



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:13 PM UTC

PDB ID : 7NNG / pdb_00007nng
Title : Crystal structure of the SARS-CoV-2 helicase in complex with Z2327226104
Authors : Newman, J.A.; Yosaatmadja, Y.; Douangamath, A.; Bountra, C.; Gileadi, O.
Deposited on : 2021-02-24
Resolution : 2.38 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)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

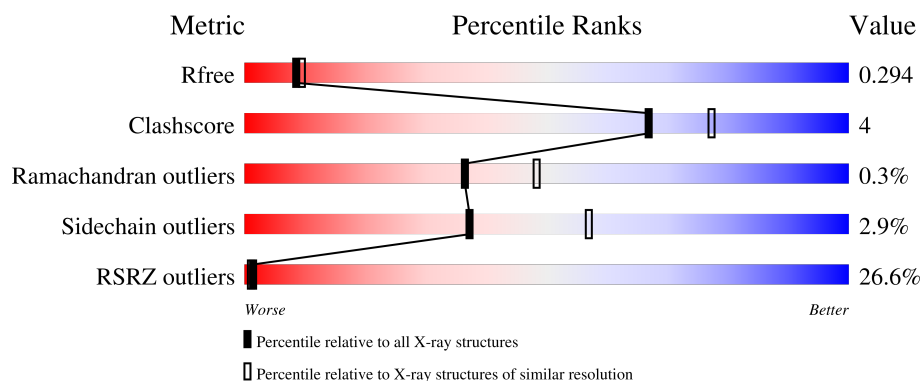
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	 33% 85% 10% 5%
1	B	601	 18% 85% 12% •

2 Entry composition [i](#)

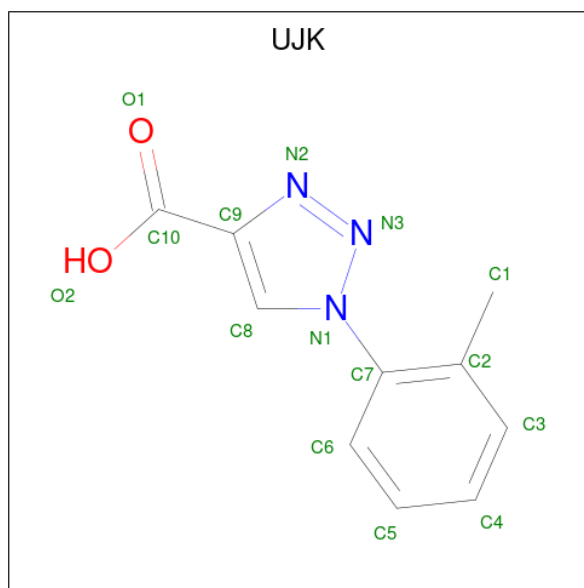
There are 5 unique types of molecules in this entry. The entry contains 9114 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SARS-CoV-2 helicase NSP13.

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 1-(2-methylphenyl)-1,2,3-triazole-4-carboxylic acid (CCD ID: UJK) (formula: C₁₀H₉N₃O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			15	10	3	2		
2	A	1	Total	C	N	O	0	0
			15	10	3	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		
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		

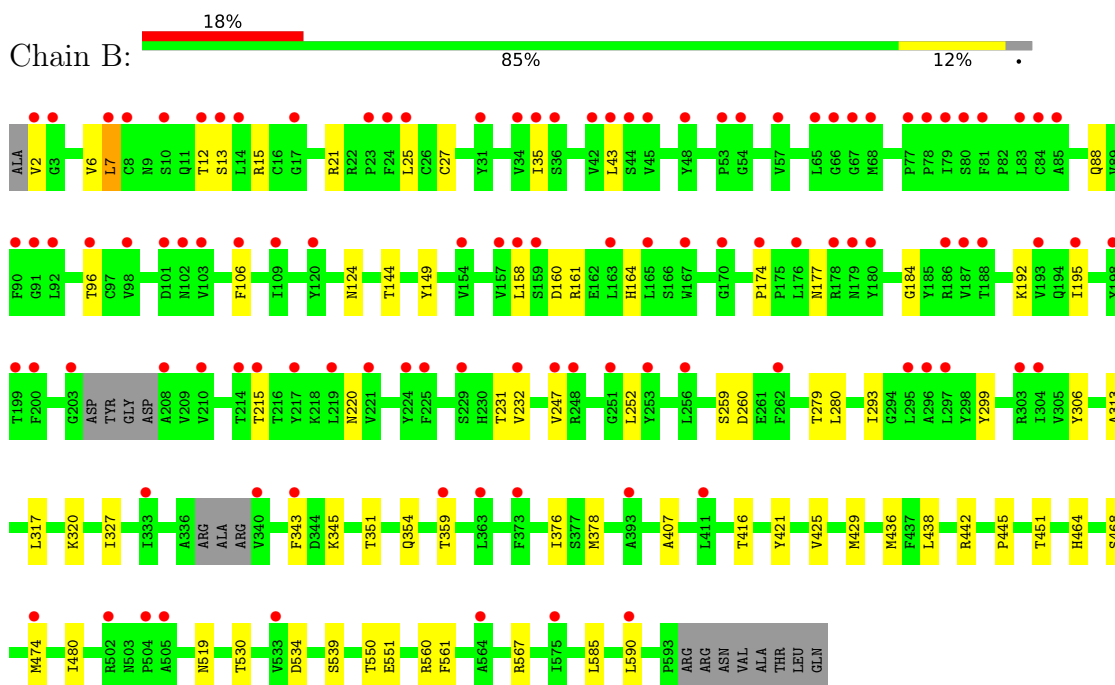
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	75	Total	O	0	0
			75	75		
5	A	58	Total	O	0	0
			58	58		

