



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:25 AM UTC

PDB ID : 5RM2 / pdb_00005rm2
Title : PanDDA analysis group deposition – Crystal Structure of SARS-CoV-2 heli-
case in complex with Z1741964527
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 : 1.82 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)

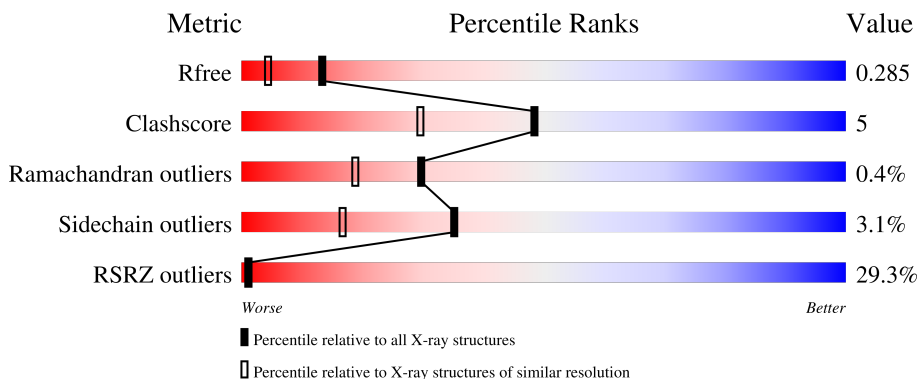
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9438 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

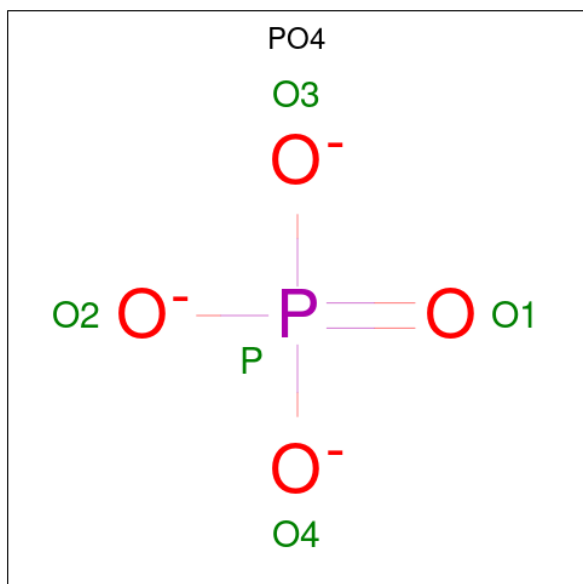
- Molecule 1 is a protein called Helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	572	Total	C	N	O	S	0	0	0
			4417	2816	737	832	32			
1	B	585	Total	C	N	O	S	0	1	0
			4508	2875	750	848	35			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

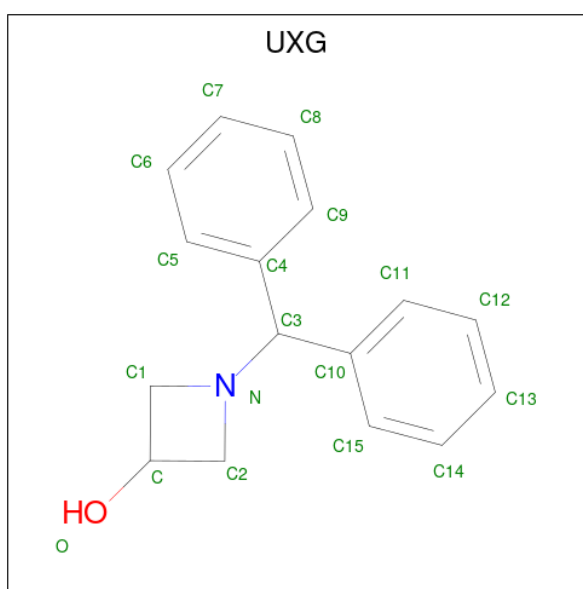
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	3	Total	Zn	0	0
			3	3		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 4 is 1-(diphenylmethyl)azetidin-3-ol (CCD ID: UXG) (formula: C₁₆H₁₇NO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 18 16 1 1	0	0
4	B	1	Total C N O 18 16 1 1	0	0

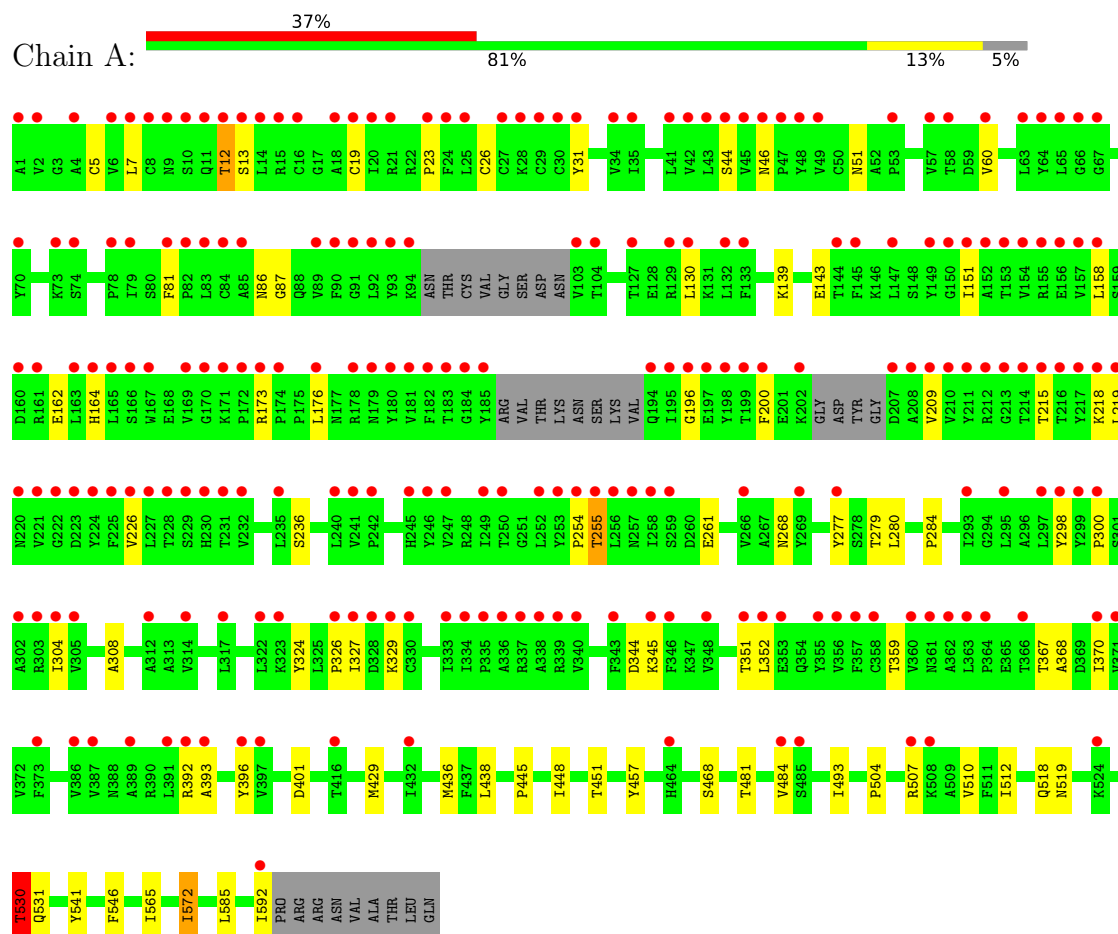
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	205	Total O 205 205	0	0
5	B	246	Total O 246 246	0	0

