



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:36 AM UTC

PDB ID : 5RMJ / pdb_00005rmj
Title : PanDDA analysis group deposition – Crystal Structure of SARS-CoV-2 heli-
case 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)

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)

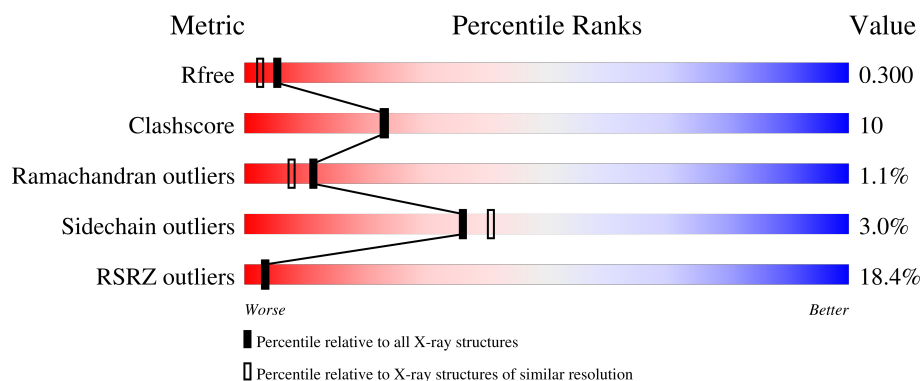
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 $\leq 5\%$. 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	24% 72% 23% 5%
1	B	601	11% 73% 23% ..

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
3	ZN	B	703	-	-	X	-

2 Entry composition [i](#)

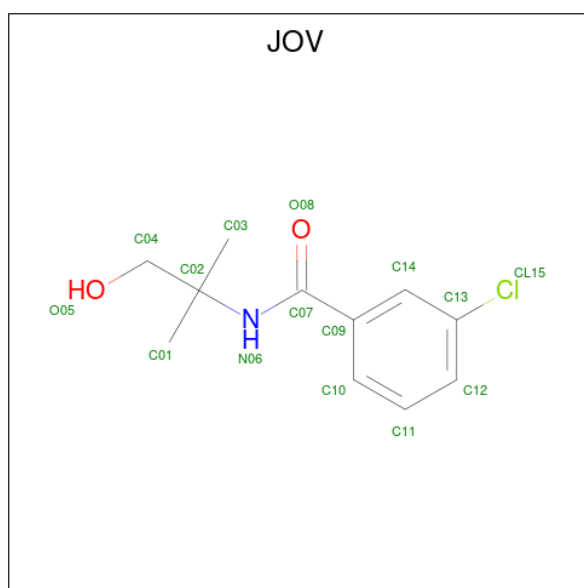
There are 5 unique types of molecules in this entry. The entry contains 9421 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	B	585	Total	C	N	O	S	0	1	0
			4508	2875	750	848	35			
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 (CCD ID: JOV) (formula: $C_{11}H_{14}ClNO_2$) (labeled as "Ligand of Interest" by depositor).