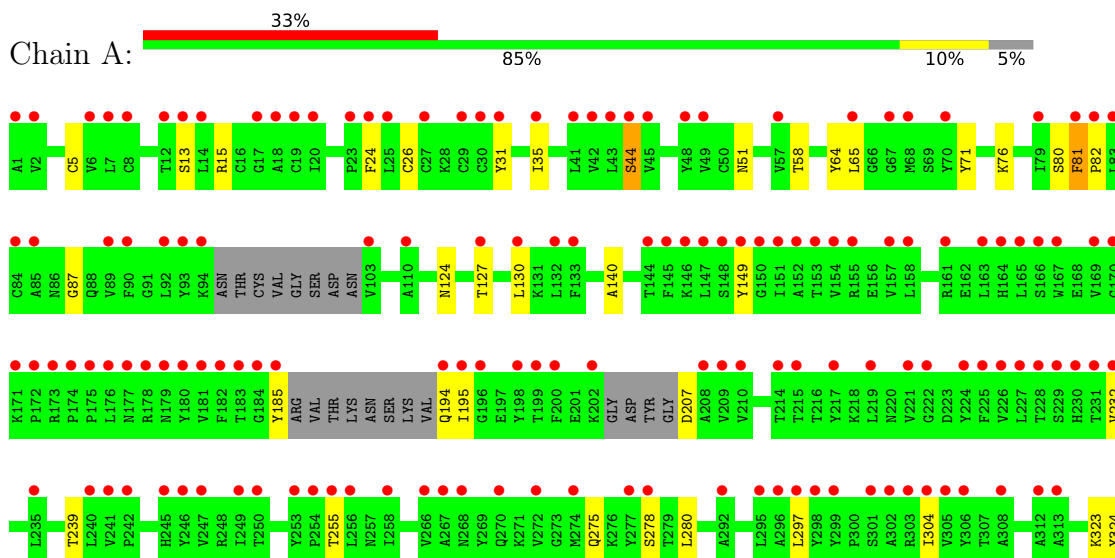
3 Residue-property plots

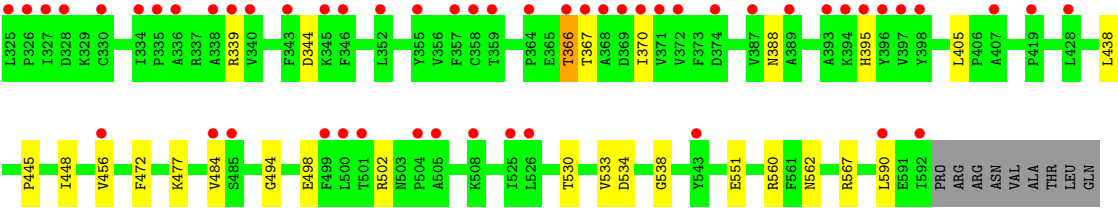
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: SARS-CoV-2 helicase NSP13



• Molecule 1: SARS-CoV-2 helicase NSP13





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.20Å 70.35Å 85.50Å 103.16° 96.10° 112.04°	Depositor
Resolution (Å)	81.35 – 2.38 81.35 – 2.38	Depositor EDS
% Data completeness (in resolution range)	87.5 (81.35-2.38) 87.6 (81.35-2.38)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.245 , 0.295 0.247 , 0.294	Depositor DCC
R_{free} test set	2174 reflections (4.45%)	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 29.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9114	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.75% 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: UJK, 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	0.10	0/4517	0.29	0/6156
1	B	0.11	0/4610	0.33	1/6283 (0.0%)
All	All	0.10	0/9127	0.31	1/12439 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	247	VAL	N-CA-C	-5.13	107.42	113.42

There are no chirality outliers.

