



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:44 AM EDT

PDB ID : 5RLK / pdb_00005rlk
Title : PanDDA analysis group deposition – Crystal Structure of SARS-CoV-2 heli-
case in complex with Z1509882419
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 ⓘ](#)) 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)

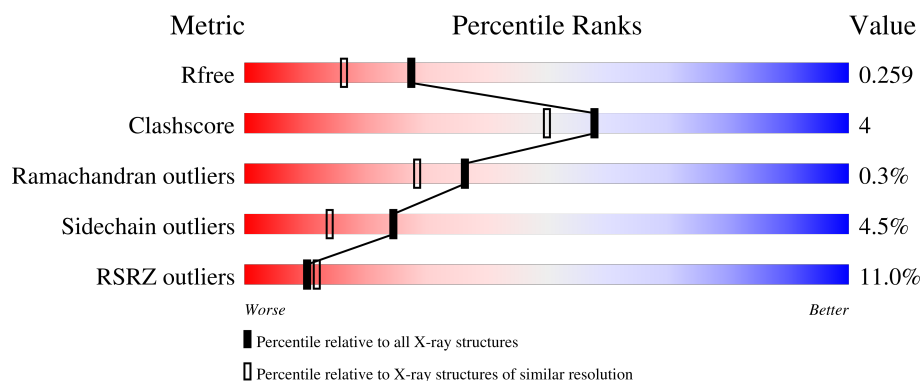
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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	16% 80% 14% • 5%
1	B	601	5% 83% 13% ••

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

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

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	B	706	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9446 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.

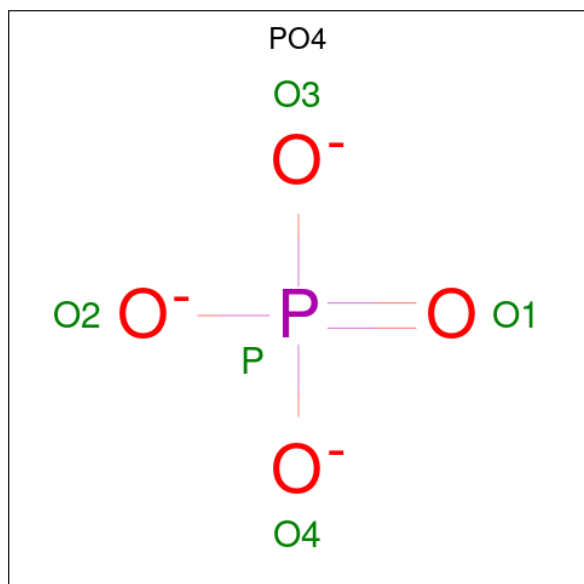
- Molecule 1 is a protein called Helicase.

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	588	Total	C	N	O	S	0	1	0
			4535	2890	759	851	35			

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

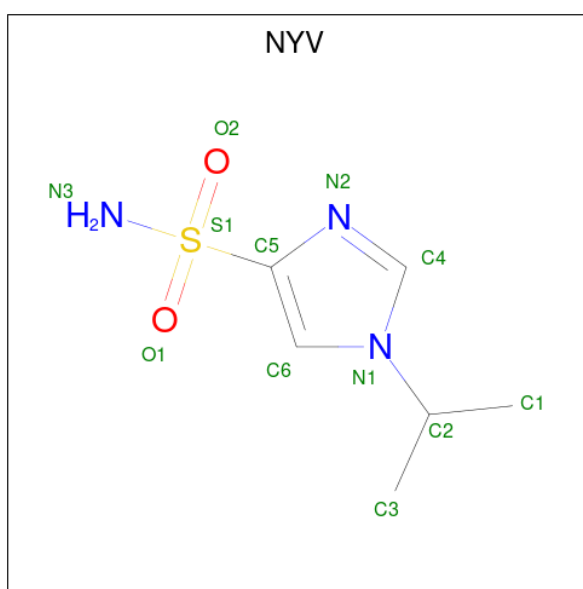
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	3	Total	Zn	0	0
			3	3		