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

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

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

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

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



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

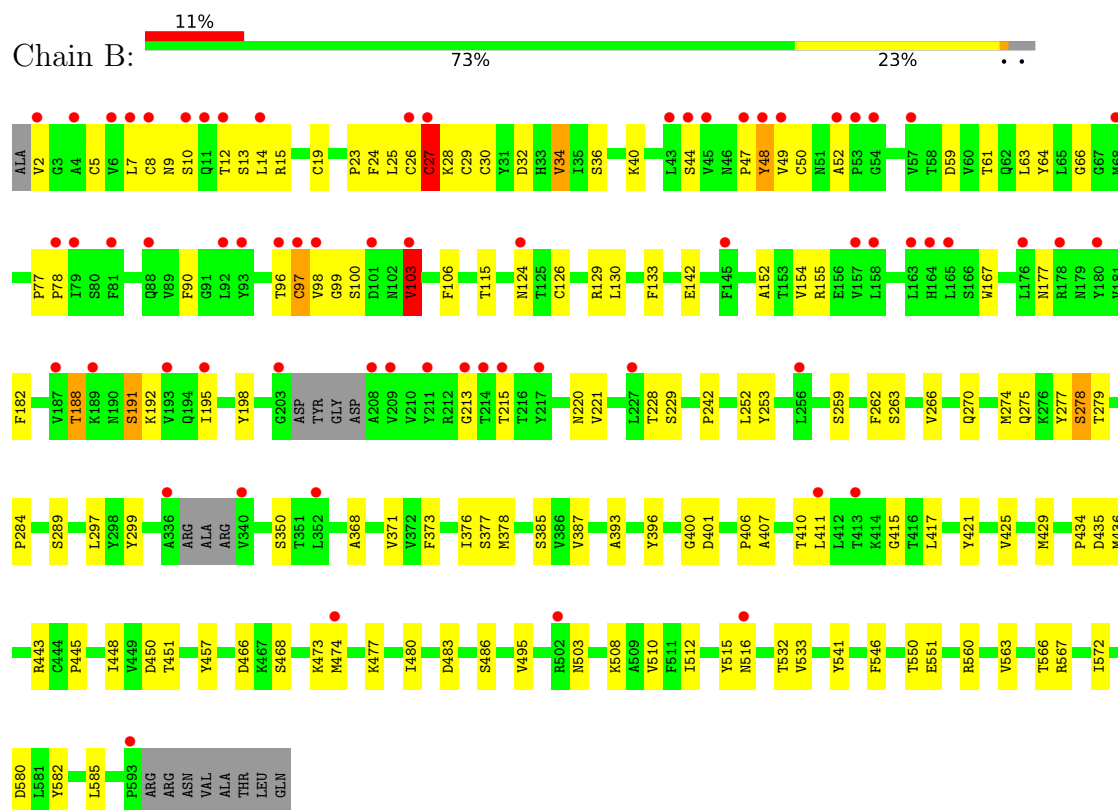
- Molecule 5 is water.