There are no planarity outliers.

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.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4417	0	4321	30	0
1	B	4508	0	4424	35	0
2	A	15	0	0	0	0
2	B	15	0	0	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	58	0	0	2	0
5	B	75	0	0	3	0
All	All	9114	0	8745	65	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (65) 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:445:PRO:HD2	1:A:448:ILE:HD12	1.73	0.70
1:B:293:ILE:HG13	1:B:320:LYS:HB3	1.76	0.67
1:A:5:CYS:HB2	1:A:26:CYS:HB3	1.80	0.63
1:B:474[B]:MET:HG2	1:B:590:LEU:HB2	1.80	0.63
1:B:534:ASP:OD2	5:B:801:HOH:O	2.16	0.62
1:B:6:VAL:HG23	1:B:7:LEU:HD23	1.83	0.61
1:B:306:TYR:HB3	1:B:317:LEU:HD13	1.84	0.59
1:B:124:ASN:HD22	1:B:421:TYR:HA	1.71	0.56
1:A:339:ARG:NH2	5:A:808:HOH:O	2.40	0.55
1:B:21:ARG:NH2	1:B:232:VAL:O	2.40	0.54
1:B:480:ILE:HD13	1:B:550:THR:HG22	1.90	0.54
1:A:140:ALA:HA	1:A:232:VAL:HG21	1.90	0.53
1:A:65:LEU:N	1:A:81:PHE:O	2.40	0.53
1:B:445:PRO:HB3	1:B:468:SER:HB3	1.90	0.53
1:B:560:ARG:NE	5:B:801:HOH:O	2.33	0.53
1:A:127:THR:HG22	1:A:130:LEU:HB2	1.91	0.52
1:B:279:THR:HB	1:B:429:MET:HE2	1.92	0.51
1:B:158:LEU:HD13	1:B:164:HIS:HB2	1.92	0.51
1:B:519:ASN:HB3	1:B:530:THR:HB	1.92	0.51
1:B:12:THR:HG21	1:B:25:LEU:O	2.11	0.50
1:A:477:LYS:NZ	1:A:551:GLU:OE2	2.44	0.50
1:B:280:LEU:HD11	1:B:438:LEU:HG	1.94	0.49
1:B:442:ARG:HA	1:B:464:HIS:HB3	1.95	0.49
1:A:280:LEU:HD11	1:A:438:LEU:HG	1.93	0.48
1:B:15:ARG:N	1:B:43:LEU:O	2.37	0.48
1:A:13:SER:O	1:A:44:SER:HA	2.15	0.47
1:A:472:PHE:HB3	1:A:590:LEU:HG	1.96	0.47
1:B:7:LEU:HD21	1:B:106:PHE:HB2	1.96	0.46
1:A:297:LEU:HD11	1:A:324:TYR:HB3	1.96	0.46
1:B:451:THR:HG21	1:B:585:LEU:HD23	1.97	0.46
1:B:2:VAL:HG22	1:B:13:SER:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:ALA:O	5:B:802:HOH:O	2.21	0.46
1:A:304:ILE:HG12	1:A:370:ILE:HB	1.98	0.46
1:B:27:CYS:HB3	1:B:88:GLN:HB3	1.97	0.46
1:B:320:LYS:NZ	2:B:701:UJK:N2	2.64	0.46
1:A:533:VAL:HG11	1:A:560:ARG:HG3	1.97	0.46
1:A:456:VAL:HG21	1:A:562:ASN:ND2	2.31	0.45
1:B:280:LEU:HB2	1:B:436:MET:HE3	1.97	0.45
1:A:494:GLY:O	1:A:498:GLU:HG2	2.18	0.44
1:B:149:TYR:HB3	1:B:174:PRO:HD3	1.99	0.44
1:A:64:TYR:HA	1:A:82:PRO:HA	1.99	0.44
1:B:149:TYR:CD2	1:B:174:PRO:HB3	2.53	0.43
1:A:64:TYR:N	1:A:71:TYR:O	2.47	0.43
1:A:124:ASN:ND2	5:A:813:HOH:O	2.50	0.43
1:B:378:MET:O	1:B:407:ALA:HB2	2.19	0.43
1:A:366:THR:OG1	1:A:367:THR:N	2.51	0.43
1:B:539:SER:O	1:B:567:ARG:HD3	2.19	0.43
1:A:5:CYS:HA	1:A:24:PHE:O	2.19	0.43
1:B:252:LEU:HB3	1:B:299:TYR:CD1	2.53	0.42
1:A:76:LYS:HD2	1:A:80:SER:OG	2.19	0.42
1:A:275:GLN:O	1:A:395:HIS:ND1	2.47	0.42
1:B:343:PHE:CZ	1:B:345:LYS:HB2	2.53	0.42
1:A:239:THR:O	1:A:388:ASN:ND2	2.53	0.42
1:A:15:ARG:HD3	1:A:24:PHE:CE1	2.55	0.41
1:A:405:LEU:HD21	1:A:560:ARG:HB2	2.02	0.41
1:B:376:ILE:HG12	1:B:425:VAL:HG11	2.02	0.41
1:A:31:TYR:CD2	1:A:87:GLY:HA2	2.55	0.41
1:A:538:GLY:H	1:A:567:ARG:NH1	2.17	0.41
1:B:561:PHE:HZ	1:B:585:LEU:HD11	1.86	0.41
1:A:405:LEU:HD13	1:A:534:ASP:OD1	2.21	0.41
1:A:185:TYR:HE2	1:A:194:GLN:HG3	1.86	0.41
1:B:260:ASP:N	1:B:260:ASP:OD1	2.52	0.40
1:B:184:GLY:C	1:B:195:ILE:HG22	2.46	0.40
1:B:160:ASP:OD2	1:B:161:ARG:N	2.54	0.40
1:A:185:TYR:CE2	1:A:194:GLN:HG3	2.56	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%)	532 (94%)	29 (5%)	3 (0%)	24	34
1	B	580/601 (96%)	539 (93%)	40 (7%)	1 (0%)	43	56
All	All	1144/1202 (95%)	1071 (94%)	69 (6%)	4 (0%)	36	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	484	VAL
1	B	354	GLN
1	A	44	SER
1	A	195	ILE