- 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 1-(propan-2-yl)-1H-imidazole-4-sulfonamide (CCD ID: NYV) (formula: $C_6H_{11}N_3O_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O S 12 6 3 2 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	204	Total O 204 204	0	0
5	B	252	Total O 252 252	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.13Å 70.19Å 85.56Å 102.74° 96.23° 112.41°	Depositor
Resolution (Å)	81.53 – 1.96 81.53 – 1.96	Depositor EDS
% Data completeness (in resolution range)	95.3 (81.53-1.96) 95.3 (81.53-1.96)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 1.95Å)	Xtriage
Refinement program	BUSTER 2.10.3 (20-MAY-2020)	Depositor
R, R_{free}	0.172 , 0.240 0.196 , 0.259	Depositor DCC
R_{free} test set	4266 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.0	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	0.97	EDS
Total number of atoms	9446	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NYV, 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	0.88	0/4517	1.12	12/6156 (0.2%)
1	B	0.89	0/4638	1.13	9/6321 (0.1%)
All	All	0.89	0/9155	1.13	21/12477 (0.2%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	ASN	CA-CB-CG	7.06	119.66	112.60
1	B	103	VAL	CA-C-N	6.56	129.07	120.28
1	B	103	VAL	C-N-CA	6.56	129.07	120.28
1	B	344	ASP	CA-CB-CG	6.55	119.15	112.60
1	A	591	GLU	CA-C-N	6.53	133.46	121.70
1	A	591	GLU	C-N-CA	6.53	133.46	121.70
1	B	580	ASP	CA-CB-CG	6.52	119.12	112.60
1	B	561	PHE	CA-CB-CG	-6.34	107.46	113.80
1	A	561	PHE	CA-CB-CG	-6.29	107.51	113.80
1	B	374	ASP	CA-CB-CG	6.13	118.73	112.60
1	A	260	ASP	CA-C-N	6.10	128.74	120.38
1	A	260	ASP	C-N-CA	6.10	128.74	120.38
1	B	532	THR	N-CA-C	-6.07	102.70	110.53
1	A	466	ASP	CA-CB-CG	6.04	118.64	112.60
1	B	45	VAL	N-CA-C	-5.45	105.06	110.62
1	A	405	LEU	N-CA-C	5.36	116.64	109.83
1	A	374	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	516	ASN	CA-CB-CG	5.22	117.82	112.60
1	A	580	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	587	PHE	CA-CB-CG	5.09	118.89	113.80
1	B	95	ASN	CA-CB-CG	5.04	117.64	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	33	0
1	B	4535	0	4457	47	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	2	0
4	B	12	0	0	2	0
5	A	204	0	0	0	0
5	B	252	0	0	3	0
All	All	9446	0	8778	79	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 4.

