



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:03 AM UTC

PDB ID : 5RLU / pdb_00005rlu
Title : PanDDA analysis group deposition – Crystal Structure of SARS-CoV-2 heli-
case in complex with Z744754722
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 : 2.35 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)

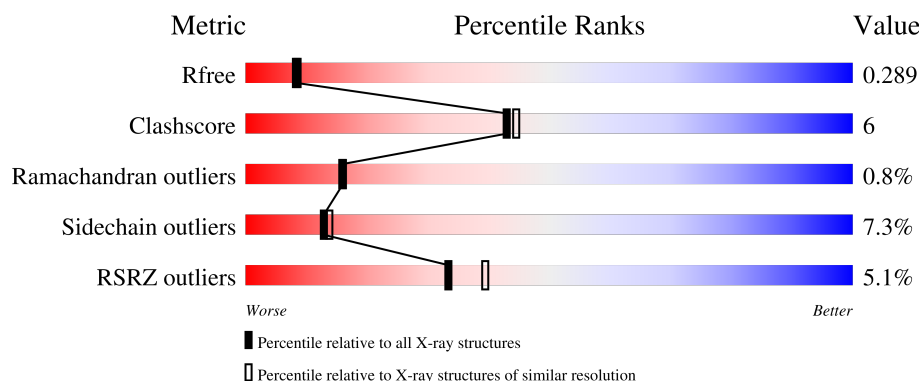
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

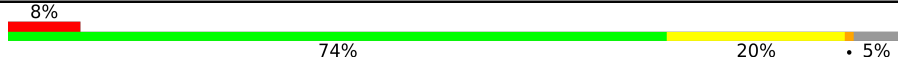
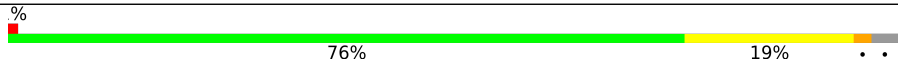
The reported resolution of this entry is 2.35 Å.

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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	
1	B	601	

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
2	JG4	B	701	-	-	X	-

2 Entry composition [i](#)

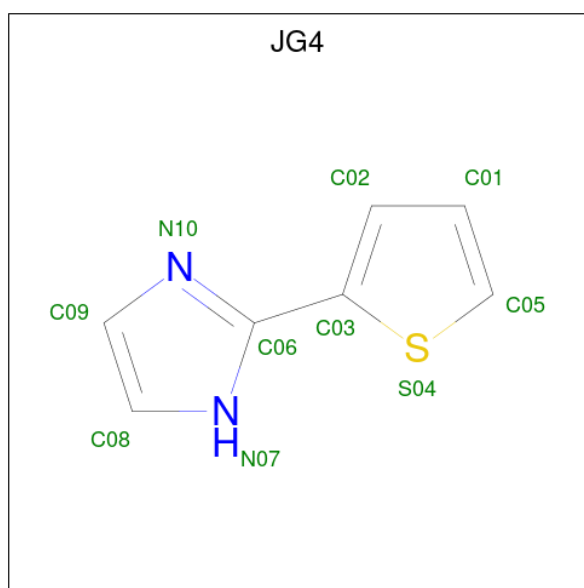
There are 5 unique types of molecules in this entry. The entry contains 9423 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2-(thiophen-2-yl)-1H-imidazole (CCD ID: JG4) (formula: $C_7H_6N_2S$) (labeled as "Ligand of Interest" by depositor).

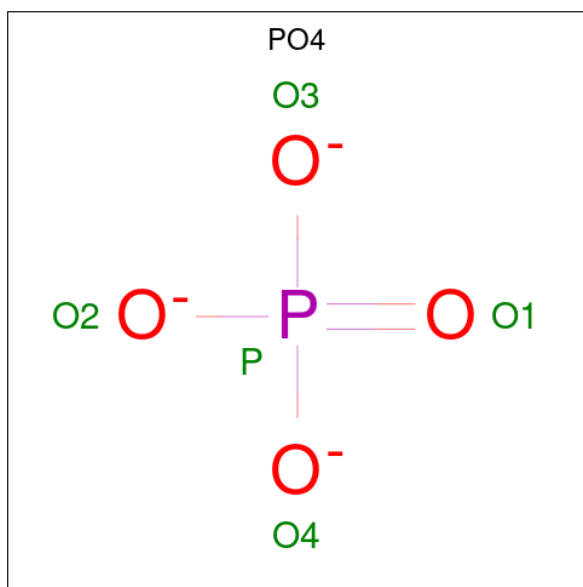


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	S	0	0
			10	7	2	1		
2	B	1	Total	C	N	S	0	0
			10	7	2	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