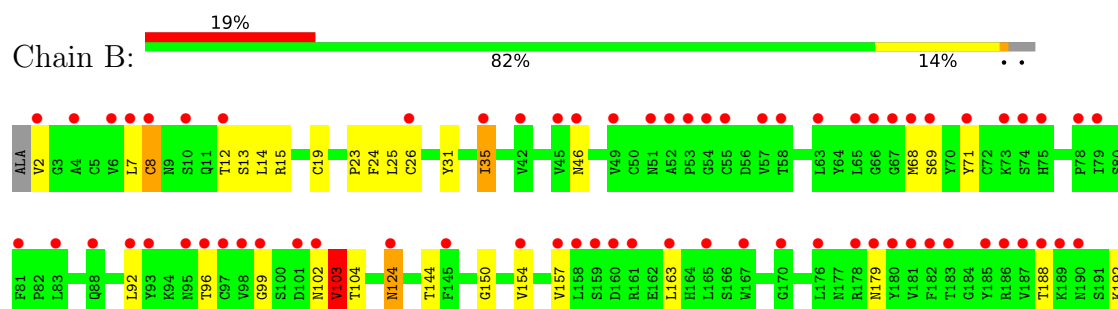
3 Residue-property plots [i](#)

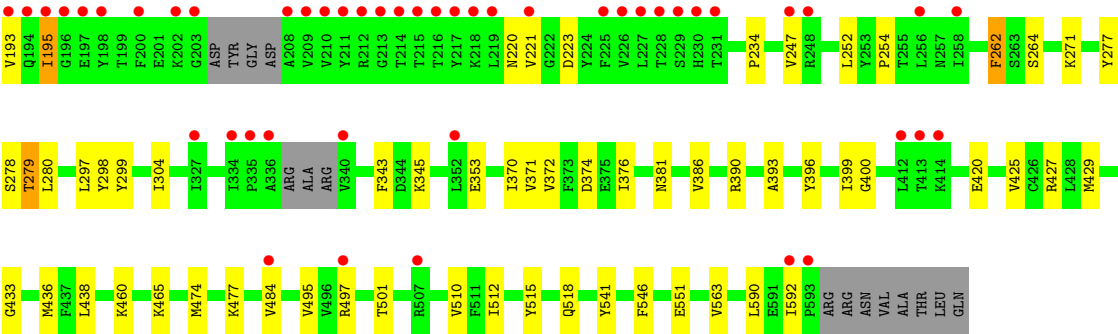
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Helicase



• Molecule 1: Helicase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	58.99Å 70.15Å 85.13Å 102.34° 96.21° 112.56°	Depositor
Resolution (Å)	81.29 – 1.82 81.29 – 1.82	Depositor EDS
% Data completeness (in resolution range)	90.5 (81.29-1.82) 90.7 (81.29-1.82)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.231 , 0.273 0.243 , 0.285	Depositor DCC
R_{free} test set	5538 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.448	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9438	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% 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: ZN, PO4, UXG

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	1.08	0/4517	1.41	5/6156 (0.1%)
1	B	1.09	2/4610 (0.0%)	1.40	8/6283 (0.1%)
All	All	1.08	2/9127 (0.0%)	1.40	13/12439 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	563	VAL	C-O	6.47	1.31	1.24
1	B	515	TYR	C-O	5.61	1.30	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	279	THR	CB-CA-C	5.67	119.52	109.72
1	A	493	ILE	CA-C-N	5.63	126.08	119.94
1	A	493	ILE	C-N-CA	5.63	126.08	119.94
1	B	374	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	196	GLY	CA-C-O	-5.41	118.25	122.52
1	B	150	GLY	CA-C-N	5.29	128.26	120.91
1	B	150	GLY	C-N-CA	5.29	128.26	120.91
1	B	262	PHE	CA-C-N	5.13	127.15	120.28
1	B	262	PHE	C-N-CA	5.13	127.15	120.28
1	A	530	THR	CB-CA-C	5.11	119.46	109.35
1	A	481	THR	N-CA-C	-5.01	102.78	110.14
1	B	103	VAL	CA-C-N	5.00	126.94	120.44
1	B	103	VAL	C-N-CA	5.00	126.94	120.44

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	4321	43	0
1	B	4508	0	4424	56	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	10	0	0	1	0
3	B	10	0	0	0	0
4	B	36	0	0	0	0
5	A	205	0	0	2	0
5	B	246	0	0	5	0
All	All	9438	0	8745	97	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 5.

