



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:52 AM UTC

PDB ID : 5RMK / pdb_00005rmk
Title : PanDDA analysis group deposition – Crystal Structure of SARS-CoV-2 heli-
case in complex with Z1273312153
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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 : 2.08 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)

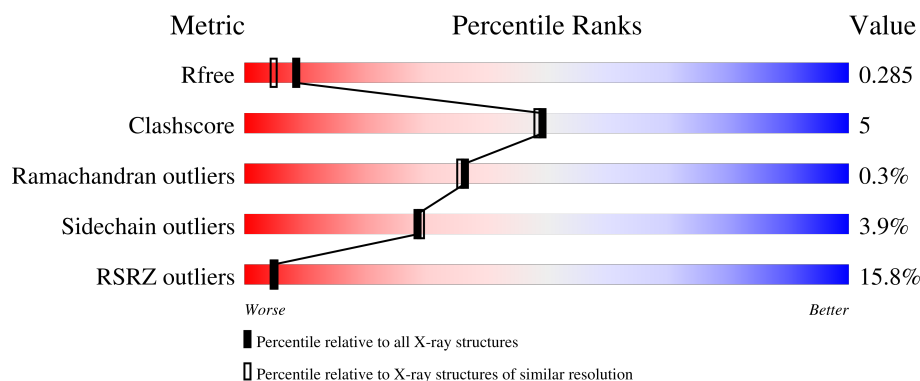
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

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	24% 80% 14% • 5%
1	B	601	7% 82% 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 9416 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).

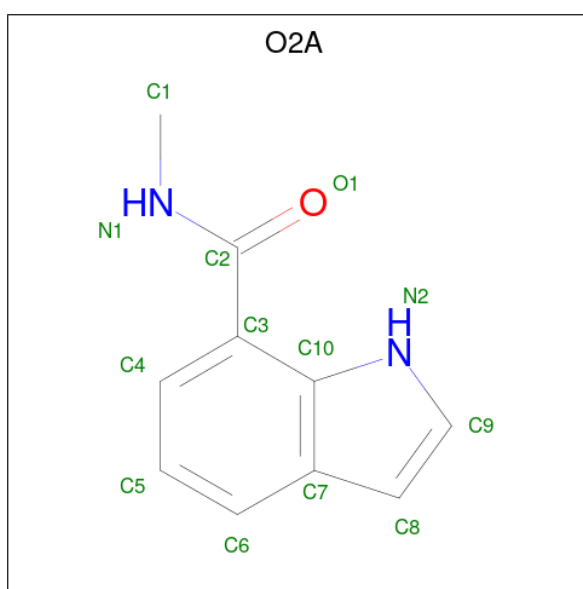
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	3	Total	Zn	0	0
			3	3		

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



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

- Molecule 4 is N-methyl-1H-indole-7-carboxamide (CCD ID: O2A) (formula: C₁₀H₁₀N₂O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			13	10	2	1		

