



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:06 PM UTC

PDB ID : 5RLC / pdb_00005rlc
Title : PanDDA analysis group deposition – Crystal Structure of SARS-CoV-2 heli-
case in complex with Z56923284
Authors : Newman, J.A.; Yosaatmadja, Y.; Douangamath, A.; Aimon, A.; Powell, A.J.;
Dias, A.; Fearon, D.; Dunnett, L.; Brandao-Neto, J.; Krojer, T.; Skyner, R.;
Gorrie-Stone, T.; Thompson, W.; von Delft, F.; Arrowsmith, C.H.; Edwards,
A.; Bountra, C.; Gileadi, O.
Deposited on : 2020-09-16
Resolution : 1.92 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)

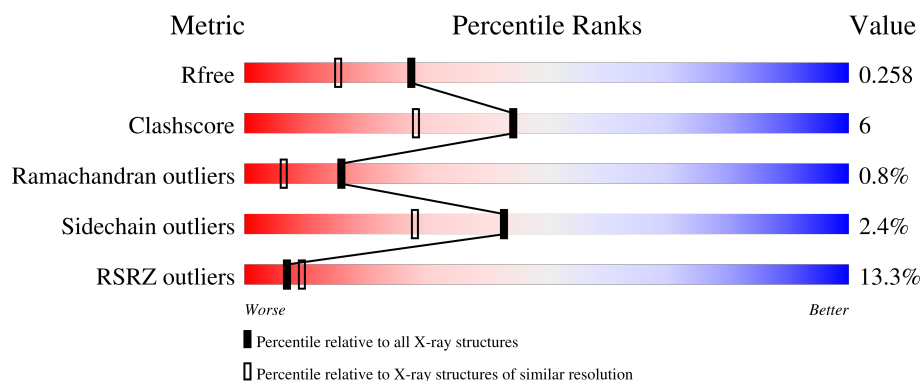
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	601	17% 81% 13% • 5%
1	B	601	9% 81% 15% • •

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9423 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.

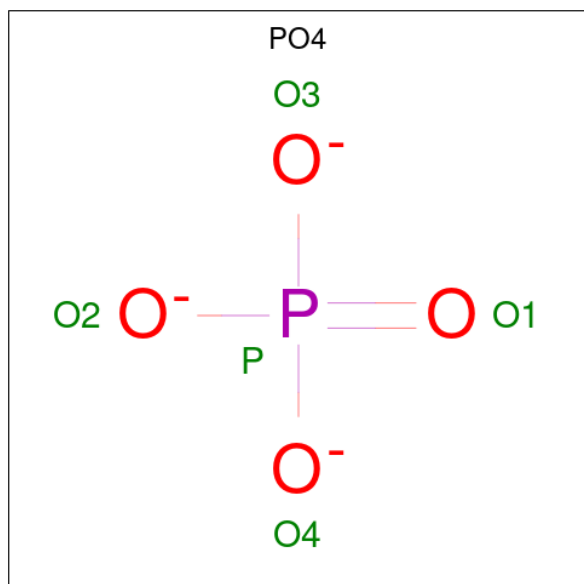
- Molecule 1 is a protein called Helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	572	Total	C	N	O	S	0	0	0
			4417	2816	737	832	32			
1	B	585	Total	C	N	O	S	0	1	0
			4508	2875	750	848	35			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

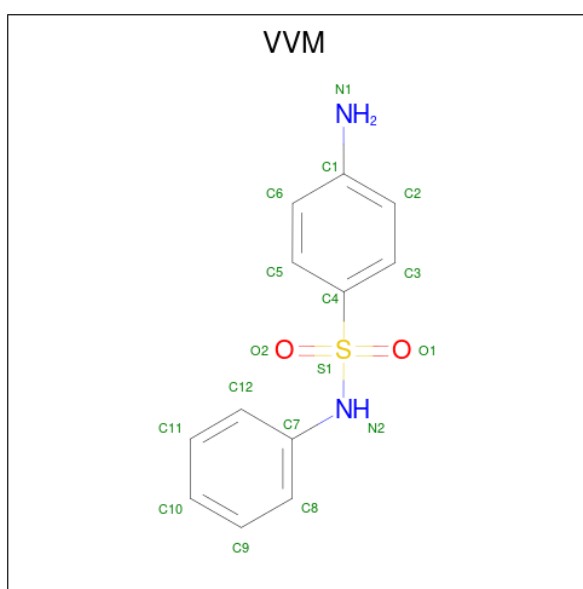
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	3	Total	Zn	0	0
			3	3		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 4 is 4-amino-N-phenylbenzene-1-sulfonamide (CCD ID: VVM) (formula: $C_{12}H_{12}N_2O_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O S 17 12 2 2 1	0	0

