WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Sep 1, 2022 – 12:05 PM EDT

PDB ID	:	5RMJ
Title	:	PanDDA analysis group deposition – Crystal Structure of SARS-CoV-2 helicase in complex with Z68299550
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	:	2.10 Å(reported)

The following versions of software and data (see references ①) were used in the production of this report:

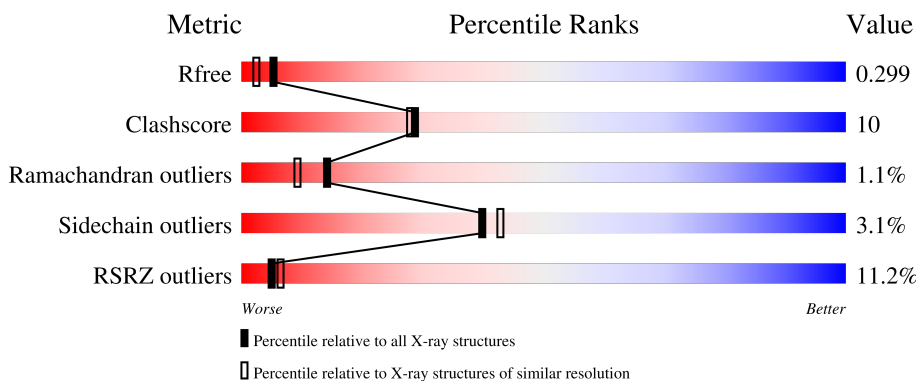|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 2.10 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	Percentile Ranks	Value
Rfree		0.299
Clashscore		10
Ramachandran outliers		1.1%
Sidechain outliers		3.1%
RSRZ outliers		11.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	601	16% 73% 21% • 5%
1	B	601	5% 76% 20% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

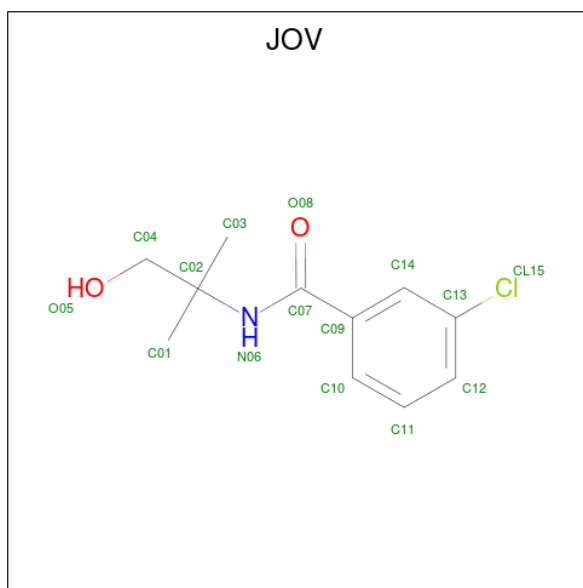| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZN	B	703	-	-	X	-

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
			Total	C	N	O	S			
1	B	585	4508	2875	750	848	35	0	1	0
1	A	572	Total	C	N	O	S	0	0	0
			4417	2816	737	832	32			

- Molecule 2 is 3-chloro-N-(1-hydroxy-2-methylpropan-2-yl)benzamide (three-letter code: JOV) (formula: $C_{11}H_{14}ClNO_2$) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
2	B	1	15	11	1	1	2	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

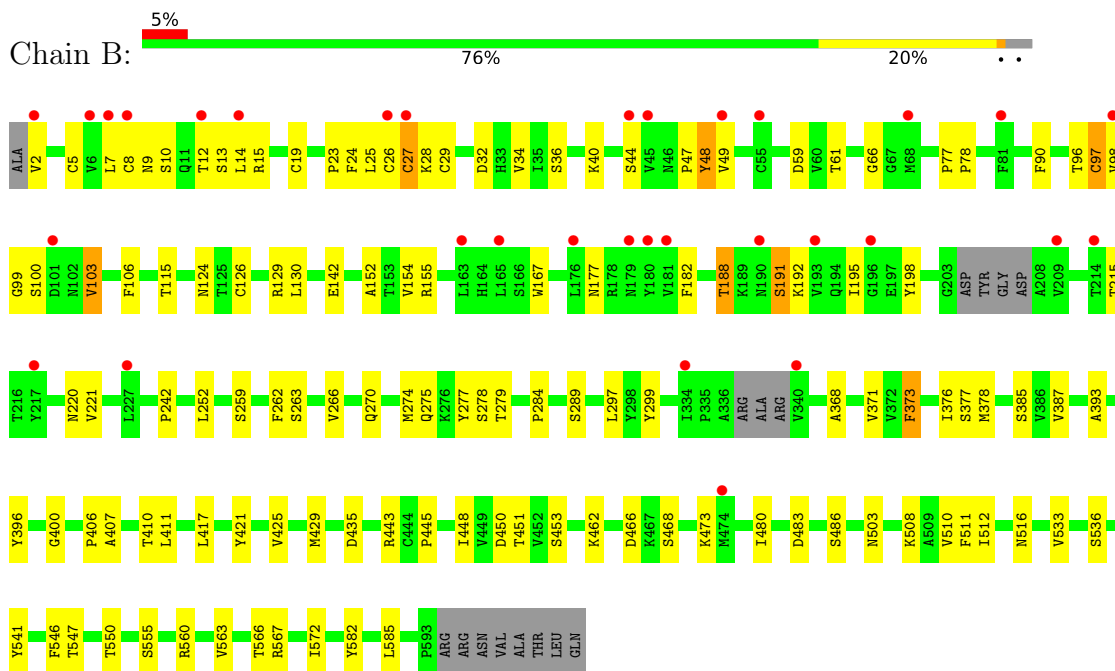| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total O P 5 4 1			0	0
4	B	1	Total O P 5 4 1			0	0
4	A	1	Total O P 5 4 1			0	0
4	A	1	Total O P 5 4 1			0	0

