



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 1, 2022 – 12:43 PM EDT

PDB ID : 5RLG
Title : PanDDA analysis group deposition – Crystal Structure of SARS-CoV-2 heli-
case in complex with Z19739650
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 : 1.96 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.29
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

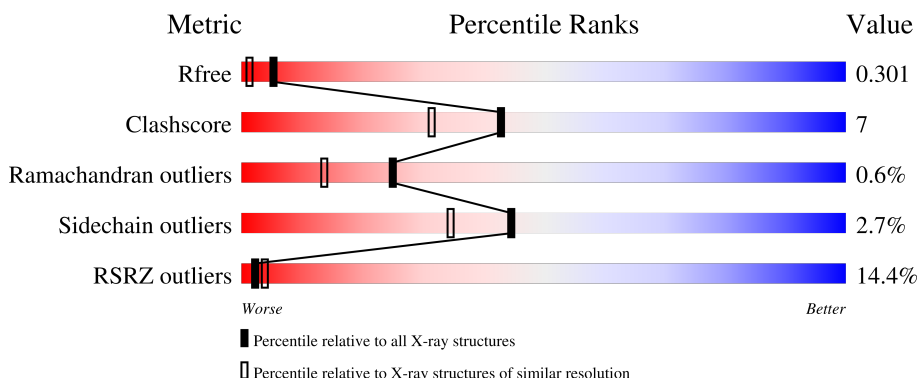
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	<div style="display: flex; align-items: center;"> <div style="width: 20%; 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: grey;"></div> </div>
1	B	601	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 83%; 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: grey;"></div> </div>

2 Entry composition [i](#)

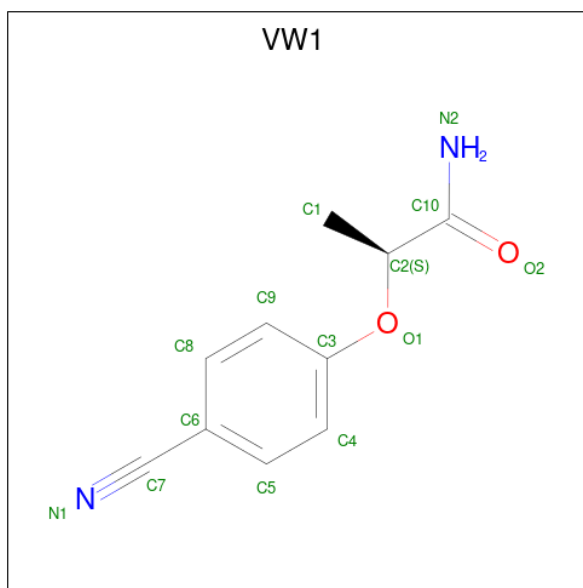
There are 5 unique types of molecules in this entry. The entry contains 9418 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	B	585	Total 4508	C 2875	N 750	O 848	S 35	0	1	0
1	A	572	Total 4417	C 2816	N 737	O 832	S 32	0	0	0

- Molecule 2 is (2S)-2-(4-cyanophenoxy)propanamide (three-letter code: VW1) (formula: C₁₀H₁₀N₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	Total 14	C 10	N 2	O 2	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

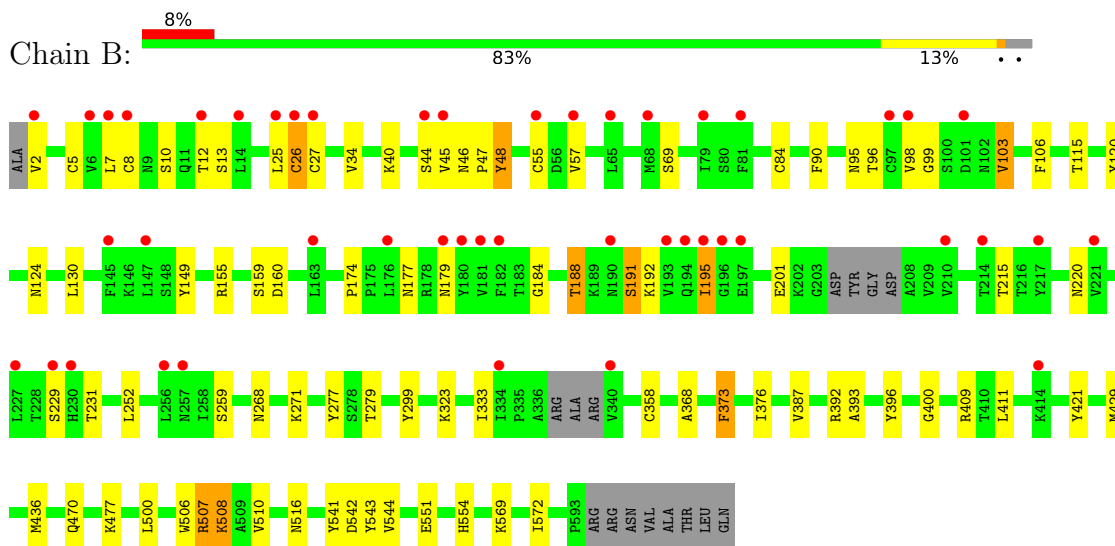
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	250	Total O 250 250	0	0
5	A	203	Total O 203 203	0	0

