



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:58 AM UTC

PDB ID : 5RM6 / pdb_00005rm6
Title : PanDDA analysis group deposition – Crystal Structure of SARS-CoV-2 heli-
case in complex with Z396380540
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 : 2.13 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)

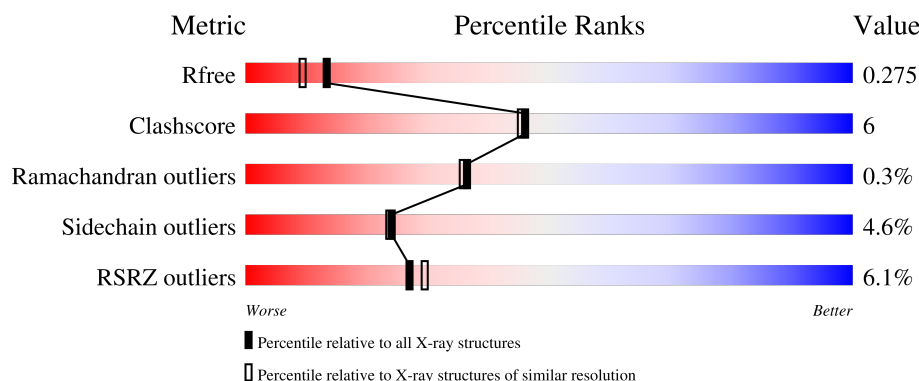
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	9% 79% 15% • 5%
1	B	601	2% 80% 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 9421 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).

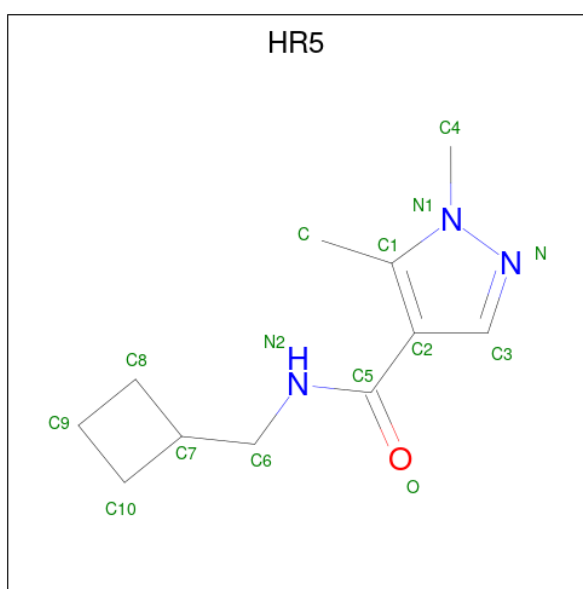
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	3	Total	Zn	0	0
			3	3		

- 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}-(cyclobutylmethyl)-1,5-dimethyl-pyrazole-4-carboxamide (CCD ID: HR5) (formula: C₁₁H₁₇N₃O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 15 11 3 1	0	0

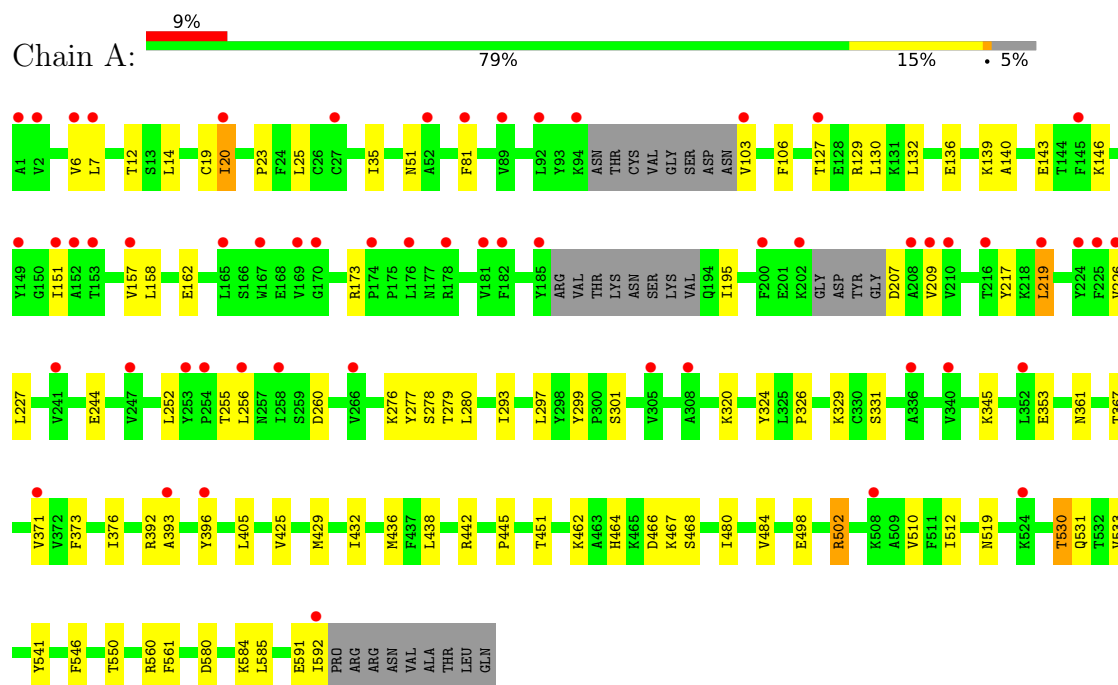
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	205	Total O 205 205	0	0
5	B	250	Total O 250 250	0	0

