



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:13 PM UTC

PDB ID : 5RM7 / pdb_00005rm7
Title : PanDDA analysis group deposition – Crystal Structure of SARS-CoV-2 heli-
case in complex with Z69118333
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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 : 1.84 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)

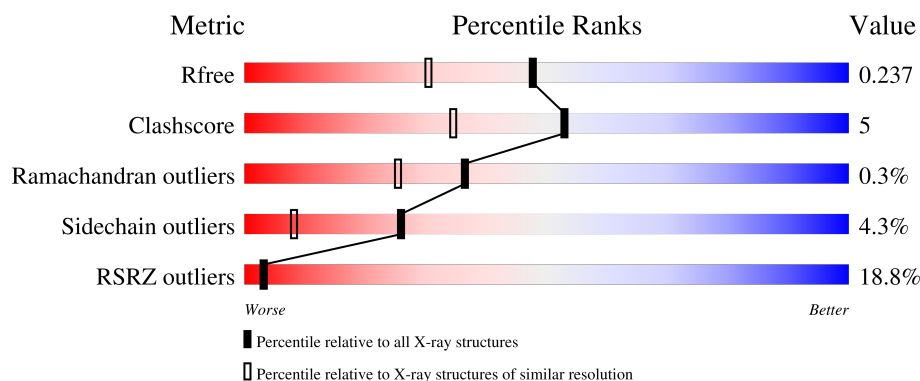
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	601	27% 81%14%5%
1	B	601	9% 82%14%..

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 9425 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).

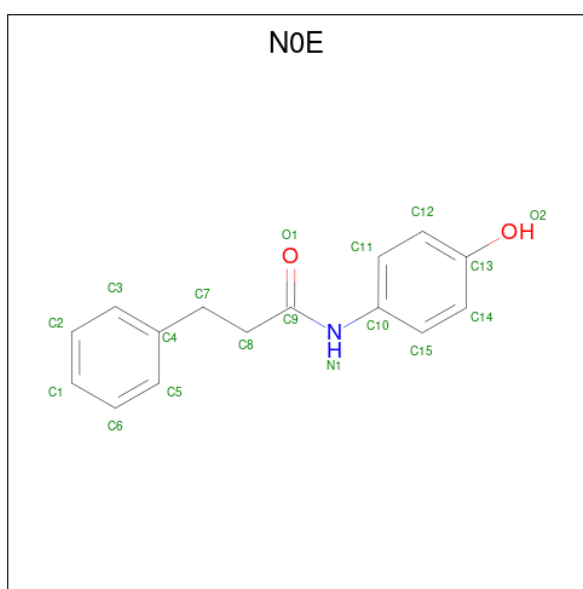
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	3	Total	Zn	0	0
			3	3		

- 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 {N}-(4-hydroxyphenyl)-3-phenyl-propanamide (CCD ID: N0E) (formula: C₁₅H₁₅NO₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 18 15 1 2	0	0