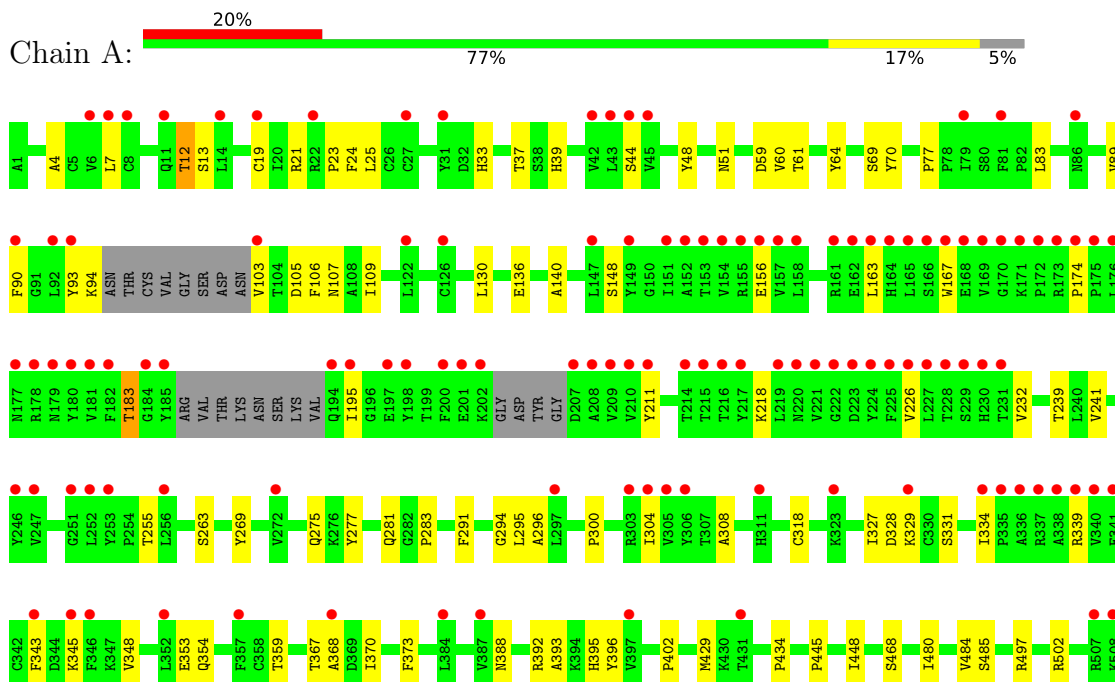
3 Residue-property plots [i](#)

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





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.18Å 70.31Å 85.68Å 103.01° 96.26° 112.07°	Depositor
Resolution (Å)	81.54 – 1.96 81.54 – 1.96	Depositor EDS
% Data completeness (in resolution range)	94.0 (81.54-1.96) 94.1 (81.54-1.96)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 1.97Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.246 , 0.286 0.263 , 0.301	Depositor DCC
R_{free} test set	4222 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtrriage
Anisotropy	0.219	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.3	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	0.93	EDS
Total number of atoms	9418	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% 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: ZN, VW1, PO4

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	0.72	0/4517	0.82	0/6156
1	B	0.69	0/4610	0.84	0/6283
All	All	0.71	0/9127	0.83	0/12439

There are no bond length outliers.