- Molecule 5 is water.

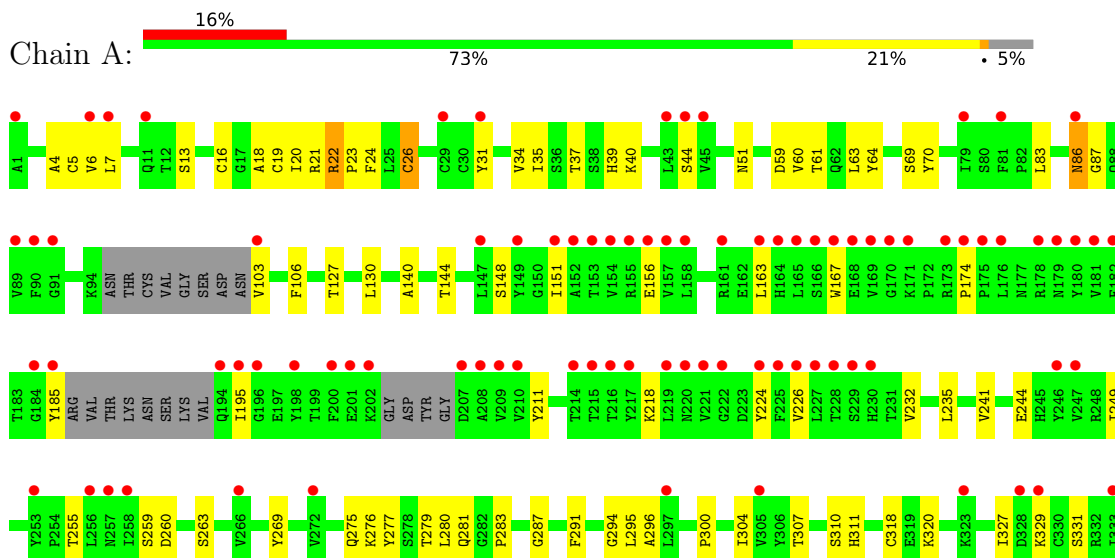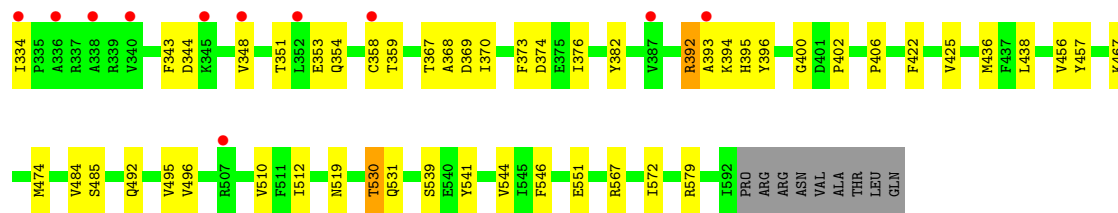| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	250	Total O 250 250		0	0
5	A	205	Total O 205 205		0	0

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

Chain B:

- Molecule 1: Helicase

Chain A:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	58.84Å 70.14Å 85.26Å 103.14° 95.74° 112.26°	Depositor
Resolution (Å)	81.23 – 2.10 81.23 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.9 (81.23-2.10) 95.9 (81.23-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.233 , 0.296 0.249 , 0.299	Depositor DCC
R_{free} test set	3479 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å^2)	34.7	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.7	EDS
L-test for twinning[2]	$< |L| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9421	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.99% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, JOV, 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	0.72	0/4517	0.82	0/6156
1	B	0.70	0/4610	0.84	0/6283
All	All	0.71	0/9127	0.83	0/12439

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	443	ARG	Peptide

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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4417	0	4321	74	0
1	B	4508	0	4426	97	0
2	B	15	0	0	1	0
3	A	3	0	0	0	0
3	B	3	0	0	4	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
5	A	205	0	0	11	1
5	B	250	0	0	14	1
All	All	9421	0	8747	171	1

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 10.