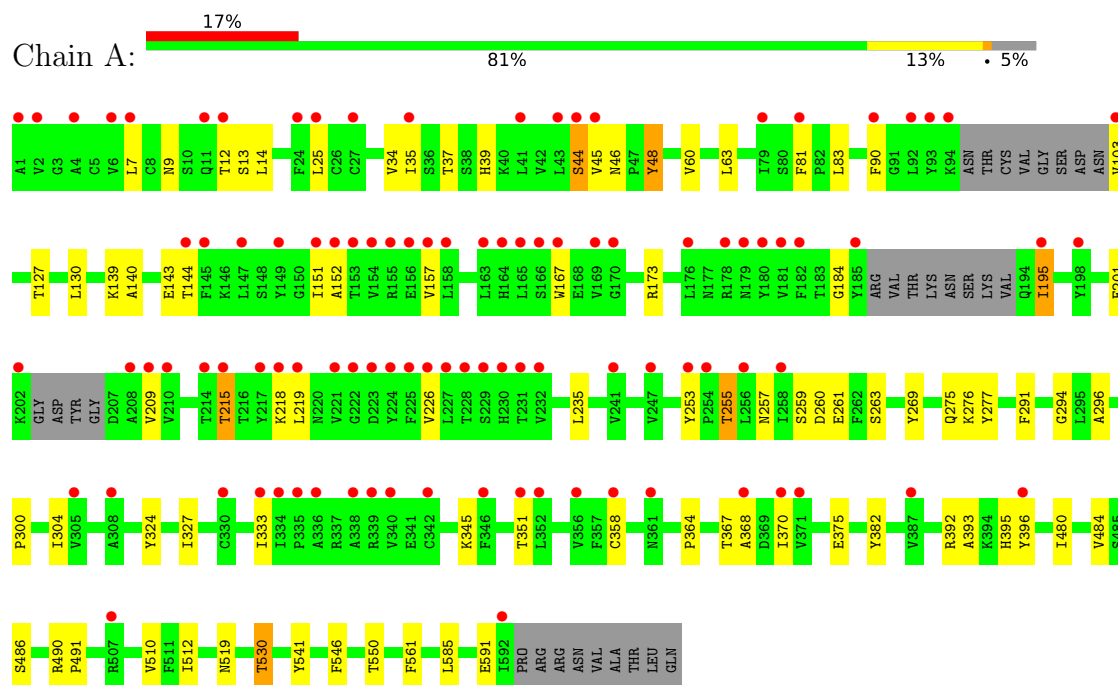
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	207	Total O 207 207	0	0
5	B	248	Total O 248 248	0	0

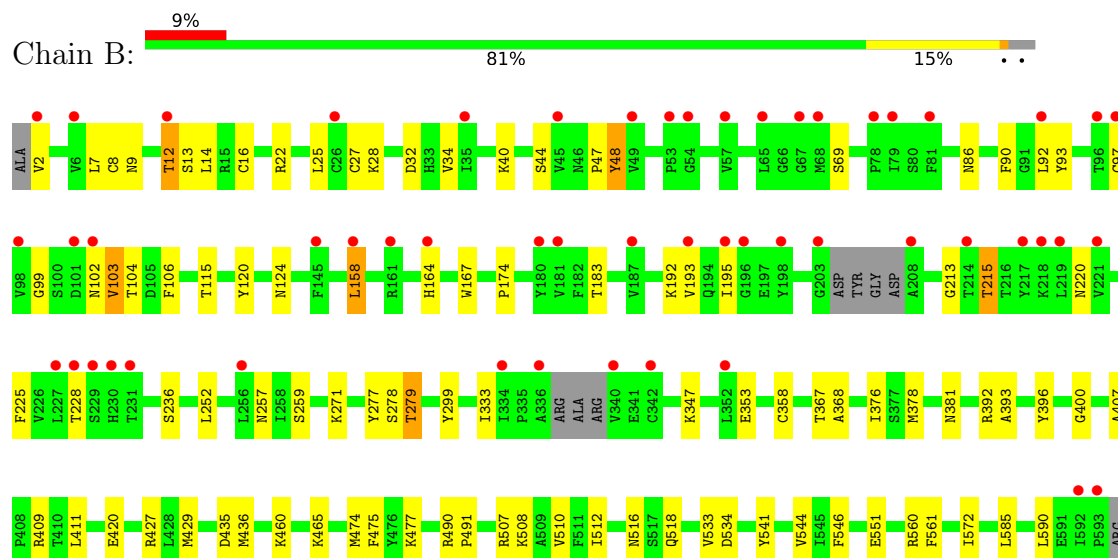
3 Residue-property plots [i](#)