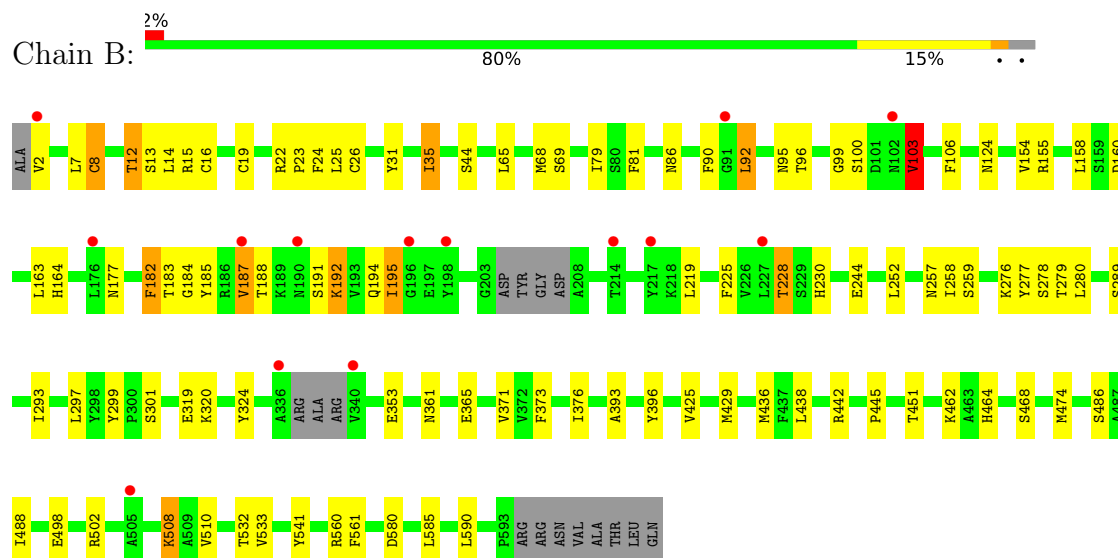
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Helicase