All (97) 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:2:VAL:N	5:B:801:HOH:O	2.00	0.93
1:B:12:THR:HG22	1:B:14:LEU:H	1.38	0.89
1:B:460:LYS:NZ	5:B:802:HOH:O	2.16	0.78
1:B:12:THR:HG21	1:B:25:LEU:O	1.82	0.78
1:B:510:VAL:HG21	1:B:541:TYR:CD1	2.21	0.75
1:B:279:THR:HB	1:B:429:MET:HE2	1.73	0.69
1:A:510:VAL:HG21	1:A:541:TYR:CD1	2.30	0.66
1:B:46:ASN:ND2	5:B:805:HOH:O	2.28	0.66
1:B:271:LYS:NZ	5:B:806:HOH:O	2.30	0.64
1:A:215:THR:HG22	1:B:193:VAL:HG21	1.81	0.63
1:B:195:ILE:HG23	1:B:195:ILE:O	1.98	0.62
1:B:512:ILE:O	1:B:546:PHE:HA	2.02	0.59
1:B:124:ASN:OD1	1:B:381:ASN:ND2	2.37	0.57
1:B:277:TYR:HA	1:B:396:TYR:O	2.05	0.56
1:B:474[B]:MET:HG2	1:B:590:LEU:HB2	1.87	0.56
1:B:280:LEU:HD11	1:B:438:LEU:HG	1.87	0.56
1:A:368:ALA:O	1:A:393:ALA:HA	2.06	0.56
1:A:60:VAL:HB	5:A:871:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:THR:OG1	1:B:26:CYS:HA	2.07	0.55
1:B:425:VAL:HG12	1:B:429:MET:HE3	1.90	0.54
1:A:445:PRO:HB3	1:A:468:SER:HB3	1.90	0.54
1:A:512:ILE:O	1:A:546:PHE:HA	2.08	0.54
1:B:262:PHE:CE2	1:B:297:LEU:HD12	2.44	0.53
1:A:519:ASN:HB3	1:A:530:THR:HG23	1.91	0.53
1:B:220:ASN:O	1:B:223:ASP:OD2	2.27	0.52
1:B:474[A]:MET:SD	1:B:495:VAL:HG11	2.49	0.52
1:A:401:ASP:OD2	1:A:457:TYR:OH	2.22	0.52
1:A:277:TYR:HA	1:A:396:TYR:O	2.10	0.52
1:B:8:CYS:SG	1:B:99:GLY:N	2.83	0.52
1:B:252:LEU:HB3	1:B:299:TYR:CD1	2.45	0.51
1:A:352:LEU:HD11	1:B:234:PRO:HD3	1.91	0.51
1:B:376:ILE:HG22	1:B:400:GLY:HA3	1.93	0.51
1:A:565:ILE:HA	1:A:572:ILE:HD13	1.92	0.50
1:B:102:ASN:C	1:B:104:THR:H	2.19	0.50
1:A:448:ILE:HD13	1:A:565:ILE:O	2.10	0.50
1:A:518:GLN:HA	1:A:518:GLN:OE1	2.12	0.49
1:B:69:SER:HB2	1:B:71:TYR:CE2	2.48	0.48
1:B:477:LYS:NZ	1:B:551:GLU:OE2	2.30	0.48
1:B:195:ILE:O	1:B:195:ILE:CG2	2.61	0.48
1:B:371:VAL:HG23	1:B:393:ALA:HB2	1.95	0.48
1:A:13:SER:OG	1:A:44:SER:OG	2.18	0.48
1:A:139:LYS:O	1:A:143:GLU:HG2	2.13	0.48
1:B:8:CYS:SG	1:B:99:GLY:O	2.71	0.48
1:B:304:ILE:HA	1:B:370:ILE:O	2.13	0.48
1:B:386:VAL:O	1:B:390:ARG:HG2	2.12	0.48
1:A:5:CYS:SG	1:A:26:CYS:N	2.79	0.47
1:A:13:SER:O	1:A:44:SER:HA	2.13	0.47
1:A:151:ILE:HG12	1:A:226:VAL:HG22	1.97	0.47
1:A:367:THR:HA	1:A:392:ARG:O	2.15	0.47
1:B:154:VAL:HG12	1:B:221:VAL:HA	1.96	0.47
1:B:372:VAL:HG13	1:B:399:ILE:HD12	1.97	0.47
1:A:451:THR:HG21	1:A:585:LEU:HD23	1.97	0.47
1:B:157:VAL:HA	1:B:163:LEU:HD23	1.97	0.47
1:B:372:VAL:CG1	1:B:399:ILE:HD12	2.46	0.46
1:B:13:SER:HB2	1:B:92:LEU:HB2	1.97	0.46
1:A:19:CYS:HB2	1:A:23:PRO:HD2	1.98	0.46
1:B:103:VAL:O	1:B:103:VAL:CG1	2.64	0.45
1:B:278:SER:HB2	1:B:436:MET:HE2	1.98	0.45
1:A:284:PRO:HA	3:A:705:PO4:O2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:PRO:O	1:A:507:ARG:HB2	2.17	0.45
1:B:12:THR:HG22	1:B:14:LEU:N	2.19	0.45
1:A:304:ILE:HA	1:A:370:ILE:O	2.17	0.45
1:B:15:ARG:HG3	1:B:24:PHE:CD2	2.52	0.44
1:B:154:VAL:HG13	1:B:163:LEU:HD22	1.99	0.44
1:B:420:GLU:OE1	1:B:427:ARG:NH1	2.47	0.44
1:A:12:THR:HG21	1:A:26:CYS:HA	2.00	0.43
1:A:326:PRO:HG2	1:A:329:LYS:NZ	2.33	0.43
1:B:343:PHE:CE2	1:B:345:LYS:HB2	2.53	0.43
1:A:519:ASN:HB3	1:A:530:THR:CG2	2.49	0.43
1:B:497:ARG:O	1:B:501:THR:HG23	2.17	0.43
1:B:220:ASN:OD1	1:B:220:ASN:N	2.51	0.43
1:A:261:GLU:OE1	1:A:324:TYR:OH	2.31	0.42
1:A:327:ILE:HD11	1:A:345:LYS:O	2.19	0.42
1:B:7:LEU:HD13	1:B:103:VAL:HG22	2.01	0.42
1:A:158:LEU:HD21	1:A:164:HIS:ND1	2.34	0.42
1:B:31:TYR:CZ	1:B:35:ILE:HG21	2.54	0.42
1:B:429:MET:O	1:B:433:GLY:HA2	2.19	0.42
1:A:130:LEU:HD23	1:A:130:LEU:HA	1.92	0.42
1:A:531:GLN:HE21	1:A:531:GLN:HB2	1.69	0.42
1:A:176:LEU:HD22	1:A:200:PHE:HB2	2.01	0.42
1:A:255:THR:HG23	1:A:300:PRO:HG3	2.02	0.42
1:A:31:TYR:CE2	1:A:87:GLY:HA2	2.55	0.42
1:A:268:ASN:HB3	1:A:436:MET:SD	2.60	0.42
1:B:465:LYS:NZ	5:B:840:HOH:O	2.53	0.42
1:A:280:LEU:HD11	1:A:438:LEU:HG	2.01	0.41
1:B:280:LEU:HD23	1:B:399:ILE:HG12	2.02	0.41
1:B:19:CYS:HB2	1:B:23:PRO:HD2	2.01	0.41
1:A:279:THR:HB	1:A:429:MET:HE2	2.02	0.41
1:B:254:PRO:HB3	1:B:298:TYR:CE2	2.56	0.41
1:B:343:PHE:CZ	1:B:345:LYS:HB2	2.56	0.41
1:A:236:SER:OG	5:A:801:HOH:O	2.22	0.41
1:B:376:ILE:HD12	1:B:376:ILE:HA	1.94	0.41
1:A:512:ILE:HA	1:A:531:GLN:O	2.21	0.40
1:A:158:LEU:HD21	1:A:164:HIS:CE1	2.55	0.40
1:A:308:ALA:O	1:A:359:THR:HA	2.22	0.40
1:B:518:GLN:HA	1:B:518:GLN:OE1	2.22	0.40
1:A:254:PRO:HA	1:A:298:TYR:O	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%)	538 (95%)	22 (4%)	4 (1%)	18	8
1	B	580/601 (96%)	548 (94%)	31 (5%)	1 (0%)	43	33
All	All	1144/1202 (95%)	1086 (95%)	53 (5%)	5 (0%)	30	19