There are no bond angle outliers.

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	57	0
1	B	4508	0	4426	64	0
2	B	14	0	0	5	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
5	A	203	0	0	10	1
5	B	250	0	0	10	1
All	All	9418	0	8747	121	1

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 (121) 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:47:PRO:O	5:B:801:HOH:O	1.79	1.01
1:B:27:CYS:SG	5:B:956:HOH:O	1.99	0.95
1:A:60:VAL:HB	5:A:920:HOH:O	1.68	0.93
1:B:8:CYS:SG	1:B:99:GLY:N	2.43	0.91
1:B:2:VAL:N	5:B:803:HOH:O	2.03	0.90
1:B:392:ARG:CB	5:B:1040:HOH:O	2.35	0.74
1:A:368:ALA:O	1:A:393:ALA:HA	1.87	0.73
1:B:12:THR:HG21	1:B:26:CYS:HA	1.69	0.73
1:B:376:ILE:HG22	1:B:400:GLY:HA3	1.71	0.72
1:A:510:VAL:HG21	1:A:541:TYR:CD1	2.26	0.70
1:A:537:GLN:O	5:A:802:HOH:O	2.10	0.69
1:B:508:LYS:HG2	2:B:701:VW1:N1	2.10	0.67
1:B:12:THR:HG21	1:B:25:LEU:O	1.96	0.65
1:A:334:ILE:HD12	1:A:348:VAL:HG13	1.79	0.65
1:A:13:SER:OG	1:A:44:SER:HB2	1.97	0.65
1:B:12:THR:CG2	1:B:26:CYS:HA	2.27	0.65
1:A:468:SER:O	5:A:803:HOH:O	2.15	0.65
1:A:331:SER:HB2	1:A:353:GLU:HG3	1.79	0.65
1:B:115:THR:HA	1:B:411:LEU:O	1.99	0.63
1:B:510:VAL:HG21	1:B:541:TYR:CD1	2.36	0.61
1:B:48:TYR:OH	1:B:90:PHE:O	2.08	0.60
1:B:201:GLU:OE2	5:B:804:HOH:O	2.17	0.60
1:B:13:SER:O	1:B:44:SER:HA	2.02	0.59
1:A:163:LEU:HD23	1:A:211:TYR:CD2	2.38	0.59
1:A:497:ARG:HG2	5:A:883:HOH:O	2.05	0.57
1:B:7:LEU:HD12	1:B:103:VAL:HG22	1.87	0.57
1:A:367:THR:HA	1:A:392:ARG:O	2.05	0.56
1:B:44:SER:N	1:B:46:ASN:O	2.35	0.56
1:B:8:CYS:SG	1:B:99:GLY:O	2.64	0.55
1:A:480:ILE:HG12	1:A:550:THR:HG22	1.88	0.55
1:A:269:TYR:OH	1:A:294:GLY:HA3	2.07	0.54
1:B:7:LEU:CD1	1:B:103:VAL:HG22	2.38	0.54
1:B:477:LYS:NZ	1:B:551:GLU:OE2	2.30	0.54
1:A:7:LEU:HD13	1:A:103:VAL:HG22	1.89	0.54
1:A:519:ASN:HB3	1:A:530:THR:HG23	1.90	0.54
1:B:34:VAL:O	1:B:40:LYS:NZ	2.37	0.53
1:A:140:ALA:HA	1:A:232:VAL:HG21	1.90	0.53
1:A:269:TYR:CD1	1:A:295:LEU:HD13	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:LYS:HG2	2:B:701:VW1:C7	2.40	0.52
1:B:252:LEU:HB3	1:B:299:TYR:CD1	2.44	0.52
1:B:508:LYS:CG	2:B:701:VW1:N1	2.72	0.52
1:A:93:TYR:O	1:A:94:LYS:O	2.27	0.52
1:B:271:LYS:NZ	5:B:802:HOH:O	1.95	0.52
1:B:188:THR:HG1	1:B:191:SER:H	1.59	0.51
1:B:277:TYR:HA	1:B:396:TYR:O	2.11	0.50
1:A:4:ALA:O	1:A:24:PHE:HB2	2.12	0.50
1:B:103:VAL:CG1	1:B:103:VAL:O	2.59	0.50
1:B:323:LYS:O	1:B:323:LYS:HG2	2.11	0.50
1:B:554:HIS:ND1	5:B:811:HOH:O	2.35	0.50
1:A:130:LEU:HD12	5:A:874:HOH:O	2.11	0.50
1:B:177:ASN:HB3	1:B:516:ASN:ND2	2.26	0.50
1:B:184:GLY:C	1:B:195:ILE:HG22	2.31	0.50
1:A:277:TYR:HA	1:A:396:TYR:O	2.12	0.49
1:B:220:ASN:N	1:B:220:ASN:OD1	2.45	0.49
1:A:519:ASN:HB3	1:A:530:THR:CG2	2.42	0.49
1:A:296:ALA:O	1:A:300:PRO:HA	2.13	0.49
1:B:506:TRP:HA	2:B:701:VW1:N1	2.28	0.48
1:A:304:ILE:HG12	1:A:370:ILE:HB	1.95	0.48