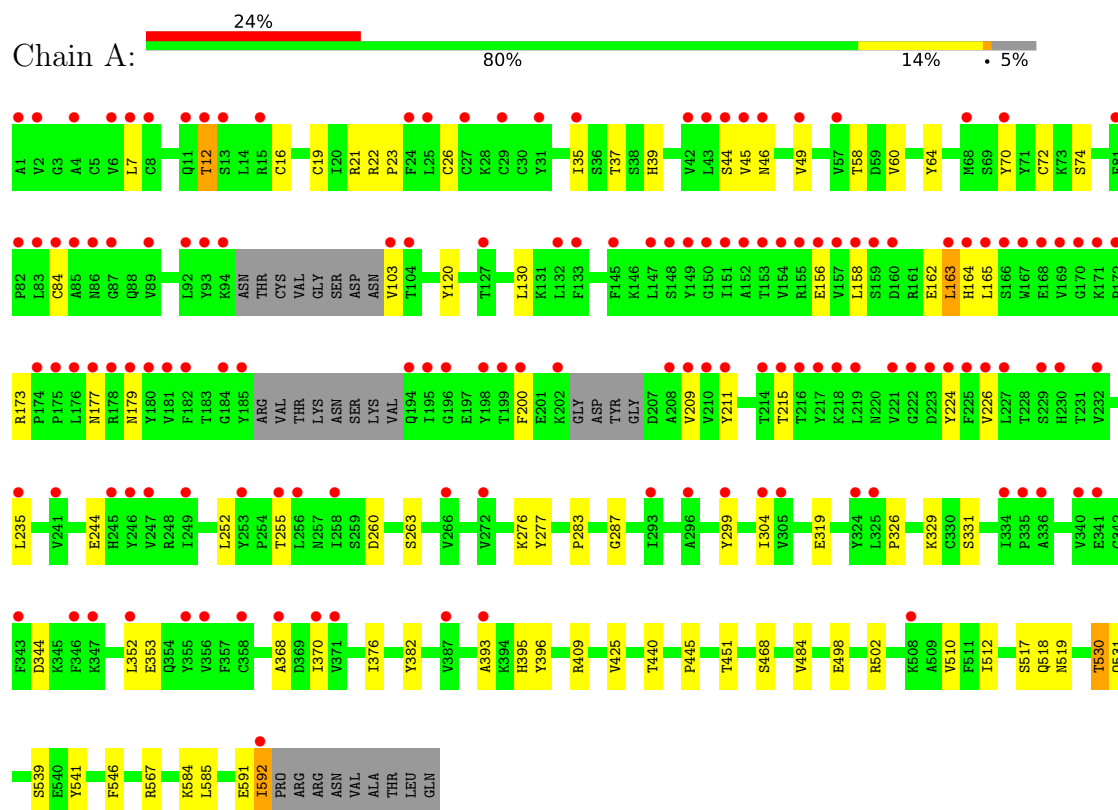
- Molecule 5 is water.

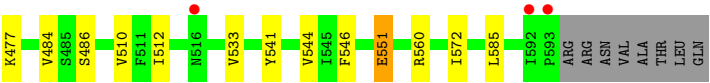
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	205	Total	O	0	0
			205	205		
5	B	247	Total	O	0	0
			247	247		

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





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.03Å 70.04Å 85.32Å 102.81° 96.07° 112.42°	Depositor
Resolution (Å)	81.32 – 2.08 81.32 – 2.08	Depositor EDS
% Data completeness (in resolution range)	96.8 (81.32-2.08) 96.9 (81.32-2.08)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.222 , 0.274 0.238 , 0.285	Depositor DCC
R_{free} test set	3730 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9416	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.43% 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, PO4, O2A

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	1.04	0/4517	1.39	0/6156
1	B	1.03	0/4610	1.36	3/6283 (0.0%)
All	All	1.03	0/9127	1.38	3/12439 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	253	TYR	CB-CA-C	5.38	117.34	110.34
1	B	415	GLY	CA-C-O	-5.32	117.98	122.29
1	B	270	GLN	N-CA-C	-5.01	105.73	111.14

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	51	0
1	B	4508	0	4424	46	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	13	0	0	0	0
5	A	205	0	0	6	1
5	B	247	0	0	4	1
All	All	9416	0	8745	95	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 5.