All (79) 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:27:CYS:SG	5:B:894:HOH:O	2.12	1.05
1:A:158:LEU:HD21	1:A:164:HIS:ND1	1.95	0.81
1:B:442:ARG:HH11	1:B:464:HIS:CE1	2.02	0.77
1:A:331:SER:HB2	1:A:353:GLU:HG3	1.66	0.76
1:B:474[B]:MET:HG2	1:B:590:LEU:HB2	1.79	0.64
1:B:279:THR:HB	1:B:429:MET:HE3	1.82	0.61
1:A:215:THR:HG22	1:B:193:VAL:HG21	1.84	0.59
1:A:7:LEU:HD21	1:A:106:PHE:HB2	1.83	0.59
1:A:158:LEU:HD12	1:A:162:GLU:HB3	1.85	0.59
1:B:335:PRO:HG3	4:B:701:NYV:N3	2.19	0.58
1:B:7:LEU:HD21	1:B:106:PHE:HB2	1.86	0.57
1:B:271:LYS:NZ	5:B:802:HOH:O	2.33	0.56
1:A:326:PRO:HG2	1:A:329:LYS:HE2	1.88	0.56
1:A:445:PRO:HD2	1:A:448:ILE:HD12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:THR:HB	1:A:429:MET:HE3	1.88	0.55
3:B:705:PO4:O2	3:B:706:PO4:O3	2.25	0.54
1:B:335:PRO:CG	4:B:701:NYV:N3	2.71	0.53
1:A:157:VAL:HG23	1:A:221:VAL:HG22	1.91	0.53
1:B:510:VAL:HG21	1:B:541:TYR:CD1	2.44	0.53
1:B:445:PRO:HD2	1:B:448:ILE:HD12	1.89	0.53
1:B:158:LEU:HD11	1:B:164:HIS:ND1	2.25	0.52
1:B:183:THR:OG1	1:B:228:THR:OG1	2.27	0.52
1:B:252:LEU:HB3	1:B:299:TYR:CD1	2.45	0.52
1:A:140:ALA:O	1:A:144:THR:HG23	2.10	0.52
1:B:13:SER:O	1:B:44:SER:HA	2.10	0.52
1:B:230:HIS:CE1	1:B:339:ARG:HH22	2.27	0.51
1:B:504:PRO:HB3	1:B:507:ARG:NH2	2.25	0.51
1:B:371:VAL:HG23	1:B:393:ALA:HB2	1.93	0.51
1:A:12:THR:HG21	1:A:26:CYS:HA	1.91	0.51
1:B:504:PRO:HB3	1:B:507:ARG:HH21	1.76	0.50
1:B:12:THR:HG21	1:B:26:CYS:HA	1.92	0.50
1:A:510:VAL:HG21	1:A:541:TYR:CD1	2.46	0.49
1:B:249:ILE:HG23	1:B:273:GLY:HA3	1.95	0.49
1:A:19:CYS:HB2	1:A:23:PRO:HD2	1.95	0.48
1:A:442:ARG:HH11	1:A:464:HIS:CE1	2.31	0.48
1:B:228:THR:HG22	1:B:230:HIS:NE2	2.28	0.48
1:B:335:PRO:HB2	1:B:337:ARG:HG3	1.95	0.47
1:B:511:PHE:HB3	1:B:530:THR:HG22	1.97	0.47
1:A:13:SER:HB2	1:A:92:LEU:HD12	1.95	0.47
1:A:352:LEU:HD11	1:B:234:PRO:HD3	1.96	0.46
1:B:8:CYS:SG	1:B:99:GLY:N	2.89	0.46
1:B:158:LEU:CD1	1:B:164:HIS:ND1	2.79	0.46
1:A:519:ASN:HB3	1:A:530:THR:CG2	2.46	0.45
1:B:538:GLY:HA2	3:B:706:PO4:O1	2.16	0.45
1:B:460:LYS:NZ	5:B:813:HOH:O	2.49	0.45
1:A:139:LYS:O	1:A:143:GLU:HG2	2.17	0.45
1:A:280:LEU:HD11	1:A:438:LEU:HG	1.98	0.45
1:B:184:GLY:HA3	1:B:195:ILE:HG22	1.98	0.45
1:B:19:CYS:HB2	1:B:23:PRO:HD2	1.98	0.44
1:B:442:ARG:NH1	1:B:464:HIS:CE1	2.79	0.44
1:A:176:LEU:HD22	1:A:200:PHE:HB2	1.99	0.44
1:A:7:LEU:HD13	1:A:103:VAL:HG22	2.01	0.43
1:A:249:ILE:HG23	1:A:273:GLY:HA3	1.99	0.43
1:A:252:LEU:HB3	1:A:299:TYR:CD2	2.53	0.43
1:A:297:LEU:HD11	1:A:324:TYR:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:CYS:SG	1:B:99:GLY:O	2.77	0.43
1:B:143:GLU:HA	1:B:146:LYS:HE2	2.00	0.43
1:A:121:ILE:HG23	1:A:421:TYR:CE1	2.54	0.43
1:A:266:VAL:O	1:A:270:GLN:HG3	2.19	0.42
1:A:512:ILE:O	1:A:546:PHE:HA	2.19	0.42
1:B:266:VAL:O	1:B:270:GLN:HG3	2.18	0.42
1:A:278:SER:HB2	1:A:436:MET:HE2	2.01	0.42
1:A:7:LEU:HD12	1:A:29:CYS:HB3	2.01	0.42
1:B:230:HIS:HE1	1:B:339:ARG:HH22	1.67	0.42
1:A:442:ARG:NH1	1:A:464:HIS:CE1	2.88	0.42
1:B:453:SER:HA	1:B:457:TYR:HB2	2.01	0.42
1:A:462:LYS:HA	1:A:462:LYS:HD3	1.88	0.41
1:B:512:ILE:O	1:B:546:PHE:HA	2.20	0.41
1:A:146:LYS:HE2	1:A:227:LEU:HB3	2.01	0.41
1:B:278:SER:HB2	1:B:436:MET:HE2	2.01	0.41
1:B:49:VAL:HG23	1:B:58:THR:HG22	2.02	0.41
1:B:195:ILE:HG23	1:B:195:ILE:O	2.21	0.41
1:B:12:THR:CG2	1:B:26:CYS:HA	2.51	0.40
1:B:175:PRO:HD2	1:B:180:TYR:CE2	2.55	0.40
1:B:297:LEU:HD11	1:B:324:TYR:HB3	2.03	0.40
1:B:451:THR:HG21	1:B:585:LEU:HD23	2.03	0.40
1:B:460:LYS:HB2	1:B:460:LYS:HE3	1.91	0.40
1:A:371:VAL:HG23	1:A:393:ALA:HB2	2.03	0.40
1:B:102:ASN:C	1:B:104:THR:H	2.30	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	564/601 (94%)	547 (97%)	14 (2%)	3 (0%)	24 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	585/601 (97%)	560 (96%)	25 (4%)	0	100	100
All	All	1149/1202 (96%)	1107 (96%)	39 (3%)	3 (0%)	36	28