1:B:279:THR:HB	1:B:429:MET:CE	2.45	0.47
1:B:368:ALA:O	1:B:393:ALA:HA	2.15	0.47
1:B:500:LEU:HB3	1:B:507:ARG:HD2	1.97	0.47
1:B:120:TYR:CE2	1:B:409:ARG:HG2	2.50	0.46
1:A:318:CYS:HB3	1:A:343:PHE:CD2	2.51	0.46
1:A:83:LEU:O	1:A:89:VAL:HA	2.16	0.46
1:A:329:LYS:HE2	1:A:354:GLN:OE1	2.16	0.46
1:B:44:SER:OG	1:B:45:VAL:N	2.46	0.45
1:B:551:GLU:HG3	5:B:938:HOH:O	2.15	0.45
1:A:241:VAL:HG12	5:A:999:HOH:O	2.16	0.45
1:B:7:LEU:HD21	1:B:106:PHE:HB2	1.99	0.45
1:B:7:LEU:CD2	1:B:130:LEU:HD21	2.47	0.45
1:B:8:CYS:SG	1:B:98:VAL:HB	2.57	0.45
1:B:506:TRP:HA	2:B:701:VW1:C7	2.47	0.45
1:A:591:GLU:O	1:A:592:ILE:HB	2.17	0.45
1:A:445:PRO:HD2	1:A:448:ILE:HD12	1.98	0.45
1:A:7:LEU:HD21	1:A:106:PHE:HB2	2.00	0.44
1:A:77:PRO:HB2	5:A:914:HOH:O	2.17	0.44
1:A:512:ILE:O	1:A:546:PHE:HA	2.17	0.44
1:A:183:THR:N	1:A:226:VAL:O	2.40	0.44
1:A:239:THR:O	1:A:388:ASN:ND2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:SER:OG	1:B:160:ASP:O	2.35	0.44
1:B:333:ILE:HB	1:B:358:CYS:SG	2.58	0.44
1:A:48:TYR:OH	1:A:90:PHE:O	2.23	0.44
1:A:339:ARG:NH2	5:A:828:HOH:O	2.50	0.43
1:A:105:ASP:O	1:A:109:ILE:HG13	2.17	0.43
1:A:59:ASP:OD1	1:A:61:THR:OG1	2.35	0.43
1:A:269:TYR:OH	1:A:294:GLY:CA	2.66	0.43
1:A:308:ALA:O	1:A:359:THR:HA	2.19	0.43
1:A:281:GLN:HG3	1:A:402:PRO:HD2	2.01	0.43
1:A:291:PHE:C	1:A:291:PHE:CD1	2.92	0.43
1:A:327:ILE:HD11	1:A:345:LYS:O	2.19	0.42
1:B:268:ASN:ND2	1:B:436:MET:HG2	2.34	0.42
1:A:12:THR:HG21	1:A:25:LEU:O	2.19	0.42
1:A:37:THR:OG1	1:A:39:HIS:HB2	2.18	0.42
1:A:328:ASP:HA	5:A:870:HOH:O	2.20	0.42
1:A:64:TYR:O	1:A:70:TYR:HA	2.19	0.42
1:A:544:VAL:O	1:A:572:ILE:HA	2.20	0.42
1:B:470:GLN:NE2	1:B:543:TYR:OH	2.53	0.42
1:B:7:LEU:HD21	1:B:130:LEU:HD21	2.02	0.41
1:B:95:ASN:OD1	1:B:95:ASN:N	2.48	0.41
1:B:516:ASN:ND2	5:B:833:HOH:O	2.53	0.41
1:A:21:ARG:NE	1:A:136:GLU:OE2	2.47	0.41
1:A:167:TRP:CZ3	1:A:174:PRO:HD2	2.55	0.41
1:B:149:TYR:HB3	1:B:174:PRO:HD3	2.02	0.41
1:B:542:ASP:OD1	1:B:569:LYS:HE3	2.20	0.41
1:A:19:CYS:HB2	1:A:23:PRO:HD2	2.01	0.41
1:A:269:TYR:OH	1:A:294:GLY:C	2.59	0.41
1:B:5:CYS:HB2	1:B:26:CYS:HB3	2.03	0.41
1:B:124:ASN:HD22	1:B:421:TYR:HA	1.85	0.41
1:B:373:PHE:CE1	1:B:387:VAL:HG21	2.56	0.41
1:B:55:CYS:SG	1:B:57:VAL:HG23	2.60	0.41
1:A:33:HIS:HA	1:A:107:ASN:OD1	2.21	0.41
1:B:179:ASN:HD22	1:B:179:ASN:HA	1.76	0.41
1:B:195:ILE:HG23	1:B:195:ILE:O	2.21	0.41
1:B:544:VAL:O	1:B:572:ILE:HA	2.21	0.41
1:B:48:TYR:CZ	1:B:90:PHE:O	2.74	0.41
1:B:8:CYS:SG	1:B:99:GLY:CA	3.08	0.40
1:A:429:MET:HG2	1:A:434:PRO:HB3	2.03	0.40
1:A:275:GLN:O	1:A:395:HIS:ND1	2.48	0.40
1:B:13:SER:O	1:B:13:SER:OG	2.38	0.40
1:A:263:SER:N	5:A:830:HOH:O	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:CYS:HB3	5:B:929:HOH:O	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1021:HOH:O	5:A:835:HOH:O[1_556]	2.09	0.11

