



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 03:37 PM UTC

PDB ID : 5RL6 / pdb_00005rl6
Title : PanDDA analysis group deposition – Crystal Structure of SARS-CoV-2 heli-
case in complex with Z198195770
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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 : 1.92 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

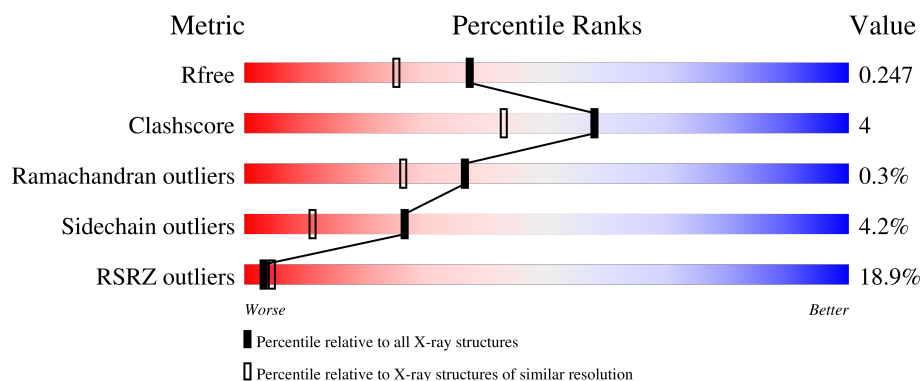
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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

Mol	Chain	Length	Quality of chain
1	A	601	30% 81% 14% • 5%
1	B	601	6% 86% 10% • •

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 9419 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).

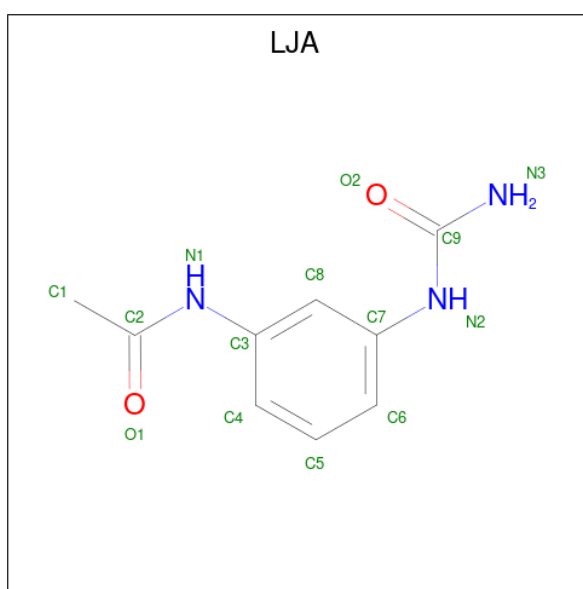
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	3	Total	Zn	0	0
			3	3		

- 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-[3-(carbamoylamino)phenyl]acetamide (CCD ID: LJA) (formula: $C_9H_{11}N_3O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 14 9 3 2	0	0