All (171) 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:8:CYS:SG	1:B:99:GLY:N	2.43	0.90
1:A:13:SER:OG	1:A:44:SER:HB2	1.76	0.86
1:B:12:THR:HG21	1:B:26:CYS:HA	1.60	0.82
1:B:26:CYS:HG	3:B:703:ZN:ZN	0.94	0.79
1:B:8:CYS:SG	1:B:99:GLY:O	2.43	0.77
1:B:5:CYS:SG	3:B:703:ZN:ZN	1.71	0.77
1:B:385:SER:OG	5:B:801:HOH:O	2.00	0.75
1:A:287:GLY:HA2	5:A:886:HOH:O	1.87	0.74
1:A:60:VAL:HB	5:A:933:HOH:O	1.89	0.72
1:A:327:ILE:O	5:A:802:HOH:O	2.11	0.69
1:B:7:LEU:HD12	1:B:103:VAL:HG22	1.75	0.68
1:B:12:THR:CG2	1:B:26:CYS:HA	2.23	0.68
1:B:32:ASP:O	1:B:36:SER:OG	2.12	0.68
1:B:26:CYS:SG	3:B:703:ZN:ZN	1.83	0.67
1:B:177:ASN:HB3	1:B:516:ASN:ND2	2.09	0.66
1:B:7:LEU:CD1	1:B:103:VAL:HG22	2.27	0.64
1:B:275:GLN:NE2	1:B:435:ASP:OD2	2.29	0.63
1:B:14:LEU:HB2	1:B:25:LEU:O	1.99	0.62
1:A:368:ALA:O	1:A:393:ALA:HA	1.99	0.62
1:B:510:VAL:HG21	1:B:541:TYR:CD1	2.34	0.62
1:B:28:LYS:CB	1:B:97:CYS:SG	2.88	0.61
1:A:4:ALA:O	1:A:24:PHE:HB2	2.00	0.61
1:A:579:ARG:NE	5:A:813:HOH:O	2.32	0.60
1:B:279:THR:HB	1:B:429:MET:CE	2.33	0.59
1:B:270:GLN:O	1:B:274:MET:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:GLU:HB2	1:A:276:LYS:HB2	1.85	0.58
1:A:64:TYR:O	1:A:70:TYR:HA	2.04	0.58
1:B:13:SER:O	1:B:44:SER:HA	2.04	0.57
1:A:34:VAL:O	1:A:40:LYS:NZ	2.25	0.57
1:A:376:ILE:HG12	1:A:425:VAL:HG11	1.86	0.57
1:B:378:MET:O	1:B:407:ALA:HB2	2.03	0.57
1:A:467:LYS:NZ	5:A:809:HOH:O	2.28	0.56
1:B:48:TYR:OH	1:B:90:PHE:O	2.16	0.56
1:B:448:ILE:HD11	1:B:572:ILE:CG2	2.36	0.56
1:A:329:LYS:HE2	1:A:354:GLN:OE1	2.06	0.55
1:B:7:LEU:HD21	1:B:106:PHE:HB2	1.87	0.55
1:B:508:LYS:HD3	5:B:857:HOH:O	2.07	0.55
1:B:5:CYS:SG	1:B:29:CYS:SG	3.06	0.54
1:A:519:ASN:HB3	1:A:530:THR:HG23	1.90	0.54
1:B:26:CYS:SG	1:B:29:CYS:SG	3.06	0.54
1:A:512:ILE:O	1:A:546:PHE:HA	2.08	0.53
1:B:115:THR:HA	1:B:411:LEU:O	2.08	0.53
1:B:252:LEU:HB3	1:B:299:TYR:CD1	2.42	0.53
1:A:492:GLN:O	1:A:496:VAL:HG23	2.09	0.53
1:A:269:TYR:CD1	1:A:295:LEU:HD13	2.44	0.53
1:A:281:GLN:HG3	1:A:402:PRO:HD2	1.91	0.52
1:A:59:ASP:OD1	1:A:61:THR:OG1	2.18	0.52
1:A:280:LEU:HD12	1:A:436:MET:O	2.09	0.52
1:B:279:THR:HB	1:B:429:MET:HE2	1.90	0.52
1:A:367:THR:HA	1:A:392:ARG:O	2.10	0.52
1:A:539:SER:O	1:A:567:ARG:HD3	2.10	0.51
1:A:519:ASN:HB3	1:A:530:THR:CG2	2.40	0.51
1:B:12:THR:OG1	1:B:26:CYS:HA	2.11	0.51
1:B:195:ILE:HG23	1:B:195:ILE:O	2.11	0.51
1:B:376:ILE:HG12	1:B:425:VAL:HG11	1.92	0.51
1:B:466:ASP:HB3	5:B:990:HOH:O	2.10	0.51
1:B:27:CYS:SG	5:B:952:HOH:O	2.17	0.51