All (95) 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	1.80	0.82
1:B:279:THR:HB	1:B:429:MET:HE2	1.65	0.77
1:B:460:LYS:NZ	5:B:803:HOH:O	2.24	0.69
1:A:510:VAL:HG21	1:A:541:TYR:CD1	2.27	0.69
1:B:510:VAL:HG21	1:B:541:TYR:CD1	2.28	0.68
1:A:260:ASP:HA	1:A:263:SER:OG	1.96	0.66
1:A:326:PRO:HD2	1:A:329:LYS:HZ1	1.61	0.64
1:A:519:ASN:HB3	1:A:530:THR:HG23	1.80	0.64
1:B:12:THR:HG22	1:B:14:LEU:H	1.63	0.63
1:A:224:TYR:OH	5:A:801:HOH:O	2.11	0.63
1:B:8:CYS:SG	1:B:99:GLY:N	2.73	0.61
1:A:177:ASN:ND2	1:A:179:ASN:HD22	1.97	0.60
1:A:519:ASN:HB3	1:A:530:THR:CG2	2.31	0.60
1:A:584:LYS:NZ	5:A:807:HOH:O	2.33	0.60
1:A:512:ILE:O	1:A:546:PHE:HA	2.02	0.60
1:A:158:LEU:HD11	1:A:164:HIS:CE1	2.38	0.59
1:B:277:TYR:HA	1:B:396:TYR:O	2.03	0.59
1:A:591:GLU:O	1:A:592:ILE:HB	2.02	0.59
1:A:368:ALA:O	1:A:393:ALA:HA	2.03	0.58
1:A:498:GLU:HG3	1:A:502:ARG:NH2	2.19	0.57
1:B:278:SER:HB2	1:B:436:MET:HE2	1.85	0.57
1:B:195:ILE:HG23	1:B:195:ILE:O	2.03	0.56
1:B:12:THR:CG2	1:B:26:CYS:HA	2.36	0.55
1:B:252:LEU:HB3	1:B:299:TYR:CD1	2.42	0.55
1:A:352:LEU:HD11	1:B:234:PRO:HD3	1.90	0.54
1:A:445:PRO:HB3	1:A:468:SER:HB3	1.88	0.54
1:A:215:THR:HG22	1:B:193:VAL:HG21	1.92	0.52
1:B:13:SER:HB3	1:B:92:LEU:HB2	1.92	0.52
1:B:442:ARG:HH11	1:B:464:HIS:CE1	2.28	0.51
1:B:103:VAL:HG12	1:B:103:VAL:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:PRO:CD	1:A:329:LYS:HZ1	2.23	0.50
1:B:196:GLY:HA3	1:B:215:THR:HG21	1.93	0.50
1:A:277:TYR:HA	1:A:396:TYR:O	2.12	0.50
1:B:12:THR:HG23	1:B:26:CYS:HA	1.93	0.50
1:A:319:GLU:OE2	1:A:319:GLU:HA	2.12	0.49
1:A:19:CYS:HB2	1:A:23:PRO:HD2	1.95	0.49
1:A:304:ILE:HA	1:A:370:ILE:O	2.13	0.48
1:A:376:ILE:HG12	1:A:425:VAL:HG11	1.95	0.48
1:B:512:ILE:O	1:B:546:PHE:HA	2.14	0.47
1:B:460:LYS:CE	5:B:803:HOH:O	2.63	0.47
1:A:64:TYR:O	1:A:70:TYR:HA	2.14	0.47
1:B:12:THR:HG22	1:B:14:LEU:N	2.28	0.47
1:B:19:CYS:HB2	1:B:23:PRO:HD2	1.96	0.47
1:B:156:GLU:HB3	1:B:164:HIS:HB2	1.96	0.47
1:B:49:VAL:HG23	1:B:58:THR:HG22	1.96	0.46
1:A:130:LEU:HD12	5:A:910:HOH:O	2.15	0.46
1:B:533:VAL:HG11	1:B:560:ARG:O	2.15	0.46
1:A:16:CYS:O	1:A:22:ARG:HA	2.16	0.46