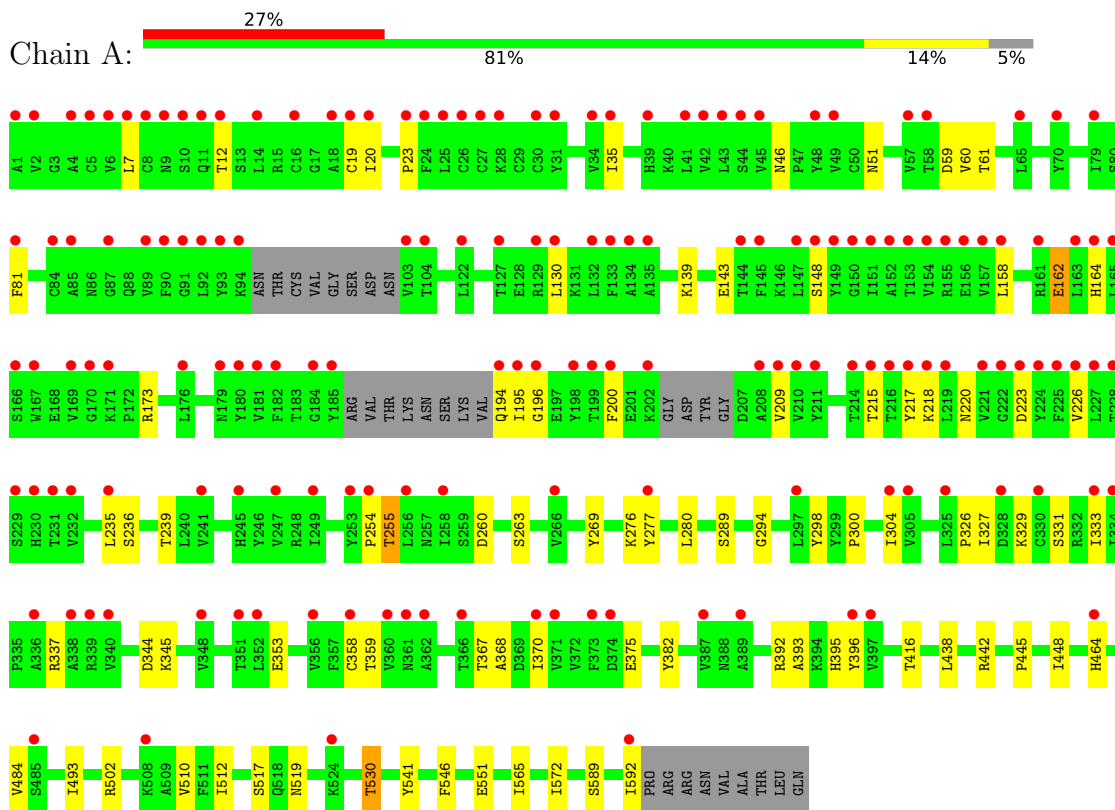
- Molecule 5 is water.

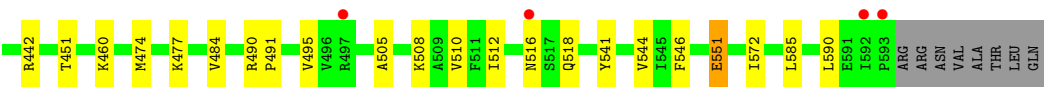
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	208	Total O 208 208	0	0
5	B	248	Total O 248 248	0	0

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





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.15Å 70.17Å 85.30Å 102.36° 96.32° 112.51°	Depositor
Resolution (Å)	81.42 – 1.84 81.42 – 1.84	Depositor EDS
% Data completeness (in resolution range)	94.1 (81.42-1.84) 92.2 (81.42-1.84)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.222 , 0.269 (Not available) , 0.237	Depositor DCC
R_{free} test set	5391 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.1	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	0.95	EDS
Total number of atoms	9425	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% 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: N0E, PO4, 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	1.08	0/4517	1.39	3/6156 (0.0%)
1	B	1.04	0/4610	1.35	10/6283 (0.2%)
All	All	1.06	0/9127	1.37	13/12439 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	THR	O-C-N	5.26	127.49	122.07
1	A	493	ILE	CA-C-N	5.24	125.76	119.94
1	A	493	ILE	C-N-CA	5.24	125.76	119.94
1	B	253	TYR	CB-CA-C	5.23	118.71	110.71
1	B	374	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	103	VAL	N-CA-C	-5.19	107.42	112.29
1	B	196	GLY	CA-C-O	-5.11	117.87	122.57
1	B	350	SER	CA-C-N	5.07	127.59	120.28
1	B	350	SER	C-N-CA	5.07	127.59	120.28
1	B	213	GLY	CA-C-N	5.01	127.00	120.28
1	B	213	GLY	C-N-CA	5.01	127.00	120.28
1	B	103	VAL	CA-C-N	5.01	126.99	120.28
1	B	103	VAL	C-N-CA	5.01	126.99	120.28

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	38	1
1	B	4508	0	4424	50	1
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
4	B	18	0	0	0	0
5	A	208	0	0	6	1
5	B	248	0	0	6	1
All	All	9425	0	8745	88	2