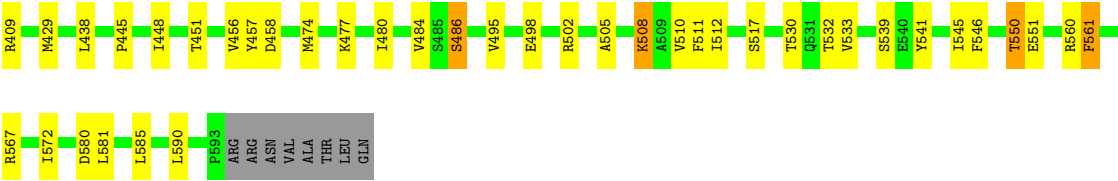
- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	202	Total 202	O 202	0	0
5	B	250	Total 250	O 250	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.21Å 70.23Å 86.04Å 103.13° 96.93° 111.98°	Depositor
Resolution (Å)	81.59 – 2.35 81.59 – 2.35	Depositor EDS
% Data completeness (in resolution range)	97.0 (81.59-2.35) 97.0 (81.59-2.35)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.34Å)	Xtriage
Refinement program	BUSTER 2.10.3 (20-MAY-2020)	Depositor
R, R_{free}	0.160 , 0.273 0.182 , 0.289	Depositor DCC
R_{free} test set	2541 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 83.3	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	9423	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.04% 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: PO4, ZN, JG4