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	LYS
1	A	484	VAL
1	A	219	LEU
1	A	351	THR
1	B	103	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%)	471 (97%)	14 (3%)	37	19
1	B	498/523 (95%)	482 (97%)	16 (3%)	34	16
All	All	983/1046 (94%)	953 (97%)	30 (3%)	35	17

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

Mol	Chain	Res	Type
1	A	7	LEU

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Mol	Chain	Res	Type
1	A	12	THR
1	A	46	ASN
1	A	51	ASN
1	A	81	PHE
1	A	86	ASN
1	A	162	GLU
1	A	173	ARG
1	A	209	VAL
1	A	255	THR
1	A	344	ASP
1	A	530	THR
1	A	572	ILE
1	A	592	ILE
1	B	8	CYS
1	B	35	ILE
1	B	68	MET
1	B	96	THR
1	B	103	VAL
1	B	124	ASN
1	B	144	THR
1	B	179	ASN
1	B	188	THR
1	B	192	LYS
1	B	195	ILE
1	B	247	VAL
1	B	264	SER
1	B	353	GLU
1	B	484	VAL
1	B	592	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	275	GLN
1	A	404	GLN
1	B	179	ASN
1	B	245	HIS
1	B	268	ASN
1	B	404	GLN
1	B	459	ASN
1	B	516	ASN

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	$\# Z > 2$
3	PO4	B	707	-	4,4,4	0.89	0	6,6,6	0.43	0
3	PO4	B	706	-	4,4,4	0.77	0	6,6,6	0.47	0
4	UXG	B	702	-	20,20,20	0.44	0	19,27,27	0.68	0
3	PO4	A	704	-	4,4,4	0.46	0	6,6,6	0.63	0
4	UXG	B	701	-	20,20,20	0.59	0	19,27,27	1.31	2 (10%)
3	PO4	A	705	-	4,4,4	1.05	0	6,6,6	0.71	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
4	UXG	B	701	-	-	0/12/20/20	0/3/3/3
4	UXG	B	702	-	-	0/12/20/20	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	701	UXG	C4-C3-N	-3.71	106.10	111.50
4	B	701	UXG	C10-C3-N	3.69	116.88	111.50

There are no chirality outliers.