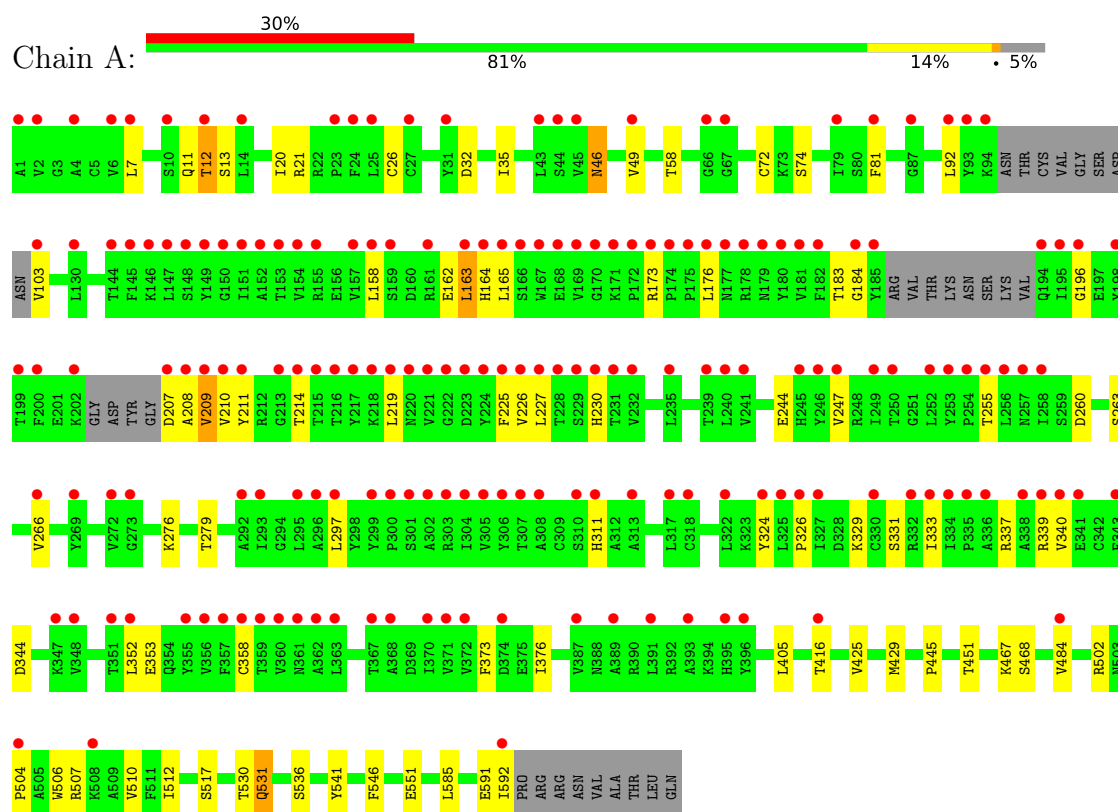
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	202	Total O 202 202	0	0
5	B	252	Total O 252 252	0	0

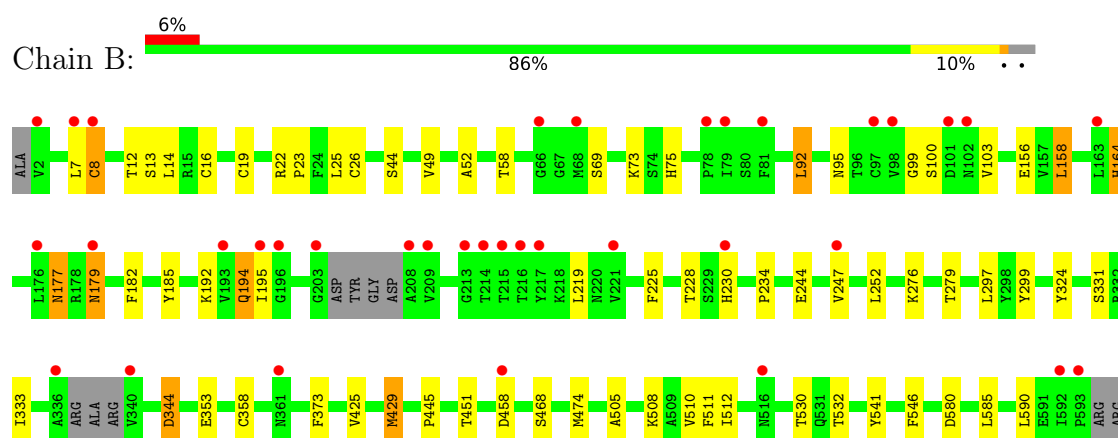
3 Residue-property plots

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



ASN
VAL
ALA
THR
LEU
GLN

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.36Å 70.30Å 85.93Å 103.23° 96.43° 112.23°	Depositor
Resolution (Å)	81.59 – 1.92 81.59 – 1.92	Depositor EDS
% Data completeness (in resolution range)	95.2 (81.59-1.92) 95.2 (81.59-1.92)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 1.92Å)	Xtriage
Refinement program	BUSTER 2.10.3 (20-MAY-2020)	Depositor
R, R_{free}	0.178 , 0.249 (Not available) , 0.247	Depositor DCC
R_{free} test set	4497 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	39.0	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 59.6	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	0.96	EDS
Total number of atoms	9419	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, ZN, LJA