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%)	472 (97%)	13 (3%)	39	59
1	B	498/523 (95%)	483 (97%)	15 (3%)	36	56
All	All	983/1046 (94%)	955 (97%)	28 (3%)	37	58

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	7	LEU
1	B	35	ILE

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Mol	Chain	Res	Type
1	B	96	THR
1	B	144	THR
1	B	177	ASN
1	B	192	LYS
1	B	215	THR
1	B	220	ASN
1	B	231	THR
1	B	259	SER
1	B	327	ILE
1	B	351	THR
1	B	359	THR
1	B	416	THR
1	B	551	GLU
1	A	35	ILE
1	A	51	ASN
1	A	58	THR
1	A	81	PHE
1	A	149	TYR
1	A	207	ASP
1	A	255	THR
1	A	278	SER
1	A	323	LYS
1	A	344	ASP
1	A	366	THR
1	A	502	ARG
1	A	530	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	51	ASN
1	B	88	GLN
1	B	164	HIS
1	B	179	ASN
1	B	194	GLN
1	B	268	ASN
1	A	11	GLN
1	A	88	GLN
1	A	116	ASN
1	A	404	GLN
1	A	459	ASN
1	A	531	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 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	B	706	-	4,4,4	0.99	0	6,6,6	0.45	0
4	PO4	B	705	-	4,4,4	1.02	0	6,6,6	0.45	0
2	UJK	A	701	-	16,16,16	0.84	1 (6%)	22,22,22	1.01	2 (9%)
4	PO4	A	705	-	4,4,4	1.01	0	6,6,6	0.46	0
2	UJK	B	701	-	16,16,16	0.85	1 (6%)	22,22,22	0.99	2 (9%)
4	PO4	A	706	-	4,4,4	0.93	0	6,6,6	0.49	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	UJK	B	701	-	-	0/8/8/8	0/2/2/2
2	UJK	A	701	-	-	0/8/8/8	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	UJK	O2-C10	-3.25	1.21	1.30
2	A	701	UJK	O2-C10	-3.20	1.21	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	UJK	O1-C10-C9	-2.77	117.65	122.02
2	A	701	UJK	O1-C10-C9	-2.75	117.67	122.02
2	B	701	UJK	O2-C10-C9	2.54	117.48	113.40
2	A	701	UJK	O2-C10-C9	2.52	117.45	113.40

There are no chirality outliers.