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: Helicase



• Molecule 1: Helicase



ARG
ASN
VAL
ALA
THR
LEU
GLN

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.23Å 70.19Å 85.17Å 102.63° 95.94° 112.44°	Depositor
Resolution (Å)	81.30 – 1.92 81.30 – 1.92	Depositor EDS
% Data completeness (in resolution range)	95.7 (81.30-1.92) 95.9 (81.30-1.92)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.206 , 0.252 0.220 , 0.258	Depositor DCC
R_{free} test set	4747 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	34.2	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 29.7	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	9423	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% 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: PO4, VVM, ZN

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	1.07	0/4517	1.39	1/6156 (0.0%)
1	B	1.05	0/4610	1.36	3/6283 (0.0%)
All	All	1.06	0/9127	1.38	4/12439 (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	534	ASP	CB-CA-C	5.77	119.94	110.88
1	A	253	TYR	CB-CA-C	5.59	117.61	110.34
1	B	279	THR	CB-CA-C	5.47	119.18	109.72
1	B	507	ARG	N-CA-C	-5.12	106.86	113.01

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	4417	0	4321	47	0
1	B	4508	0	4424	61	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	0	0	0
4	B	17	0	0	1	0
5	A	207	0	0	4	0
5	B	248	0	0	11	0
All	All	9423	0	8745	107	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 (107) 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:12:THR:HG21	1:B:25:LEU:O	1.74	0.86
1:B:183:THR:OG1	1:B:228:THR:OG1	1.82	0.82
1:A:60:VAL:HB	5:A:928:HOH:O	1.80	0.81
1:B:102:ASN:O	1:B:104:THR:N	2.13	0.80
1:B:2:VAL:N	5:B:802:HOH:O	2.14	0.80
1:B:510:VAL:HG21	1:B:541:TYR:CD1	2.20	0.77
1:B:271:LYS:NZ	5:B:804:HOH:O	2.22	0.72
1:B:102:ASN:C	1:B:104:THR:H	1.96	0.72
1:A:375:GLU:OE2	5:A:801:HOH:O	2.08	0.72
1:A:327:ILE:O	5:A:802:HOH:O	2.10	0.70
1:B:47:PRO:O	5:B:801:HOH:O	2.13	0.67
1:B:460:LYS:NZ	5:B:805:HOH:O	2.26	0.67
1:B:183:THR:HG1	1:B:228:THR:HG1	1.07	0.65
1:A:486:SER:OG	5:A:803:HOH:O	2.15	0.64
1:A:255:THR:HG23	1:A:300:PRO:HG3	1.79	0.62
1:B:257:ASN:HB2	5:B:809:HOH:O	2.00	0.62
1:A:260:ASP:HA	1:A:263:SER:OG	1.99	0.62
1:A:48:TYR:OH	1:A:90:PHE:O	2.16	0.60
1:A:13:SER:O	1:A:44:SER:HA	2.02	0.60
1:B:8:CYS:SG	1:B:99:GLY:O	2.60	0.60
1:A:510:VAL:HG21	1:A:541:TYR:CD1	2.37	0.59
1:A:235:LEU:HD21	1:A:382:TYR:CE2	2.38	0.58
1:B:279:THR:HB	1:B:429:MET:CE	2.34	0.58
1:B:278:SER:HB2	1:B:436:MET:HE2	1.86	0.57
1:B:120:TYR:CE2	1:B:409:ARG:HG2	2.40	0.57
1:A:277:TYR:HA	1:A:396:TYR:O	2.05	0.56
1:B:279:THR:HB	1:B:429:MET:HE3	1.86	0.56
1:A:127:THR:HG22	1:A:130:LEU:HD12	1.88	0.56
1:A:368:ALA:O	1:A:393:ALA:HA	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:TYR:OH	1:A:294:GLY:HA3	2.05	0.55
1:A:44:SER:OG	1:A:45:VAL:N	2.37	0.55
1:A:276:LYS:O	1:A:395:HIS:HA	2.07	0.54
1:B:277:TYR:HA	1:B:396:TYR:O	2.08	0.54
1:B:103:VAL:CG1	1:B:103:VAL:O	2.56	0.53
1:A:367:THR:HA	1:A:392:ARG:O	2.09	0.53
1:B:124:ASN:OD1	1:B:381:ASN:ND2	2.37	0.53
1:B:86:ASN:HB3	5:B:1021:HOH:O	2.08	0.52
1:B:92:LEU:HB3	1:B:93:TYR:CD2	2.45	0.52