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	0.87	0/4517	1.13	13/6156 (0.2%)
1	B	0.91	1/4610 (0.0%)	1.12	9/6283 (0.1%)
All	All	0.89	1/9127 (0.0%)	1.12	22/12439 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	429	MET	SD-CE	-6.25	1.64	1.79

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	177	ASN	CA-CB-CG	7.16	119.76	112.60
1	A	506	TRP	CA-C-N	7.10	130.11	120.38
1	A	506	TRP	C-N-CA	7.10	130.11	120.38
1	B	373	PHE	CA-CB-CG	6.46	120.27	113.80
1	A	373	PHE	CA-CB-CG	6.01	119.81	113.80
1	B	103	VAL	CA-C-N	5.98	128.61	120.54
1	B	103	VAL	C-N-CA	5.98	128.61	120.54
1	A	13	SER	CA-C-N	5.66	128.87	120.95
1	A	13	SER	C-N-CA	5.66	128.87	120.95
1	A	591	GLU	CA-C-N	5.63	131.84	121.70
1	A	591	GLU	C-N-CA	5.63	131.84	121.70
1	B	344	ASP	CA-CB-CG	5.61	118.21	112.60
1	A	165	LEU	N-CA-C	5.59	118.36	109.81
1	A	46	ASN	CA-CB-CG	5.54	118.14	112.60
1	B	179	ASN	CA-CB-CG	5.35	117.95	112.60
1	A	260	ASP	CA-C-N	5.29	127.63	120.38
1	A	260	ASP	C-N-CA	5.29	127.63	120.38
1	A	405	LEU	N-CA-C	5.19	116.37	109.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	532	THR	N-CA-C	-5.12	103.92	110.53
1	B	580	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	183	THR	CB-CA-C	5.09	117.93	109.53
1	B	95	ASN	CA-CB-CG	5.05	117.65	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	41	0
1	B	4508	0	4424	40	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
4	B	14	0	0	1	0
5	A	202	0	0	1	0
5	B	252	0	0	1	0
All	All	9419	0	8745	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:A:352:LEU:HD11	1:B:234:PRO:HD3	1.50	0.91
1:B:12:THR:HG21	1:B:25:LEU:O	1.74	0.87
1:B:279:THR:HB	1:B:429:MET:HE2	1.59	0.84
1:A:326:PRO:HB2	1:A:329:LYS:HZ3	1.46	0.80
1:A:279:THR:HB	1:A:429:MET:HE2	1.63	0.80
1:B:12:THR:HG22	1:B:14:LEU:H	1.47	0.79
1:A:158:LEU:HD11	1:A:164:HIS:NE2	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:LEU:HD11	1:A:164:HIS:CE1	2.27	0.69
1:A:158:LEU:HB2	1:A:163:LEU:HA	1.76	0.67
1:A:352:LEU:CD1	1:B:234:PRO:HD3	2.21	0.67
1:A:504:PRO:O	1:A:507:ARG:HB2	1.95	0.66
1:A:326:PRO:HB2	1:A:329:LYS:NZ	2.11	0.66
1:A:32:ASP:HB3	1:A:103:VAL:HG11	1.80	0.62
1:A:184:GLY:HA2	1:A:225:PHE:HD1	1.64	0.62
1:A:467:LYS:NZ	5:A:801:HOH:O	2.29	0.62
1:B:13:SER:HB3	1:B:92:LEU:HB2	1.80	0.62
1:B:474[B]:MET:HG2	1:B:590:LEU:HB2	1.81	0.61
1:B:510:VAL:HG21	1:B:541:TYR:CD1	2.37	0.59
1:B:158:LEU:HD11	1:B:164:HIS:ND1	2.19	0.58
1:A:184:GLY:HA2	1:A:225:PHE:CD1	2.39	0.57
1:A:20:ILE:HG23	1:A:21:ARG:HG2	1.87	0.56
1:B:12:THR:CG2	1:B:26:CYS:HA	2.36	0.55
1:A:510:VAL:HG21	1:A:541:TYR:CD1	2.42	0.53
1:B:19:CYS:CB	1:B:23:PRO:HD2	2.38	0.53
1:A:12:THR:HG21	1:A:26:CYS:HA	1.90	0.53