1:B:15:ARG:HA	1:B:23:PRO:O	2.11	0.51
1:B:5:CYS:O	1:B:9:ASN:N	2.36	0.51
1:A:374:ASP:OD2	5:A:803:HOH:O	2.19	0.51
1:A:260:ASP:HA	1:A:263:SER:OG	2.11	0.50
1:B:483:ASP:O	5:B:804:HOH:O	2.20	0.50
1:B:26:CYS:O	1:B:29:CYS:N	2.45	0.50
1:B:277:TYR:HA	1:B:396:TYR:O	2.12	0.50
1:B:47:PRO:O	1:B:49:VAL:HG12	2.12	0.50
1:A:167:TRP:CZ3	1:A:174:PRO:HD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:VAL:N	5:B:828:HOH:O	2.45	0.50
1:A:86:ASN:N	1:A:86:ASN:HD22	2.09	0.50
1:B:47:PRO:O	5:B:805:HOH:O	2.20	0.49
1:A:510:VAL:HG21	1:A:541:TYR:CD1	2.47	0.49
1:B:8:CYS:SG	1:B:98:VAL:HB	2.52	0.49
1:B:142:GLU:OE2	5:B:803:HOH:O	2.19	0.49
1:B:445:PRO:HG2	1:B:448:ILE:HD12	1.95	0.49
1:B:448:ILE:HD11	1:B:572:ILE:HG21	1.96	0.48
1:A:275:GLN:O	1:A:395:HIS:ND1	2.43	0.48
1:B:124:ASN:HD22	1:B:421:TYR:HA	1.79	0.48
1:B:19:CYS:HB2	1:B:23:PRO:HD2	1.94	0.48
1:A:279:THR:HG21	5:A:850:HOH:O	2.13	0.48
1:B:103:VAL:CG1	1:B:103:VAL:O	2.61	0.48
1:A:296:ALA:O	1:A:300:PRO:HA	2.13	0.48
1:B:377:SER:O	1:B:406:PRO:HA	2.14	0.47
1:B:410:THR:HG23	5:B:895:HOH:O	2.13	0.47
1:B:462:LYS:NZ	5:B:829:HOH:O	2.45	0.47
1:B:373:PHE:CE1	1:B:387:VAL:HG21	2.49	0.47
1:B:371:VAL:HG23	1:B:393:ALA:HB2	1.95	0.47
1:A:277:TYR:HA	1:A:396:TYR:O	2.14	0.47
1:B:188:THR:HG1	1:B:191:SER:H	1.63	0.47
1:A:4:ALA:O	1:A:24:PHE:CB	2.61	0.47
1:B:7:LEU:CD2	1:B:130:LEU:HD21	2.46	0.46
1:B:368:ALA:O	1:B:393:ALA:HA	2.16	0.46
1:B:510:VAL:HG21	1:B:541:TYR:CG	2.51	0.46
1:B:445:PRO:HB3	1:B:468:SER:HB3	1.96	0.46
1:A:163:LEU:HD23	1:A:211:TYR:CD2	2.50	0.46
1:A:7:LEU:HD21	1:A:130:LEU:HD21	1.97	0.46
1:B:376:ILE:HG22	1:B:400:GLY:HA3	1.98	0.46
1:B:473:LYS:HE3	1:B:582:TYR:CZ	2.50	0.46
1:A:19:CYS:HB2	1:A:23:PRO:HD2	1.98	0.46
1:A:5:CYS:SG	1:A:26:CYS:HB3	2.56	0.46
1:A:21:ARG:O	1:A:22:ARG:HB2	2.16	0.45
1:A:280:LEU:HD11	1:A:438:LEU:HG	1.98	0.45
1:B:220:ASN:N	1:B:220:ASN:OD1	2.49	0.45
1:A:320:LYS:NZ	5:A:815:HOH:O	2.34	0.45
1:A:7:LEU:HD13	1:A:103:VAL:HG22	1.99	0.45
1:A:318:CYS:HB3	1:A:343:PHE:CD2	2.52	0.45
1:A:331:SER:HB2	1:A:353:GLU:HG3	1.99	0.45
1:B:503:ASN:ND2	2:B:701:JOV:O08	2.40	0.45
1:B:182:PHE:N	1:B:198:TYR:O	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:GLU:HG3	5:A:897:HOH:O	2.17	0.44
1:A:291:PHE:C	1:A:291:PHE:CD1	2.90	0.44
1:B:5:CYS:SG	1:B:29:CYS:HB2	2.58	0.44
1:B:279:THR:HB	1:B:429:MET:HE3	2.00	0.44
1:B:451:THR:HG21	1:B:585:LEU:HD23	2.00	0.44
1:B:59:ASP:OD1	1:B:61:THR:OG1	2.30	0.44
1:B:5:CYS:HG	3:B:703:ZN:ZN	1.27	0.44