1:B:333:ILE:HB	1:B:358:CYS:SG	2.49	0.52
1:B:465:LYS:NZ	5:B:818:HOH:O	2.42	0.52
1:B:508:LYS:HD3	5:B:995:HOH:O	2.11	0.51
1:B:518:GLN:HA	1:B:518:GLN:OE1	2.11	0.51
1:A:151:ILE:HG12	1:A:226:VAL:HG22	1.93	0.50
1:B:8:CYS:SG	1:B:99:GLY:N	2.84	0.50
1:B:167:TRP:CZ3	1:B:174:PRO:HD2	2.46	0.50
1:B:28:LYS:O	1:B:32:ASP:OD1	2.29	0.50
1:B:34:VAL:O	1:B:40:LYS:NZ	2.36	0.50
1:A:275:GLN:O	1:A:395:HIS:ND1	2.44	0.49
1:A:63:LEU:HB3	1:A:83:LEU:HD12	1.95	0.49
1:A:296:ALA:O	1:A:300:PRO:HA	2.13	0.49
1:B:13:SER:O	1:B:44:SER:HA	2.13	0.49
1:A:140:ALA:O	1:A:144:THR:HG23	2.13	0.49
1:B:102:ASN:C	1:B:104:THR:N	2.65	0.48
1:B:474[B]:MET:HG2	1:B:590:LEU:HB2	1.96	0.48
1:A:152:ALA:HB2	1:A:167:TRP:CZ3	2.49	0.48
1:A:37:THR:OG1	1:A:39:HIS:HB2	2.14	0.48
1:A:215:THR:HG22	1:B:193:VAL:HG21	1.96	0.47
1:A:139:LYS:O	1:A:143:GLU:HG2	2.13	0.47
1:A:304:ILE:HA	1:A:370:ILE:O	2.14	0.47
1:A:184:GLY:C	1:A:195:ILE:HG12	2.39	0.47
1:B:13:SER:OG	1:B:44:SER:OG	2.33	0.47
1:B:48:TYR:OH	1:B:90:PHE:O	2.24	0.47
1:A:14:LEU:HB2	1:A:25:LEU:O	2.14	0.47
1:B:27:CYS:HB2	1:B:97:CYS:SG	2.55	0.47
1:B:368:ALA:O	1:B:393:ALA:HA	2.14	0.47
1:B:7:LEU:HD21	1:B:106:PHE:HB2	1.98	0.46
1:B:278:SER:HA	1:B:435:ASP:OD1	2.14	0.46
1:A:327:ILE:HD11	1:A:345:LYS:O	2.16	0.46
1:B:236:SER:O	4:B:701:VVM:C10	2.63	0.46
1:A:7:LEU:HD13	1:A:103:VAL:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:GLU:OE1	1:A:324:TYR:OH	2.17	0.46
1:A:351:THR:HG23	1:A:364:PRO:HG3	1.97	0.45
1:A:512:ILE:O	1:A:546:PHE:HA	2.17	0.45
1:A:157:VAL:HG21	1:A:219:LEU:O	2.16	0.45
1:A:333:ILE:HB	1:A:358:CYS:SG	2.57	0.45
1:A:304:ILE:HG12	1:A:370:ILE:HB	1.98	0.45
1:B:475:PHE:CZ	1:B:477:LYS:HE2	2.51	0.45
1:B:533:VAL:HG11	1:B:560:ARG:O	2.17	0.45
1:B:16:CYS:O	1:B:22:ARG:HA	2.16	0.45
1:B:420:GLU:OE1	1:B:427:ARG:NH1	2.48	0.45
1:A:34:VAL:HA	1:A:39:HIS:O	2.18	0.45
1:A:480:ILE:HG21	1:A:550:THR:HG22	1.98	0.45
1:A:490:ARG:HB2	1:A:491:PRO:HD3	1.99	0.45
1:A:519:ASN:HB3	1:A:530:THR:CG2	2.46	0.45
1:B:544:VAL:O	1:B:572:ILE:HA	2.17	0.45
1:B:252:LEU:HB3	1:B:299:TYR:CD1	2.53	0.44
1:A:519:ASN:HB3	1:A:530:THR:HG23	1.99	0.44
1:B:2:VAL:N	5:B:835:HOH:O	2.50	0.44
1:B:12:THR:HG22	1:B:14:LEU:H	1.83	0.44
1:B:367:THR:HA	1:B:392:ARG:O	2.18	0.44
1:B:376:ILE:HG22	1:B:400:GLY:HA3	1.99	0.44
1:B:213:GLY:C	1:B:215:THR:H	2.26	0.43
1:B:103:VAL:O	1:B:103:VAL:HG12	2.19	0.43
1:B:512:ILE:O	1:B:546:PHE:HA	2.18	0.43
1:B:378:MET:O	1:B:407:ALA:HB2	2.19	0.43
1:B:561:PHE:CZ	1:B:585:LEU:HD21	2.53	0.43
1:A:257:ASN:C	1:A:257:ASN:HD22	2.26	0.43
1:A:291:PHE:CD1	1:A:291:PHE:C	2.96	0.42
1:A:151:ILE:HG12	1:A:226:VAL:CG2	2.50	0.42
1:B:409:ARG:NH2	5:B:827:HOH:O	2.48	0.42
1:A:561:PHE:CZ	1:A:585:LEU:HD21	2.55	0.41
1:B:48:TYR:O	5:B:803:HOH:O	2.21	0.41
1:A:130:LEU:HD23	1:A:130:LEU:HA	1.94	0.41
1:B:347:LYS:HD2	1:B:353:GLU:OE2	2.20	0.41
1:B:115:THR:HA	1:B:411:LEU:O	2.21	0.40
1:B:490:ARG:HB2	1:B:491:PRO:HD3	2.03	0.40
1:B:183:THR:O	1:B:225:PHE:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	564/601 (94%)	533 (94%)	26 (5%)	5 (1%)	14	5
1	B	580/601 (96%)	540 (93%)	36 (6%)	4 (1%)	18	9
All	All	1144/1202 (95%)	1073 (94%)	62 (5%)	9 (1%)	16	6