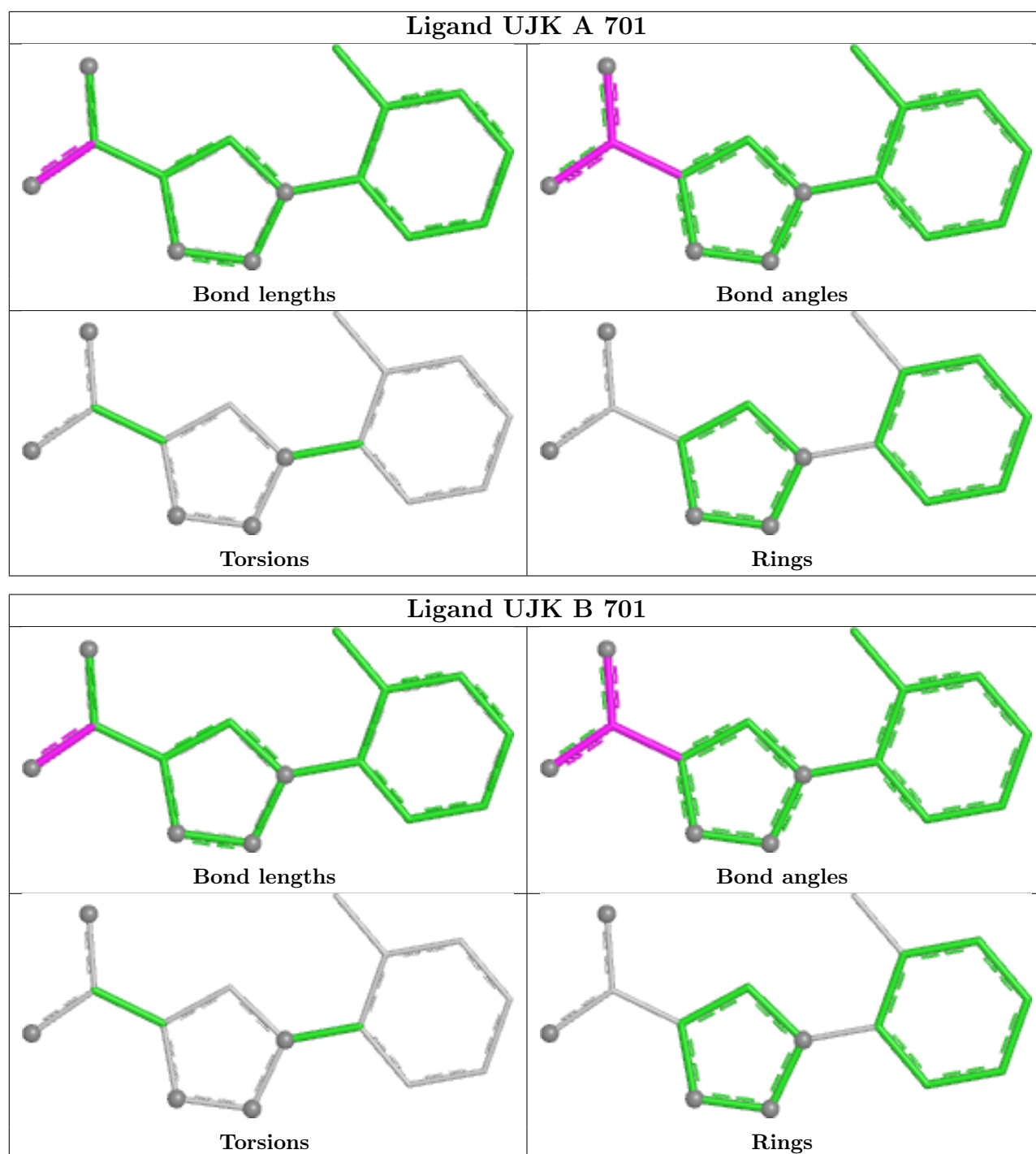
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	UJK	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%)	1.70	201 (35%)	1 0	37, 70, 133, 155	0
1	B	585/601 (97%)	1.31	107 (18%)	3 3	29, 56, 98, 123	1 (0%)
All	All	1157/1202 (96%)	1.50	308 (26%)	1 1	29, 63, 121, 155	1 (0%)