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

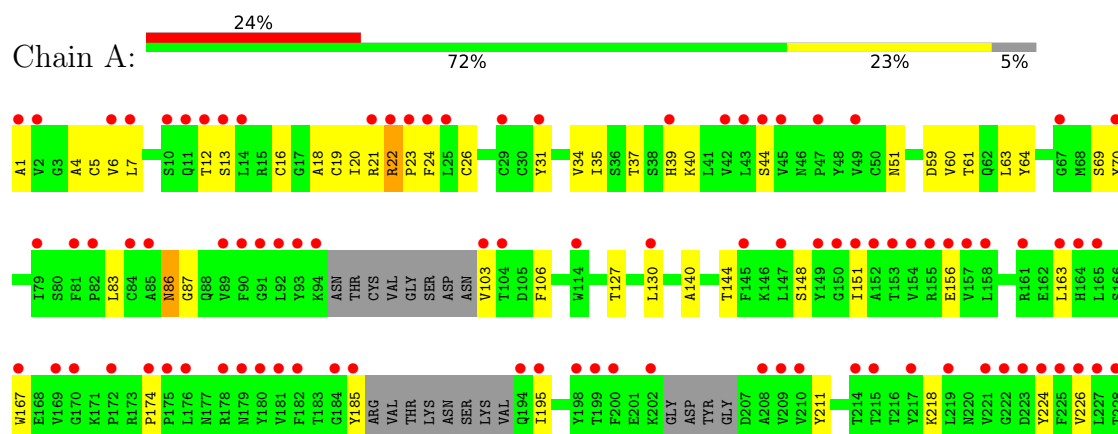
3 Residue-property plots

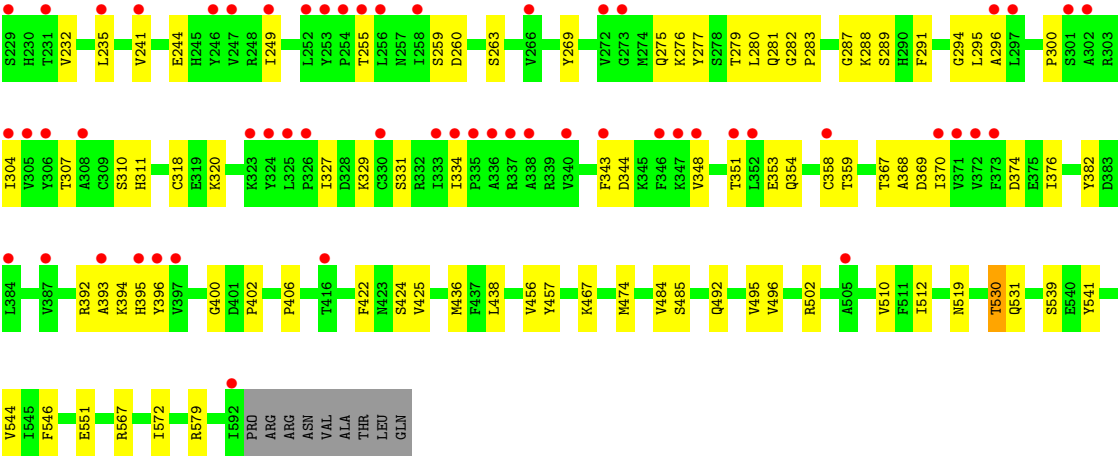
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.233 , 0.296 0.252 , 0.300	Depositor DCC
R_{free} test set	3620 reflections (5.16%)	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)	0.32 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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: JOV, 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	1.10	0/4517	1.43	2/6156 (0.0%)
1	B	1.06	0/4610	1.42	14/6283 (0.2%)
All	All	1.08	0/9127	1.42	16/12439 (0.1%)

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.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	253	TYR	CB-CA-C	6.72	117.18	110.33
1	B	415	GLY	CA-C-O	-6.19	117.96	122.23
1	B	103	VAL	N-CA-C	-6.15	106.99	112.90
1	B	34	VAL	CA-C-O	-5.47	115.26	120.95
1	A	289	SER	CA-C-N	5.38	127.75	120.38
1	A	289	SER	C-N-CA	5.38	127.75	120.38
1	B	580	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	350	SER	CA-C-N	5.26	127.59	120.38
1	B	350	SER	C-N-CA	5.26	127.59	120.38
1	B	213	GLY	CA-C-N	5.16	127.51	120.54
1	B	213	GLY	C-N-CA	5.16	127.51	120.54
1	B	434	PRO	CA-C-O	-5.12	115.62	121.86
1	B	30	CYS	CA-C-N	5.08	127.54	120.63
1	B	30	CYS	C-N-CA	5.08	127.54	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	228	THR	CB-CA-C	5.06	117.98	109.89
1	B	133	PHE	CA-C-O	-5.02	115.52	120.90

