%)
1	B	427/454 (94%)	0.73	37 (8%) 16 12	29, 52, 86, 102	1 (0%)
All	All	856/908 (94%)	0.63	53 (6%) 26 19	28, 51, 80, 102	2 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	213	PHE	5.9
1	B	530	ILE	4.2
1	B	224	LEU	4.2
1	B	302	MET	3.8
1	B	425	PRO	3.8
1	A	411	ILE	3.6
1	B	472	ILE	3.6
1	B	382	TYR	3.5
1	B	214	TYR	3.3
1	A	425	PRO	3.3
1	A	207	THR	3.3
1	B	300	GLY	3.1
1	A	289	HIS	3.1
1	A	305	GLU	3.0
1	B	170	LEU	3.0
1	B	111	VAL	3.0
1	B	308	LEU	2.9
1	A	304	VAL	2.9
1	B	234	GLY	2.8
1	A	325	LEU	2.8
1	B	410	VAL	2.7
1	B	531	PRO	2.7
1	B	465	GLY	2.7
1	B	305	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	196	GLN	2.6
1	B	223	THR	2.6
1	A	301	SER	2.6
1	A	408	ALA	2.6
1	B	169	MET	2.6
1	B	195	ARG	2.5
1	A	308	LEU	2.5
1	A	219	SER	2.5
1	B	408	ALA	2.5
1	B	206	ARG	2.4
1	B	289	HIS	2.3
1	B	217	PRO	2.3
1	B	383	ILE	2.3
1	B	301	SER	2.2
1	B	241	LYS	2.2
1	A	130	GLU	2.2
1	B	306	ALA	2.2
1	B	243	SER	2.2
1	B	85	ARG	2.1
1	B	304	VAL	2.1
1	A	278	PHE	2.1
1	B	411	ILE	2.1
1	A	312	ASN	2.1
1	B	86	ILE	2.1
1	A	131	GLY	2.1
1	A	216	SER	2.0
1	B	193	ASP	2.0
1	B	167	GLY	2.0
1	B	529	GLU	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(Å ²)	Q<0.9
1	PTR	A	527	16/17	0.95	0.09	34,42,49,65	0
1	PTR	B	527	16/17	0.95	0.11	36,53,59,60	0

6.3 Carbohydrates [i](#)

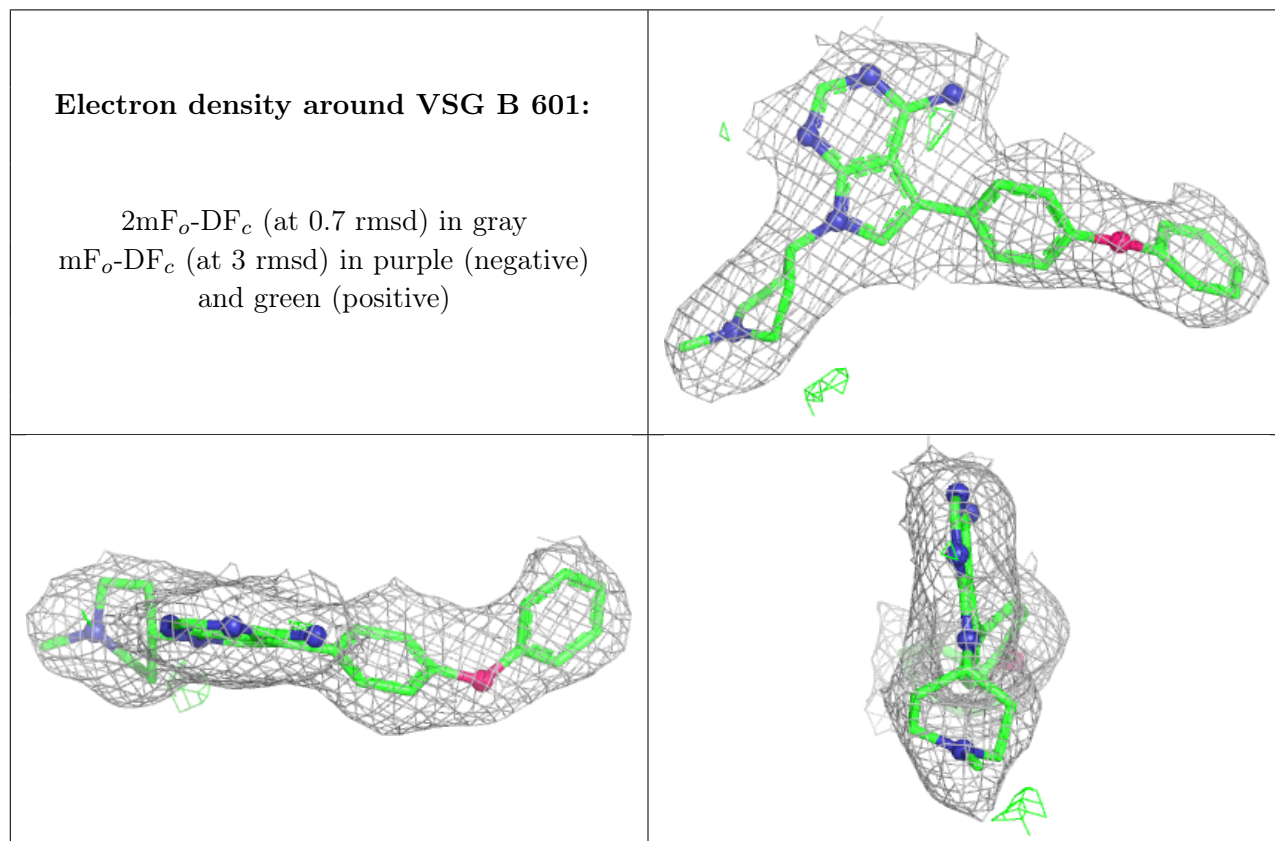
There are no oligosaccharides in this entry.