• Molecule 1: Helicase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.12Å 70.25Å 85.68Å 102.81° 96.39° 112.15°	Depositor
Resolution (Å)	81.58 – 2.13 81.58 – 2.13	Depositor EDS
% Data completeness (in resolution range)	96.7 (81.58-2.13) 96.7 (81.58-2.13)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.12Å)	Xtriage
Refinement program	BUSTER 2.10.3 (20-MAY-2020)	Depositor
R, R_{free}	0.162 , 0.251 0.190 , 0.275	Depositor DCC
R_{free} test set	3392 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	43.5	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 77.6	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	0.97	EDS
Total number of atoms	9421	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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: HR5, ZN, 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	0.89	0/4517	1.14	10/6156 (0.2%)
1	B	0.90	1/4610 (0.0%)	1.17	14/6283 (0.2%)
All	All	0.90	1/9127 (0.0%)	1.15	24/12439 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	488	ILE	CG1-CD1	-5.78	1.29	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	VAL	CA-C-N	7.36	130.14	120.28
1	B	103	VAL	C-N-CA	7.36	130.14	120.28
1	B	580	ASP	CA-CB-CG	6.96	119.56	112.60
1	A	466	ASP	CA-CB-CG	6.90	119.50	112.60
1	A	591	GLU	CA-C-N	6.35	133.13	121.70
1	A	591	GLU	C-N-CA	6.35	133.13	121.70
1	A	561	PHE	CA-CB-CG	-6.23	107.57	113.80
1	B	561	PHE	CA-CB-CG	-6.20	107.60	113.80
1	A	361	ASN	CA-CB-CG	6.14	118.74	112.60
1	B	95	ASN	CA-CB-CG	6.02	118.62	112.60
1	B	361	ASN	CA-CB-CG	5.99	118.59	112.60
1	A	256	LEU	N-CA-C	-5.87	105.78	113.12
1	B	86	ASN	CA-CB-CG	5.76	118.36	112.60
1	B	373	PHE	CA-CB-CG	5.72	119.53	113.80
1	B	90	PHE	CA-CB-CG	-5.68	108.11	113.80
1	B	532	THR	N-CA-C	-5.38	103.28	110.55
1	A	373	PHE	CA-CB-CG	5.36	119.16	113.80
1	A	405	LEU	N-CA-C	5.25	116.50	109.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	319	GLU	CB-CG-CD	5.13	121.32	112.60
1	B	182	PHE	CA-CB-CG	-5.03	108.77	113.80
1	B	2	VAL	CA-C-N	5.01	126.62	120.51
1	B	2	VAL	C-N-CA	5.01	126.62	120.51
1	A	260	ASP	CA-C-N	5.00	127.24	120.38
1	A	260	ASP	C-N-CA	5.00	127.24	120.38

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	4322	51	0
1	B	4508	0	4425	51	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	15	0	0	0	0
5	A	205	0	0	1	0
5	B	250	0	0	1	0
All	All	9421	0	8747	102	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 6.