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 ⓘ

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	78	0
1	B	4508	0	4426	104	0
2	B	15	0	0	1	0
3	A	3	0	0	0	0
3	B	3	0	0	3	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
5	A	205	0	0	13	1
5	B	250	0	0	13	1
All	All	9421	0	8747	182	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 (182) 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	0.93	0.80
1:B:8:CYS:SG	1:B:99:GLY:O	2.43	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:279:THR:HB	1:B:429:MET:HE2	1.69	0.74
1:A:60:VAL:HB	5:A:933:HOH:O	1.89	0.72
1:A:224:TYR:OH	5:A:801:HOH:O	2.09	0.69
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:A:467:LYS:NZ	5:A:809:HOH:O	2.28	0.66
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:A:59:ASP:OD1	1:A:61:THR:OG1	2.18	0.62
1:B:28:LYS:CB	1:B:97:CYS:SG	2.88	0.61
1:A:320:LYS:NZ	5:A:815:HOH:O	2.34	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
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:B:278:SER:HB2	1:B:436:MET:HE2	1.85	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:280:LEU:HD12	1:A:436:MET:O	2.09	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: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:195:ILE:HG23	1:B:195:ILE:O	2.11	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:B:401:ASP:OD2	1:B:457:TYR:OH	2.25	0.50
1:A:167:TRP:CZ3	1:A:174:PRO:HD2	2.46	0.50
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:477:LYS:NZ	1:B:551:GLU:OE2	2.30	0.49
1:A:291:PHE:C	1:A:291:PHE:CD1	2.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:THR:HG23	5:B:895:HOH:O	2.13	0.47
1:A:1:ALA:N	5:A:816:HOH:O	2.40	0.47
1:B:373:PHE:CE1	1:B:387:VAL:HG21	2.49	0.47
1:B:188:THR:HG1	1:B:191:SER:H	1.62	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: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:B:474[B]:MET:HE2	1:B:474[B]:MET:HB3	1.64	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: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
1:A:5:CYS:C	1:A:7:LEU:H	2.25	0.44
1:A:551:GLU:HG3	5:A:897:HOH:O	2.17	0.44
1:B:5:CYS:SG	1:B:29:CYS:HB2	2.58	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:A:21:ARG:NH1	5:A:836:HOH:O	2.51	0.44
1:B:275:GLN:HE22	1:B:435:ASP:CG	2.24	0.43
1:A:37:THR:OG1	1:A:39:HIS:HB2	2.18	0.43
1:A:282:GLY:O	1:A:288:LYS:NZ	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:515:TYR:HH	1:B:550:THR:HG1	1.66	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:A:241:VAL:HG22	5:A:840:HOH:O	2.19	0.43
1:B:26:CYS:O	1:B:27:CYS:C	2.62	0.42
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:B:532:THR:O	1:B:533:VAL:C	2.62	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
1:A:406:PRO:HG3	1:A:422:PHE:CE1	2.55	0.42
1:B:59:ASP:OD1	1:B:59:ASP:C	2.62	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:CYS:C	1:B:52:ALA:H	2.28	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:B:63:LEU:C	1:B:64:TYR:CD1	3.00	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	564/601 (94%)	517 (92%)	39 (7%)	8 (1%)	9	5
1	B	580/601 (96%)	532 (92%)	43 (7%)	5 (1%)	14	10
All	All	1144/1202 (95%)	1049 (92%)	82 (7%)	13 (1%)	11	8

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%)	35	39
1	B	498/523 (95%)	484 (97%)	14 (3%)	38	43
All	All	983/1046 (94%)	954 (97%)	29 (3%)	36	41

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	27	CYS
1	B	96	THR
1	B	103	VAL
1	B	155	ARG
1	B	188	THR
1	B	191	SER
1	B	192	LYS
1	B	215	THR
1	B	229	SER
1	B	259	SER
1	B	278	SER

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Mol	Chain	Res	Type
1	B	289	SER
1	B	486	SER
1	B	495	VAL
1	A	12	THR
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	424	SER
1	A	485	SER
1	A	502	ARG
1	A	530	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) 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	270	GLN
1	B	459	ASN
1	B	470	GLN
1	B	516	ASN
1	A	86	ASN
1	A	179	ASN
1	A	220	ASN
1	A	275	GLN
1	A	404	GLN
1	A	459	ASN
1	A	482	HIS

5.3.3 RNA ⓘ

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	$\# Z > 2$
4	PO4	A	704	-	4,4,4	0.76	0	6,6,6	0.48	0
4	PO4	A	705	-	4,4,4	0.83	0	6,6,6	0.61	0
4	PO4	B	705	-	4,4,4	1.11	0	6,6,6	0.44	0
2	JOV	B	701	-	15,15,15	0.35	0	21,21,21	0.42	0
4	PO4	B	706	-	4,4,4	1.24	0	6,6,6	0.55	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:

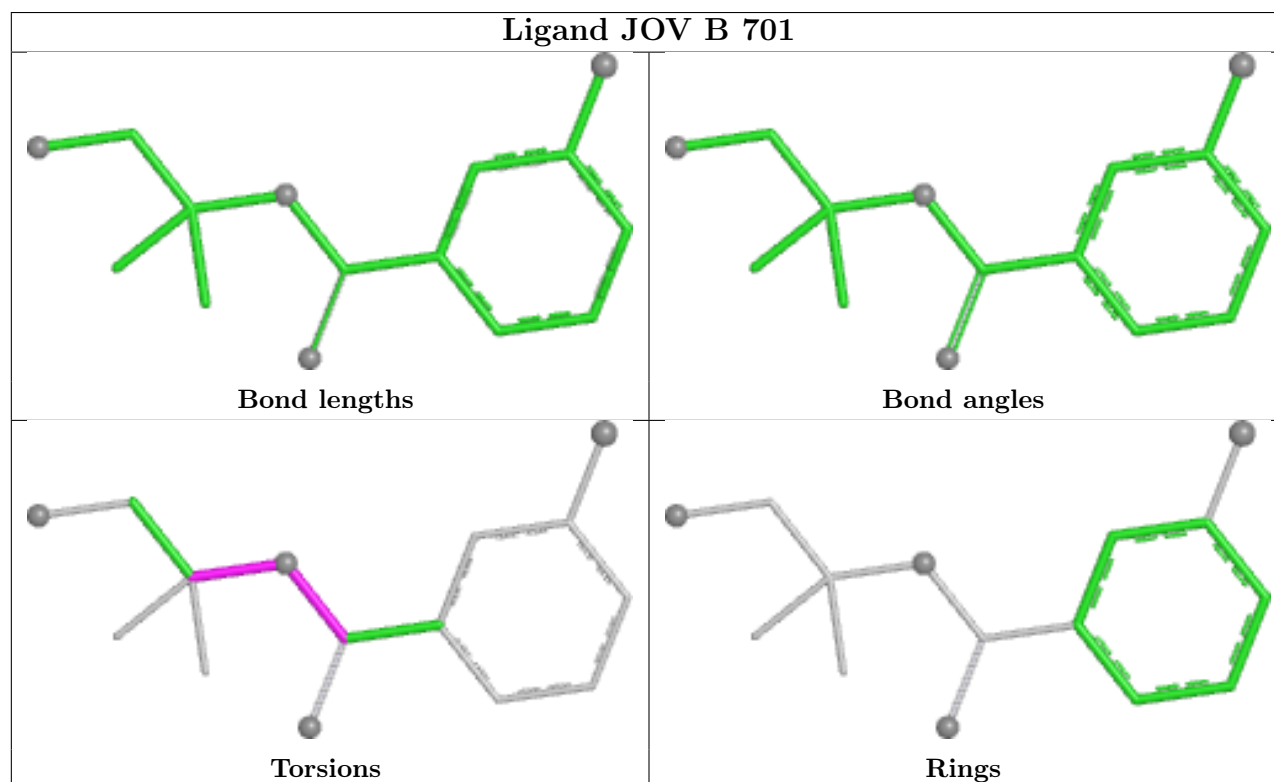
Mol	Chain	Res	Type	Atoms
2	B	701	JOV	C09-C07-N06-C02
2	B	701	JOV	C01-C02-N06-C07
2	B	701	JOV	O08-C07-N06-C02
2	B	701	JOV	C03-C02-N06-C07

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 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%)	1.23	147 (25%)  	26, 65, 142, 188	0
1	B	585/601 (97%)	0.68	66 (11%)  	10, 48, 105, 133	2 (0%)
All	All	1157/1202 (96%)	0.95	213 (18%)  	10, 54, 128, 188	2 (0%)