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	103	VAL
1	A	9	ASN
1	A	218	LYS
1	A	484	VAL
1	B	158	LEU
1	A	48	TYR
1	B	9	ASN
1	B	48	TYR
1	A	195	ILE

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	485/523 (93%)	472 (97%)	13 (3%)	39	24
1	B	498/523 (95%)	487 (98%)	11 (2%)	45	32
All	All	983/1046 (94%)	959 (98%)	24 (2%)	43	28

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	35	ILE
1	A	44	SER
1	A	46	ASN
1	A	81	PHE
1	A	173	ARG
1	A	201	GLU
1	A	209	VAL
1	A	215	THR
1	A	255	THR
1	A	259	SER
1	A	530	THR
1	A	591	GLU
1	B	12	THR
1	B	69	SER
1	B	158	LEU
1	B	164	HIS
1	B	192	LYS
1	B	195	ILE
1	B	215	THR
1	B	220	ASN
1	B	259	SER
1	B	516	ASN
1	B	551	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	164	HIS
1	A	257	ASN
1	A	404	GLN
1	A	586	GLN
1	B	51	ASN
1	B	88	GLN
1	B	179	ASN
1	B	404	GLN
1	B	459	ASN
1	B	464	HIS
1	B	482	HIS
1	B	516	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 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	$\# Z > 2$
3	PO4	B	706	-	4,4,4	1.61	2 (50%)	6,6,6	0.49	0
4	VVM	B	701	-	18,18,18	0.59	0	25,25,25	0.85	1 (4%)
3	PO4	A	705	-	4,4,4	1.46	0	6,6,6	0.59	0
3	PO4	A	704	-	4,4,4	0.82	0	6,6,6	0.77	0
3	PO4	B	705	-	4,4,4	0.77	0	6,6,6	0.60	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	VVM	B	701	-	-	0/11/11/11	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	706	PO4	P-O3	-2.21	1.48	1.54
3	B	706	PO4	P-O4	-2.19	1.48	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	701	VVM	O1-S1-C4	2.19	110.74	107.98

There are no chirality outliers.