1:B:8:CYS:SG	1:B:99:GLY:N	2.82	0.52
1:B:182:PHE:HB3	1:B:225:PHE:HB3	1.92	0.52
1:A:162:GLU:HG2	1:A:210:VAL:HG22	1.92	0.52
1:B:12:THR:HG23	1:B:26:CYS:HA	1.92	0.52
1:A:445:PRO:HB3	1:A:468:SER:HB3	1.92	0.51
1:B:19:CYS:HB2	1:B:23:PRO:HD2	1.91	0.50
1:B:445:PRO:HB3	1:B:468:SER:HB3	1.93	0.50
1:A:425:VAL:HG12	1:A:429:MET:HE3	1.94	0.50
1:A:158:LEU:CD1	1:A:164:HIS:CE1	2.95	0.48
1:A:244:GLU:HB2	1:A:276:LYS:HB2	1.97	0.47
1:B:12:THR:HG22	1:B:14:LEU:N	2.23	0.47
1:B:13:SER:O	1:B:44:SER:HA	2.15	0.47
1:A:297:LEU:HD11	1:A:324:TYR:HB3	1.97	0.46
1:B:505:ALA:O	1:B:508:LYS:HG2	2.15	0.46
1:A:263:SER:O	1:A:266:VAL:HG22	2.15	0.46
1:A:352:LEU:HD11	1:B:234:PRO:CD	2.36	0.46
1:B:228:THR:HG22	1:B:230:HIS:CE1	2.51	0.46
4:B:701:LJA:C1	4:B:701:LJA:C8	2.93	0.46
1:B:195:ILE:O	1:B:195:ILE:HG22	2.16	0.46
1:B:158:LEU:CD1	1:B:164:HIS:ND1	2.79	0.45
1:B:451:THR:HG21	1:B:585:LEU:HD23	1.99	0.45
1:A:331:SER:HB2	1:A:353:GLU:HG3	1.99	0.45
1:B:52:ALA:CB	1:B:75:HIS:CG	2.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:SER:HB2	1:B:353:GLU:HG3	1.98	0.45
1:B:425:VAL:HG12	1:B:429:MET:HE3	1.99	0.45
1:A:158:LEU:CD1	1:A:164:HIS:NE2	2.78	0.45
1:B:244:GLU:HB2	1:B:276:LYS:HB2	1.99	0.44
1:B:195:ILE:O	1:B:195:ILE:CG2	2.64	0.44
1:A:512:ILE:O	1:A:546:PHE:HA	2.18	0.43
1:A:164:HIS:CD2	1:A:208:ALA:HA	2.53	0.43
1:B:185:TYR:CE2	1:B:194:GLN:HG2	2.53	0.43
1:A:311:HIS:HE2	1:A:339:ARG:NH2	2.17	0.43
1:A:49:VAL:HG23	1:A:58:THR:HG22	2.00	0.43
1:A:176:LEU:HD13	1:A:209:VAL:HG21	2.01	0.43
1:B:508:LYS:HD2	5:B:906:HOH:O	2.17	0.43
1:B:8:CYS:SG	1:B:99:GLY:O	2.77	0.43
1:A:214:THR:HG21	1:A:340:VAL:HG12	2.00	0.42
1:B:297:LEU:HD11	1:B:324:TYR:HB3	2.00	0.42
1:B:49:VAL:HG23	1:B:58:THR:HG22	2.01	0.42
1:A:163:LEU:HD11	1:A:211:TYR:HB3	2.01	0.42
1:B:512:ILE:O	1:B:546:PHE:HA	2.20	0.42
1:B:156:GLU:HB3	1:B:164:HIS:HB2	2.00	0.42
1:A:333:ILE:HB	1:A:358:CYS:HB2	2.01	0.42
1:B:252:LEU:HB3	1:B:299:TYR:CD1	2.55	0.42
1:A:158:LEU:CG	1:A:164:HIS:CE1	3.03	0.41
1:A:326:PRO:CB	1:A:329:LYS:NZ	2.79	0.41
1:B:16:CYS:O	1:B:22:ARG:HA	2.20	0.41
1:A:451:THR:HG21	1:A:585:LEU:HD23	2.03	0.41
1:A:12:THR:CG2	1:A:26:CYS:HA	2.49	0.41
1:B:511:PHE:HB3	1:B:530:THR:HG22	2.03	0.41
1:A:72:CYS:SG	1:A:74:SER:HB2	2.61	0.41
1:A:376:ILE:HG12	1:A:425:VAL:HG11	2.03	0.41
1:A:531:GLN:HG2	1:A:536:SER:HB3	2.03	0.40
1:B:333:ILE:HB	1:B:358:CYS:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	564/601 (94%)	541 (96%)	20 (4%)	3 (0%)	24	14
1	B	580/601 (96%)	561 (97%)	19 (3%)	0	100	100
All	All	1144/1202 (95%)	1102 (96%)	39 (3%)	3 (0%)	36	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	GLY
1	A	484	VAL
1	A	219	LEU