All (308) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	151	ILE	5.8
1	A	219	LEU	5.6
1	A	149	TYR	5.4
1	A	225	PHE	5.2
1	A	167	TRP	5.0
1	A	200	PHE	4.9
1	A	179	ASN	4.9
1	A	393	ALA	4.8
1	A	182	PHE	4.8
1	A	152	ALA	4.7
1	A	592	ILE	4.7
1	A	266	VAL	4.6
1	A	221	VAL	4.6
1	A	195	ILE	4.6
1	A	327	ILE	4.5
1	A	49	VAL	4.3
1	A	208	ALA	4.3
1	A	178	ARG	4.2
1	A	247	VAL	4.2
1	A	304	ILE	4.2
1	A	371	VAL	4.2
1	A	90	PHE	4.1
1	A	154	VAL	4.1
1	A	370	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	296	ALA	4.0
1	A	165	LEU	3.9
1	B	84	CYS	3.9
1	A	81	PHE	3.9
1	B	187	VAL	3.9
1	A	352	LEU	3.8
1	A	6	VAL	3.8
1	A	181	VAL	3.8
1	A	202	LYS	3.8
1	A	258	ILE	3.8
1	A	305	VAL	3.8
1	B	57	VAL	3.7
1	A	169	VAL	3.7
1	B	214	THR	3.7
1	B	2	VAL	3.7
1	A	1	ALA	3.7
1	B	200	PHE	3.6
1	B	193	VAL	3.6
1	A	172	PRO	3.6
1	B	83	LEU	3.6
1	A	94	LYS	3.6
1	B	45	VAL	3.6
1	A	292	ALA	3.6
1	B	79	ILE	3.5
1	A	7	LEU	3.5
1	A	226	VAL	3.5
1	B	340	VAL	3.5
1	A	42	VAL	3.5
1	A	336	ALA	3.5
1	B	167	TRP	3.5
1	B	109	ILE	3.5
1	B	373	PHE	3.5
1	B	157	VAL	3.4
1	A	368	ALA	3.4
1	B	262	PHE	3.4
1	A	147	LEU	3.4
1	A	224	TYR	3.4
1	A	387	VAL	3.4
1	A	92	LEU	3.4
1	A	170	GLY	3.4
1	B	81	PHE	3.3
1	A	228	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	227	LEU	3.3
1	A	345	LYS	3.3
1	A	217	TYR	3.3
1	A	246	TYR	3.3
1	B	98	VAL	3.3
1	B	92	LEU	3.2
1	B	256	LEU	3.2
1	A	176	LEU	3.2
1	A	153	THR	3.2
1	A	396	TYR	3.2
1	B	203	GLY	3.2
1	B	78	PRO	3.2
1	A	185	TYR	3.2
1	A	41	LEU	3.2
1	A	163	LEU	3.2
1	A	199	THR	3.2
1	A	145	PHE	3.2
1	A	146	LYS	3.2
1	A	18	ALA	3.2
1	B	165	LEU	3.2
1	A	13	SER	3.1
1	A	407	ALA	3.1
1	A	157	VAL	3.1
1	A	180	TYR	3.1
1	B	14	LEU	3.1
1	B	90	PHE	3.1
1	A	308	ALA	3.1
1	A	389	ALA	3.1
1	A	103	VAL	3.1
1	A	158	LEU	3.1
1	A	334	ILE	3.1
1	A	93	TYR	3.1
1	A	150	GLY	3.1
1	B	210	VAL	3.1
1	A	306	TYR	3.0
1	A	229	SER	3.0
1	A	209	VAL	3.0
1	A	231	THR	3.0
1	A	245	HIS	3.0
1	A	19	CYS	3.0
1	A	27	CYS	3.0
1	B	10	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	163	LEU	3.0
1	A	256	LEU	3.0
1	A	295	LEU	3.0
1	A	31	TYR	3.0
1	A	328	ASP	3.0
1	A	25	LEU	2.9
1	A	30	CYS	2.9
1	A	84	CYS	2.9
1	A	79	ILE	2.9
1	B	217	TYR	2.9
1	A	241	VAL	2.9
1	B	8	CYS	2.9
1	B	359	THR	2.9
1	B	48	TYR	2.9
1	A	24	PHE	2.9
1	B	34	VAL	2.9
1	B	91	GLY	2.9
1	A	133	PHE	2.9
1	A	338	ALA	2.9
1	A	89	VAL	2.9
1	A	346	PHE	2.8
1	A	456	VAL	2.8
1	A	355	TYR	2.8
1	B	564	ALA	2.8
1	B	215	THR	2.8
1	A	214	THR	2.8
1	A	222	GLY	2.8
1	B	176	LEU	2.8
1	B	363	LEU	2.8
1	A	65	LEU	2.8
1	A	500	LEU	2.8
1	B	195	ILE	2.8
1	A	12	THR	2.8
1	B	66	GLY	2.8
1	A	330	CYS	2.8
1	A	70	TYR	2.8
1	B	219	LEU	2.7
1	B	208	ALA	2.7
1	A	20	ILE	2.7
1	A	184	GLY	2.7
1	A	278	SER	2.7
1	B	297	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	14	LEU	2.7
1	A	130	LEU	2.7
1	A	398	TYR	2.7
1	A	313	ALA	2.7
1	B	24	PHE	2.7
1	A	366	THR	2.7
1	A	132	LEU	2.7
1	A	235	LEU	2.7
1	A	325	LEU	2.7
1	A	171	LYS	2.6
1	A	299	TYR	2.6
1	A	17	GLY	2.6
1	A	43	LEU	2.6
1	B	179	ASN	2.6
1	A	177	ASN	2.6
1	A	198	TYR	2.6
1	B	42	VAL	2.6
1	A	23	PRO	2.6
1	A	174	PRO	2.6
1	A	166	SER	2.6
1	A	358	CYS	2.6
1	B	474[A]	MET	2.6
1	B	12	THR	2.6
1	A	357	PHE	2.6
1	B	533	VAL	2.6
1	A	232	VAL	2.6
1	B	44	SER	2.6
1	B	198	TYR	2.6
1	A	249	ILE	2.6
1	A	339	ARG	2.5
1	A	215	THR	2.5
1	A	57	VAL	2.5
1	A	485	SER	2.5
1	A	253	TYR	2.5
1	B	7	LEU	2.5
1	B	96	THR	2.5
1	A	270	GLN	2.5
1	A	298	TYR	2.5
1	B	504	PRO	2.5
1	A	254	PRO	2.5
1	B	304	ILE	2.5
1	A	45	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	180	TYR	2.5
1	B	590	LEU	2.5
1	A	68	MET	2.5
1	A	374	ASP	2.5
1	B	3	GLY	2.5
1	A	504	PRO	2.5
1	A	230	HIS	2.4
1	B	77	PRO	2.4
1	A	367	THR	2.4
1	A	499	PHE	2.4
1	B	25	LEU	2.4
1	A	240	LEU	2.4
1	B	35	ILE	2.4
1	A	82	PRO	2.4
1	A	419	PRO	2.4
1	A	394	LYS	2.4
1	A	148	SER	2.4
1	B	225	PHE	2.4
1	A	343	PHE	2.4
1	A	297	LEU	2.4
1	A	48	TYR	2.3
1	B	53	PRO	2.3
1	B	170	GLY	2.3
1	B	85	ALA	2.3
1	B	13	SER	2.3
1	A	301	SER	2.3
1	B	333	ILE	2.3
1	A	303	ARG	2.3
1	B	158	LEU	2.3
1	B	251	GLY	2.3
1	B	178	ARG	2.3
1	B	295	LEU	2.3
1	A	268	ASN	2.3
1	A	364	PRO	2.3
1	B	188	THR	2.3
1	A	194	GLN	2.3
1	B	575	ILE	2.3
1	A	340	VAL	2.3
1	A	8	CYS	2.3
1	B	174	PRO	2.3
1	B	502	ARG	2.3
1	A	85	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	359	THR	2.3
1	B	80	SER	2.3
1	A	508	LYS	2.3
1	B	103	VAL	2.3
1	A	175	PRO	2.2
1	A	505	ALA	2.2
1	B	199	THR	2.2
1	B	36	SER	2.2
1	A	590	LEU	2.2
1	A	29	CYS	2.2
1	B	31	TYR	2.2
1	B	229	SER	2.2
1	A	44	SER	2.2
1	A	428	LEU	2.2
1	A	2	VAL	2.2
1	B	106	PHE	2.2
1	A	155	ARG	2.2
1	B	68	MET	2.2
1	B	54	GLY	2.2
1	B	67	GLY	2.2
1	B	296	ALA	2.2
1	B	159	SER	2.2
1	A	127	THR	2.2
1	A	302	ALA	2.2
1	A	543	TYR	2.2
1	B	232	VAL	2.2
1	A	397	VAL	2.2
1	A	274	MET	2.2
1	B	505	ALA	2.2
1	A	525	ILE	2.1
1	B	154	VAL	2.1
1	B	221	VAL	2.1
1	A	272	VAL	2.1
1	A	242	PRO	2.1
1	B	393	ALA	2.1
1	A	110	ALA	2.1
1	A	255	THR	2.1
1	B	186	ARG	2.1
1	B	120	TYR	2.1
1	B	102	ASN	2.1
1	A	335	PRO	2.1
1	B	17	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	196	GLY	2.1
1	A	183	THR	2.1
1	B	65	LEU	2.1
1	A	83	LEU	2.1
1	B	253	TYR	2.1
1	A	210	VAL	2.1
1	A	326	PRO	2.1
1	B	343	PHE	2.1
1	B	303	ARG	2.1
1	A	250	THR	2.1
1	B	411	LEU	2.1
1	A	35	ILE	2.1
1	B	23	PRO	2.1
1	A	372	VAL	2.1
1	A	484	VAL	2.1
1	A	67	GLY	2.1
1	A	144	THR	2.0
1	A	312	ALA	2.0
1	A	164	HIS	2.0
1	B	43	LEU	2.0
1	B	224	TYR	2.0
1	A	277	TYR	2.0
1	B	247	VAL	2.0
1	B	248	ARG	2.0
1	A	173	ARG	2.0
1	A	501	THR	2.0
1	A	267	ALA	2.0
1	A	395	HIS	2.0
1	B	101	ASP	2.0
1	A	369	ASP	2.0
1	A	526	LEU	2.0
1	A	161	ARG	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 ⓘ