1:B:451:THR:HG21	1:B:585:LEU:HD23	1.98	0.45
1:A:60:VAL:HB	5:A:846:HOH:O	2.16	0.45
1:B:59:ASP:OD1	1:B:59:ASP:C	2.60	0.45
1:A:7:LEU:HD13	1:A:103:VAL:HG22	1.98	0.45
1:A:329:LYS:HB2	1:A:329:LYS:NZ	2.31	0.45
1:B:385:SER:OG	5:B:802:HOH:O	2.21	0.44
1:A:44:SER:OG	1:A:45:VAL:N	2.51	0.44
1:A:244:GLU:HB2	1:A:276:LYS:HB2	2.00	0.44
1:B:236:SER:OG	5:B:801:HOH:O	2.20	0.44
1:B:16:CYS:O	1:B:22:ARG:HA	2.17	0.44
1:B:442:ARG:NH1	1:B:464:HIS:CE1	2.86	0.44
1:A:49:VAL:HG23	1:A:58:THR:HG22	2.00	0.44
1:A:235:LEU:HD21	1:A:382:TYR:CE2	2.53	0.43
1:A:326:PRO:CG	1:A:329:LYS:HZ1	2.30	0.43
1:A:60:VAL:HG13	1:A:84:CYS:SG	2.57	0.43
1:A:331:SER:HB2	1:A:353:GLU:HG3	1.99	0.43
1:B:92:LEU:HB3	1:B:93:TYR:CD2	2.53	0.43
1:A:165:LEU:HD11	1:A:200:PHE:CZ	2.53	0.43
1:B:120:TYR:CE2	1:B:409:ARG:HG2	2.53	0.43
1:A:530:THR:CG2	5:A:919:HOH:O	2.66	0.43
1:A:163:LEU:HG	1:A:211:TYR:HB3	2.01	0.42
1:A:120:TYR:CE2	1:A:409:ARG:HG2	2.53	0.42
1:A:304:ILE:HG12	1:A:370:ILE:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:ILE:HA	1:B:370:ILE:O	2.19	0.42
1:A:287:GLY:HA2	5:A:914:HOH:O	2.17	0.42
1:B:307:THR:HA	1:B:358:CYS:O	2.19	0.42
1:B:188:THR:O	1:B:189:LYS:C	2.63	0.42
1:A:37:THR:C	1:A:39:HIS:H	2.28	0.42
1:A:276:LYS:O	1:A:395:HIS:HA	2.19	0.42
1:B:477:LYS:NZ	1:B:551:GLU:OE2	2.36	0.42
1:A:72:CYS:SG	1:A:74:SER:HB2	2.60	0.41
1:A:518:GLN:HA	1:A:518:GLN:OE1	2.20	0.41
1:B:544:VAL:O	1:B:572:ILE:HA	2.20	0.41
1:B:65:LEU:HD23	1:B:81:PHE:CZ	2.55	0.41
1:B:376:ILE:HG12	1:B:425:VAL:HG11	2.02	0.41
1:A:21:ARG:O	1:A:22:ARG:C	2.63	0.41
1:B:278:SER:HA	1:B:435:ASP:OD1	2.19	0.41
1:B:167:TRP:CZ3	1:B:174:PRO:HD2	2.56	0.41
1:B:13:SER:O	1:B:44:SER:HA	2.21	0.41
1:B:228:THR:HG22	1:B:230:HIS:NE2	2.35	0.41
1:A:376:ILE:HD12	1:A:376:ILE:HA	1.93	0.41
1:B:154:VAL:HG13	1:B:163:LEU:HD22	2.02	0.41
1:A:539:SER:O	1:A:567:ARG:HD3	2.21	0.41
1:A:252:LEU:HB3	1:A:299:TYR:CD2	2.56	0.40
1:A:12:THR:HG21	1:A:26:CYS:HA	2.02	0.40
1:A:451:THR:HG21	1:A:585:LEU:HD23	2.02	0.40
1:B:409:ARG:HD3	1:B:417:LEU:HD22	2.03	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:A:943:HOH:O	5:B:992:HOH:O[1_554]	2.08	0.12