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	0.92	0/4517	1.19	17/6156 (0.3%)
1	B	0.94	1/4610 (0.0%)	1.21	19/6283 (0.3%)
All	All	0.93	1/9127 (0.0%)	1.20	36/12439 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	550	THR	CA-C	5.10	1.59	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	591	GLU	CA-C-N	7.69	135.53	121.70
1	A	591	GLU	C-N-CA	7.69	135.53	121.70
1	B	95	ASN	CA-CB-CG	6.93	119.53	112.60
1	B	344	ASP	CA-CB-CG	6.89	119.49	112.60
1	B	580	ASP	CA-CB-CG	6.69	119.29	112.60
1	B	361	ASN	CA-CB-CG	6.54	119.14	112.60
1	A	317	LEU	CA-C-N	6.49	128.98	120.28
1	A	317	LEU	C-N-CA	6.49	128.98	120.28
1	A	545	ILE	N-CA-CB	6.33	119.87	111.90
1	A	466	ASP	CA-CB-CG	6.16	118.76	112.60
1	A	580	ASP	CA-CB-CG	5.97	118.57	112.60
1	B	532	THR	N-CA-C	-5.96	102.85	110.53
1	B	314	VAL	CA-C-N	5.88	128.15	120.28
1	B	314	VAL	C-N-CA	5.88	128.15	120.28
1	B	373	PHE	CA-CB-CG	5.83	119.64	113.80
1	A	45	VAL	N-CA-C	-5.66	105.21	110.53
1	B	545	ILE	N-CA-CB	5.51	118.84	111.90
1	A	4	ALA	CA-C-N	5.50	128.52	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	ALA	C-N-CA	5.50	128.52	120.71
1	B	157	VAL	CA-C-N	5.42	127.80	120.65
1	B	157	VAL	C-N-CA	5.42	127.80	120.65
1	A	136	GLU	CA-C-N	5.41	127.47	120.44
1	A	136	GLU	C-N-CA	5.41	127.47	120.44
1	B	103	VAL	CA-C-N	5.39	127.45	120.44
1	B	103	VAL	C-N-CA	5.39	127.45	120.44
1	A	314	VAL	CA-C-N	5.32	127.40	120.28
1	A	314	VAL	C-N-CA	5.32	127.40	120.28
1	A	587	PHE	CA-CB-CG	5.31	119.11	113.80
1	A	561	PHE	CA-CB-CG	-5.29	108.51	113.80
1	B	350	SER	CA-C-N	5.22	128.00	120.38
1	B	350	SER	C-N-CA	5.22	128.00	120.38
1	A	373	PHE	CA-CB-CG	5.21	119.01	113.80
1	B	561	PHE	CA-CB-CG	-5.17	108.63	113.80
1	B	177	ASN	CA-CB-CG	5.11	117.71	112.60
1	B	59	ASP	CA-CB-CG	5.05	117.65	112.60
1	B	56	ASP	CA-CB-CG	5.03	117.63	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	4322	57	0
1	B	4508	0	4424	53	0
2	A	10	0	0	0	0
2	B	10	0	0	4	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
5	A	202	0	0	3	0
5	B	250	0	0	0	0
All	All	9423	0	8746	110	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 (110) 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:158:LEU:HD11	1:A:164:HIS:CE1	2.13	0.83
1:B:505:ALA:O	1:B:508:LYS:HE3	1.82	0.78
1:A:326:PRO:HG2	1:A:329:LYS:HZ1	1.48	0.77
1:B:226:VAL:HG21	2:B:701:JG4:C02	2.14	0.77
1:A:158:LEU:HD21	1:A:164:HIS:CE1	2.20	0.76
1:A:326:PRO:CG	1:A:329:LYS:HZ1	1.99	0.75
1:A:158:LEU:HD21	1:A:164:HIS:HE1	1.53	0.74
1:A:333:ILE:HB	1:A:358:CYS:HB2	1.78	0.66
1:B:498:GLU:HG3	1:B:502:ARG:HH21	1.62	0.64
1:A:158:LEU:HD11	1:A:164:HIS:HE1	1.59	0.63
1:B:333:ILE:HB	1:B:358:CYS:HB2	1.80	0.62
1:A:326:PRO:HB2	1:A:329:LYS:HZ2	1.65	0.61
1:B:510:VAL:HG21	1:B:541:TYR:CD1	2.36	0.60
1:A:467:LYS:NZ	5:A:809:HOH:O	2.34	0.59
1:B:279:THR:HB	1:B:429:MET:HE3	1.85	0.58
1:A:326:PRO:HB2	1:A:329:LYS:NZ	2.18	0.58
1:A:202:LYS:HA	1:A:209:VAL:HG23	1.86	0.57
1:B:259:SER:HB2	1:B:261:GLU:HG3	1.86	0.57
1:A:451:THR:HG21	1:A:585:LEU:HD23	1.87	0.57
1:A:279:THR:HB	1:A:429:MET:HE3	1.87	0.57
1:A:510:VAL:HG21	1:A:541:TYR:CD1	2.40	0.57
1:A:480:ILE:HG21	1:A:550:THR:HG22	1.87	0.57
1:A:363:LEU:HD22	1:A:391:LEU:HD21	1.87	0.56
1:B:451:THR:HG21	1:B:585:LEU:HD23	1.88	0.56
1:B:13:SER:HB2	1:B:92:LEU:HB2	1.86	0.56
1:B:252:LEU:HB3	1:B:299:TYR:CD1	2.41	0.56
1:B:445:PRO:HD2	1:B:448:ILE:HD12	1.88	0.55
1:A:332:ARG:HG2	1:A:343:PHE:HB3	1.89	0.54
1:A:139:LYS:NZ	5:A:813:HOH:O	2.41	0.53
1:A:445:PRO:HD2	1:A:448:ILE:HD12	1.89	0.53
1:B:363:LEU:HD22	1:B:391:LEU:HD21	1.90	0.53
1:B:226:VAL:HG11	2:B:701:JG4:S04	2.48	0.53
1:A:533:VAL:HG11	1:A:560:ARG:HG3	1.91	0.53