All (102) 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:326:PRO:CG	1:A:329:LYS:HZ1	1.92	0.82
1:A:467:LYS:NZ	5:A:801:HOH:O	2.11	0.80
1:B:279:THR:HB	1:B:429:MET:HE2	1.69	0.75
1:A:326:PRO:HG2	1:A:329:LYS:HZ1	1.54	0.72
1:A:279:THR:HB	1:A:429:MET:HE2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:SER:HB2	1:A:353:GLU:HG3	1.73	0.69
1:A:326:PRO:HB2	1:A:329:LYS:HZ2	1.59	0.67
1:A:326:PRO:CD	1:A:329:LYS:HZ1	2.11	0.63
1:A:19:CYS:HB2	1:A:23:PRO:HD2	1.81	0.63
1:A:326:PRO:HB2	1:A:329:LYS:NZ	2.14	0.63
1:A:326:PRO:HD2	1:A:329:LYS:NZ	2.15	0.61
1:A:244:GLU:HB2	1:A:276:LYS:HB2	1.82	0.61
1:A:151:ILE:HG12	1:A:226:VAL:HG22	1.82	0.61
1:B:445:PRO:HB3	1:B:468:SER:HB3	1.83	0.60
1:A:445:PRO:HB3	1:A:468:SER:HB3	1.83	0.59
1:A:326:PRO:HD2	1:A:329:LYS:HZ1	1.67	0.59
1:B:19:CYS:HB2	1:B:23:PRO:HD2	1.83	0.59
1:B:244:GLU:HB2	1:B:276:LYS:HB2	1.84	0.58
1:B:12:THR:HG21	1:B:26:CYS:HA	1.88	0.55
1:B:451:THR:HG21	1:B:585:LEU:HD23	1.89	0.55
1:A:7:LEU:HD13	1:A:103:VAL:HG22	1.89	0.55
1:A:293:ILE:HG13	1:A:320:LYS:HB3	1.88	0.54
1:B:474[B]:MET:HG2	1:B:590:LEU:HB2	1.90	0.54
1:B:15:ARG:HG3	1:B:24:PHE:CD2	2.43	0.54
1:A:7:LEU:HD21	1:A:106:PHE:HB2	1.90	0.53
1:A:297:LEU:HD11	1:A:324:TYR:HB3	1.90	0.53
1:B:7:LEU:HD21	1:B:106:PHE:HB2	1.91	0.53
1:A:425:VAL:HG12	1:A:429:MET:HE3	1.91	0.53
1:A:519:ASN:HB3	1:A:530:THR:CG2	2.38	0.52
1:B:13:SER:HB3	1:B:92:LEU:HB2	1.90	0.52
1:A:451:THR:HG21	1:A:585:LEU:HD23	1.91	0.52
1:B:100:SER:HB2	1:B:103:VAL:HG23	1.92	0.52
1:A:146:LYS:HE2	1:A:227:LEU:HB3	1.93	0.51
1:B:13:SER:O	1:B:44:SER:HA	2.11	0.50
1:B:371:VAL:HG23	1:B:393:ALA:HB2	1.93	0.50
1:B:185:TYR:CE2	1:B:194:GLN:HG2	2.46	0.50
1:B:293:ILE:HG13	1:B:320:LYS:HB3	1.93	0.50
1:B:155:ARG:HE	1:B:164:HIS:CD2	2.29	0.50
1:B:425:VAL:HG12	1:B:429:MET:HE3	1.95	0.49
1:B:252:LEU:HB3	1:B:299:TYR:CD1	2.48	0.48
1:B:297:LEU:HD11	1:B:324:TYR:HB3	1.94	0.48
1:A:20:ILE:HD11	1:A:140:ALA:HB1	1.95	0.48
1:B:228:THR:HG22	1:B:230:HIS:CE1	2.49	0.48
1:A:132:LEU:O	1:A:136:GLU:HG3	2.13	0.48
1:B:498:GLU:HG3	1:B:502:ARG:NH2	2.28	0.48
1:A:371:VAL:HG23	1:A:393:ALA:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:VAL:HG21	1:B:541:TYR:CD1	2.49	0.48
1:B:12:THR:OG1	1:B:26:CYS:HA	2.13	0.47
1:A:19:CYS:CB	1:A:23:PRO:HD2	2.45	0.47
1:A:280:LEU:HD11	1:A:438:LEU:HG	1.95	0.46
1:B:8:CYS:SG	1:B:99:GLY:O	2.73	0.46
1:A:498:GLU:HG3	1:A:502:ARG:NH2	2.30	0.46
1:A:519:ASN:HB3	1:A:530:THR:HG23	1.97	0.46
1:B:7:LEU:HD13	1:B:103:VAL:HG22	1.98	0.46
1:B:8:CYS:SG	1:B:99:GLY:N	2.89	0.46
1:B:19:CYS:CB	1:B:23:PRO:HD2	2.45	0.46
1:A:326:PRO:CB	1:A:329:LYS:NZ	2.78	0.46
1:B:192:LYS:H	1:B:192:LYS:HD2	1.81	0.46
1:B:192:LYS:HD2	1:B:192:LYS:N	2.31	0.46
1:B:278:SER:HB2	1:B:436:MET:HE2	1.98	0.46
1:B:508:LYS:HD2	5:B:869:HOH:O	2.16	0.46
1:B:12:THR:CG2	1:B:26:CYS:HA	2.46	0.46
1:B:13:SER:CB	1:B:92:LEU:HB2	2.46	0.45
1:A:326:PRO:CG	1:A:329:LYS:NZ	2.73	0.45
1:A:510:VAL:HG21	1:A:541:TYR:CD1	2.51	0.45
1:A:157:VAL:HG21	1:A:219:LEU:O	2.16	0.45
1:B:183:THR:OG1	1:B:228:THR:OG1	2.28	0.45
1:B:65:LEU:HD23	1:B:81:PHE:CZ	2.52	0.45
1:B:154:VAL:HG22	1:B:163:LEU:HD13	1.99	0.44
1:A:158:LEU:HD12	1:A:162:GLU:HB3	2.00	0.44
1:A:277:TYR:HA	1:A:396:TYR:O	2.17	0.44
1:A:580:ASP:OD1	1:A:584:LYS:HE2	2.17	0.44
1:B:182:PHE:HB3	1:B:225:PHE:HB3	1.99	0.44
1:B:462:LYS:HA	1:B:462:LYS:HD3	1.86	0.44
1:B:184:GLY:HA3	1:B:195:ILE:HG22	2.00	0.43
1:A:252:LEU:HB3	1:A:299:TYR:CD2	2.53	0.43
1:A:139:LYS:O	1:A:143:GLU:HG2	2.19	0.43
1:B:13:SER:OG	1:B:44:SER:OG	2.30	0.43
1:A:329:LYS:NZ	1:A:329:LYS:HB2	2.34	0.43
1:A:6:VAL:HA	1:A:129:ARG:HD2	2.01	0.43
1:A:367:THR:HG22	1:A:392:ARG:HB3	2.00	0.43
1:A:14:LEU:HB2	1:A:25:LEU:O	2.19	0.43
1:A:127:THR:HG23	1:A:130:LEU:H	1.83	0.43
1:B:16:CYS:O	1:B:22:ARG:HA	2.18	0.43
1:B:258:ILE:HG13	1:B:259:SER:N	2.34	0.42
1:A:278:SER:HB2	1:A:436:MET:HE2	2.01	0.42
1:A:480:ILE:HG21	1:A:550:THR:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:LEU:HB2	1:B:25:LEU:O	2.19	0.42
1:A:326:PRO:CD	1:A:329:LYS:NZ	2.78	0.42
1:B:31:TYR:CZ	1:B:35:ILE:HG21	2.55	0.42
1:B:154:VAL:HG13	1:B:163:LEU:HD22	2.01	0.42
1:B:376:ILE:HD12	1:B:376:ILE:HA	1.94	0.41
1:B:533:VAL:HG11	1:B:560:ARG:O	2.19	0.41
1:A:442:ARG:HA	1:A:464:HIS:HB3	2.02	0.41
1:B:280:LEU:HD11	1:B:438:LEU:HG	2.02	0.41
1:B:442:ARG:HA	1:B:464:HIS:HB3	2.02	0.41
1:A:512:ILE:O	1:A:546:PHE:HA	2.21	0.41
1:A:519:ASN:HB3	1:A:530:THR:HG21	2.02	0.41
1:B:474[B]:MET:CG	1:B:590:LEU:HB2	2.49	0.41
1:A:533:VAL:HG11	1:A:560:ARG:O	2.21	0.41
1:B:277:TYR:HA	1:B:396:TYR:O	2.21	0.41
1:A:462:LYS:HD3	1:A:462:LYS:HA	1.89	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%)	543 (96%)	18 (3%)	3 (0%)	24	22
1	B	580/601 (96%)	557 (96%)	22 (4%)	1 (0%)	43	44
All	All	1144/1202 (95%)	1100 (96%)	40 (4%)	4 (0%)	36	36