All (213) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	45	VAL	5.8
1	B	7	LEU	5.8
1	A	157	VAL	5.8
1	A	169	VAL	5.4
1	A	592	ILE	5.0
1	B	12	THR	5.0
1	A	225	PHE	4.7
1	A	151	ILE	4.6
1	B	6	VAL	4.5
1	B	193	VAL	4.5
1	A	149	TYR	4.4
1	A	6	VAL	4.4
1	A	219	LEU	4.4
1	A	210	VAL	4.4
1	B	2	VAL	4.2
1	A	7	LEU	4.2
1	A	393	ALA	4.2
1	A	181	VAL	4.1
1	B	214	THR	4.1
1	A	304	ILE	4.1
1	A	152	ALA	4.1
1	A	221	VAL	4.0
1	A	185	TYR	4.0
1	A	70	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	247	VAL	3.8
1	A	81	PHE	3.8
1	A	103	VAL	3.8
1	A	222	GLY	3.8
1	B	27	CYS	3.7
1	A	158	LEU	3.7
1	A	195	ILE	3.7
1	B	14	LEU	3.7
1	A	229	SER	3.6
1	A	154	VAL	3.6
1	A	305	VAL	3.6
1	B	81	PHE	3.6
1	B	98	VAL	3.6
1	A	226	VAL	3.6
1	A	326	PRO	3.6
1	A	352	LEU	3.5
1	B	217	TYR	3.5
1	A	14	LEU	3.5
1	A	347	LYS	3.4
1	B	187	VAL	3.4
1	B	474[A]	MET	3.4
1	A	336	ALA	3.4
1	A	227	LEU	3.4
1	A	208	ALA	3.4
1	A	258	ILE	3.4
1	A	224	TYR	3.4
1	A	200	PHE	3.4
1	B	340	VAL	3.3
1	A	45	VAL	3.3
1	A	296	ALA	3.3
1	A	90	PHE	3.3
1	A	306	TYR	3.3
1	A	387	VAL	3.3
1	A	334	ILE	3.3
1	A	333	ILE	3.3
1	A	182	PHE	3.3
1	A	145	PHE	3.2
1	A	266	VAL	3.2
1	A	348	VAL	3.2
1	A	94	LYS	3.2
1	B	163	LEU	3.2
1	A	43	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	97	CYS	3.2
1	A	49	VAL	3.1
1	A	371	VAL	3.1
1	A	180	TYR	3.1
1	A	254	PRO	3.1
1	A	167	TRP	3.1
1	B	502	ARG	3.1
1	A	253	TYR	3.1
1	B	101	ASP	3.1
1	A	370	ILE	3.1
1	A	170	GLY	3.0
1	A	25	LEU	3.0
1	A	228	THR	3.0
1	A	335	PRO	3.0
1	B	8	CYS	3.0
1	B	336	ALA	3.0
1	A	44	SER	3.0
1	B	96	THR	3.0
1	A	198	TYR	3.0
1	A	217	TYR	3.0
1	A	92	LEU	3.0
1	A	12	THR	3.0
1	B	208	ALA	2.9
1	A	330	CYS	2.9
1	A	2	VAL	2.9
1	A	209	VAL	2.9
1	A	147	LEU	2.8
1	A	396	TYR	2.8
1	B	165	LEU	2.8
1	B	53	PRO	2.8
1	B	44	SER	2.8
1	A	297	LEU	2.8
1	A	153	THR	2.8
1	A	255	THR	2.8
1	B	47	PRO	2.8
1	A	256	LEU	2.8
1	B	103	VAL	2.8
1	A	397	VAL	2.8
1	A	172	PRO	2.7
1	A	272	VAL	2.7
1	A	346	PHE	2.7