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	484	VAL
1	A	219	LEU
1	A	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%)	462 (95%)	23 (5%)	23	12
1	B	500/523 (96%)	479 (96%)	21 (4%)	26	16
All	All	985/1046 (94%)	941 (96%)	44 (4%)	24	14

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	20	ILE
1	A	35	ILE
1	A	69	SER
1	A	81	PHE
1	A	127	THR
1	A	148	SER
1	A	149	TYR
1	A	158	LEU
1	A	173	ARG
1	A	179	ASN
1	A	207	ASP
1	A	209	VAL

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Mol	Chain	Res	Type
1	A	217	TYR
1	A	226	VAL
1	A	230	HIS
1	A	255	THR
1	A	337	ARG
1	A	416	THR
1	A	502	ARG
1	A	516	ASN
1	A	530	THR
1	A	592	ILE
1	B	11	GLN
1	B	12	THR
1	B	68	MET
1	B	69	SER
1	B	92	LEU
1	B	96	THR
1	B	103	VAL
1	B	160	ASP
1	B	164	HIS
1	B	192	LYS
1	B	195	ILE
1	B	219	LEU
1	B	220	ASN
1	B	247	VAL
1	B	259	SER
1	B	337	ARG
1	B	339	ARG
1	B	344	ASP
1	B	347	LYS
1	B	353	GLU
1	B	516	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	62	GLN
1	A	116	ASN
1	A	220	ASN
1	A	245	HIS
1	A	275	GLN
1	A	459	ASN

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Mol	Chain	Res	Type
1	A	464	HIS
1	A	516	ASN
1	B	116	ASN
1	B	177	ASN
1	B	245	HIS
1	B	265	ASN
1	B	268	ASN
1	B	404	GLN
1	B	459	ASN
1	B	464	HIS
1	B	516	ASN

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	2.49	1 (25%)	6,6,6	0.38	0
4	NYV	B	701	-	11,12,12	0.64	0	13,18,18	1.19	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	A	705	-	4,4,4	2.52	2 (50%)	6,6,6	1.03	0
3	PO4	A	704	-	4,4,4	2.60	3 (75%)	6,6,6	0.89	0
3	PO4	B	706	-	4,4,4	2.52	1 (25%)	6,6,6	0.84	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	NYV	B	701	-	-	3/6/10/10	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	704	PO4	P-O1	4.31	1.60	1.50
3	B	706	PO4	P-O1	4.25	1.60	1.50
3	B	705	PO4	P-O1	4.19	1.60	1.50
3	A	705	PO4	P-O1	4.02	1.59	1.50
3	A	705	PO4	P-O3	2.27	1.61	1.54
3	A	704	PO4	P-O3	2.06	1.60	1.54
3	A	704	PO4	P-O4	2.04	1.60	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	701	NYV	C4-N2-C5	3.70	106.80	103.39

There are no chirality outliers.