1:A:21:ARG:NH1	5:A:836:HOH:O	2.51	0.44
1:A:37:THR:OG1	1:A:39:HIS:HB2	2.18	0.43
1:B:12:THR:HG21	1:B:25:LEU:O	2.17	0.43
1:B:512:ILE:O	1:B:546:PHE:HA	2.19	0.43
1:B:533:VAL:HG11	1:B:560:ARG:O	2.18	0.43
1:A:151:ILE:HG12	1:A:226:VAL:HG22	1.99	0.43
1:A:140:ALA:HA	1:A:232:VAL:HG21	2.01	0.43
1:B:284:PRO:HG2	1:B:566:THR:HG21	2.01	0.43
1:B:417:LEU:HA	5:B:868:HOH:O	2.18	0.43
1:B:450:ASP:OD1	5:B:806:HOH:O	2.21	0.43
1:B:563:VAL:O	1:B:567:ARG:HG2	2.19	0.43
1:A:370:ILE:HA	1:A:395:HIS:O	2.19	0.43
1:B:511:PHE:HZ	1:B:547:THR:HG1	1.63	0.43
1:A:241:VAL:HG22	5:A:840:HOH:O	2.19	0.43
1:B:66:GLY:HA3	1:B:77:PRO:CG	2.49	0.42
1:A:307:THR:HA	1:A:358:CYS:O	2.19	0.42
1:B:480:ILE:HD13	1:B:550:THR:HG22	2.00	0.42
1:A:31:TYR:CE2	1:A:87:GLY:HA2	2.53	0.42
1:A:456:VAL:HG23	1:A:457:TYR:CD2	2.54	0.42
1:B:7:LEU:HD21	1:B:130:LEU:HD21	2.00	0.42
1:A:20:ILE:HD11	1:A:144:THR:HG21	2.01	0.42
1:A:235:LEU:HD21	1:A:382:TYR:CE2	2.54	0.42
1:A:304:ILE:HG12	1:A:370:ILE:HB	2.01	0.42
1:A:474:MET:SD	1:A:495:VAL:HG11	2.59	0.42
1:A:7:LEU:HD21	1:A:106:PHE:HB2	2.01	0.42
1:A:276:LYS:O	1:A:395:HIS:HA	2.19	0.42
1:B:154:VAL:HG12	1:B:221:VAL:HA	2.02	0.42
1:B:480:ILE:HG21	1:B:550:THR:HG22	2.00	0.42
1:B:262:PHE:CE2	1:B:297:LEU:HD12	2.54	0.42
1:A:334:ILE:HD12	1:A:348:VAL:HG13	2.02	0.42
1:B:12:THR:HG21	1:B:26:CYS:CA	2.42	0.42
1:B:14:LEU:O	1:B:24:PHE:HA	2.20	0.42
1:A:127:THR:HG22	1:A:130:LEU:HB2	2.01	0.42
1:A:369:ASP:O	1:A:394:LYS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:PRO:HG3	1:A:422:PHE:CE1	2.55	0.42
1:B:263:SER:HA	1:B:266:VAL:HG23	2.02	0.41
1:B:15:ARG:HG3	1:B:24:PHE:CD2	2.55	0.41
1:B:242:PRO:HA	5:B:968:HOH:O	2.20	0.41
1:B:373:PHE:CD1	1:B:387:VAL:HG21	2.55	0.41
1:B:13:SER:O	1:B:13:SER:OG	2.37	0.41
1:B:34:VAL:O	1:B:40:LYS:NZ	2.48	0.41
1:A:86:ASN:HD22	1:A:86:ASN:H	1.68	0.41
1:A:269:TYR:OH	1:A:294:GLY:HA3	2.20	0.41
1:B:19:CYS:CB	1:B:23:PRO:HD2	2.51	0.41
1:B:129:ARG:HA	1:B:129:ARG:HD2	1.83	0.41
1:A:512:ILE:HA	1:A:531:GLN:O	2.20	0.41
1:B:152:ALA:HB2	1:B:167:TRP:CZ3	2.55	0.41
1:A:185:TYR:HB2	1:A:224:TYR:CZ	2.55	0.41
1:A:281:GLN:HA	1:A:400:GLY:O	2.21	0.41
1:A:311:HIS:ND1	1:A:359:THR:HG21	2.36	0.40
1:A:544:VAL:O	1:A:572:ILE:HA	2.21	0.40
1:A:63:LEU:HB3	1:A:83:LEU:HD12	2.03	0.40
1:B:516:ASN:ND2	5:B:851:HOH:O	2.55	0.40
1:B:77:PRO:HB2	1:B:78:PRO:HD2	2.03	0.40
1:B:99:GLY:O	1:B:100:SER:OG	2.34	0.40
1:A:16:CYS:SG	1:A:18:ALA:HB3	2.62	0.40
1:A:140:ALA:O	1:A:144:THR:HG23	2.21	0.40