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%)	460 (95%)	25 (5%)	21	7
1	B	498/523 (95%)	482 (97%)	16 (3%)	34	18
All	All	983/1046 (94%)	942 (96%)	41 (4%)	26	11

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	11	GLN
1	A	12	THR
1	A	35	ILE
1	A	46	ASN
1	A	81	PHE
1	A	92	LEU
1	A	163	LEU
1	A	173	ARG
1	A	207	ASP

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Mol	Chain	Res	Type
1	A	209	VAL
1	A	226	VAL
1	A	227	LEU
1	A	230	HIS
1	A	247	VAL
1	A	255	THR
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	531	GLN
1	A	551	GLU
1	A	592	ILE
1	B	7	LEU
1	B	8	CYS
1	B	69	SER
1	B	73	LYS
1	B	92	LEU
1	B	100	SER
1	B	158	LEU
1	B	164	HIS
1	B	177	ASN
1	B	179	ASN
1	B	192	LYS
1	B	194	GLN
1	B	219	LEU
1	B	247	VAL
1	B	344	ASP
1	B	458	ASP

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	177	ASN
1	A	245	HIS
1	A	257	ASN
1	A	275	GLN
1	A	404	GLN
1	A	459	ASN
1	A	464	HIS

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Mol	Chain	Res	Type
1	B	230	HIS
1	B	245	HIS
1	B	268	ASN
1	B	404	GLN
1	B	459	ASN
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	2.61	2 (50%)	6,6,6	0.76	0
3	PO4	A	704	-	4,4,4	2.62	3 (75%)	6,6,6	0.81	0
3	PO4	A	705	-	4,4,4	2.62	2 (50%)	6,6,6	0.51	0
4	LJA	B	701	-	14,14,14	0.36	0	18,18,18	0.88	0
3	PO4	B	705	-	4,4,4	2.49	1 (25%)	6,6,6	0.61	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	LJA	B	701	-	-	2/8/8/8	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	704	PO4	P-O1	4.35	1.60	1.50
3	A	705	PO4	P-O1	4.28	1.60	1.50
3	B	705	PO4	P-O1	4.15	1.60	1.50
3	B	706	PO4	P-O1	4.03	1.60	1.50
3	B	706	PO4	P-O2	2.12	1.60	1.54
3	A	705	PO4	P-O3	2.11	1.60	1.54
3	A	704	PO4	P-O3	2.00	1.60	1.54
3	A	704	PO4	P-O4	2.00	1.60	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