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%)	541 (96%)	21 (4%)	2 (0%)	30	28
1	B	580/601 (96%)	544 (94%)	35 (6%)	1 (0%)	43	44
All	All	1144/1202 (95%)	1085 (95%)	56 (5%)	3 (0%)	36	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	484	VAL
1	B	215	THR
1	A	283	PRO

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%)	469 (97%)	16 (3%)	33	35
1	B	498/523 (95%)	476 (96%)	22 (4%)	25	25
All	All	983/1046 (94%)	945 (96%)	38 (4%)	28	29

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	35	ILE
1	A	46	ASN
1	A	156	GLU
1	A	162	GLU
1	A	163	LEU
1	A	173	ARG
1	A	209	VAL
1	A	226	VAL
1	A	255	THR
1	A	344	ASP

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Mol	Chain	Res	Type
1	A	440	THR
1	A	517	SER
1	A	530	THR
1	A	531	GLN
1	A	592	ILE
1	B	8	CYS
1	B	11	GLN
1	B	68	MET
1	B	69	SER
1	B	95	ASN
1	B	96	THR
1	B	124	ASN
1	B	144	THR
1	B	158	LEU
1	B	162	GLU
1	B	164	HIS
1	B	166	SER
1	B	191	SER
1	B	192	LYS
1	B	226	VAL
1	B	289	SER
1	B	328	ASP
1	B	353	GLU
1	B	458	ASP
1	B	484	VAL
1	B	486	SER
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	11	GLN
1	A	164	HIS
1	A	179	ASN
1	A	230	HIS
1	A	245	HIS
1	A	404	GLN
1	B	46	ASN
1	B	62	GLN
1	B	245	HIS
1	B	268	ASN
1	B	459	ASN

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Mol	Chain	Res	Type
1	B	464	HIS
1	B	470	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	705	-	4,4,4	0.60	0	6,6,6	0.55	0
3	PO4	A	704	-	4,4,4	0.75	0	6,6,6	0.39	0
3	PO4	B	706	-	4,4,4	1.19	0	6,6,6	0.41	0
4	O2A	B	701	-	14,14,14	0.51	0	18,19,19	1.11	1 (5%)
3	PO4	A	705	-	4,4,4	0.93	0	6,6,6	0.50	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	O2A	B	701	-	-	2/6/6/6	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	701	O2A	C10-C3-C2	3.56	124.45	120.85

There are no chirality outliers.