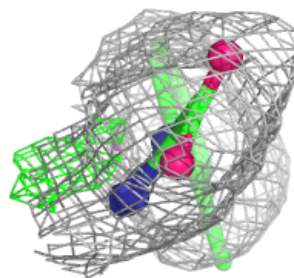
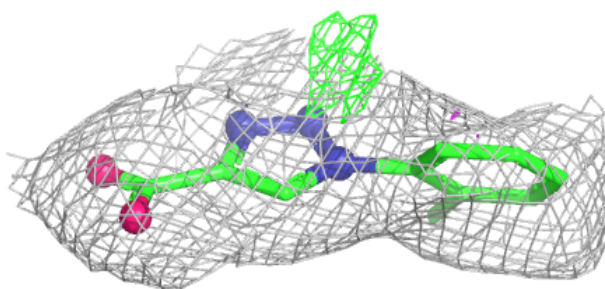
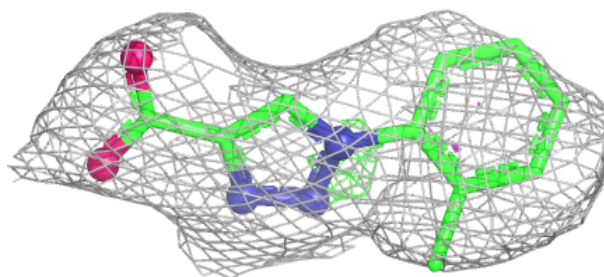
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	UJK	B	701	15/15	0.84	0.14	41,53,64,82	0
3	ZN	B	703	1/1	0.86	0.09	90,90,90,90	0
2	UJK	A	701	15/15	0.88	0.10	53,61,70,74	0
4	PO4	B	705	5/5	0.88	0.11	47,49,62,63	0
4	PO4	A	705	5/5	0.89	0.11	40,47,54,60	0
4	PO4	A	706	5/5	0.89	0.09	37,44,60,62	0
4	PO4	B	706	5/5	0.92	0.10	37,39,53,54	0
3	ZN	A	702	1/1	0.93	0.07	71,71,71,71	0
3	ZN	B	702	1/1	0.95	0.06	56,56,56,56	0
3	ZN	A	704	1/1	0.95	0.06	102,102,102,102	0
3	ZN	A	703	1/1	0.96	0.06	68,68,68,68	0
3	ZN	B	704	1/1	0.97	0.04	102,102,102,102	0