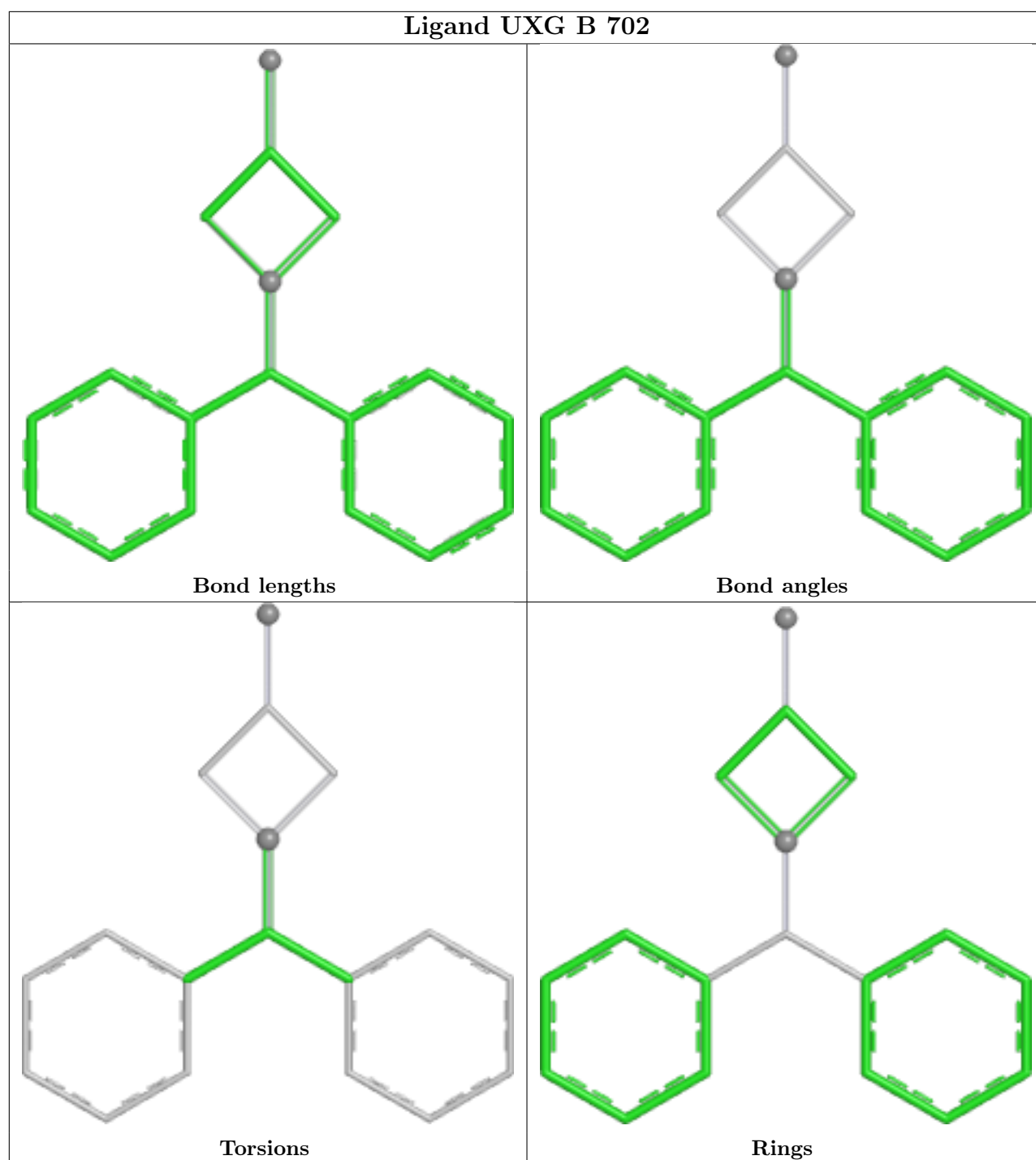
There are no torsion outliers.

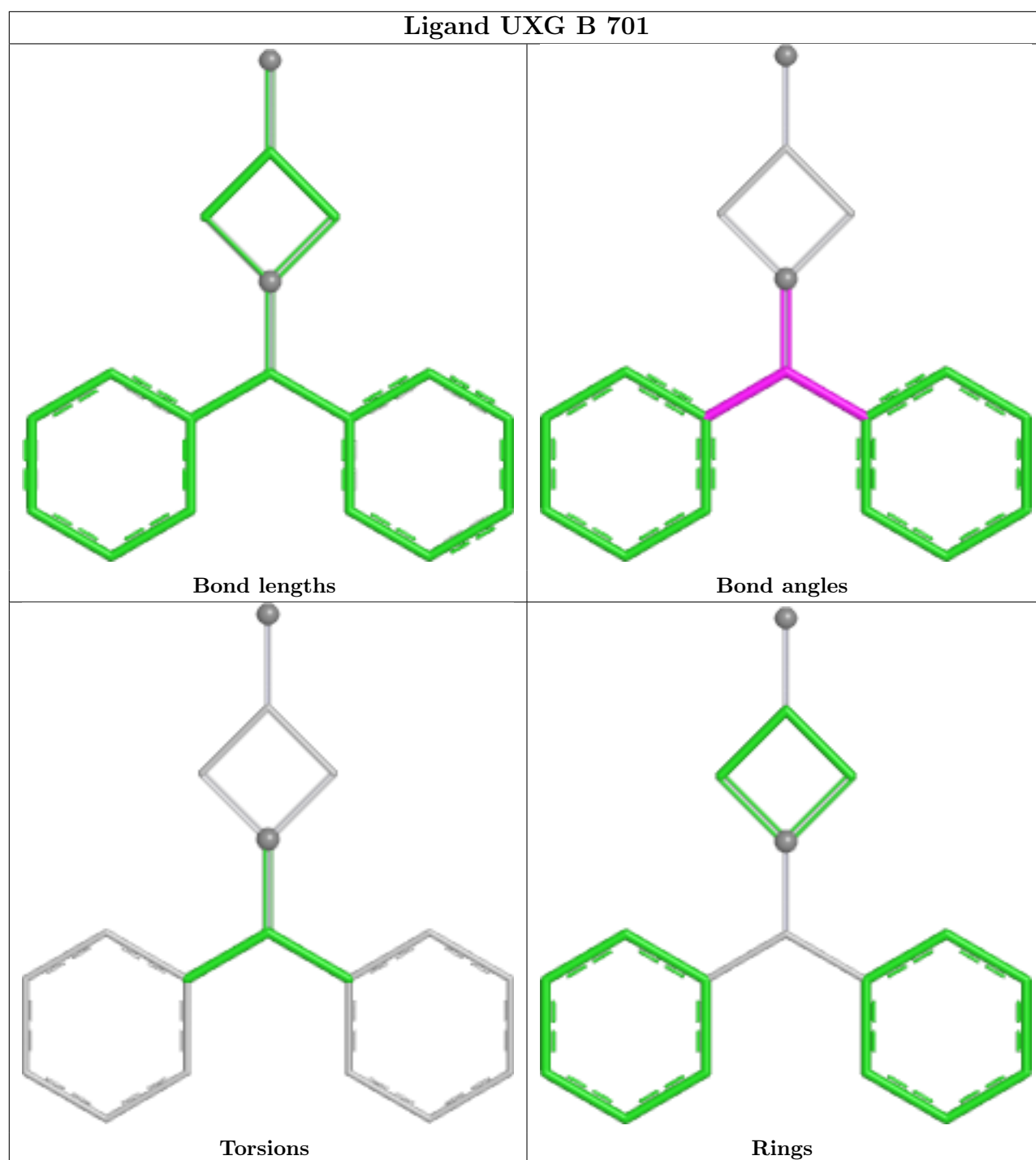
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	705	PO4	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%)	1.73	223 (38%)	1 0	21, 52, 111, 134	0
1	B	585/601 (97%)	1.01	116 (19%)	3 3	17, 39, 89, 125	1 (0%)
All	All	1157/1202 (96%)	1.37	339 (29%)	1 1	17, 45, 101, 134	1 (0%)