1	A	358	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	413	THR	2.6
1	A	165	LEU	2.6
1	A	246	TYR	2.6
1	B	195	ILE	2.6
1	A	42	VAL	2.6
1	B	209	VAL	2.6
1	B	26	CYS	2.6
1	A	199	THR	2.6
1	B	78	PRO	2.6
1	B	145	PHE	2.6
1	A	84	CYS	2.6
1	A	174	PRO	2.6
1	B	43	LEU	2.6
1	A	155	ARG	2.5
1	B	215	THR	2.5
1	B	158	LEU	2.5
1	A	231	THR	2.5
1	A	13	SER	2.5
1	A	156	GLU	2.5
1	A	202	LYS	2.5
1	A	416	THR	2.5
1	B	4	ALA	2.5
1	A	338	ALA	2.5
1	B	352	LEU	2.5
1	A	241	VAL	2.4
1	A	104	THR	2.4
1	A	82	PRO	2.4
1	A	252	LEU	2.4
1	A	89	VAL	2.4
1	B	92	LEU	2.4
1	B	88	GLN	2.4
1	A	184	GLY	2.4
1	A	178	ARG	2.4
1	A	340	VAL	2.4
1	A	93	TYR	2.3
1	B	176	LEU	2.3
1	A	235	LEU	2.3
1	B	203	GLY	2.3
1	A	343	PHE	2.3
1	B	180	TYR	2.3
1	A	308	ALA	2.3
1	A	176	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	24	PHE	2.3
1	A	301	SER	2.3
1	A	23	PRO	2.3
1	B	52	ALA	2.3
1	B	178	ARG	2.3
1	A	91	GLY	2.3
1	B	11	GLN	2.3
1	A	85	ALA	2.3
1	A	223	ASP	2.3
1	B	256	LEU	2.3
1	A	130	LEU	2.3
1	A	325	LEU	2.3
1	A	249	ILE	2.2
1	A	214	THR	2.2
1	A	179	ASN	2.2
1	B	48	TYR	2.2
1	B	10	SER	2.2
1	B	68	MET	2.2
1	A	31	TYR	2.2
1	A	324	TYR	2.2
1	B	49	VAL	2.2
1	B	213	GLY	2.2
1	B	164	HIS	2.2
1	A	164	HIS	2.2
1	B	227	LEU	2.2
1	B	411	LEU	2.2
1	A	163	LEU	2.2
1	A	47	PRO	2.1
1	B	79	ILE	2.1
1	B	157	VAL	2.1
1	A	39	HIS	2.1
1	A	302	ALA	2.1
1	A	337	ARG	2.1
1	A	351	THR	2.1
1	A	194	GLN	2.1
1	A	323	LYS	2.1
1	A	215	THR	2.1
1	A	22	ARG	2.1
1	A	79	ILE	2.1
1	A	372	VAL	2.1
1	A	1	ALA	2.1
1	A	505	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	93	TYR	2.1
1	A	175	PRO	2.1
1	B	54	GLY	2.1
1	A	67	GLY	2.1
1	B	57	VAL	2.1
1	A	373	PHE	2.1
1	A	114	TRP	2.1
1	A	10	SER	2.1
1	A	384	LEU	2.0
1	B	516	ASN	2.0
1	A	11	GLN	2.0
1	A	161	ARG	2.0
1	A	395	HIS	2.0
1	B	593	PRO	2.0
1	B	189	LYS	2.0
1	A	150	GLY	2.0
1	A	273	GLY	2.0
1	B	124	ASN	2.0
1	A	21	ARG	2.0
1	A	29	CYS	2.0
1	B	211	TYR	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.