1:A:263:SER:HA	1:A:266:VAL:HG13	1.91	0.52
1:A:198:TYR:HE2	1:A:211:TYR:HD1	1.57	0.52
1:A:519:ASN:HB3	1:A:530:THR:CG2	2.40	0.52
1:B:7:LEU:HD21	1:B:106:PHE:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:THR:OG1	1:B:228:THR:OG1	2.27	0.51
1:B:486:SER:HB3	1:B:517:SER:HB2	1.91	0.51
1:A:163:LEU:HG	1:A:211:TYR:CD2	2.45	0.51
1:B:21:ARG:HD3	1:B:140:ALA:HB2	1.92	0.51
1:B:297:LEU:HD11	1:B:324:TYR:HB3	1.94	0.50
1:B:474[B]:MET:CG	1:B:590:LEU:HB2	2.41	0.50
1:A:280:LEU:HD11	1:A:438:LEU:HG	1.94	0.50
1:B:226:VAL:HG21	2:B:701:JG4:C03	2.41	0.49
1:A:7:LEU:HD21	1:A:106:PHE:HB2	1.93	0.49
1:A:297:LEU:HD11	1:A:324:TYR:HB3	1.94	0.49
1:B:533:VAL:HG11	1:B:560:ARG:HG3	1.94	0.49
1:A:504:PRO:O	1:A:507:ARG:HB2	2.13	0.48
1:B:480:ILE:HG21	1:B:550:THR:HG22	1.95	0.48
1:B:157:VAL:HG21	1:B:220:ASN:HA	1.94	0.48
1:A:448:ILE:HD11	1:A:572:ILE:CG2	2.44	0.48
1:B:183:THR:HG1	1:B:228:THR:HG1	1.57	0.48
1:B:195:ILE:HG23	1:B:195:ILE:O	2.13	0.48
1:A:409:ARG:NH2	1:A:422:PHE:O	2.43	0.48
1:A:326:PRO:CG	1:A:329:LYS:NZ	2.75	0.47
1:A:534:ASP:OD2	5:A:801:HOH:O	2.20	0.47
1:B:511:PHE:HB3	1:B:530:THR:HG22	1.96	0.47
1:B:184:GLY:HA3	1:B:195:ILE:HG22	1.97	0.46
1:A:313:ALA:HB2	1:A:375:GLU:OE1	2.14	0.46
1:B:19:CYS:HB2	1:B:23:PRO:HD2	1.97	0.46
1:A:19:CYS:HB2	1:A:23:PRO:HD2	1.96	0.46
1:B:474[B]:MET:HG2	1:B:590:LEU:HB2	1.96	0.46
1:B:477:LYS:HE2	1:B:551:GLU:OE2	2.16	0.46
1:B:386:VAL:O	1:B:390:ARG:HG2	2.16	0.46
1:A:139:LYS:HG2	1:A:232:VAL:HG22	1.99	0.45
1:B:448:ILE:HD11	1:B:572:ILE:CG2	2.46	0.45
1:A:376:ILE:HG22	1:A:400:GLY:HA3	1.98	0.45
1:B:376:ILE:HG22	1:B:400:GLY:HA3	1.99	0.45
1:A:326:PRO:CD	1:A:329:LYS:HZ1	2.30	0.45
1:A:363:LEU:O	1:A:390:ARG:HD3	2.16	0.45
1:A:39:HIS:NE2	1:A:111:THR:HG22	2.32	0.45
1:A:185:TYR:HA	1:A:194:GLN:N	2.32	0.44
1:A:326:PRO:HD2	1:A:329:LYS:NZ	2.32	0.44
1:A:512:ILE:O	1:A:546:PHE:HA	2.18	0.44
1:A:139:LYS:O	1:A:143:GLU:HG2	2.18	0.44
1:A:120:TYR:CE2	1:A:409:ARG:HG2	2.52	0.44
1:A:448:ILE:HD11	1:A:572:ILE:HG22	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:SER:O	1:B:567:ARG:HD3	2.18	0.43
1:B:7:LEU:HD12	1:B:103:VAL:HG22	1.99	0.43
1:A:456:VAL:HG23	1:A:457:TYR:CE2	2.53	0.43
1:B:120:TYR:CE2	1:B:409:ARG:HG2	2.53	0.43
1:B:280:LEU:HD11	1:B:438:LEU:HG	2.00	0.43
1:B:12:THR:OG1	1:B:26:CYS:HA	2.19	0.43
1:A:561:PHE:CD2	1:A:581:LEU:HD22	2.54	0.43
1:B:39:HIS:NE2	1:B:111:THR:HG22	2.34	0.43
1:B:561:PHE:CD2	1:B:581:LEU:HD22	2.53	0.43
1:B:192:LYS:H	1:B:192:LYS:HD2	1.84	0.43
1:B:52:ALA:HB1	1:B:75:HIS:CD2	2.54	0.42
1:B:226:VAL:HG11	2:B:701:JG4:C03	2.49	0.42
1:B:448:ILE:HD11	1:B:572:ILE:HG22	2.00	0.42
1:B:331:SER:OG	1:B:347:LYS:O	2.30	0.42
1:B:456:VAL:HG23	1:B:457:TYR:CE2	2.55	0.42
1:A:480:ILE:CG2	1:A:550:THR:HG22	2.48	0.42
1:B:31:TYR:CE2	1:B:35:ILE:HD13	2.55	0.42
1:B:377:SER:O	1:B:406:PRO:HA	2.20	0.42
1:A:539:SER:O	1:A:567:ARG:HD3	2.20	0.42
1:A:326:PRO:CB	1:A:329:LYS:NZ	2.82	0.42
1:B:158:LEU:CD1	1:B:164:HIS:ND1	2.83	0.42
1:A:127:THR:HG23	1:A:130:LEU:H	1.85	0.41
1:A:378:MET:O	1:A:407:ALA:HB2	2.20	0.41
1:A:472:PHE:HB3	1:A:590:LEU:HG	2.01	0.41
1:A:446:ALA:HB3	1:A:467:LYS:HG3	2.02	0.41
1:A:12:THR:OG1	1:A:26:CYS:HA	2.21	0.41
1:B:303:ARG:NH1	1:B:353:GLU:O	2.53	0.41
1:A:162:GLU:HG2	1:A:210:VAL:HG22	2.04	0.40
1:A:480:ILE:HG12	1:A:550:THR:HG22	2.04	0.40
1:B:512:ILE:O	1:B:546:PHE:HA	2.22	0.40
1:B:357:PHE:CD1	1:B:357:PHE:N	2.89	0.40
1:B:378:MET:O	1:B:407:ALA:HB2	2.21	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%)	535 (95%)	22 (4%)	7 (1%)	10	8
1	B	580/601 (96%)	548 (94%)	30 (5%)	2 (0%)	36	41
All	All	1144/1202 (95%)	1083 (95%)	52 (4%)	9 (1%)	16	16