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	484	VAL
1	A	219	LEU
1	A	195	ILE

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Mol	Chain	Res	Type
1	B	187	VAL

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%)	467 (96%)	18 (4%)	30	31
1	B	498/523 (95%)	471 (95%)	27 (5%)	20	18
All	All	983/1046 (94%)	938 (95%)	45 (5%)	24	24

All (45) 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	51	ASN
1	A	81	PHE
1	A	173	ARG
1	A	207	ASP
1	A	209	VAL
1	A	217	TYR
1	A	255	THR
1	A	301	SER
1	A	345	LYS
1	A	376	ILE
1	A	432	ILE
1	A	502	ARG
1	A	530	THR
1	A	531	GLN
1	A	592	ILE
1	B	8	CYS
1	B	12	THR
1	B	35	ILE
1	B	68	MET

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Mol	Chain	Res	Type
1	B	69	SER
1	B	79	ILE
1	B	92	LEU
1	B	96	THR
1	B	103	VAL
1	B	124	ASN
1	B	158	LEU
1	B	160	ASP
1	B	177	ASN
1	B	187	VAL
1	B	188	THR
1	B	191	SER
1	B	192	LYS
1	B	195	ILE
1	B	219	LEU
1	B	228	THR
1	B	257	ASN
1	B	289	SER
1	B	301	SER
1	B	353	GLU
1	B	365	GLU
1	B	486	SER
1	B	508	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	116	ASN
1	A	220	ASN
1	A	230	HIS
1	A	245	HIS
1	A	265	ASN
1	A	275	GLN
1	A	464	HIS
1	A	531	GLN
1	B	51	ASN
1	B	177	ASN
1	B	230	HIS
1	B	245	HIS
1	B	265	ASN
1	B	268	ASN

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Mol	Chain	Res	Type
1	B	404	GLN

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	A	704	-	4,4,4	2.56	2 (50%)	6,6,6	0.66	0
3	PO4	A	705	-	4,4,4	2.59	3 (75%)	6,6,6	0.69	0
3	PO4	B	706	-	4,4,4	2.46	1 (25%)	6,6,6	0.64	0
3	PO4	B	705	-	4,4,4	2.58	1 (25%)	6,6,6	0.74	0
4	HR5	B	701	-	16,16,16	0.53	0	21,22,22	1.33	1 (4%)

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	HR5	B	701	-	-	4/9/15/15	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	705	PO4	P-O1	4.25	1.60	1.50
3	A	704	PO4	P-O1	4.25	1.60	1.50
3	B	705	PO4	P-O1	4.25	1.60	1.50
3	B	706	PO4	P-O1	4.16	1.60	1.50
3	A	705	PO4	P-O3	2.09	1.60	1.54
3	A	704	PO4	P-O4	2.03	1.60	1.54
3	A	705	PO4	P-O4	2.00	1.60	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	701	HR5	C1-N1-N	-5.32	111.03	112.91

There are no chirality outliers.