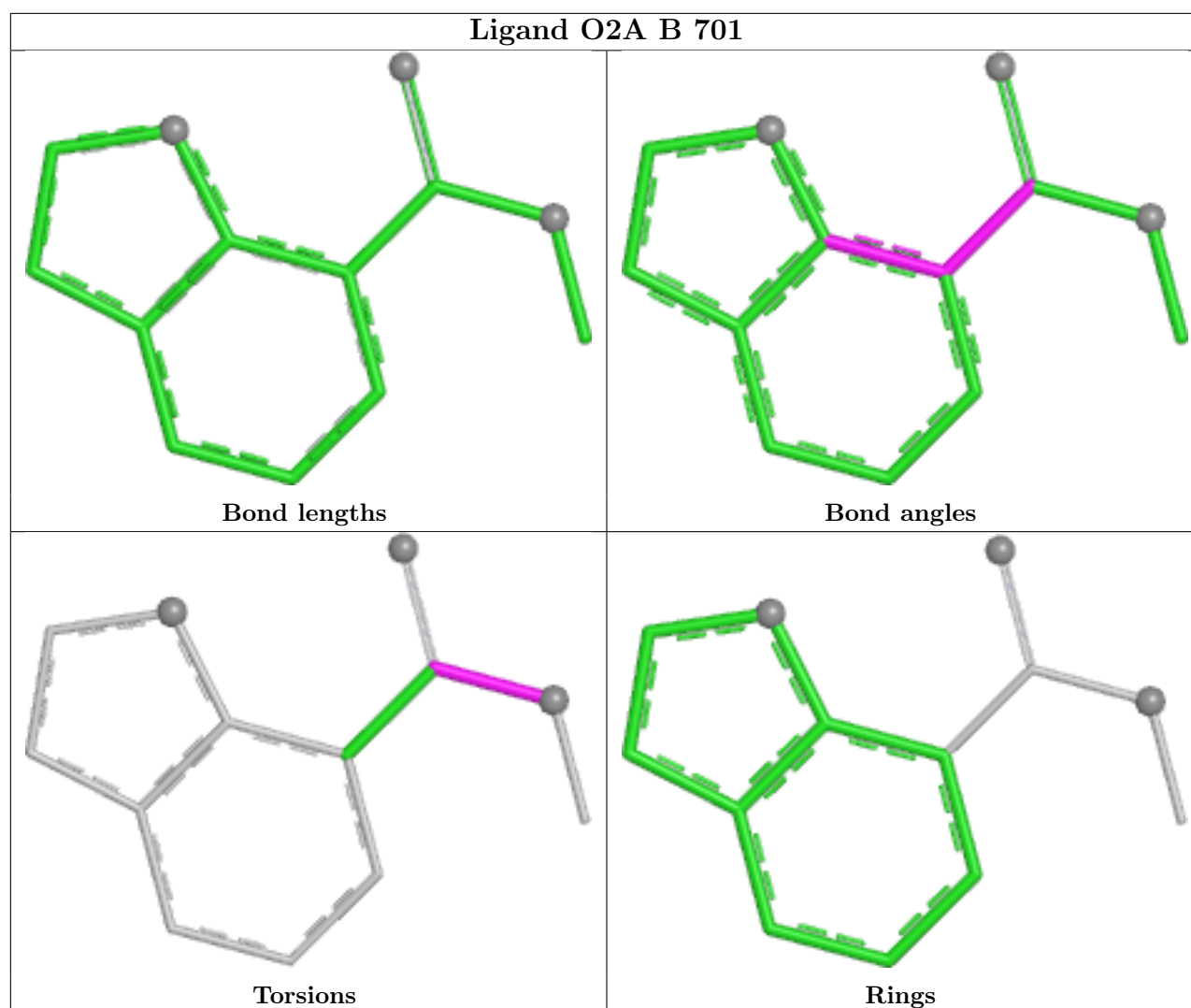
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	701	O2A	O1-C2-N1-C1
4	B	701	O2A	C3-C2-N1-C1

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	1.19	142 (24%) 2 2	25, 61, 155, 225	0
1	B	585/601 (97%)	0.45	41 (7%) 22 23	21, 43, 92, 129	1 (0%)
All	All	1157/1202 (96%)	0.82	183 (15%) 5 5	21, 51, 128, 225	1 (0%)