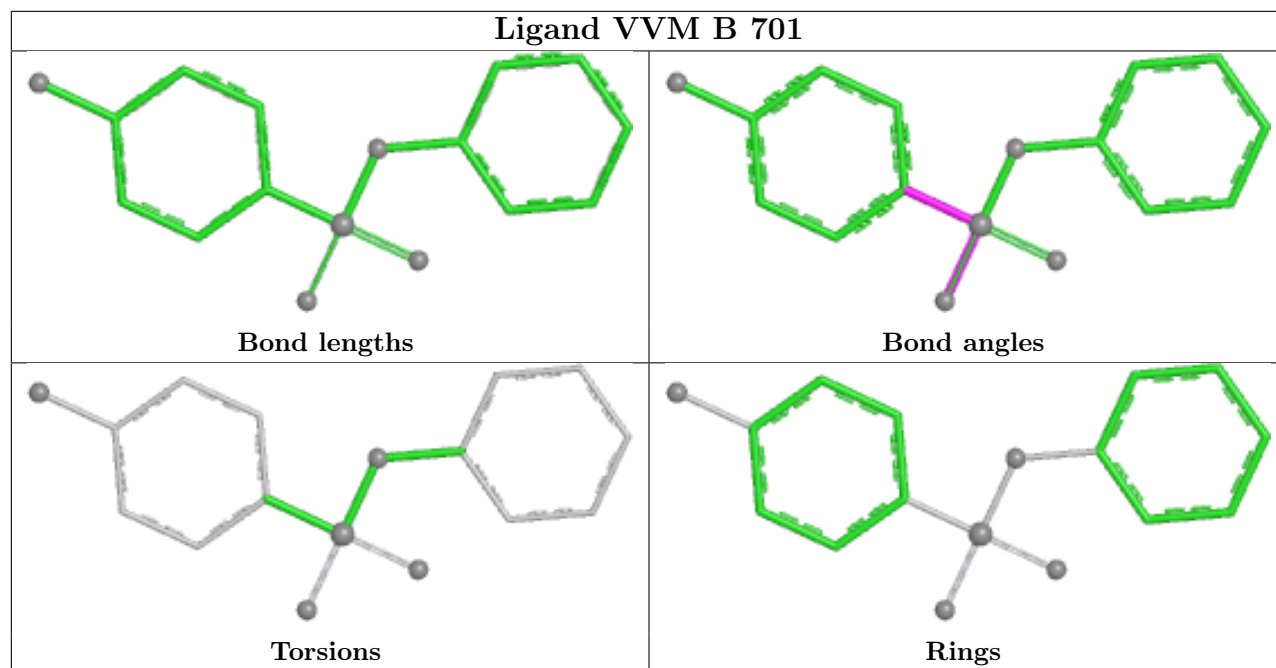
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	701	VVM	1	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	572/601 (95%)	0.99	101 (17%) 4 5	24, 52, 104, 144	0
1	B	585/601 (97%)	0.44	53 (9%) 15 18	18, 40, 87, 136	1 (0%)
All	All	1157/1202 (96%)	0.71	154 (13%) 7 9	18, 47, 97, 144	1 (0%)