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	564/601 (94%)	528 (94%)	32 (6%)	4 (1%)	22	11
1	B	580/601 (96%)	540 (93%)	37 (6%)	3 (0%)	29	17
All	All	1144/1202 (95%)	1068 (93%)	69 (6%)	7 (1%)	25	14

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	ILE
1	A	218	LYS
1	A	484	VAL
1	B	10	SER
1	B	48	TYR
1	A	283	PRO
1	B	195	ILE

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	485/523 (93%)	473 (98%)	12 (2%)	47	38
1	B	498/523 (95%)	483 (97%)	15 (3%)	41	30
All	All	983/1046 (94%)	956 (97%)	27 (3%)	44	34

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	26	CYS
1	B	69	SER
1	B	96	THR
1	B	103	VAL
1	B	155	ARG
1	B	188	THR
1	B	191	SER
1	B	192	LYS
1	B	215	THR
1	B	229	SER
1	B	231	THR
1	B	259	SER
1	B	373	PHE
1	B	507	ARG
1	B	508	LYS
1	A	12	THR
1	A	51	ASN
1	A	69	SER
1	A	148	SER
1	A	156	GLU
1	A	183	THR
1	A	255	THR
1	A	373	PHE
1	A	485	SER
1	A	502	ARG
1	A	517	SER
1	A	530	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	179	ASN
1	B	268	ASN
1	B	404	GLN
1	B	470	GLN
1	B	516	ASN
1	A	86	ASN
1	A	179	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 monosaccharides 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	$\# Z > 2$
4	PO4	A	705	-	4,4,4	1.09	0	6,6,6	0.59	0
4	PO4	A	704	-	4,4,4	0.64	0	6,6,6	0.66	0
4	PO4	B	705	-	4,4,4	1.33	1 (25%)	6,6,6	0.34	0
2	VW1	B	701	-	14,14,14	0.22	0	16,18,18	0.64	0
4	PO4	B	706	-	4,4,4	1.17	0	6,6,6	0.55	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	VW1	B	701	-	-	0/10/10/10	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	705	PO4	P-O1	2.00	1.55	1.50

There are no bond angle outliers.

There are no chirality outliers.