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	169	VAL	7.4
1	A	592	ILE	7.2
1	A	151	ILE	6.1
1	A	225	PHE	5.5
1	A	149	TYR	5.3
1	A	200	PHE	5.2
1	A	167	TRP	5.2
1	A	154	VAL	4.9
1	A	224	TYR	4.9
1	A	176	LEU	4.8
1	A	340	VAL	4.7
1	A	157	VAL	4.7
1	B	2	VAL	4.6
1	A	103	VAL	4.6
1	A	165	LEU	4.6
1	A	6	VAL	4.5
1	A	210	VAL	4.5
1	A	152	ALA	4.3
1	A	226	VAL	4.3
1	A	170	GLY	4.3
1	A	209	VAL	4.2
1	A	208	ALA	4.2
1	A	153	THR	4.1
1	A	45	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	217	TYR	4.0
1	A	7	LEU	4.0
1	A	195	ILE	3.8
1	A	84	CYS	3.8
1	B	208	ALA	3.8
1	A	2	VAL	3.8
1	A	181	VAL	3.8
1	B	340	VAL	3.8
1	A	1	ALA	3.8
1	A	148	SER	3.7
1	A	256	LEU	3.7
1	B	592	ILE	3.7
1	A	258	ILE	3.7
1	A	221	VAL	3.7
1	A	247	VAL	3.7
1	A	336	ALA	3.6
1	A	185	TYR	3.6
1	A	202	LYS	3.6
1	A	132	LEU	3.6
1	A	182	PHE	3.5
1	B	98	VAL	3.4
1	B	203	GLY	3.4
1	B	176	LEU	3.4
1	B	187	VAL	3.4
1	A	229	SER	3.4
1	A	219	LEU	3.4
1	A	272	VAL	3.3
1	A	43	LEU	3.3
1	A	249	ILE	3.3
1	A	168	GLU	3.2
1	A	92	LEU	3.2
1	B	227	LEU	3.2
1	B	336	ALA	3.2
1	A	222	GLY	3.2
1	B	193	VAL	3.2
1	A	352	LEU	3.2
1	A	49	VAL	3.1
1	A	147	LEU	3.1
1	A	241	VAL	3.1
1	A	158	LEU	3.1
1	A	508	LYS	3.1
1	A	180	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	194	GLN	3.1
1	B	214	THR	3.0
1	A	305	VAL	3.0
1	A	150	GLY	3.0
1	A	178	ARG	3.0
1	A	94	LYS	3.0
1	A	166	SER	3.0
1	A	217	TYR	3.0
1	A	235	LEU	3.0
1	A	184	GLY	3.0
1	B	195	ILE	2.9
1	A	31	TYR	2.9
1	A	81	PHE	2.9
1	A	163	LEU	2.8
1	A	24	PHE	2.8
1	A	179	ASN	2.8
1	A	198	TYR	2.8
1	A	12	THR	2.8
1	A	174	PRO	2.8
1	A	211	TYR	2.8
1	A	393	ALA	2.8
1	A	42	VAL	2.7
1	B	157	VAL	2.7
1	B	53	PRO	2.7
1	A	266	VAL	2.7
1	A	223	ASP	2.7
1	A	218	LYS	2.7
1	B	593	PRO	2.7
1	A	227	LEU	2.6
1	B	7	LEU	2.6
1	A	355	TYR	2.6
1	A	155	ARG	2.6
1	A	230	HIS	2.6
1	A	296	ALA	2.6
1	B	4	ALA	2.6
1	B	102	ASN	2.6
1	A	82	PRO	2.6
1	A	70	TYR	2.6
1	A	246	TYR	2.6
1	A	27	CYS	2.6
1	B	97	CYS	2.6
1	A	216	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	175	PRO	2.6
1	A	232	VAL	2.5
1	A	304	ILE	2.5
1	A	177	ASN	2.5
1	B	202	LYS	2.5
1	B	101	ASP	2.5
1	A	44	SER	2.5
1	B	256	LEU	2.5
1	A	334	ILE	2.5
1	A	8	CYS	2.5
1	B	81	PHE	2.5
1	A	253	TYR	2.4
1	A	199	THR	2.4
1	A	85	ALA	2.4
1	A	171	LYS	2.4
1	B	228	THR	2.4
1	A	133	PHE	2.4
1	A	346	PHE	2.4
1	A	214	THR	2.4
1	A	325	LEU	2.3
1	B	103	VAL	2.3
1	B	230	HIS	2.3
1	B	175	PRO	2.3
1	A	93	TYR	2.3
1	A	347	LYS	2.3
1	A	35	ILE	2.3
1	A	46	ASN	2.3
1	A	358	CYS	2.3
1	A	25	LEU	2.3
1	B	178	ARG	2.3
1	A	156	GLU	2.3
1	B	145	PHE	2.3
1	A	356	VAL	2.3
1	A	371	VAL	2.3
1	A	215	THR	2.3
1	B	163	LEU	2.3
1	A	245	HIS	2.2
1	A	15	ARG	2.2
1	A	160	ASP	2.2
1	A	341	GLU	2.2
1	B	189	LYS	2.2
1	B	516	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	57	VAL	2.2
1	A	29	CYS	2.2
1	B	165	LEU	2.2
1	A	13	SER	2.2
1	A	255	THR	2.2
1	A	11	GLN	2.1
1	A	87	GLY	2.1
1	A	4	ALA	2.1
1	A	324	TYR	2.1
1	A	104	THR	2.1
1	A	127	THR	2.1
1	A	335	PRO	2.1
1	A	145	PHE	2.1
1	A	293	ILE	2.1
1	A	343	PHE	2.1
1	A	196	GLY	2.1
1	B	210	VAL	2.1
1	A	86	ASN	2.1
1	A	172	PRO	2.1
1	A	370	ILE	2.1
1	A	89	VAL	2.1
1	A	387	VAL	2.1
1	A	368	ALA	2.1
1	A	159	SER	2.1
1	A	164	HIS	2.1
1	B	196	GLY	2.1
1	B	57	VAL	2.1
1	A	68	MET	2.0
1	A	83	LEU	2.0
1	A	299	TYR	2.0
1	B	218	LYS	2.0
1	B	323	LYS	2.0
1	B	209	VAL	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