All (1) 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)
5:B:944:HOH:O	5:A:917:HOH:O[1_556]	2.16	0.04

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%)	517 (92%)	39 (7%)	8 (1%)	11	6
1	B	580/601 (96%)	532 (92%)	43 (7%)	5 (1%)	17	12
All	All	1144/1202 (95%)	1049 (92%)	82 (7%)	13 (1%)	14	9

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	ILE
1	A	351	THR
1	B	126	CYS
1	A	195	ILE
1	A	283	PRO
1	A	484	VAL
1	B	27	CYS
1	B	48	TYR
1	B	97	CYS
1	B	10	SER
1	A	218	LYS
1	A	22	ARG
1	A	6	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%)	470 (97%)	15 (3%)	40	43
1	B	498/523 (95%)	483 (97%)	15 (3%)	41	44
All	All	983/1046 (94%)	953 (97%)	30 (3%)	40	43

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	96	THR
1	B	103	VAL
1	B	155	ARG

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Mol	Chain	Res	Type
1	B	188	THR
1	B	191	SER
1	B	192	LYS
1	B	215	THR
1	B	259	SER
1	B	278	SER
1	B	289	SER
1	B	373	PHE
1	B	453	SER
1	B	486	SER
1	B	536	SER
1	B	555	SER
1	A	26	CYS
1	A	35	ILE
1	A	51	ASN
1	A	69	SER
1	A	86	ASN
1	A	148	SER
1	A	156	GLU
1	A	255	THR
1	A	259	SER
1	A	310	SER
1	A	344	ASP
1	A	373	PHE
1	A	392	ARG
1	A	485	SER
1	A	530	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	51	ASN
1	B	62	GLN
1	B	179	ASN
1	B	268	ASN
1	B	470	GLN
1	B	516	ASN
1	A	86	ASN
1	A	116	ASN
1	A	179	ASN
1	A	275	GLN
1	A	503	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
4	PO4	B	705	-	4,4,4	1.05	0	6,6,6	0.42	0
4	PO4	A	705	-	4,4,4	0.80	0	6,6,6	0.58	0
4	PO4	B	706	-	4,4,4	1.19	0	6,6,6	0.52	0
2	JOV	B	701	-	15,15,15	0.33	0	21,21,21	0.40	0
4	PO4	A	704	-	4,4,4	0.71	0	6,6,6	0.46	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	JOV	B	701	-	-	4/12/12/12	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.
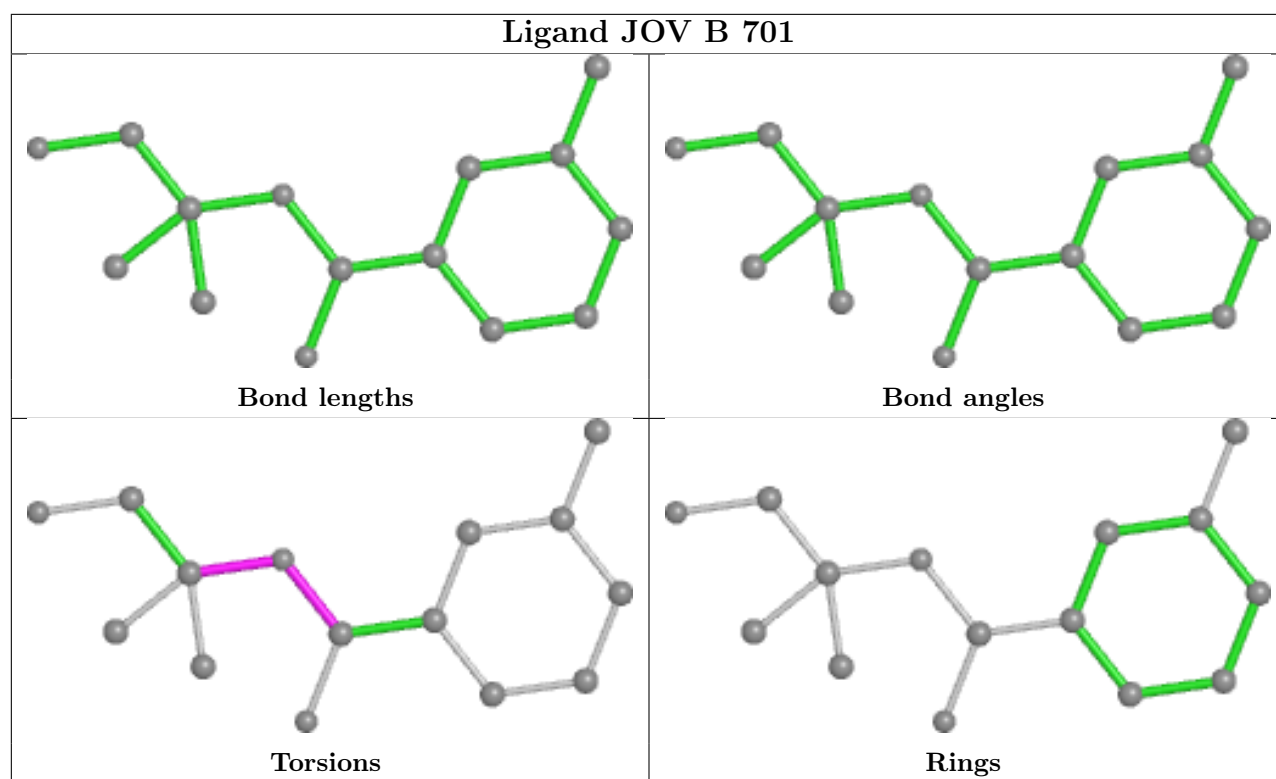
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	JOV	C09-C07-N06-C02
2	B	701	JOV	C01-C02-N06-C07
2	B	701	JOV	O08-C07-N06-C02
2	B	701	JOV	C03-C02-N06-C07

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	JOV	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 then 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.