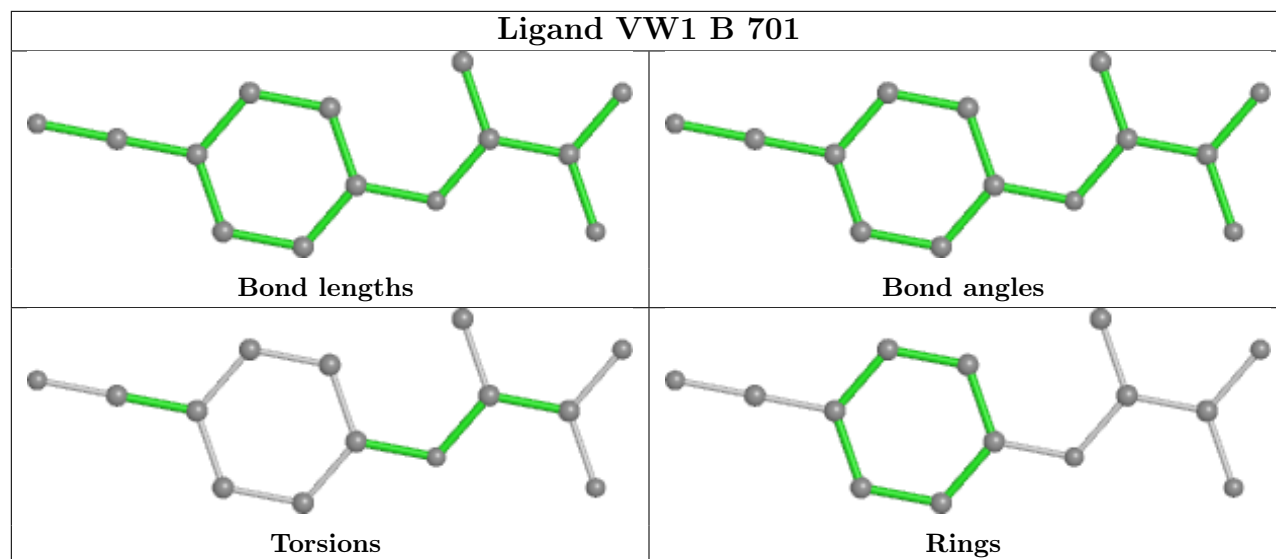
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	VW1	5	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 [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	572/601 (95%)	1.31	121 (21%) 0 1	28, 57, 136, 177	0
1	B	585/601 (97%)	0.62	46 (7%) 12 19	26, 43, 94, 128	0
All	All	1157/1202 (96%)	0.96	167 (14%) 2 4	26, 50, 120, 177	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	207	ASP	15.6
1	A	219	LEU	12.7
1	A	229	SER	11.2
1	A	225	PHE	10.2
1	B	214	THR	10.0
1	A	182	PHE	10.0
1	A	176	LEU	9.2
1	A	336	ALA	9.2
1	A	202	LYS	9.1
1	A	208	ALA	8.9
1	A	167	TRP	8.2
1	B	217	TYR	8.2
1	A	228	THR	8.1
1	A	154	VAL	8.0
1	A	200	PHE	7.7
1	B	45	VAL	7.5
1	A	149	TYR	7.5
1	A	221	VAL	7.2
1	B	193	VAL	7.2
1	A	152	ALA	7.2
1	A	178	ARG	7.1
1	A	215	THR	7.1
1	B	340	VAL	6.9
1	A	216	THR	6.9