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 (88) 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	1.82	0.80
1:B:12:THR:HG22	1:B:14:LEU:H	1.55	0.72
1:A:60:VAL:HB	5:A:908:HOH:O	1.90	0.71
1:B:510:VAL:HG21	1:B:541:TYR:CD1	2.32	0.65
1:A:368:ALA:O	1:A:393:ALA:HA	1.99	0.61
1:A:519:ASN:HB3	1:A:530:THR:CG2	2.29	0.61
1:A:519:ASN:HB3	1:A:530:THR:HG23	1.82	0.59
1:B:12:THR:CG2	1:B:26:CYS:HA	2.33	0.59
1:A:375:GLU:OE2	5:A:801:HOH:O	2.17	0.58
1:A:255:THR:HG23	1:A:300:PRO:HG3	1.86	0.57
1:A:510:VAL:HG21	1:A:541:TYR:CD1	2.41	0.56
1:B:12:THR:HG22	1:B:14:LEU:N	2.20	0.56
1:A:200:PHE:N	5:A:810:HOH:O	2.38	0.56
1:A:277:TYR:HA	1:A:396:TYR:O	2.07	0.55
1:A:331:SER:HB2	1:A:353:GLU:HG3	1.89	0.54
1:B:92:LEU:HB3	1:B:93:TYR:CD2	2.43	0.53
1:B:195:ILE:HG23	1:B:195:ILE:O	2.10	0.52
1:A:158:LEU:HD12	1:A:162:GLU:HB3	1.92	0.52
1:B:8:CYS:SG	1:B:99:GLY:N	2.80	0.52
1:B:277:TYR:HA	1:B:396:TYR:O	2.11	0.51
1:A:236:SER:OG	5:A:802:HOH:O	2.19	0.51
1:A:235:LEU:HD21	1:A:382:TYR:CE2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474[B]:MET:HG2	1:B:590:LEU:HB2	1.94	0.50
1:A:359:THR:OG1	5:A:803:HOH:O	2.19	0.50
1:B:252:LEU:HB3	1:B:299:TYR:CD1	2.47	0.50
1:B:279:THR:HB	1:B:429:MET:CE	2.42	0.49
1:A:512:ILE:O	1:A:546:PHE:HA	2.13	0.49
1:B:371:VAL:HG23	1:B:393:ALA:HB2	1.95	0.49
1:B:460:LYS:NZ	5:B:808:HOH:O	2.42	0.48
1:A:326:PRO:HB2	1:A:329:LYS:HZ3	1.79	0.48
1:B:143:GLU:HA	1:B:146:LYS:HE2	1.96	0.48
1:B:69:SER:HB2	1:B:71:TYR:CE2	2.49	0.48
1:B:477:LYS:NZ	1:B:551:GLU:OE2	2.39	0.48
1:A:260:ASP:HA	1:A:263:SER:OG	2.14	0.48
1:A:158:LEU:HD21	1:A:164:HIS:ND1	2.30	0.47
1:B:347:LYS:HD2	1:B:353:GLU:OE2	2.15	0.46
1:B:460:LYS:CE	5:B:808:HOH:O	2.63	0.46
1:A:442:ARG:HA	1:A:464:HIS:HB3	1.98	0.46
1:B:505:ALA:O	1:B:508:LYS:HG2	2.16	0.46
1:B:16:CYS:O	1:B:22:ARG:HA	2.16	0.45
1:A:333:ILE:HB	1:A:358:CYS:SG	2.57	0.45
1:B:376:ILE:HD12	1:B:376:ILE:HA	1.89	0.45
1:A:519:ASN:HB3	1:A:530:THR:HG21	1.98	0.45