Ligand JOV B 701

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	572/601 (95%)	0.91	98 (17%)	1	1	26, 65, 142, 188	0
1	B	585/601 (97%)	0.29	32 (5%)	25	31	26, 48, 105, 133	2 (0%)
All	All	1157/1202 (96%)	0.60	130 (11%)	5	6	26, 54, 128, 188	2 (0%)

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	169	VAL	14.6
1	A	219	LEU	13.4
1	A	178	ARG	9.5
1	A	225	PHE	9.2
1	A	167	TRP	8.3
1	A	149	TYR	8.0
1	A	221	VAL	7.9
1	A	176	LEU	7.6
1	A	207	ASP	7.4
1	B	45	VAL	7.4
1	A	152	ALA	7.4
1	A	202	LYS	7.3
1	B	163	LEU	7.1
1	A	229	SER	7.0
1	A	170	GLY	6.9
1	A	200	PHE	6.8
1	A	228	THR	6.5
1	B	7	LEU	6.0
1	A	182	PHE	5.8
1	B	217	TYR	5.5
1	A	156	GLU	5.3
1	A	216	THR	5.1
1	A	247	VAL	5.1
1	A	222	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	154	VAL	5.0
1	A	210	VAL	4.9
1	A	157	VAL	4.8
1	A	90	PHE	4.7
1	B	81	PHE	4.6
1	A	215	THR	4.6
1	A	158	LEU	4.5
1	A	155	ARG	4.5
1	A	340	VAL	4.5
1	A	336	ALA	4.3
1	A	81	PHE	4.2
1	A	195	ILE	4.2
1	A	334	ILE	4.2
1	A	184	GLY	4.2
1	A	224	TYR	4.2
1	B	179	ASN	4.1
1	A	305	VAL	4.1
1	B	2	VAL	4.1
1	B	214	THR	4.1
1	B	6	VAL	4.0
1	B	176	LEU	3.9
1	A	153	THR	3.8
1	A	230	HIS	3.8
1	A	227	LEU	3.6
1	A	253	TYR	3.6
1	B	12	THR	3.5
1	A	214	THR	3.4
1	A	45	VAL	3.4
1	A	174	PRO	3.4
1	A	7	LEU	3.4
1	A	161	ARG	3.3
1	A	352	LEU	3.3
1	A	168	GLU	3.3
1	B	101	ASP	3.2
1	B	27	CYS	3.2
1	A	185	TYR	3.2
1	A	256	LEU	3.1
1	A	151	ILE	3.1
1	A	181	VAL	3.1
1	A	91	GLY	3.1
1	A	165	LEU	3.1
1	B	181	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	209	VAL	3.1
1	A	198	TYR	3.1
1	A	345	LYS	3.0
1	A	297	LEU	3.0
1	B	68	MET	3.0
1	A	44	SER	3.0
1	A	86	ASN	3.0
1	A	179	ASN	3.0
1	A	180	TYR	2.9
1	B	8	CYS	2.9
1	A	209	VAL	2.9
1	A	208	ALA	2.9
1	A	147	LEU	2.9
1	B	98	VAL	2.8