All (3) torsion outliers are listed below:

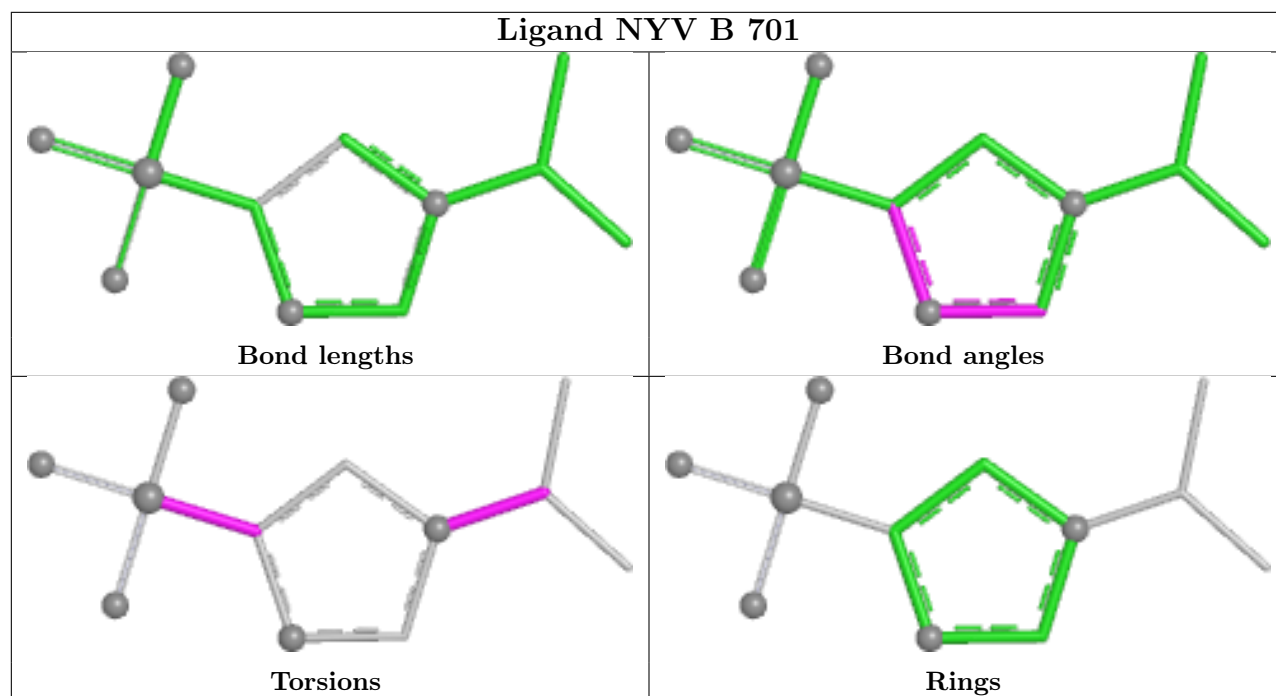
Mol	Chain	Res	Type	Atoms
4	B	701	NYV	C6-C5-S1-O2
4	B	701	NYV	C1-C2-N1-C6
4	B	701	NYV	C1-C2-N1-C4

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	705	PO4	1	0
4	B	701	NYV	2	0
3	B	706	PO4	2	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%)	0.84	95 (16%) 4 4	32, 65, 133, 166	0
1	B	588/601 (97%)	0.39	33 (5%) 30 35	24, 53, 105, 138	1 (0%)
All	All	1160/1202 (96%)	0.61	128 (11%) 10 12	24, 58, 123, 166	1 (0%)