1:B:167:TRP:CZ3	1:B:174:PRO:HD2	2.51	0.45
1:A:254:PRO:HA	1:A:298:TYR:O	2.17	0.44
1:A:304:ILE:HA	1:A:370:ILE:O	2.16	0.44
1:B:184:GLY:HA3	1:B:195:ILE:HG22	2.00	0.44
1:B:253:TYR:O	5:B:801:HOH:O	2.20	0.44
1:B:368:ALA:O	1:B:393:ALA:HA	2.17	0.44
1:B:162:GLU:HG2	1:B:210:VAL:HG22	1.99	0.44
1:B:187:VAL:HG23	5:B:872:HOH:O	2.17	0.44
1:A:20:ILE:HG22	5:A:873:HOH:O	2.17	0.43
1:B:12:THR:HG23	1:B:26:CYS:HA	2.00	0.43
1:A:276:LYS:O	1:A:395:HIS:HA	2.18	0.43
1:A:280:LEU:HD11	1:A:438:LEU:HG	1.99	0.43
1:A:19:CYS:HB2	1:A:23:PRO:HD2	1.99	0.43
1:A:367:THR:HA	1:A:392:ARG:O	2.17	0.43
1:B:516:ASN:ND2	5:B:814:HOH:O	2.50	0.43
1:B:279:THR:HB	1:B:429:MET:HE3	2.01	0.43
1:B:474[A]:MET:SD	1:B:495:VAL:HG11	2.58	0.43
1:A:130:LEU:HD23	1:A:130:LEU:HA	1.94	0.43
1:A:327:ILE:HD11	1:A:345:LYS:O	2.18	0.43
1:B:311:HIS:CD2	1:B:340:VAL:HG11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:ILE:HG23	1:B:273:GLY:HA3	2.01	0.42
1:B:63:LEU:C	1:B:64:TYR:CD1	2.98	0.42
1:A:565:ILE:HA	1:A:572:ILE:CD1	2.50	0.42
1:B:19:CYS:HB2	1:B:23:PRO:HD2	2.01	0.42
1:A:59:ASP:CG	1:A:61:THR:HG1	2.21	0.42
1:A:139:LYS:O	1:A:143:GLU:HG2	2.20	0.42
1:A:194:GLN:C	1:A:196:GLY:H	2.28	0.42
1:B:268:ASN:HD22	1:B:268:ASN:HA	1.53	0.42
1:B:278:SER:HA	1:B:435:ASP:OD1	2.20	0.42
1:B:64:TYR:CD1	1:B:64:TYR:N	2.88	0.41
1:B:512:ILE:O	1:B:546:PHE:HA	2.20	0.41
1:B:544:VAL:O	1:B:572:ILE:HA	2.20	0.41
1:A:220:ASN:HB2	1:A:223:ASP:CG	2.45	0.41
1:B:490:ARG:N	1:B:491:PRO:CD	2.84	0.41
1:A:269:TYR:OH	1:A:294:GLY:HA3	2.20	0.41
1:B:451:THR:HG21	1:B:585:LEU:HD23	2.03	0.41
1:B:129:ARG:HD2	1:B:129:ARG:HA	1.81	0.41
1:B:14:LEU:HB2	1:B:25:LEU:O	2.20	0.40
1:B:94:LYS:CB	5:B:861:HOH:O	2.70	0.40
1:B:115:THR:HA	1:B:411:LEU:O	2.21	0.40
1:B:518:GLN:HA	1:B:518:GLN:OE1	2.21	0.40
1:A:158:LEU:HD21	1:A:164:HIS:CE1	2.56	0.40
1:A:445:PRO:HD2	1:A:448:ILE:HD12	2.02	0.40
1:B:27:CYS:HB2	1:B:97:CYS:SG	2.62	0.40
1:B:376:ILE:HG22	1:B:400:GLY:HA3	2.04	0.40