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	ILE
1	A	484	VAL
1	B	161	ARG
1	A	44	SER
1	A	219	LEU
1	A	228	THR
1	A	339	ARG
1	A	258	ILE
1	B	221	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%)	451 (93%)	34 (7%)	14	15
1	B	498/523 (95%)	460 (92%)	38 (8%)	12	13
All	All	983/1046 (94%)	911 (93%)	72 (7%)	13	14

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	12	THR
1	A	35	ILE

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Mol	Chain	Res	Type
1	A	46	ASN
1	A	49	VAL
1	A	69	SER
1	A	74	SER
1	A	76	LYS
1	A	81	PHE
1	A	92	LEU
1	A	147	LEU
1	A	156	GLU
1	A	157	VAL
1	A	163	LEU
1	A	169	VAL
1	A	173	ARG
1	A	225	PHE
1	A	226	VAL
1	A	230	HIS
1	A	247	VAL
1	A	255	THR
1	A	289	SER
1	A	307	THR
1	A	340	VAL
1	A	353	GLU
1	A	392	ARG
1	A	485	SER
1	A	495	VAL
1	A	502	ARG
1	A	508	LYS
1	A	530	THR
1	A	531	GLN
1	A	551	GLU
1	A	592	ILE
1	B	2	VAL
1	B	9	ASN
1	B	11	GLN
1	B	12	THR
1	B	49	VAL
1	B	65	LEU
1	B	69	SER
1	B	73	LYS
1	B	74	SER
1	B	76	LYS
1	B	92	LEU