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	219	LEU	5.8
1	A	225	PHE	5.5
1	A	592	ILE	5.2
1	A	195	ILE	4.8
1	B	2	VAL	4.5
1	A	167	TRP	4.4
1	A	1	ALA	4.3
1	A	210	VAL	4.2
1	A	209	VAL	4.1
1	A	152	ALA	4.1
1	A	200	PHE	3.9
1	A	340	VAL	3.9
1	B	214	THR	3.9
1	A	229	SER	3.8
1	A	258	ILE	3.8
1	A	182	PHE	3.8
1	A	352	LEU	3.7
1	A	151	ILE	3.6
1	A	226	VAL	3.5
1	A	157	VAL	3.5
1	A	149	TYR	3.5
1	A	202	LYS	3.5
1	A	6	VAL	3.4
1	A	221	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	169	VAL	3.4
1	A	227	LEU	3.3
1	B	217	TYR	3.3
1	A	208	ALA	3.2
1	A	371	VAL	3.2
1	A	7	LEU	3.2
1	A	224	TYR	3.2
1	A	181	VAL	3.2
1	A	247	VAL	3.2
1	B	215	THR	3.1
1	B	203	GLY	3.0
1	A	220	ASN	3.0
1	A	163	LEU	3.0
1	B	340	VAL	2.9
1	B	593	PRO	2.9
1	B	98	VAL	2.9
1	A	178	ARG	2.9
1	A	176	LEU	2.9
1	B	592	ILE	2.9
1	A	214	THR	2.8
1	A	305	VAL	2.8
1	A	249	ILE	2.8
1	A	145	PHE	2.8
1	A	158	LEU	2.8
1	B	7	LEU	2.8
1	A	217	TYR	2.8
1	A	256	LEU	2.8
1	B	208	ALA	2.7
1	B	97	CYS	2.7
1	A	230	HIS	2.7
1	A	81	PHE	2.7
1	A	215	THR	2.7
1	B	96	THR	2.7
1	A	266	VAL	2.7
1	A	27	CYS	2.7
1	A	336	ALA	2.6
1	A	185	TYR	2.6
1	A	179	ASN	2.6
1	A	20	ILE	2.6
1	B	24	PHE	2.6
1	B	12	THR	2.6
1	B	198	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	24	PHE	2.6
1	A	228	THR	2.6
1	A	165	LEU	2.5
1	A	45	VAL	2.5
1	A	150	GLY	2.5
1	A	154	VAL	2.5
1	A	508	LYS	2.5
1	A	252	LEU	2.5
1	A	184	GLY	2.4
1	A	12	THR	2.4
1	A	232	VAL	2.4
1	A	241	VAL	2.4
1	A	94	LYS	2.4
1	B	247	VAL	2.4
1	A	180	TYR	2.4
1	A	153	THR	2.4
1	B	35	ILE	2.4
1	A	103	VAL	2.4
1	A	222	GLY	2.4
1	B	45	VAL	2.3
1	B	92	LEU	2.3
1	A	223	ASP	2.3
1	A	2	VAL	2.3
1	B	102	ASN	2.3
1	A	92	LEU	2.3
1	A	253	TYR	2.2
1	A	393	ALA	2.2
1	A	524	LYS	2.2
1	B	8	CYS	2.2
1	A	231	THR	2.2
1	A	43	LEU	2.2
1	B	3	GLY	2.2
1	B	178	ARG	2.2
1	B	339	ARG	2.2
1	A	183	THR	2.2
1	A	396	TYR	2.2
1	B	90	PHE	2.2
1	B	211	TYR	2.2
1	A	245	HIS	2.2
1	A	89	VAL	2.2
1	B	187	VAL	2.2
1	A	255	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	146	LYS	2.2
1	A	339	ARG	2.2
1	A	304	ILE	2.1
1	B	193	VAL	2.1
1	A	147	LEU	2.1
1	A	218	LYS	2.1
1	A	296	ALA	2.1
1	A	216	THR	2.1
1	B	176	LEU	2.1
1	A	198	TYR	2.1
1	A	306	TYR	2.1
1	A	199	THR	2.1
1	B	53	PRO	2.1
1	A	170	GLY	2.0
1	A	174	PRO	2.0
1	B	78	PRO	2.0
1	B	79	ILE	2.0
1	A	194	GLN	2.0
1	A	351	THR	2.0
1	A	31	TYR	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.