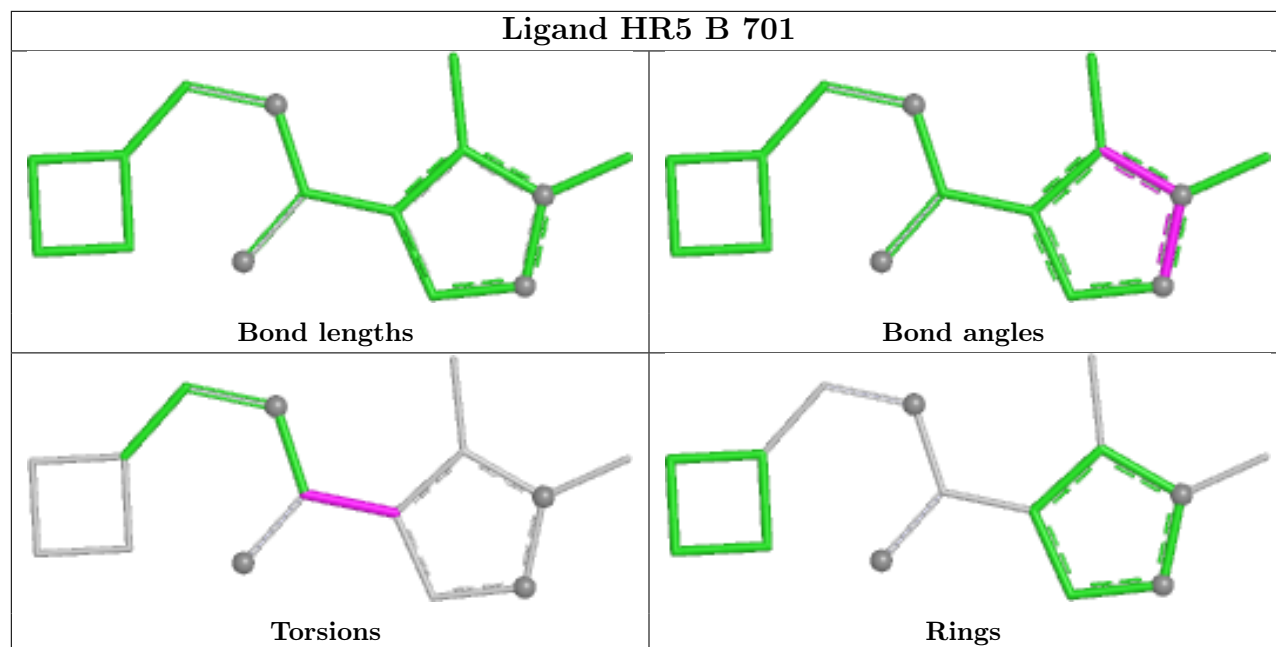
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	701	HR5	C3-C2-C5-O
4	B	701	HR5	C3-C2-C5-N2
4	B	701	HR5	C1-C2-C5-O
4	B	701	HR5	C1-C2-C5-N2