All (339) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	219	LEU	7.4
1	A	592	ILE	7.2
1	B	340	VAL	6.4
1	B	193	VAL	6.2
1	A	152	ALA	5.8
1	A	81	PHE	5.6
1	B	219	LEU	5.6
1	A	154	VAL	5.3
1	A	256	LEU	5.2
1	A	90	PHE	5.2
1	A	247	VAL	5.2
1	B	217	TYR	5.1
1	A	336	ALA	5.1
1	A	7	LEU	5.1
1	B	187	VAL	5.1
1	A	338	ALA	5.0
1	A	165	LEU	5.0
1	A	92	LEU	5.0
1	A	151	ILE	5.0
1	A	352	LEU	5.0
1	A	221	VAL	5.0
1	A	181	VAL	4.9
1	A	169	VAL	4.9
1	A	215	THR	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	225	PHE	4.8
1	A	333	ILE	4.8
1	A	340	VAL	4.8
1	A	258	ILE	4.8
1	B	336	ALA	4.8
1	A	185	TYR	4.7
1	A	210	VAL	4.6
1	A	79	ILE	4.6
1	B	592	ILE	4.6
1	A	167	TRP	4.6
1	A	182	PHE	4.5
1	A	226	VAL	4.5
1	B	98	VAL	4.5
1	A	334	ILE	4.5
1	A	170	GLY	4.5
1	A	253	TYR	4.4
1	A	147	LEU	4.4
1	A	145	PHE	4.4
1	A	195	ILE	4.4
1	A	91	GLY	4.3
1	A	176	LEU	4.3
1	A	14	LEU	4.3
1	A	180	TYR	4.3
1	A	217	TYR	4.3
1	A	200	PHE	4.2
1	A	49	VAL	4.2
1	A	1	ALA	4.2
1	A	42	VAL	4.2
1	B	195	ILE	4.2
1	B	208	ALA	4.2
1	B	157	VAL	4.2
1	A	224	TYR	4.2
1	B	210	VAL	4.1
1	A	94	LYS	4.1
1	B	593	PRO	4.1
1	B	229	SER	4.0
1	A	27	CYS	4.0
1	A	6	VAL	4.0
1	A	208	ALA	4.0
1	A	202	LYS	4.0
1	A	155	ARG	4.0
1	B	2	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	232	VAL	4.0
1	B	231	THR	3.9
1	A	335	PRO	3.9
1	A	222	GLY	3.9
1	A	227	LEU	3.9
1	B	196	GLY	3.9
1	A	209	VAL	3.9
1	B	57	VAL	3.9
1	A	158	LEU	3.9
1	B	53	PRO	3.9
1	A	184	GLY	3.8
1	A	149	TYR	3.8
1	B	214	THR	3.8
1	B	158	LEU	3.8
1	A	153	THR	3.8
1	A	228	THR	3.7
1	A	2	VAL	3.7
1	B	78	PRO	3.7
1	A	230	HIS	3.7
1	B	45	VAL	3.7
1	A	93	TYR	3.7
1	B	97	CYS	3.7
1	B	203	GLY	3.7
1	A	89	VAL	3.6
1	A	163	LEU	3.6
1	B	211	TYR	3.6
1	A	330	CYS	3.6
1	A	166	SER	3.6
1	A	229	SER	3.6
1	A	198	TYR	3.6
1	A	304	ILE	3.6
1	A	216	THR	3.6
1	A	249	ILE	3.5
1	A	57	VAL	3.5
1	A	157	VAL	3.5
1	B	35	ILE	3.5
1	B	230	HIS	3.5
1	A	144	THR	3.4
1	B	228	THR	3.4
1	A	45	VAL	3.4
1	B	181	VAL	3.4
1	A	214	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	79	ILE	3.4
1	A	317	LEU	3.4
1	A	199	THR	3.4
1	B	216	THR	3.4
1	A	339	ARG	3.4
1	B	67	GLY	3.4
1	A	348	VAL	3.4
1	B	81	PHE	3.4
1	A	84	CYS	3.3
1	B	92	LEU	3.3
1	A	218	LYS	3.3
1	B	215	THR	3.3
1	A	254	PRO	3.3
1	A	327	ILE	3.3
1	A	356	VAL	3.3
1	B	209	VAL	3.3
1	B	163	LEU	3.3
1	A	48	TYR	3.2
1	A	65	LEU	3.2
1	A	485	SER	3.2
1	A	211	TYR	3.2
1	A	246	TYR	3.2
1	A	387	VAL	3.2
1	A	346	PHE	3.2
1	B	221	VAL	3.2
1	B	213	GLY	3.2
1	A	293	ILE	3.1
1	A	370	ILE	3.1
1	A	295	LEU	3.1
1	A	392	ARG	3.1
1	B	96	THR	3.1
1	B	183	THR	3.1
1	A	47	PRO	3.1
1	B	102	ASN	3.1
1	A	12	THR	3.1
1	A	252	LEU	3.1
1	A	24	PHE	3.1
1	A	4	ALA	3.1
1	B	327	ILE	3.0
1	A	28	LYS	3.0
1	A	31	TYR	3.0
1	B	7	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	34	VAL	3.0
1	A	19	CYS	3.0
1	B	218	LYS	3.0
1	B	179	ASN	3.0
1	B	256	LEU	3.0
1	A	103	VAL	3.0
1	A	364	PRO	3.0
1	A	305	VAL	2.9
1	A	351	THR	2.9
1	A	302	ALA	2.9
1	A	25	LEU	2.9
1	A	63	LEU	2.9
1	B	414	LYS	2.9
1	B	49	VAL	2.9
1	A	363	LEU	2.9
1	A	391	LEU	2.9
1	A	60	VAL	2.9
1	B	247	VAL	2.9
1	A	396	TYR	2.9
1	A	53	PRO	2.9
1	A	362	ALA	2.9
1	A	178	ARG	2.9
1	B	186	ARG	2.9
1	A	43	LEU	2.9
1	A	297	LEU	2.9
1	A	11	GLN	2.8
1	A	161	ARG	2.8
1	B	198	TYR	2.8
1	A	85	ALA	2.8
1	A	179	ASN	2.8
1	B	484	VAL	2.8
1	A	16	CYS	2.8
1	A	345	LYS	2.8
1	A	41	LEU	2.8
1	B	176	LEU	2.8
1	A	223	ASP	2.8
1	A	484	VAL	2.8
1	A	245	HIS	2.7
1	B	75	HIS	2.7
1	A	255	THR	2.7
1	A	35	ILE	2.7
1	A	78	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	6	VAL	2.7
1	A	70	TYR	2.7
1	B	66	GLY	2.7
1	A	343	PHE	2.7
1	A	18	ALA	2.7
1	A	277	TYR	2.7
1	B	93	TYR	2.7
1	A	357	PHE	2.7
1	A	266	VAL	2.7
1	A	196	GLY	2.6
1	A	389	ALA	2.6
1	A	231	THR	2.6
1	B	188	THR	2.6
1	A	44	SER	2.6
1	B	73	LYS	2.6
1	A	46	ASN	2.6
1	B	178	ARG	2.6
1	A	29	CYS	2.6
1	A	358	CYS	2.6
1	A	235	LEU	2.6
1	A	240	LEU	2.6
1	A	328	ASP	2.6
1	A	156	GLU	2.6
1	A	220	ASN	2.6
1	B	225	PHE	2.6
1	A	173	ARG	2.6
1	A	337	ARG	2.6
1	A	323	LYS	2.6
1	B	10	SER	2.6
1	A	183	THR	2.6
1	A	15	ARG	2.5
1	A	300	PRO	2.5
1	A	83	LEU	2.5
1	A	10	SER	2.5
1	B	248	ARG	2.5
1	A	174	PRO	2.5
1	A	298	TYR	2.5
1	B	185	TYR	2.5
1	B	200	PHE	2.5
1	A	130	LEU	2.5
1	B	159	SER	2.5
1	B	12	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	64	TYR	2.5
1	B	180	TYR	2.5
1	A	432	ILE	2.5
1	A	58	THR	2.5
1	B	189	LYS	2.5
1	B	202	LYS	2.5
1	A	73	LYS	2.4
1	A	127	THR	2.4
1	A	508	LYS	2.4
1	A	355	TYR	2.4
1	B	65	LEU	2.4
1	B	165	LEU	2.4
1	A	524	LYS	2.4
1	A	82	PRO	2.4
1	A	9	ASN	2.4
1	A	150	GLY	2.4
1	B	54	GLY	2.4
1	B	170	GLY	2.4
1	B	26	CYS	2.4
1	B	68	MET	2.4
1	A	132	LEU	2.4
1	B	197	GLU	2.4
1	A	361	ASN	2.4
1	B	42	VAL	2.4
1	A	8	CYS	2.4
1	B	161	ARG	2.3
1	A	393	ALA	2.3
1	A	257	ASN	2.3
1	A	213	GLY	2.3
1	A	13	SER	2.3
1	A	259	SER	2.3
1	B	227	LEU	2.3
1	B	71	TYR	2.3
1	B	182	PHE	2.3
1	B	46	ASN	2.3
1	B	334	ILE	2.3
1	A	242	PRO	2.3
1	B	83	LEU	2.3
1	A	353	GLU	2.3
1	A	164	HIS	2.3
1	B	95	ASN	2.3
1	A	23	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	52	ALA	2.2
1	A	314	VAL	2.2
1	A	212	ARG	2.2
1	B	58	THR	2.2
1	A	194	GLN	2.2
1	A	207	ASP	2.2
1	B	101	ASP	2.2
1	B	160	ASP	2.2
1	A	269	TYR	2.2
1	A	329	LYS	2.2
1	B	212	ARG	2.2
1	A	104	THR	2.2
1	B	88	GLN	2.2
1	B	352	LEU	2.2
1	A	299	TYR	2.2
1	A	373	PHE	2.2
1	A	20	ILE	2.2
1	B	167	TRP	2.2
1	A	241	VAL	2.2
1	A	250	THR	2.2
1	A	366	THR	2.2
1	B	413	THR	2.2
1	A	160	ASP	2.2
1	A	30	CYS	2.2
1	A	67	GLY	2.2
1	A	312	ALA	2.2
1	B	4	ALA	2.2
1	A	129	ARG	2.2
1	B	497	ARG	2.2
1	A	133	PHE	2.1
1	B	194	GLN	2.1
1	A	371	VAL	2.1
1	A	74	SER	2.1
1	A	303	ARG	2.1
1	A	197	GLU	2.1
1	B	145	PHE	2.1
1	B	69	SER	2.1
1	A	397	VAL	2.1
1	A	507	ARG	2.1
1	B	226	VAL	2.1
1	A	464	HIS	2.1
1	B	55	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	335	PRO	2.1
1	B	507	ARG	2.1
1	B	51	ASN	2.1
1	B	124	ASN	2.1
1	B	154	VAL	2.1
1	A	172	PRO	2.1
1	A	171	LYS	2.0
1	A	416	THR	2.0
1	A	66	GLY	2.0
1	A	322	LEU	2.0
1	B	8	CYS	2.0
1	B	63	LEU	2.0
1	B	412	LEU	2.0
1	B	74	SER	2.0
1	B	258	ILE	2.0
1	B	99	GLY	2.0
1	B	190	ASN	2.0
1	A	326	PRO	2.0
1	A	21	ARG	2.0
1	A	360	VAL	2.0
1	A	386	VAL	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
4	UXG	B	701	18/18	0.86	0.13	15,18,22,22	18
4	UXG	B	702	18/18	0.87	0.16	22,24,33,33	18