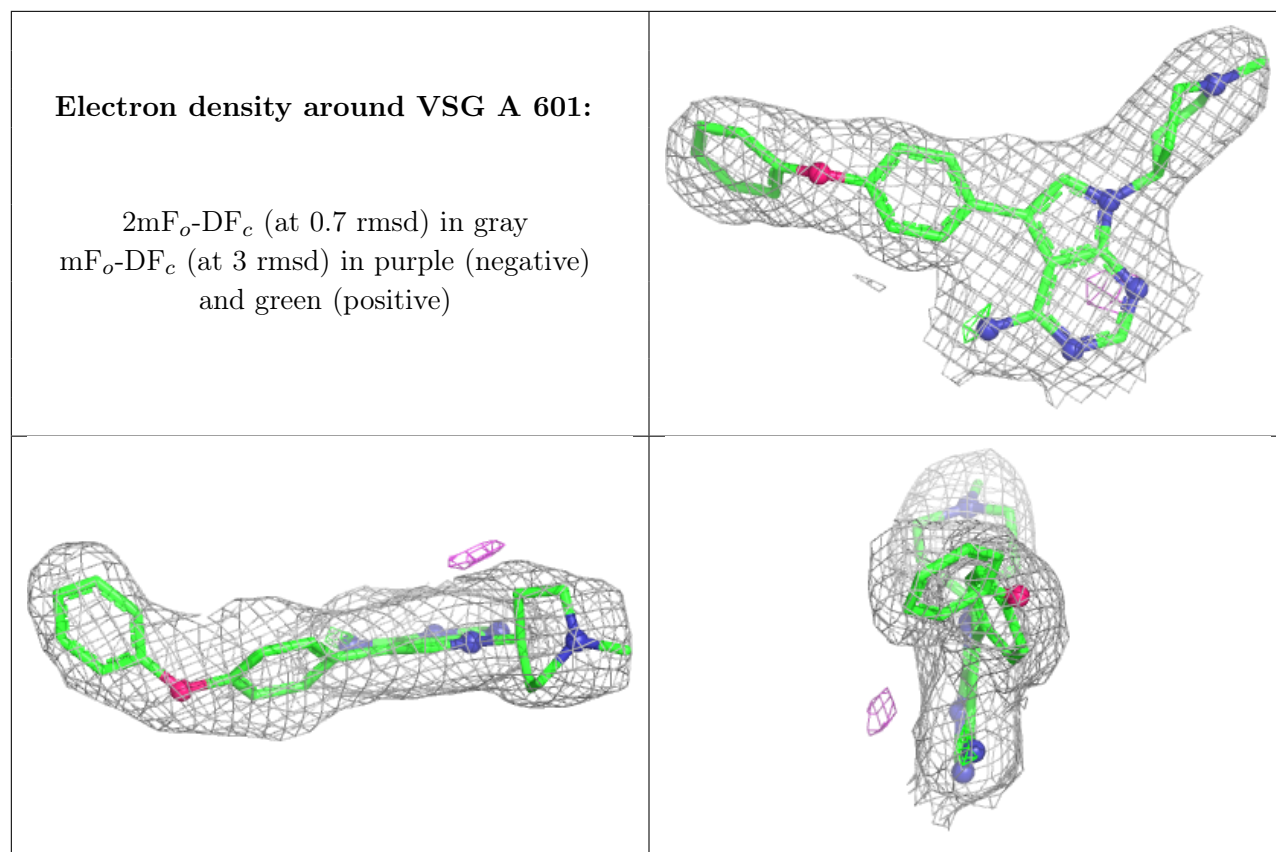
6.4 Ligands [i](#)

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	CA	A	602	1/1	0.70	0.20	66,66,66,66	0
3	CA	B	602	1/1	0.74	0.19	71,71,71,71	0
2	VSG	B	601	30/30	0.93	0.14	50,60,66,69	0
2	VSG	A	601	30/30	0.95	0.15	45,59,65,71	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.