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	219	LEU	8.3
1	A	592	ILE	7.4
1	A	202	LYS	5.1
1	A	229	SER	4.9
1	A	336	ALA	4.7
1	B	336	ALA	4.7
1	A	215	THR	4.5
1	B	187	VAL	4.5
1	B	340	VAL	4.5
1	A	208	ALA	4.4
1	A	92	LEU	4.4
1	A	6	VAL	4.3
1	A	157	VAL	4.3
1	B	217	TYR	4.2
1	A	154	VAL	4.1
1	A	2	VAL	4.1
1	A	81	PHE	4.1
1	A	94	LYS	4.1
1	A	222	GLY	4.1
1	B	208	ALA	4.0
1	A	209	VAL	4.0
1	A	226	VAL	3.9
1	A	163	LEU	3.8
1	A	352	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	2	VAL	3.8
1	A	7	LEU	3.8
1	A	155	ARG	3.8
1	B	592	ILE	3.8
1	A	170	GLY	3.7
1	A	247	VAL	3.7
1	B	203	GLY	3.6
1	A	169	VAL	3.6
1	A	195	ILE	3.6
1	A	334	ILE	3.6
1	A	103	VAL	3.6
1	A	224	TYR	3.5
1	B	196	GLY	3.5
1	B	81	PHE	3.5
1	A	149	TYR	3.5
1	A	179	ASN	3.5
1	A	45	VAL	3.5
1	A	185	TYR	3.4
1	A	221	VAL	3.4
1	B	193	VAL	3.4
1	A	158	LEU	3.4
1	A	165	LEU	3.3
1	A	12	THR	3.3
1	A	152	ALA	3.2
1	A	145	PHE	3.2
1	A	258	ILE	3.2
1	A	181	VAL	3.2
1	B	593	PRO	3.1
1	A	230	HIS	3.1
1	B	57	VAL	3.1
1	B	78	PRO	3.0
1	A	333	ILE	3.0
1	B	219	LEU	2.9
1	B	101	ASP	2.9
1	A	90	PHE	2.9
1	A	1	ALA	2.9
1	A	44	SER	2.9
1	A	43	LEU	2.9
1	A	151	ILE	2.9
1	A	227	LEU	2.9
1	B	98	VAL	2.8
1	A	217	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	256	LEU	2.8
1	A	361	ASN	2.8
1	A	178	ARG	2.8
1	B	230	HIS	2.8
1	A	305	VAL	2.8
1	A	153	THR	2.8
1	A	218	LYS	2.8
1	A	93	TYR	2.8
1	A	180	TYR	2.8
1	B	45	VAL	2.8
1	B	49	VAL	2.8
1	A	182	PHE	2.7
1	A	358	CYS	2.7
1	A	164	HIS	2.7
1	B	53	PRO	2.7
1	A	210	VAL	2.7
1	A	335	PRO	2.7
1	B	102	ASN	2.7
1	A	167	TRP	2.6
1	B	97	CYS	2.6
1	A	225	PHE	2.6
1	A	156	GLU	2.6
1	A	176	LEU	2.6
1	B	214	THR	2.6
1	A	223	ASP	2.6
1	A	198	TYR	2.6
1	A	339	ARG	2.6
1	B	67	GLY	2.6
1	A	4	ALA	2.6
1	A	340	VAL	2.6
1	A	356	VAL	2.6
1	B	181	VAL	2.6
1	B	65	LEU	2.5
1	B	158	LEU	2.5
1	B	195	ILE	2.5
1	A	24	PHE	2.5
1	B	180	TYR	2.5
1	B	231	THR	2.5
1	A	27	CYS	2.4
1	A	228	THR	2.4
1	A	254	PRO	2.4
1	B	6	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	35	ILE	2.4
1	A	144	THR	2.4
1	A	308	ALA	2.4
1	B	218	LYS	2.4
1	B	228	THR	2.4
1	B	35	ILE	2.4
1	A	387	VAL	2.4
1	A	396	TYR	2.3
1	B	145	PHE	2.3
1	A	351	THR	2.3
1	B	342	CYS	2.3
1	A	338	ALA	2.3
1	A	371	VAL	2.3
1	B	68	MET	2.3
1	B	96	THR	2.3
1	A	253	TYR	2.2
1	A	342	CYS	2.2
1	A	231	THR	2.2
1	A	166	SER	2.2
1	B	54	GLY	2.2
1	B	26	CYS	2.2
1	A	41	LEU	2.2
1	A	147	LEU	2.2
1	A	370	ILE	2.2
1	B	79	ILE	2.2
1	B	229	SER	2.2
1	A	232	VAL	2.1
1	B	12	THR	2.1
1	B	221	VAL	2.1
1	A	25	LEU	2.1
1	A	368	ALA	2.1
1	B	227	LEU	2.1
1	B	352	LEU	2.1
1	A	346	PHE	2.1
1	A	214	THR	2.1
1	A	330	CYS	2.1
1	B	161	ARG	2.1
1	A	79	ILE	2.0
1	B	334	ILE	2.0
1	B	198	TYR	2.0
1	B	164	HIS	2.0
1	A	241	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	92	LEU	2.0
1	B	256	LEU	2.0
1	A	11	GLN	2.0
1	A	507	ARG	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