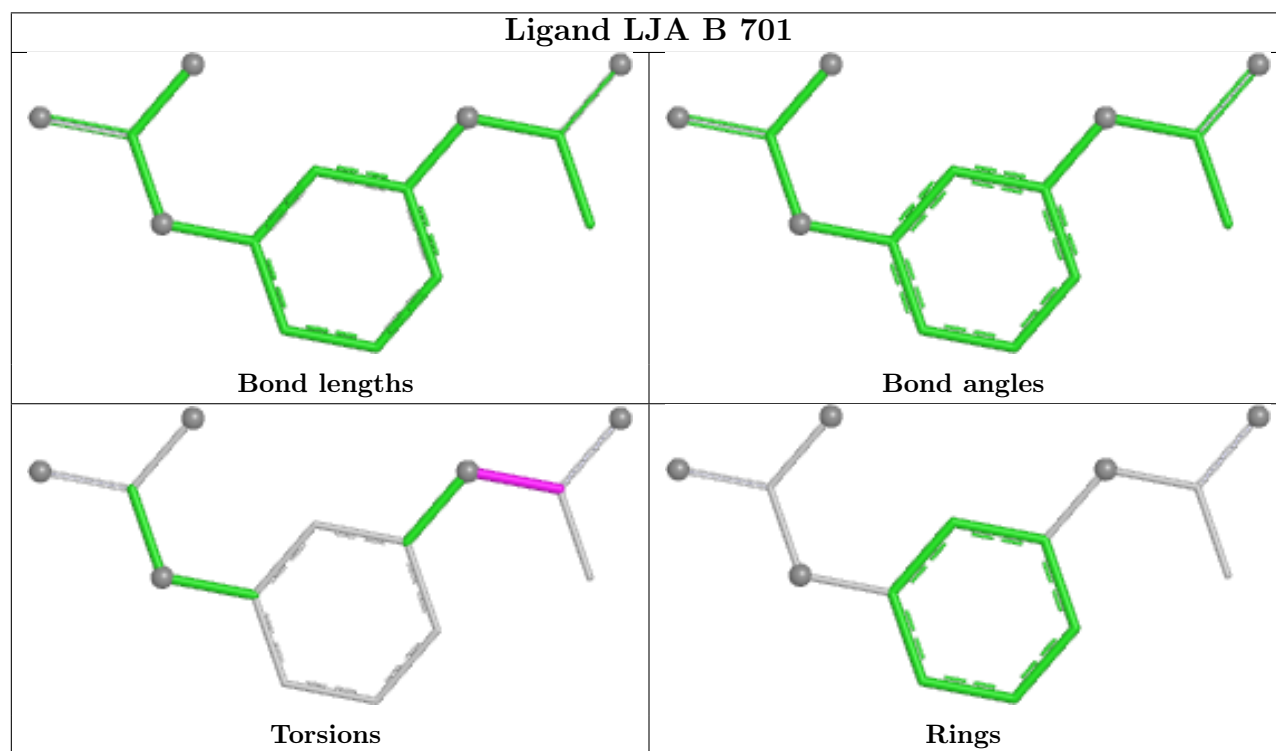
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	701	LJA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	572/601 (95%)	1.49	183 (31%) 1 1	33, 69, 175, 239	0
1	B	585/601 (97%)	0.45	36 (6%) 26 31	22, 49, 95, 134	1 (0%)
All	All	1157/1202 (96%)	0.97	219 (18%) 3 4	22, 57, 134, 239	1 (0%)