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Mol	Chain	Res	Type	RSRZ
1	A	81	PHE	6.7
1	A	217	TYR	6.7
1	A	181	VAL	6.6
1	A	184	GLY	6.3
1	A	156	GLU	6.3
1	B	196	GLY	6.1
1	A	170	GLY	6.1
1	A	165	LEU	5.8
1	A	45	VAL	5.8
1	A	224	TYR	5.7
1	A	227	LEU	5.5
1	A	158	LEU	5.4
1	A	256	LEU	5.4
1	B	190	ASN	5.4
1	A	169	VAL	5.4
1	A	195	ILE	5.2
1	B	2	VAL	5.2
1	A	7	LEU	5.1
1	B	12	THR	5.1
1	A	334	ILE	5.0
1	A	230	HIS	4.9
1	A	222	GLY	4.8
1	A	247	VAL	4.8
1	A	387	VAL	4.7
1	A	177	ASN	4.7
1	A	166	SER	4.6
1	A	11	GLN	4.6
1	A	198	TYR	4.6
1	A	157	VAL	4.4
1	A	174	PRO	4.4
1	A	209	VAL	4.3
1	A	214	THR	4.3
1	A	253	TYR	4.2
1	A	304	ILE	4.2
1	A	153	THR	4.2
1	B	98	VAL	4.1
1	A	352	LEU	4.1
1	B	163	LEU	4.0
1	A	338	ALA	4.0
1	A	155	ARG	4.0
1	A	340	VAL	4.0
1	A	197	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	171	LYS	3.8
1	A	179	ASN	3.8
1	A	337	ARG	3.7
1	A	210	VAL	3.7
1	B	8	CYS	3.7
1	B	26	CYS	3.7
1	A	185	TYR	3.6
1	B	179	ASN	3.5
1	B	97	CYS	3.5
1	A	43	LEU	3.4
1	A	220	ASN	3.4
1	B	14	LEU	3.3
1	B	7	LEU	3.3
1	A	246	TYR	3.3
1	A	151	ILE	3.2
1	A	231	THR	3.2
1	A	357	PHE	3.2
1	B	414	LYS	3.2
1	B	195	ILE	3.1
1	B	79	ILE	3.1
1	B	81	PHE	3.1
1	A	164	HIS	3.1
1	A	173	ARG	3.0
1	A	90	PHE	3.0
1	A	305	VAL	3.0
1	A	147	LEU	3.0
1	A	297	LEU	3.0
1	B	334	ILE	3.0
1	A	341	GLU	2.9
1	A	346	PHE	2.9
1	A	201	GLU	2.9
1	A	27	CYS	2.9
1	A	323	LYS	2.9
1	B	210	VAL	2.9
1	B	57	VAL	2.8
1	B	194	GLN	2.8
1	A	303	ARG	2.8
1	A	175	PRO	2.8
1	A	335	PRO	2.8
1	B	55	CYS	2.8
1	B	147	LEU	2.8
1	A	592	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	172	PRO	2.7
1	A	103	VAL	2.7
1	A	86	ASN	2.7
1	A	339	ARG	2.7
1	A	343	PHE	2.7
1	A	180	TYR	2.7
1	A	79	ILE	2.6
1	B	181	VAL	2.6
1	B	230	HIS	2.6
1	A	14	LEU	2.6
1	A	161	ARG	2.6
1	B	6	VAL	2.6
1	A	31	TYR	2.5
1	B	229	SER	2.5
1	A	223	ASP	2.5
1	A	44	SER	2.5
1	A	8	CYS	2.5
1	A	92	LEU	2.5
1	A	507	ARG	2.5
1	B	68	MET	2.5
1	A	6	VAL	2.4
1	A	345	LYS	2.4
1	A	19	CYS	2.4
1	A	311	HIS	2.4
1	B	65	LEU	2.4
1	B	101	ASP	2.4
1	A	122	LEU	2.4
1	A	163	LEU	2.4
1	B	44	SER	2.3
1	A	272	VAL	2.3
1	B	25	LEU	2.3
1	B	256	LEU	2.3
1	A	508	LYS	2.3
1	A	22	ARG	2.3
1	A	431	THR	2.3
1	A	168	GLU	2.3
1	B	27	CYS	2.3
1	A	329	LYS	2.3
1	A	211	TYR	2.2
1	A	42	VAL	2.2
1	A	93	TYR	2.2
1	A	162	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	180	TYR	2.2
1	B	197	GLU	2.1
1	B	257	ASN	2.1
1	A	368	ALA	2.1
1	B	221	VAL	2.1
1	A	126	CYS	2.1
1	B	227	LEU	2.1
1	A	194	GLN	2.1
1	A	306	TYR	2.1
1	B	182	PHE	2.1
1	B	145	PHE	2.1
1	A	397	VAL	2.1
1	B	176	LEU	2.1
1	A	251	GLY	2.0
1	A	384	LEU	2.0
1	A	226	VAL	2.0
1	A	252	LEU	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 monosaccharides 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.