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Mol	Chain	Res	Type
1	B	95	ASN
1	B	160	ASP
1	B	162	GLU
1	B	169	VAL
1	B	187	VAL
1	B	188	THR
1	B	193	VAL
1	B	194	GLN
1	B	195	ILE
1	B	201	GLU
1	B	219	LEU
1	B	220	ASN
1	B	247	VAL
1	B	256	LEU
1	B	257	ASN
1	B	258	ILE
1	B	259	SER
1	B	261	GLU
1	B	275	GLN
1	B	289	SER
1	B	307	THR
1	B	353	GLU
1	B	458	ASP
1	B	484	VAL
1	B	486	SER
1	B	495	VAL
1	B	508	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	164	HIS
1	A	177	ASN
1	A	179	ASN
1	A	245	HIS
1	A	270	GLN
1	A	349	ASN
1	A	404	GLN
1	A	516	ASN
1	B	75	HIS
1	B	245	HIS

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Mol	Chain	Res	Type
1	B	268	ASN
1	B	270	GLN
1	B	361	ASN
1	B	586	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\# Z > 2$
4	PO4	A	705	-	4,4,4	2.55	1 (25%)	6,6,6	0.57	0
2	JG4	A	701	-	11,11,11	0.31	0	13,14,14	0.61	0
4	PO4	B	705	-	4,4,4	2.69	1 (25%)	6,6,6	0.75	0
2	JG4	B	701	-	11,11,11	0.26	0	13,14,14	0.53	0
4	PO4	B	706	-	4,4,4	2.61	1 (25%)	6,6,6	0.29	0
4	PO4	A	706	-	4,4,4	2.59	2 (50%)	6,6,6	0.57	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
2	JG4	A	701	-	-	4/4/4/4	0/2/2/2
2	JG4	B	701	-	-	0/4/4/4	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	706	PO4	P-O1	4.46	1.60	1.50
4	B	705	PO4	P-O1	4.40	1.60	1.50
4	A	706	PO4	P-O1	4.33	1.60	1.50
4	A	705	PO4	P-O1	4.27	1.60	1.50
4	A	706	PO4	P-O4	2.01	1.60	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
2	A	701	JG4	S04-C03-C06-N10
2	A	701	JG4	S04-C03-C06-N07
2	A	701	JG4	C02-C03-C06-N10
2	A	701	JG4	C02-C03-C06-N07

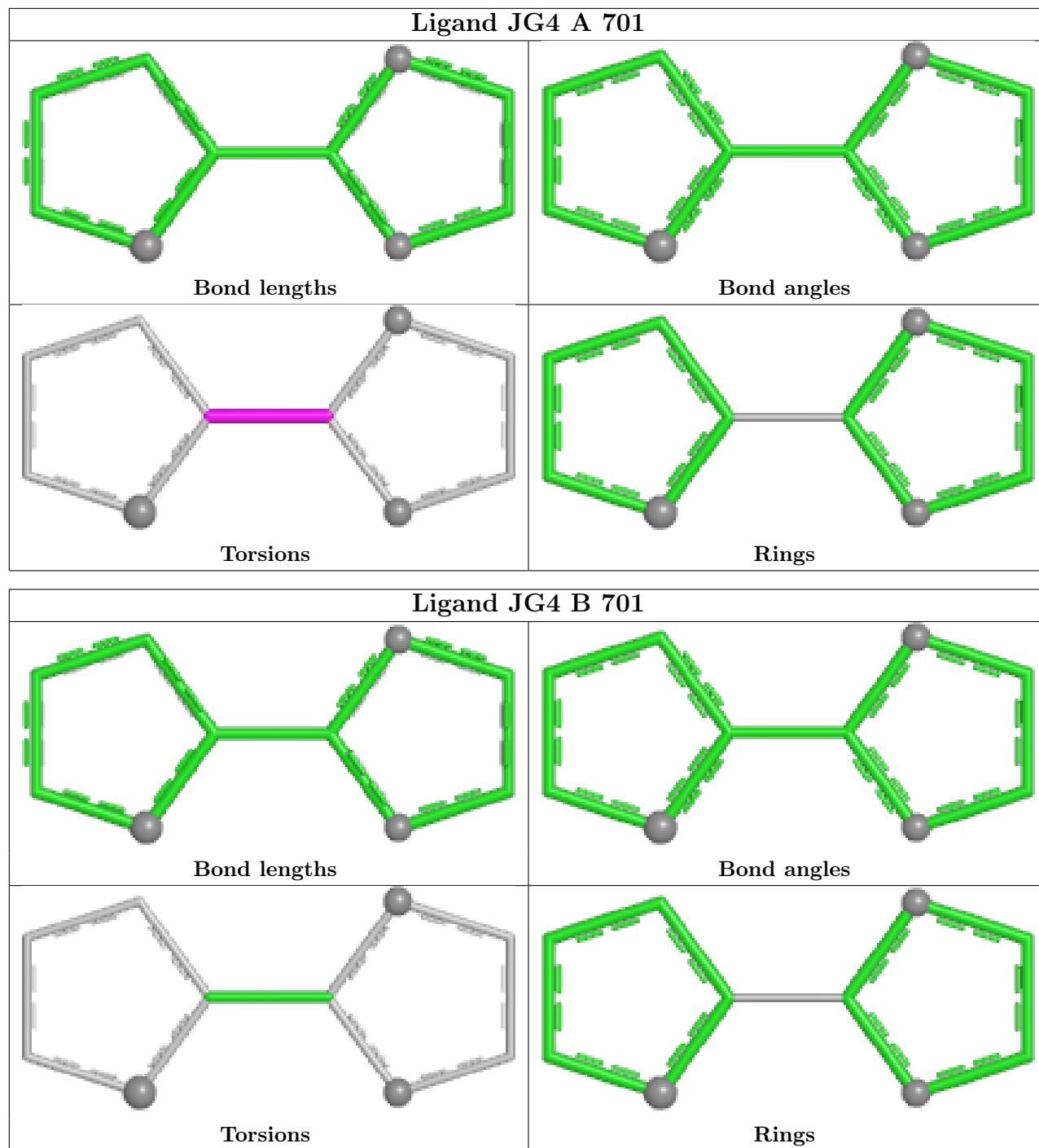
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	JG4	4	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 ⓘ