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%)	0.69	57 (9%) 12 14	39, 78, 147, 170	0
1	B	585/601 (97%)	0.23	14 (2%) 59 62	27, 61, 113, 154	1 (0%)
All	All	1157/1202 (96%)	0.46	71 (6%) 27 29	27, 69, 136, 170	1 (0%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	225	PHE	4.4
1	A	1	ALA	4.0
1	A	592	ILE	3.9
1	A	208	ALA	3.6
1	A	209	VAL	3.5
1	A	152	ALA	3.4
1	B	2	VAL	3.3
1	A	170	GLY	3.2
1	A	6	VAL	3.2
1	A	258	ILE	3.2
1	A	2	VAL	3.1
1	A	241	VAL	3.1
1	A	508	LYS	3.1
1	B	214	THR	3.1
1	A	340	VAL	3.1
1	A	210	VAL	3.0
1	B	217	TYR	3.0
1	B	340	VAL	2.9
1	A	169	VAL	2.9
1	A	176	LEU	2.9
1	A	165	LEU	2.8
1	A	157	VAL	2.8
1	A	226	VAL	2.8
1	A	200	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	52	ALA	2.8
1	A	181	VAL	2.7
1	A	7	LEU	2.6
1	A	153	THR	2.6
1	A	202	LYS	2.6
1	A	266	VAL	2.6
1	A	167	TRP	2.6
1	A	94	LYS	2.5
1	A	182	PHE	2.5
1	A	247	VAL	2.5
1	A	151	ILE	2.5
1	A	81	PHE	2.4
1	A	103	VAL	2.4
1	B	187	VAL	2.4
1	A	27	CYS	2.4
1	A	393	ALA	2.4
1	A	89	VAL	2.4
1	A	224	TYR	2.4
1	B	190	ASN	2.3
1	B	336	ALA	2.3
1	B	196	GLY	2.3
1	A	256	LEU	2.3
1	A	352	LEU	2.2
1	A	149	TYR	2.2
1	A	185	TYR	2.2
1	A	396	TYR	2.2
1	A	145	PHE	2.2
1	B	102	ASN	2.2
1	A	92	LEU	2.2
1	B	176	LEU	2.2
1	A	178	ARG	2.2
1	B	227	LEU	2.2
1	A	336	ALA	2.1
1	A	20	ILE	2.1
1	B	505	ALA	2.1
1	A	219	LEU	2.1
1	A	254	PRO	2.1
1	A	305	VAL	2.1
1	A	371	VAL	2.1
1	A	524	LYS	2.1
1	A	308	ALA	2.1
1	A	174	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	216	THR	2.1
1	A	253	TYR	2.0
1	B	198	TYR	2.0
1	A	127	THR	2.0
1	B	91	GLY	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](#)

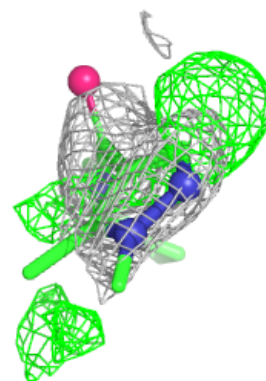
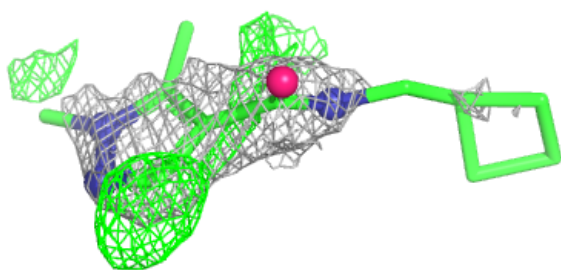
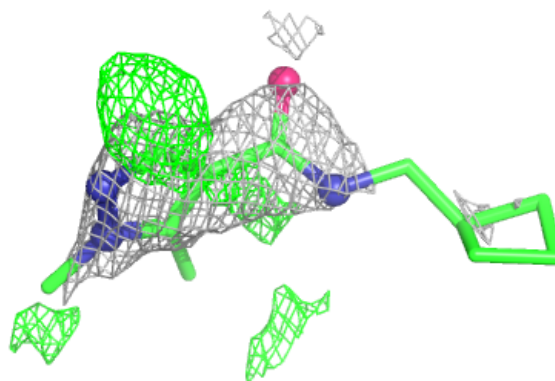
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	HR5	B	701	15/15	0.88	0.24	34,35,36,38	15
3	PO4	B	705	5/5	0.97	0.06	55,56,58,61	0
3	PO4	A	704	5/5	0.98	0.06	65,65,68,71	0
3	PO4	B	706	5/5	0.98	0.06	57,59,60,64	0
3	PO4	A	705	5/5	0.98	0.05	60,61,65,65	0
2	ZN	A	701	1/1	0.99	0.05	48,48,48,48	0
2	ZN	A	702	1/1	0.99	0.03	72,72,72,72	0
2	ZN	A	703	1/1	0.99	0.04	119,119,119,119	0
2	ZN	B	703	1/1	0.99	0.05	95,95,95,95	0
2	ZN	B	704	1/1	0.99	0.04	103,103,103,103	0
2	ZN	B	702	1/1	1.00	0.02	58,58,58,58	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 HR5 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.