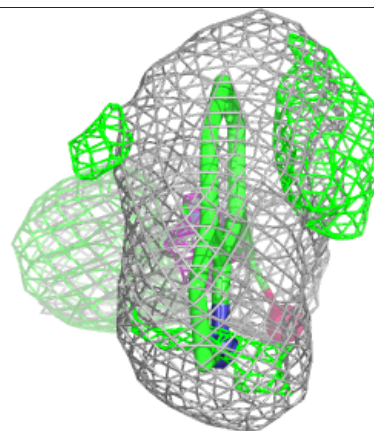
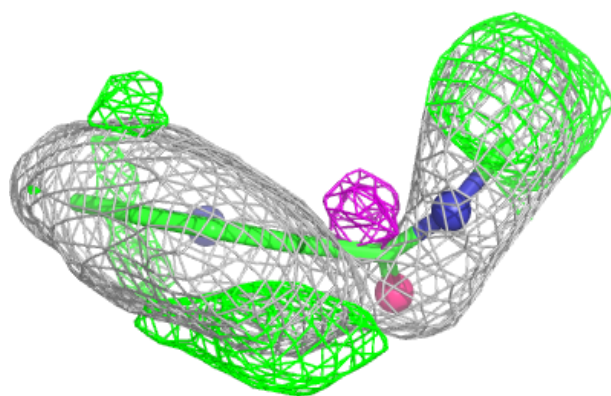
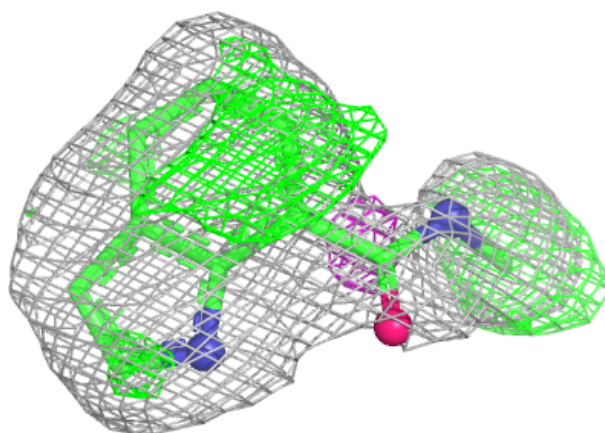
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	O2A	B	701	13/13	0.72	0.20	37,42,54,56	13
3	PO4	A	705	5/5	0.96	0.07	39,40,47,47	0
3	PO4	B	705	5/5	0.96	0.06	34,37,41,44	0
2	ZN	A	703	1/1	0.96	0.08	89,89,89,89	0
3	PO4	A	704	5/5	0.97	0.05	36,38,38,45	0
3	PO4	B	706	5/5	0.98	0.05	37,38,42,44	0
2	ZN	A	702	1/1	0.98	0.04	53,53,53,53	0
2	ZN	B	704	1/1	0.99	0.04	64,64,64,64	0
2	ZN	A	701	1/1	0.99	0.03	59,59,59,59	0
2	ZN	B	703	1/1	0.99	0.02	50,50,50,50	0
2	ZN	B	702	1/1	1.00	0.02	37,37,37,37	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around O2A B 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.