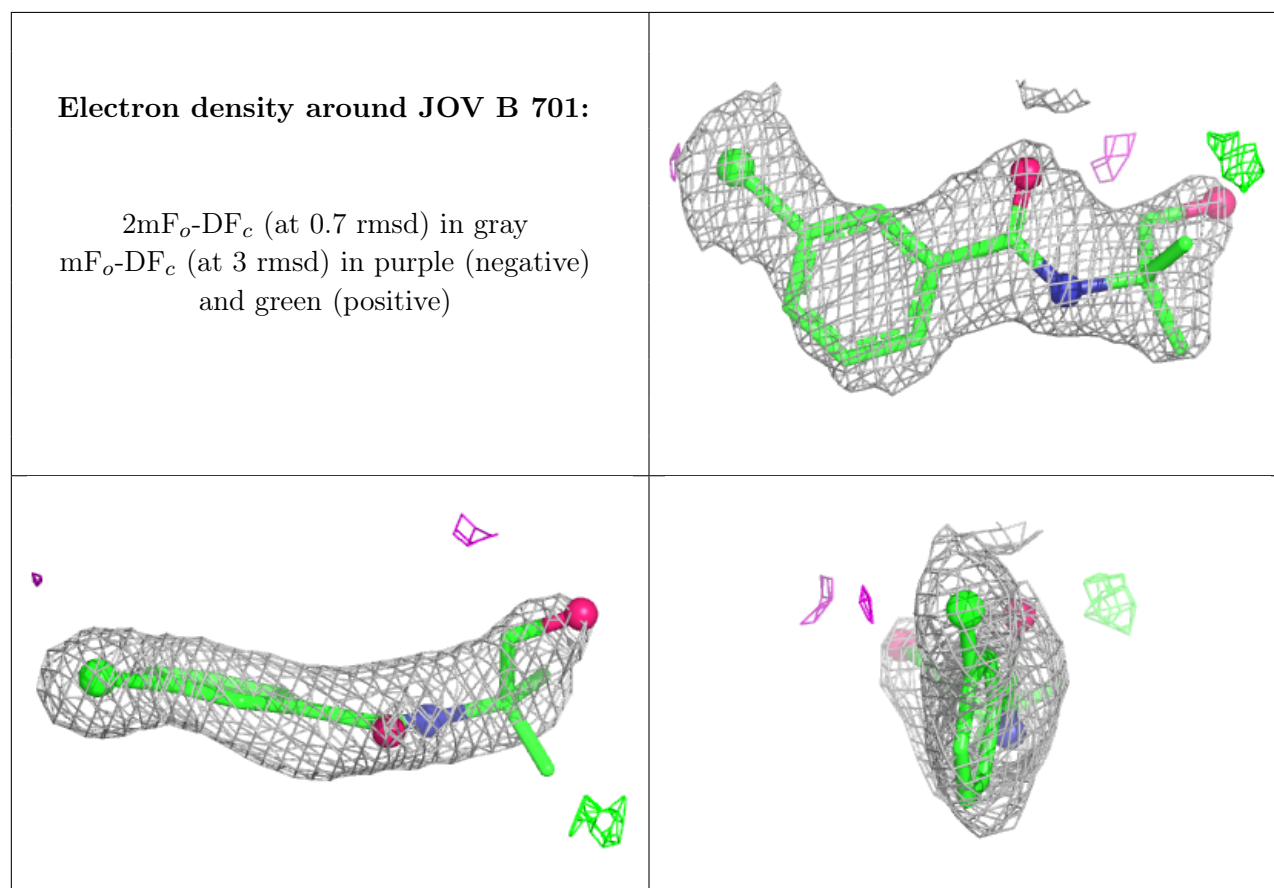
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	JOV	B	701	15/15	0.89	0.18	38,41,43,46	15
4	PO4	B	705	5/5	0.95	0.08	33,36,47,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PO4	A	705	5/5	0.95	0.07	45,48,52,60	0
3	ZN	A	703	1/1	0.96	0.05	102,102,102,102	0
3	ZN	B	704	1/1	0.97	0.05	78,78,78,78	0
4	PO4	B	706	5/5	0.97	0.07	32,34,42,42	0
4	PO4	A	704	5/5	0.97	0.06	35,39,43,48	0
3	ZN	B	703	1/1	0.97	0.05	66,66,66,66	0
3	ZN	A	702	1/1	0.98	0.04	57,57,57,57	0
3	ZN	B	702	1/1	0.99	0.02	42,42,42,42	0
3	ZN	A	701	1/1	0.99	0.03	62,62,62,62	0

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



6.5 Other polymers ⓘ

There are no such residues in this entry.