All (2) 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)
1:A:589:SER:OG	1:B:257:ASN:OD1[1_444]	2.15	0.05
5:A:928:HOH:O	5:B:1030:HOH:O[1_554]	2.16	0.04

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%)	535 (95%)	26 (5%)	3 (0%)	24	12
1	B	538/601 (90%)	516 (96%)	22 (4%)	0	100	100
All	All	1102/1202 (92%)	1051 (95%)	48 (4%)	3 (0%)	36	25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	ILE
1	A	484	VAL
1	A	218	LYS

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%)	462 (95%)	23 (5%)	23	7
1	B	442/523 (84%)	425 (96%)	17 (4%)	29	12
All	All	927/1046 (89%)	887 (96%)	40 (4%)	26	8

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	12	THR
1	A	35	ILE
1	A	46	ASN
1	A	51	ASN
1	A	81	PHE
1	A	148	SER
1	A	162	GLU
1	A	173	ARG
1	A	209	VAL

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Mol	Chain	Res	Type
1	A	215	THR
1	A	217	TYR
1	A	226	VAL
1	A	255	THR
1	A	289	SER
1	A	337	ARG
1	A	344	ASP
1	A	416	THR
1	A	502	ARG
1	A	517	SER
1	A	530	THR
1	A	551	GLU
1	A	592	ILE
1	B	8	CYS
1	B	20	ILE
1	B	68	MET
1	B	69	SER
1	B	79	ILE
1	B	95	ASN
1	B	96	THR
1	B	103	VAL
1	B	124	ASN
1	B	164	HIS
1	B	215	THR
1	B	219	LEU
1	B	289	SER
1	B	353	GLU
1	B	442	ARG
1	B	484	VAL
1	B	551	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	ASN
1	A	230	HIS
1	A	245	HIS
1	A	404	GLN
1	A	586	GLN
1	B	179	ASN
1	B	459	ASN
1	B	482	HIS

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Mol	Chain	Res	Type
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	1.65	2 (50%)	6,6,6	0.64	0
3	PO4	B	705	-	4,4,4	0.76	0	6,6,6	0.56	0
4	N0E	B	701	-	19,19,19	0.22	0	24,24,24	0.54	0
3	PO4	A	705	-	4,4,4	1.37	0	6,6,6	0.66	0
3	PO4	A	704	-	4,4,4	1.00	0	6,6,6	0.83	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	N0E	B	701	-	-	4/9/9/9	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	-2.20	1.48	1.54
3	B	706	PO4	P-O4	-2.03	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

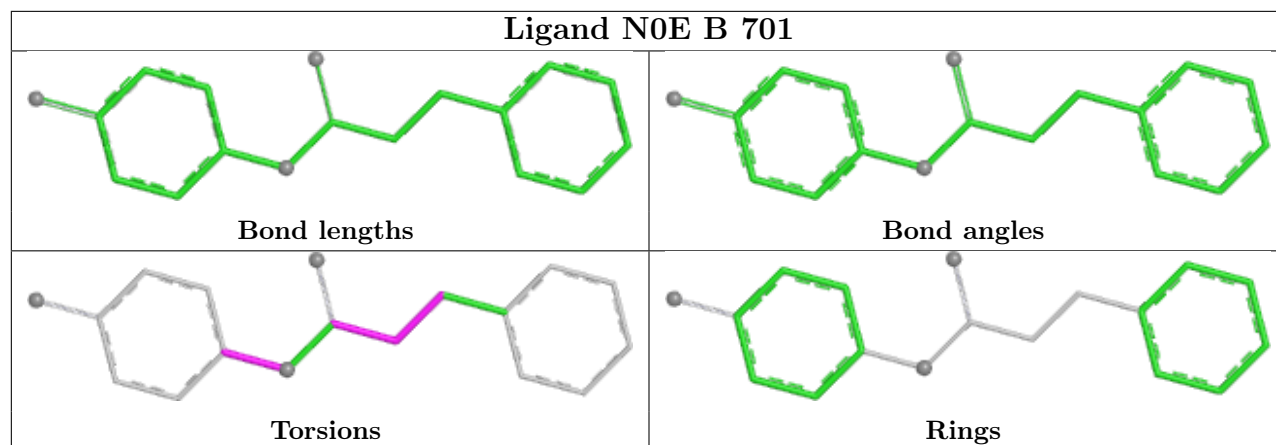
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	701	N0E	C4-C7-C8-C9
4	B	701	N0E	C7-C8-C9-O1
4	B	701	N0E	C7-C8-C9-N1
4	B	701	N0E	C15-C10-N1-C9