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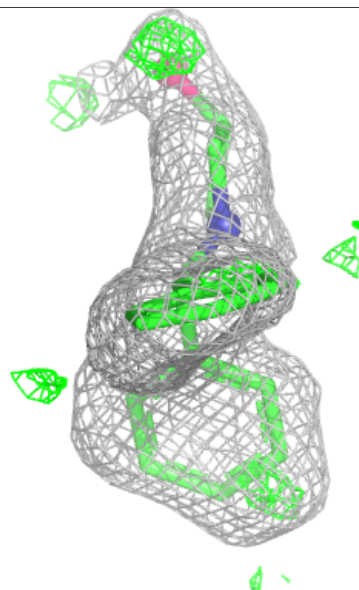
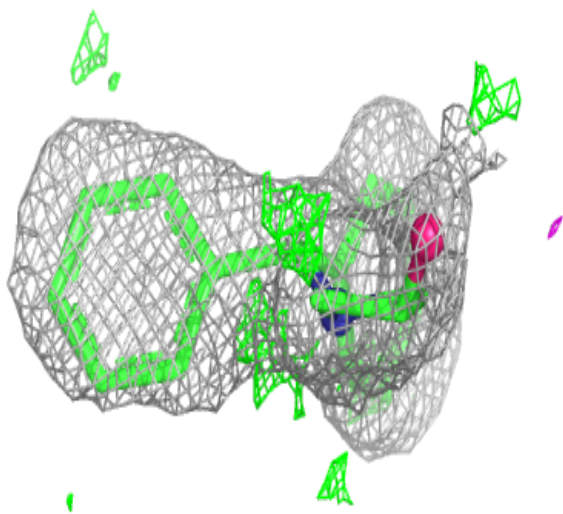
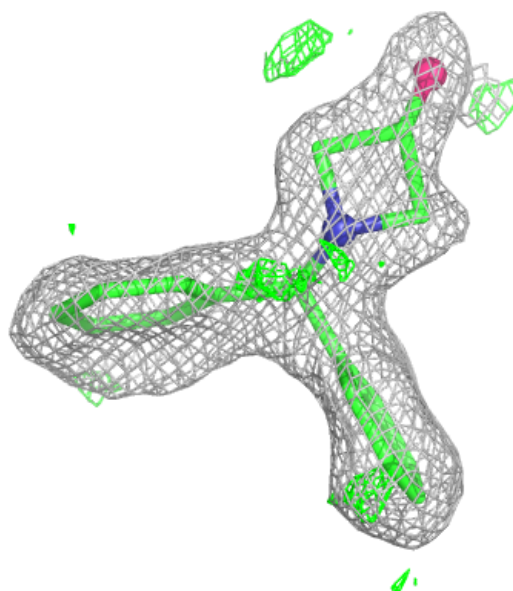
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PO4	B	706	5/5	0.93	0.10	25,27,34,38	0
2	ZN	A	702	1/1	0.94	0.07	51,51,51,51	0
3	PO4	A	704	5/5	0.94	0.08	30,33,38,45	0
3	PO4	A	705	5/5	0.94	0.08	30,36,40,43	0
2	ZN	A	703	1/1	0.96	0.06	86,86,86,86	0
3	PO4	B	707	5/5	0.96	0.08	21,27,31,31	0
2	ZN	B	704	1/1	0.98	0.04	56,56,56,56	0
2	ZN	B	705	1/1	0.98	0.06	71,71,71,71	0
2	ZN	A	701	1/1	0.98	0.04	57,57,57,57	0
2	ZN	B	703	1/1	0.98	0.03	38,38,38,38	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.