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%)	0.63	50 (8%)	16 19	49, 104, 184, 231	0
1	B	585/601 (97%)	0.11	9 (1%)	72 76	33, 74, 131, 174	1 (0%)
All	All	1157/1202 (96%)	0.36	59 (5%)	33 39	33, 86, 161, 231	1 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	219	LEU	4.3
1	A	387	VAL	4.2
1	A	272	VAL	4.0
1	A	371	VAL	3.8
1	A	252	LEU	3.8
1	A	305	VAL	3.7
1	A	592	ILE	3.5
1	A	225	PHE	3.3
1	A	170	GLY	3.1
1	A	355	TYR	3.1
1	A	169	VAL	3.1
1	A	304	ILE	3.0
1	A	209	VAL	2.9
1	A	181	VAL	2.9
1	A	258	ILE	2.9
1	A	45	VAL	2.9
1	A	306	TYR	2.8
1	A	393	ALA	2.8
1	A	151	ILE	2.8
1	A	370	ILE	2.8
1	A	6	VAL	2.7
1	B	58	THR	2.7
1	A	396	TYR	2.7
1	A	157	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	53	PRO	2.6
1	A	247	VAL	2.6
1	B	203	GLY	2.6
1	A	356	VAL	2.6
1	A	167	TRP	2.5
1	A	350	SER	2.5
1	A	273	GLY	2.5
1	A	176	LEU	2.4
1	A	226	VAL	2.4
1	A	326	PRO	2.4
1	A	330	CYS	2.4
1	A	103	VAL	2.3
1	A	241	VAL	2.3
1	A	340	VAL	2.3
1	A	31	TYR	2.3
1	A	154	VAL	2.3
1	A	227	LEU	2.2
1	A	325	LEU	2.2
1	A	292	ALA	2.2
1	B	217	TYR	2.2
1	A	254	PRO	2.2
1	A	391	LEU	2.2
1	A	49	VAL	2.2
1	A	351	THR	2.2
1	B	83	LEU	2.1
1	B	81	PHE	2.1
1	A	27	CYS	2.1
1	A	84	CYS	2.1
1	A	333	ILE	2.1
1	B	214	THR	2.1
1	B	98	VAL	2.1
1	B	340	VAL	2.1
1	A	358	CYS	2.0
1	A	249	ILE	2.0
1	A	299	TYR	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 ⓘ