1	A	333	ILE	2.8
1	B	193	VAL	2.8
1	B	474[A]	MET	2.7
1	B	334	ILE	2.7
1	A	103	VAL	2.7
1	A	217	TYR	2.7
1	A	220	ASN	2.7
1	A	163	LEU	2.7
1	A	246	TYR	2.7
1	A	173	ARG	2.7
1	A	272	VAL	2.7
1	B	44	SER	2.7
1	A	323	LYS	2.7
1	B	196	GLY	2.6
1	B	190	ASN	2.6
1	A	31	TYR	2.6
1	A	226	VAL	2.6
1	A	194	GLN	2.6
1	A	196	GLY	2.5
1	A	6	VAL	2.5
1	A	171	LYS	2.5
1	A	166	SER	2.5
1	A	89	VAL	2.5
1	A	338	ALA	2.4
1	B	227	LEU	2.4
1	A	175	PRO	2.4
1	B	55	CYS	2.4
1	A	393	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	387	VAL	2.3
1	B	14	LEU	2.3
1	B	49	VAL	2.3
1	A	11	GLN	2.3
1	A	266	VAL	2.3
1	A	43	LEU	2.3
1	B	180	TYR	2.2
1	A	348	VAL	2.2
1	A	79	ILE	2.2
1	A	328	ASP	2.2
1	A	164	HIS	2.2
1	A	1	ALA	2.2
1	A	257	ASN	2.2
1	A	258	ILE	2.2
1	B	340	VAL	2.2
1	B	165	LEU	2.1
1	A	507	ARG	2.1
1	B	26	CYS	2.1
1	A	329	LYS	2.1
1	A	29	CYS	2.1
1	A	201	GLU	2.0
1	A	358	CYS	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 monosaccharides 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.
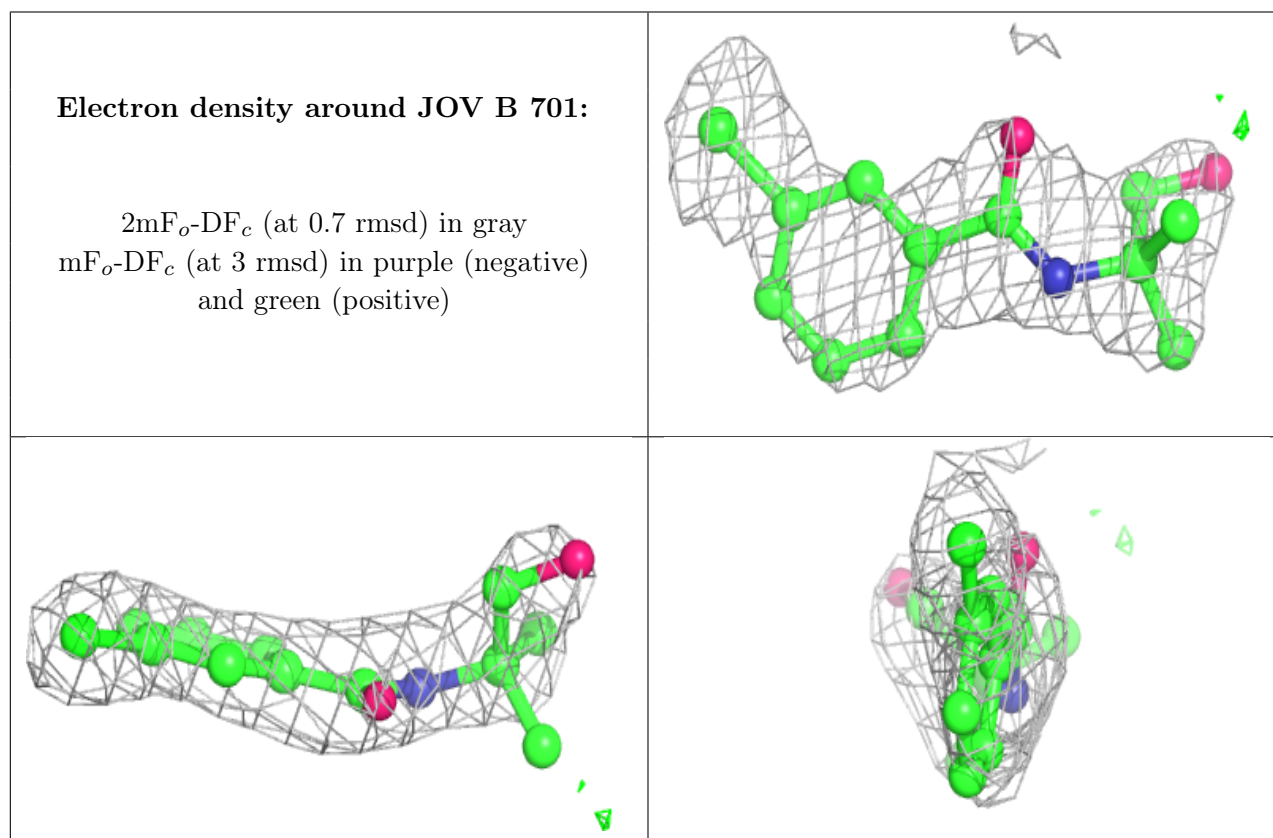
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	JOV	B	701	15/15	0.89	0.25	38,41,43,46	15

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	A	703	1/1	0.89	0.08	102,102,102,102	0
3	ZN	B	704	1/1	0.90	0.13	78,78,78,78	0
3	ZN	B	703	1/1	0.94	0.11	66,66,66,66	0
3	ZN	A	702	1/1	0.95	0.11	57,57,57,57	0
4	PO4	B	705	5/5	0.96	0.13	33,36,47,50	0
4	PO4	B	706	5/5	0.96	0.12	32,34,42,42	0
3	ZN	A	701	1/1	0.97	0.11	62,62,62,62	0
4	PO4	A	705	5/5	0.97	0.13	45,48,52,60	0
4	PO4	A	704	5/5	0.98	0.12	35,39,43,48	0
3	ZN	B	702	1/1	0.98	0.11	42,42,42,42	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 JOV 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.