All (219) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	151	ILE	8.5
1	A	149	TYR	7.7
1	A	154	VAL	6.8
1	A	219	LEU	6.7
1	A	209	VAL	6.7
1	A	150	GLY	6.5
1	A	296	ALA	6.5
1	A	200	PHE	6.3
1	A	167	TRP	6.2
1	A	170	GLY	6.2
1	A	169	VAL	6.0
1	A	157	VAL	6.0
1	A	152	ALA	6.0
1	A	592	ILE	5.9
1	A	165	LEU	5.9
1	A	181	VAL	5.6
1	A	225	PHE	5.5
1	A	340	VAL	5.3
1	A	247	VAL	5.2
1	A	355	TYR	5.1
1	A	163	LEU	5.1
1	A	153	THR	5.1
1	A	229	SER	5.0
1	A	176	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	148	SER	4.9
1	A	304	ILE	4.9
1	A	362	ALA	4.9
1	A	217	TYR	4.9
1	A	210	VAL	4.9
1	A	221	VAL	4.8
1	A	208	ALA	4.8
1	A	172	PRO	4.8
1	A	306	TYR	4.8
1	B	102	ASN	4.6
1	A	2	VAL	4.5
1	A	252	LEU	4.5
1	B	336	ALA	4.5
1	A	224	TYR	4.4
1	A	357	PHE	4.3
1	A	371	VAL	4.3
1	A	258	ILE	4.3
1	B	208	ALA	4.2
1	A	7	LEU	4.1
1	A	92	LEU	4.1
1	B	217	TYR	4.1
1	A	94	LYS	4.0
1	A	81	PHE	4.0
1	A	396	TYR	4.0
1	A	166	SER	4.0
1	A	180	TYR	4.0
1	A	305	VAL	4.0
1	A	370	ILE	3.9
1	A	1	ALA	3.9
1	A	171	LYS	3.8
1	A	230	HIS	3.8
1	A	387	VAL	3.8
1	A	147	LEU	3.8
1	A	300	PRO	3.8
1	A	302	ALA	3.8
1	A	266	VAL	3.8
1	A	158	LEU	3.7
1	A	195	ILE	3.7
1	A	232	VAL	3.7
1	A	352	LEU	3.7
1	A	308	ALA	3.6
1	A	185	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	164	HIS	3.6
1	A	226	VAL	3.6
1	A	356	VAL	3.6
1	A	145	PHE	3.6
1	A	256	LEU	3.6
1	A	214	THR	3.5
1	A	249	ILE	3.5
1	A	6	VAL	3.5
1	A	334	ILE	3.5
1	A	325	LEU	3.5
1	A	351	THR	3.5
1	A	222	GLY	3.4
1	A	231	THR	3.4
1	A	12	THR	3.4
1	A	292	ALA	3.4
1	A	223	ASP	3.3
1	A	155	ARG	3.3
1	A	228	THR	3.3
1	A	299	TYR	3.3
1	A	179	ASN	3.3
1	B	214	THR	3.3
1	A	326	PRO	3.3
1	A	253	TYR	3.3
1	A	301	SER	3.3
1	A	215	THR	3.2
1	A	168	GLU	3.2
1	B	81	PHE	3.2
1	A	198	TYR	3.2
1	A	250	THR	3.2
1	B	593	PRO	3.2
1	A	218	LYS	3.2
1	A	202	LYS	3.1
1	A	211	TYR	3.1
1	A	241	VAL	3.1
1	A	335	PRO	3.1
1	A	45	VAL	3.1
1	A	146	LYS	3.1
1	B	97	CYS	3.1
1	A	4	ALA	3.1
1	B	2	VAL	3.1
1	A	336	ALA	3.1
1	A	389	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	393	ALA	3.1
1	B	592	ILE	3.0
1	A	343	PHE	3.0
1	A	199	THR	3.0
1	A	93	TYR	3.0
1	A	175	PRO	3.0
1	A	333	ILE	3.0
1	A	227	LEU	2.9
1	A	508	LYS	2.9
1	A	255	THR	2.9
1	A	273	GLY	2.9
1	B	203	GLY	2.9
1	B	340	VAL	2.9
1	A	310	SER	2.9
1	A	361	ASN	2.8
1	A	174	PRO	2.8
1	A	246	TYR	2.8
1	B	101	ASP	2.8
1	B	215	THR	2.8
1	A	269	TYR	2.8
1	A	318	CYS	2.8
1	B	195	ILE	2.8
1	B	216	THR	2.8
1	A	240	LEU	2.8
1	A	359	THR	2.8
1	A	416	THR	2.8
1	A	196	GLY	2.7
1	A	235	LEU	2.7
1	A	178	ARG	2.7
1	B	209	VAL	2.7
1	A	24	PHE	2.7
1	B	79	ILE	2.7
1	A	257	ASN	2.7
1	A	272	VAL	2.7
1	A	67	GLY	2.7
1	A	43	LEU	2.7
1	A	391	LEU	2.7
1	A	216	THR	2.6
1	A	327	ILE	2.6
1	A	245	HIS	2.6
1	B	163	LEU	2.6
1	A	368	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	159	SER	2.6
1	A	358	CYS	2.5
1	A	184	GLY	2.5
1	A	311	HIS	2.5
1	A	239	THR	2.5
1	A	177	ASN	2.5
1	A	220	ASN	2.5
1	A	293	ILE	2.5
1	A	254	PRO	2.5
1	A	324	TYR	2.4
1	A	307	THR	2.4
1	A	103	VAL	2.4
1	A	360	VAL	2.4
1	A	372	VAL	2.4
1	B	361	ASN	2.4
1	A	297	LEU	2.4
1	A	317	LEU	2.4
1	B	176	LEU	2.4
1	A	79	ILE	2.4
1	A	322	LEU	2.4
1	A	363	LEU	2.4
1	A	395	HIS	2.4
1	A	303	ARG	2.3
1	B	7	LEU	2.3
1	A	207	ASP	2.3
1	A	339	ARG	2.3
1	B	458	ASP	2.3
1	A	182	PHE	2.3
1	B	179	ASN	2.3
1	B	230	HIS	2.3
1	A	374	ASP	2.3
1	B	98	VAL	2.3
1	A	330	CYS	2.3
1	B	8	CYS	2.3
1	A	31	TYR	2.3
1	A	213	GLY	2.3
1	B	66	GLY	2.2
1	B	78	PRO	2.2
1	B	193	VAL	2.2
1	A	161	ARG	2.2
1	A	367	THR	2.2
1	B	196	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	27	CYS	2.2
1	A	313	ALA	2.2
1	B	516	ASN	2.2
1	A	194	GLN	2.2
1	A	14	LEU	2.2
1	A	23	PRO	2.2
1	A	504	PRO	2.2
1	A	341	GLU	2.1
1	A	484	VAL	2.1
1	B	247	VAL	2.1
1	A	130	LEU	2.1
1	B	68	MET	2.1
1	A	49	VAL	2.1
1	A	332	ARG	2.1
1	A	348	VAL	2.1
1	A	25	LEU	2.1
1	A	10	SER	2.1
1	A	66	GLY	2.1
1	B	213	GLY	2.1
1	A	295	LEU	2.1
1	A	44	SER	2.0
1	A	87	GLY	2.0
1	A	338	ALA	2.0
1	A	347	LYS	2.0
1	A	144	THR	2.0
1	A	173	ARG	2.0
1	B	221	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 [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,