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%)	1.42	163 (28%) 1 1	23, 54, 125, 156	0
1	B	585/601 (97%)	0.54	54 (9%) 14 15	17, 38, 85, 132	1 (0%)
All	All	1157/1202 (96%)	0.97	217 (18%) 3 3	17, 45, 110, 156	1 (0%)

All (217) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	592	ILE	7.0
1	A	6	VAL	6.8
1	A	225	PHE	6.2
1	A	154	VAL	5.7
1	A	219	LEU	5.4
1	A	7	LEU	5.1
1	A	352	LEU	5.1
1	A	149	TYR	5.1
1	A	81	PHE	5.0
1	A	25	LEU	4.9
1	A	152	ALA	4.9
1	A	258	ILE	4.8
1	A	176	LEU	4.8
1	A	221	VAL	4.8
1	A	195	ILE	4.7
1	A	92	LEU	4.7
1	A	182	PHE	4.6
1	A	210	VAL	4.6
1	A	181	VAL	4.6
1	A	200	PHE	4.5
1	A	226	VAL	4.4
1	A	132	LEU	4.4
1	A	208	ALA	4.3
1	B	208	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	103	VAL	4.3
1	A	167	TRP	4.3
1	A	133	PHE	4.2
1	A	157	VAL	4.2
1	A	224	TYR	4.1
1	A	185	TYR	4.1
1	A	43	LEU	4.1
1	A	16	CYS	4.1
1	B	217	TYR	4.0
1	B	340	VAL	4.0
1	A	94	LYS	4.0
1	B	336	ALA	4.0
1	A	145	PHE	4.0
1	A	247	VAL	4.0
1	B	102	ASN	3.9
1	A	169	VAL	3.8
1	B	187	VAL	3.8
1	B	193	VAL	3.8
1	A	19	CYS	3.8
1	A	340	VAL	3.8
1	A	256	LEU	3.8
1	B	214	THR	3.7
1	A	151	ILE	3.7
1	A	155	ARG	3.7
1	B	45	VAL	3.7
1	A	253	TYR	3.7
1	A	232	VAL	3.7
1	A	12	THR	3.7
1	A	150	GLY	3.6
1	A	153	THR	3.6
1	B	230	HIS	3.6
1	A	222	GLY	3.6
1	A	209	VAL	3.6
1	A	23	PRO	3.6
1	A	90	PHE	3.6
1	A	228	THR	3.5
1	B	592	ILE	3.5
1	B	229	SER	3.5
1	A	254	PRO	3.5
1	B	195	ILE	3.5
1	A	27	CYS	3.4
1	B	198	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	199	THR	3.4
1	A	10	SER	3.4
1	A	215	THR	3.4
1	A	198	TYR	3.4
1	A	156	GLU	3.3
1	A	229	SER	3.3
1	A	241	VAL	3.3
1	A	266	VAL	3.3
1	B	98	VAL	3.3
1	A	8	CYS	3.3
1	A	91	GLY	3.3
1	B	196	GLY	3.3
1	A	163	LEU	3.3
1	A	202	LYS	3.2
1	A	4	ALA	3.2
1	A	147	LEU	3.2
1	A	230	HIS	3.2
1	B	221	VAL	3.2
1	A	165	LEU	3.2
1	B	176	LEU	3.2
1	A	214	THR	3.2
1	A	217	TYR	3.2
1	B	97	CYS	3.2
1	A	370	ILE	3.1
1	A	42	VAL	3.1
1	A	20	ILE	3.1
1	B	2	VAL	3.1
1	A	24	PHE	3.1
1	A	44	SER	3.1
1	B	227	LEU	3.0
1	A	48	TYR	3.0
1	A	49	VAL	3.0
1	A	164	HIS	3.0
1	A	336	ALA	3.0
1	B	181	VAL	3.0
1	B	211	TYR	3.0