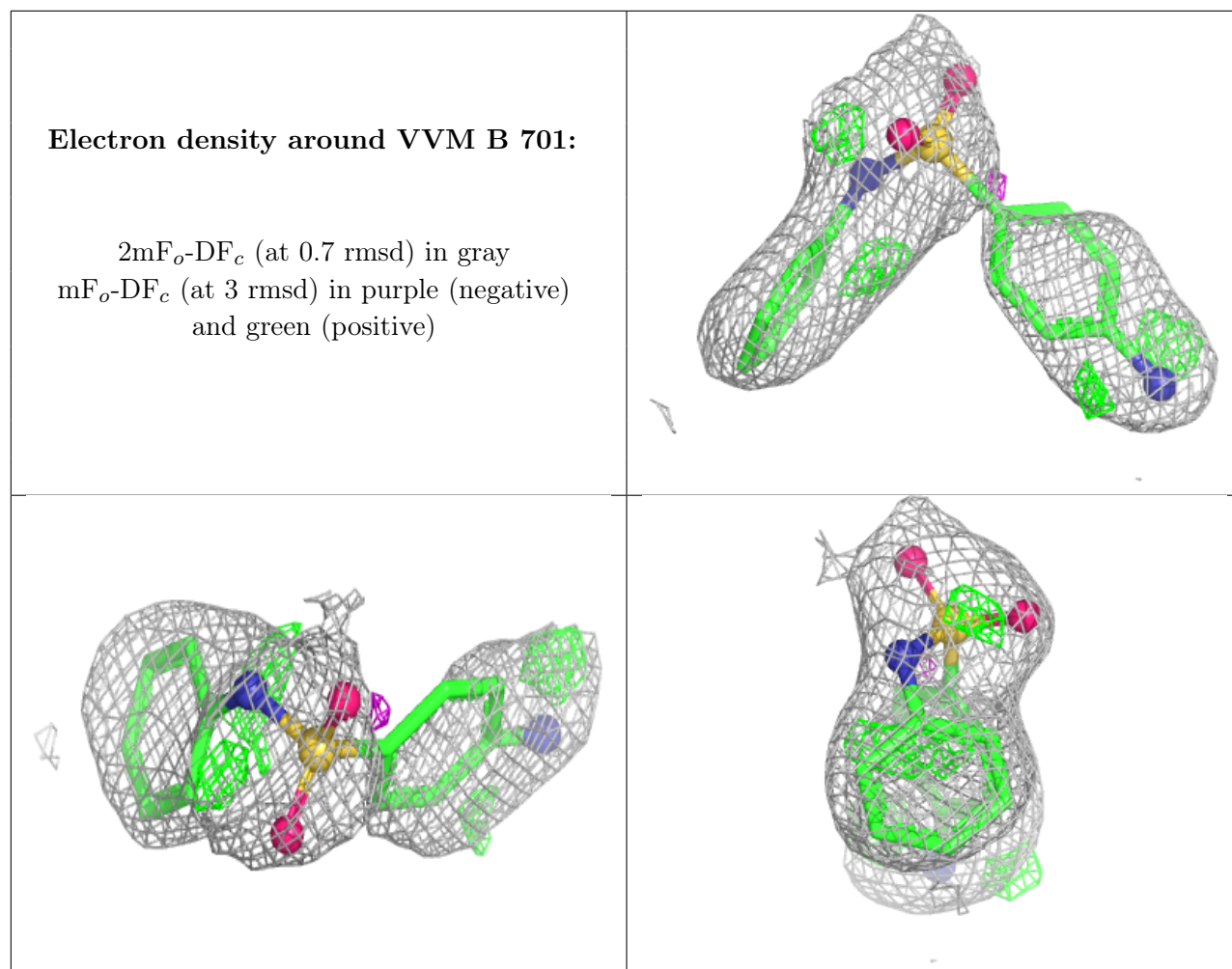
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	VVM	B	701	17/17	0.85	0.19	40,50,65,73	17
3	PO4	B	705	5/5	0.97	0.05	35,35,42,42	0
3	PO4	B	706	5/5	0.97	0.06	34,37,40,48	0
2	ZN	B	703	1/1	0.97	0.05	64,64,64,64	0
3	PO4	A	705	5/5	0.98	0.07	34,39,40,43	0
2	ZN	A	703	1/1	0.98	0.06	75,75,75,75	0
2	ZN	A	702	1/1	0.98	0.03	49,49,49,49	0
3	PO4	A	704	5/5	0.98	0.06	35,36,39,42	0
2	ZN	B	704	1/1	0.99	0.04	71,71,71,71	0
2	ZN	B	702	1/1	0.99	0.02	41,41,41,41	0
2	ZN	A	701	1/1	0.99	0.03	55,55,55,55	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 ⓘ

There are no such residues in this entry.