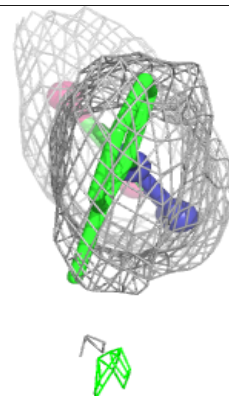
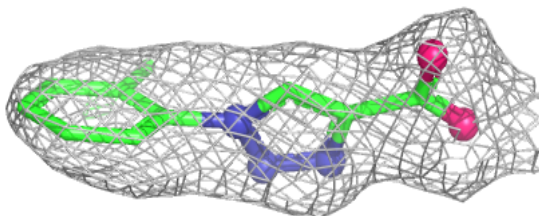
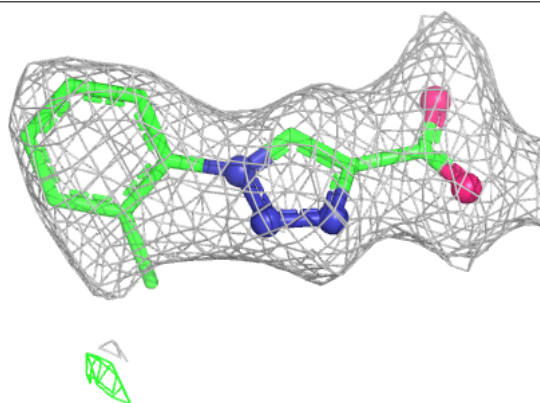
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UJK 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)

**Electron density around UJK 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.