1	A	144	THR	3.0
1	B	593	PRO	3.0
1	A	371	VAL	2.9
1	A	127	THR	2.9
1	A	18	ALA	2.9
1	A	180	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	396	TYR	2.9
1	A	1	ALA	2.9
1	A	334	ILE	2.9
1	B	158	LEU	2.9
1	A	227	LEU	2.8
1	A	28	LYS	2.8
1	A	211	TYR	2.8
1	B	203	GLY	2.8
1	A	122	LEU	2.8
1	A	158	LEU	2.8
1	B	228	THR	2.8
1	A	339	ARG	2.8
1	A	171	LYS	2.8
1	A	325	LEU	2.8
1	A	305	VAL	2.8
1	A	184	GLY	2.7
1	A	79	ILE	2.7
1	A	387	VAL	2.7
1	A	93	TYR	2.7
1	A	223	ASP	2.7
1	B	231	THR	2.7
1	A	65	LEU	2.7
1	A	235	LEU	2.7
1	A	333	ILE	2.7
1	A	11	GLN	2.7
1	A	45	VAL	2.7
1	A	57	VAL	2.7
1	A	31	TYR	2.7
1	A	277	TYR	2.7
1	A	14	LEU	2.7
1	A	245	HIS	2.7
1	A	2	VAL	2.7
1	A	348	VAL	2.7
1	A	374	ASP	2.6
1	A	170	GLY	2.6
1	A	356	VAL	2.6
1	A	389	ALA	2.6
1	B	161	ARG	2.6
1	A	508	LYS	2.6
1	A	485	SER	2.6
1	A	373	PHE	2.6
1	A	249	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	57	VAL	2.6
1	A	39	HIS	2.6
1	A	330	CYS	2.6
1	B	157	VAL	2.6
1	A	358	CYS	2.5
1	B	215	THR	2.5
1	A	89	VAL	2.5
1	B	49	VAL	2.5
1	A	297	LEU	2.4
1	A	231	THR	2.4
1	B	210	VAL	2.4
1	A	26	CYS	2.4
1	B	8	CYS	2.4
1	A	148	SER	2.4
1	B	92	LEU	2.4
1	A	104	THR	2.4
1	A	194	GLN	2.4
1	B	516	ASN	2.4
1	A	130	LEU	2.4
1	A	35	ILE	2.4
1	A	129	ARG	2.4
1	A	134	ALA	2.4
1	A	9	ASN	2.4
1	A	58	THR	2.3
1	A	338	ALA	2.3
1	A	362	ALA	2.3
1	B	73	LYS	2.3
1	A	30	CYS	2.3
1	B	7	LEU	2.3
1	B	81	PHE	2.3
1	B	52	ALA	2.3
1	A	218	LYS	2.3
1	B	53	PRO	2.3
1	B	101	ASP	2.3
1	A	179	ASN	2.3
1	B	46	ASN	2.3
1	B	91	GLY	2.2
1	A	524	LYS	2.2
1	B	186	ARG	2.2
1	A	328	ASP	2.2
1	A	161	ARG	2.2
1	A	360	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	216	THR	2.2
1	A	351	THR	2.2
1	A	464	HIS	2.2
1	A	5	CYS	2.2
1	A	87	GLY	2.2
1	B	68	MET	2.1
1	A	70	TYR	2.1
1	B	180	TYR	2.1
1	B	79	ILE	2.1
1	A	84	CYS	2.1
1	A	85	ALA	2.1
1	A	361	ASN	2.1
1	B	35	ILE	2.1
1	A	196	GLY	2.1
1	A	397	VAL	2.1
1	A	41	LEU	2.1
1	B	220	ASN	2.1
1	A	166	SER	2.0
1	A	304	ILE	2.0
1	B	218	LYS	2.0
1	A	135	ALA	2.0
1	B	497	ARG	2.0
1	A	366	THR	2.0
1	B	179	ASN	2.0
1	A	34	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