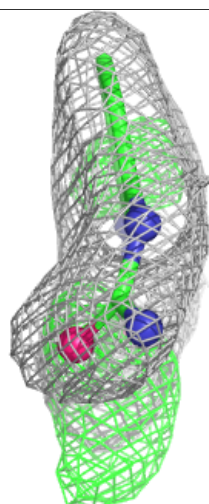
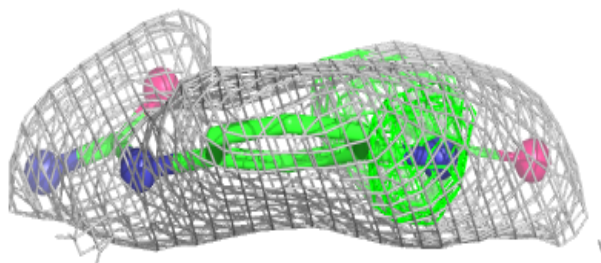
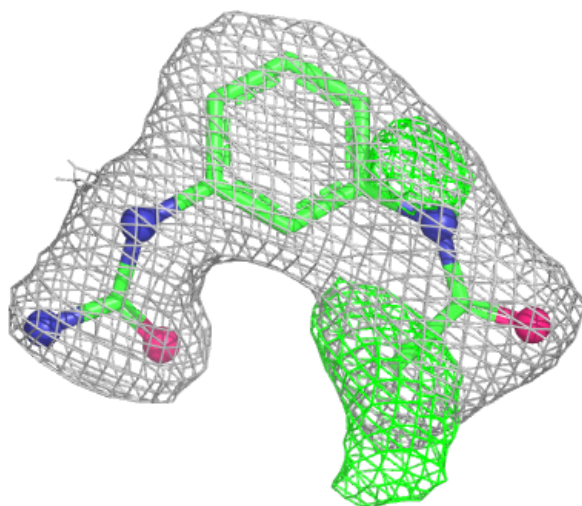
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	LJA	B	701	14/14	0.88	0.14	41,45,51,53	14
3	PO4	B	706	5/5	0.95	0.09	47,47,54,55	0
3	PO4	B	705	5/5	0.95	0.08	48,52,55,57	0
3	PO4	A	704	5/5	0.96	0.08	52,53,57,58	0
2	ZN	A	703	1/1	0.99	0.04	101,101,101,101	0
2	ZN	A	702	1/1	0.99	0.04	62,62,62,62	0
3	PO4	A	705	5/5	0.99	0.04	47,48,51,52	0
2	ZN	B	702	1/1	1.00	0.01	47,47,47,47	0
2	ZN	B	703	1/1	1.00	0.04	62,62,62,62	0
2	ZN	B	704	1/1	1.00	0.02	63,63,63,63	0
2	ZN	A	701	1/1	1.00	0.03	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.

Electron density around LJA 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 [i](#)

There are no such residues in this entry.