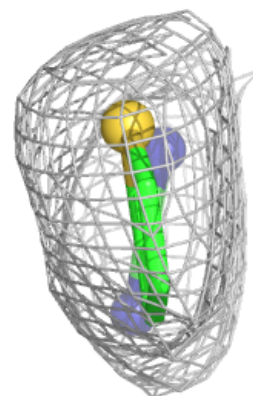
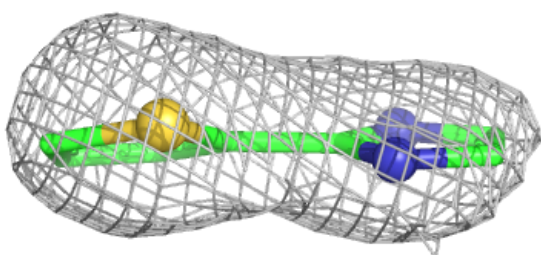
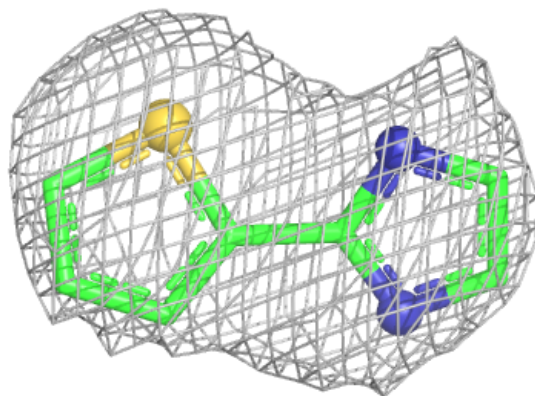
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	JG4	A	701	10/10	0.92	0.10	96,98,99,103	0
2	JG4	B	701	10/10	0.92	0.12	108,112,119,122	0
4	PO4	A	705	5/5	0.94	0.08	87,89,93,94	0
4	PO4	A	706	5/5	0.95	0.07	80,81,83,86	0
4	PO4	B	705	5/5	0.97	0.07	61,65,68,72	0
4	PO4	B	706	5/5	0.98	0.05	68,68,71,76	0
3	ZN	A	702	1/1	0.99	0.04	89,89,89,89	0
3	ZN	A	703	1/1	0.99	0.03	89,89,89,89	0
3	ZN	A	704	1/1	0.99	0.04	139,139,139,139	0
3	ZN	B	704	1/1	0.99	0.05	119,119,119,119	0
3	ZN	B	703	1/1	1.00	0.05	85,85,85,85	0
3	ZN	B	702	1/1	1.00	0.02	75,75,75,75	0

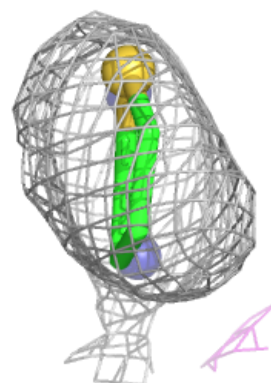
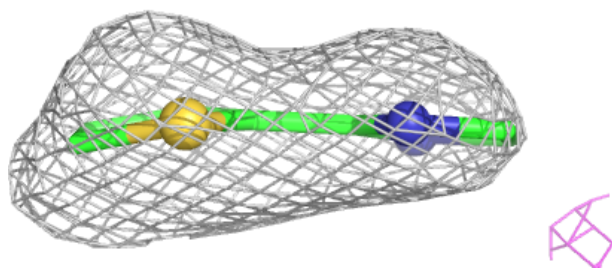
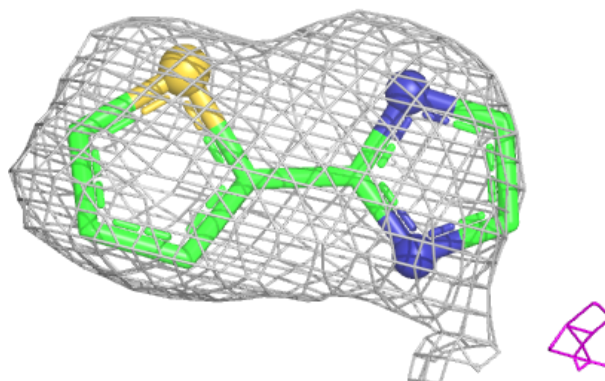
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JG4 A 701:

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

**Electron density around JG4 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.