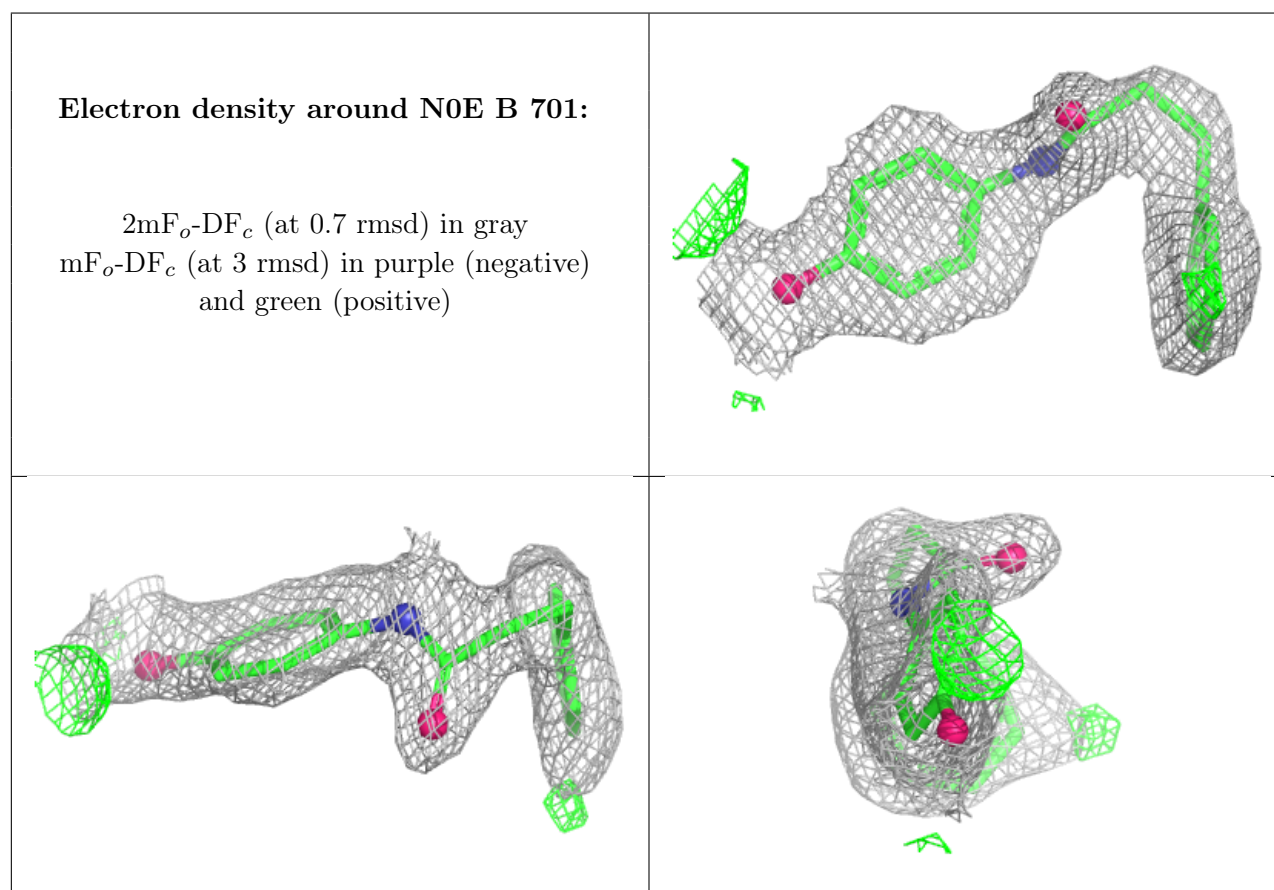
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
4	N0E	B	701	18/18	0.88	0.12	26,33,36,37	18
2	ZN	A	703	1/1	0.94	0.07	91,91,91,91	0
2	ZN	A	702	1/1	0.95	0.06	50,50,50,50	0
3	PO4	B	705	5/5	0.96	0.07	33,35,36,41	0
3	PO4	A	704	5/5	0.96	0.07	34,37,43,47	0
3	PO4	A	705	5/5	0.97	0.07	33,35,38,43	0
3	PO4	B	706	5/5	0.98	0.06	27,33,35,44	0
2	ZN	B	703	1/1	0.98	0.04	53,53,53,53	0
2	ZN	B	704	1/1	0.99	0.06	61,61,61,61	0
2	ZN	B	702	1/1	0.99	0.02	37,37,37,37	0
2	ZN	A	701	1/1	0.99	0.03	51,51,51,51	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.