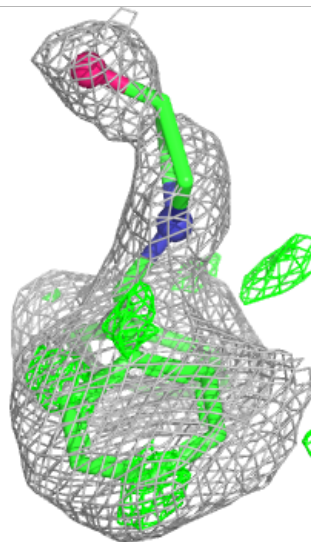
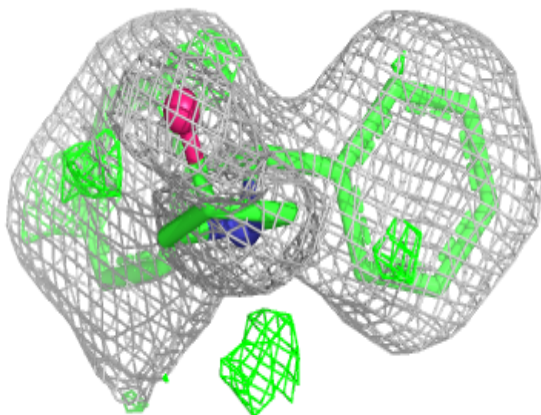
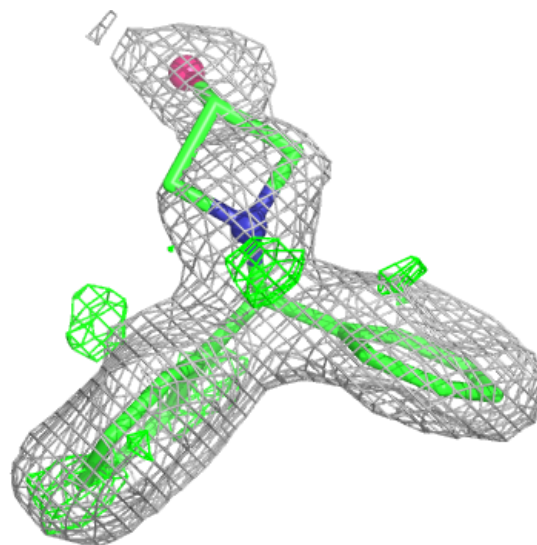
Electron density around UXG B 701:

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



Electron density around UXG B 702:

$2mF_o-DF_c$ (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.