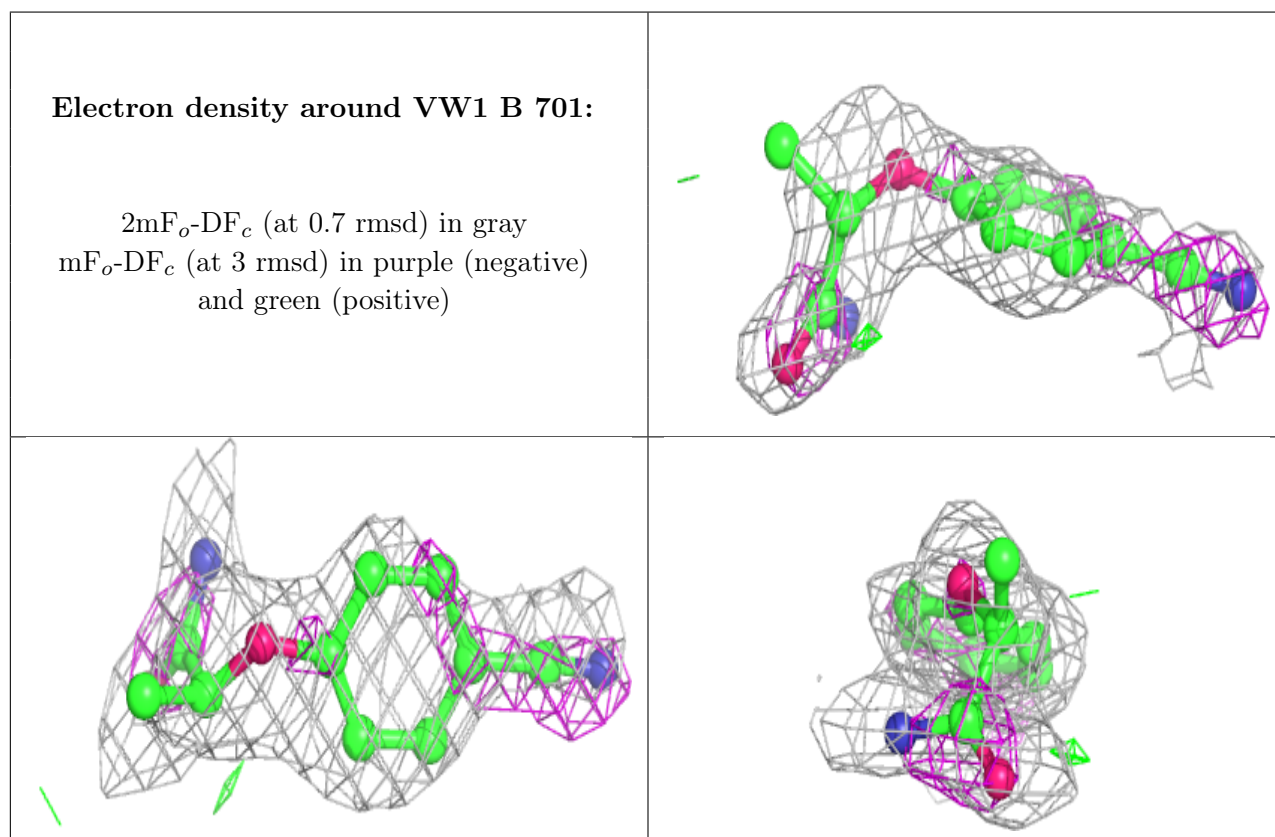
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	VW1	B	701	14/14	0.77	0.28	20,20,20,20	14
3	ZN	A	703	1/1	0.85	0.09	96,96,96,96	0
3	ZN	B	704	1/1	0.88	0.11	76,76,76,76	0
3	ZN	B	703	1/1	0.95	0.09	59,59,59,59	0
3	ZN	A	702	1/1	0.96	0.05	48,48,48,48	0
4	PO4	B	705	5/5	0.96	0.12	38,39,42,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PO4	B	706	5/5	0.96	0.13	39,40,45,51	0
4	PO4	A	705	5/5	0.96	0.11	34,39,48,49	0
4	PO4	A	704	5/5	0.97	0.10	36,40,42,47	0
3	ZN	B	702	1/1	0.97	0.10	42,42,42,42	0
3	ZN	A	701	1/1	0.98	0.08	53,53,53,53	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.