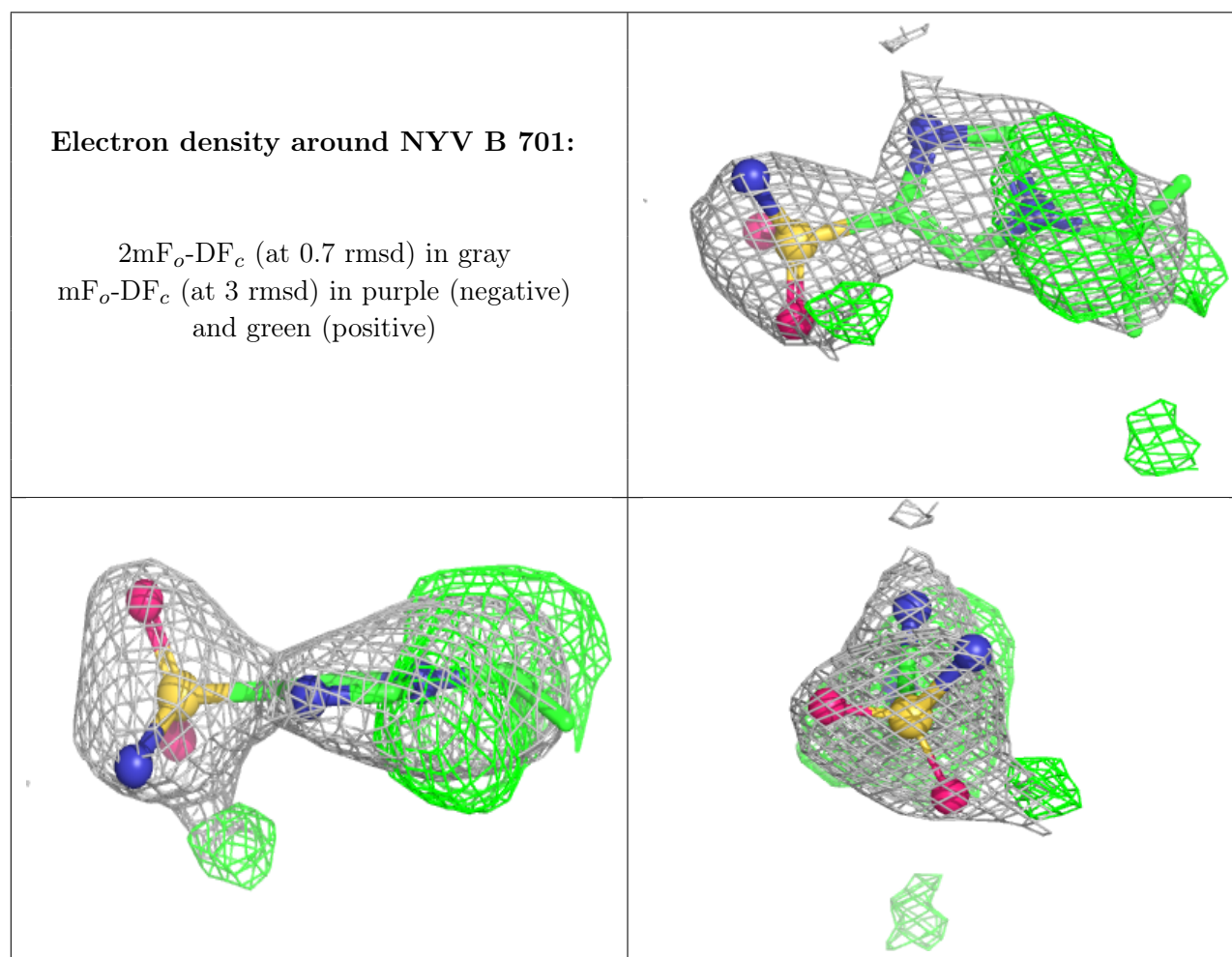
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NYV	B	701	12/12	0.90	0.19	36,38,39,40	12
3	PO4	B	705	5/5	0.97	0.06	52,52,55,55	0
3	PO4	B	706	5/5	0.97	0.06	49,50,53,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PO4	A	704	5/5	0.97	0.06	51,53,55,58	0
3	PO4	A	705	5/5	0.98	0.05	47,49,49,50	0
2	ZN	A	703	1/1	0.99	0.03	93,93,93,93	0
2	ZN	B	703	1/1	0.99	0.05	85,85,85,85	0
2	ZN	B	704	1/1	0.99	0.03	95,95,95,95	0
2	ZN	A	702	1/1	0.99	0.03	62,62,62,62	0
2	ZN	B	702	1/1	1.00	0.01	56,56,56,56	0
2	ZN	A	701	1/1	1.00	0.02	61,61,61,61	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.