



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:13 AM UTC

PDB ID : 5RLW / pdb\_00005rlw  
Title : PanDDA analysis group deposition – Crystal Structure of SARS-CoV-2 heli-  
case in complex with Z45705015  
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 : 1.97 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](mailto: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>.

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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)

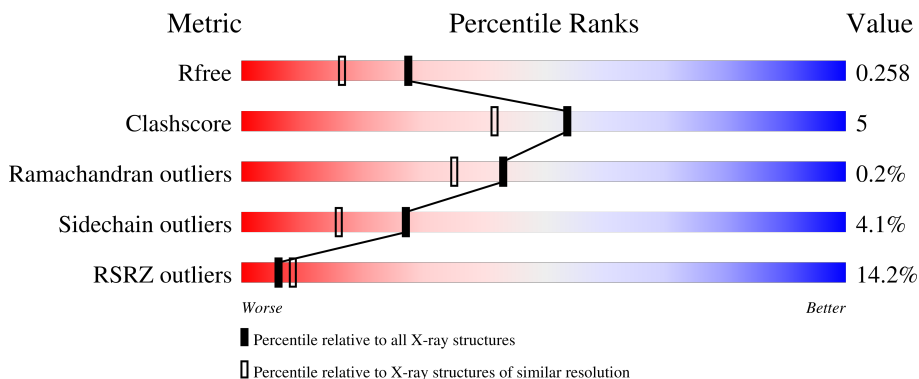
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.97 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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  $\geq 3$ , 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](#)

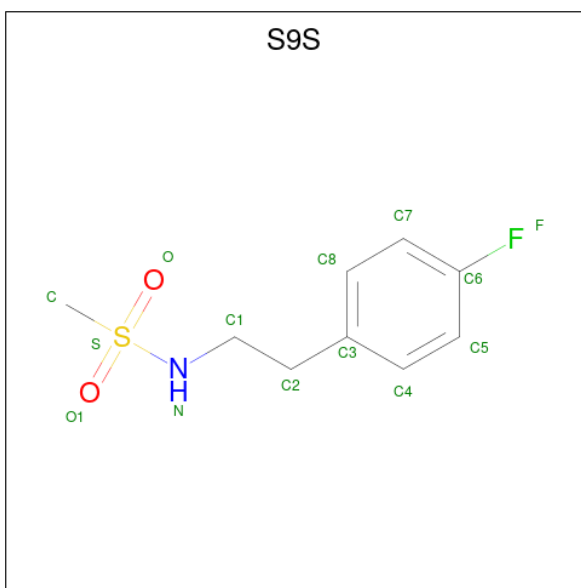
There are 5 unique types of molecules in this entry. The entry contains 9433 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 2 is {N}-[2-(4-fluorophenyl)ethyl]methanesulfonamide (CCD ID: S9S) (formula: C<sub>9</sub>H<sub>12</sub>FNO<sub>2</sub>S) (labeled as "Ligand of Interest" by depositor).

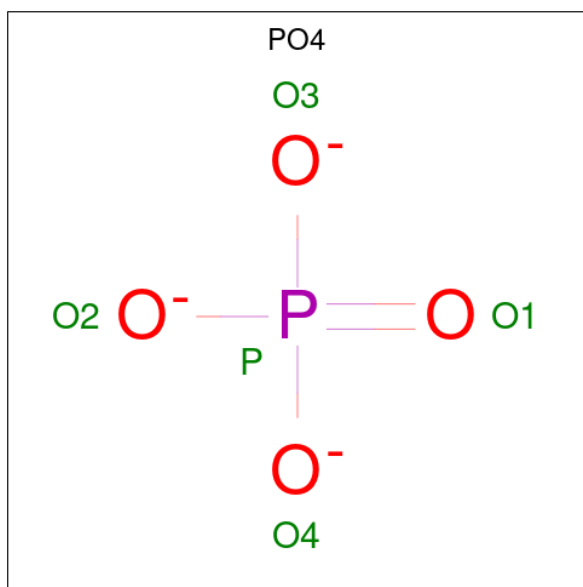


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	N	O			S
2	A	1	Total 14	C 9	F 1	N 1	O 2	S 1	0	0
2	B	1	Total 14	C 9	F 1	N 1	O 2	S 1	0	0

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

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

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



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

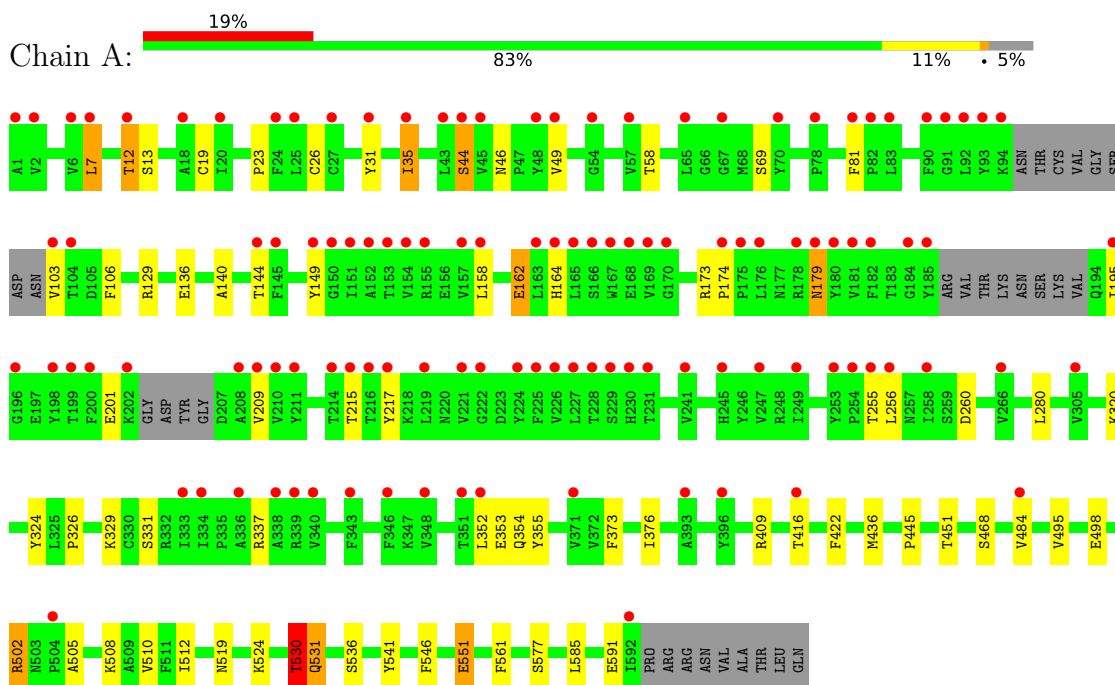
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	204	Total	O	0	0
			204	204		
5	B	250	Total	O	0	0
			250	250		

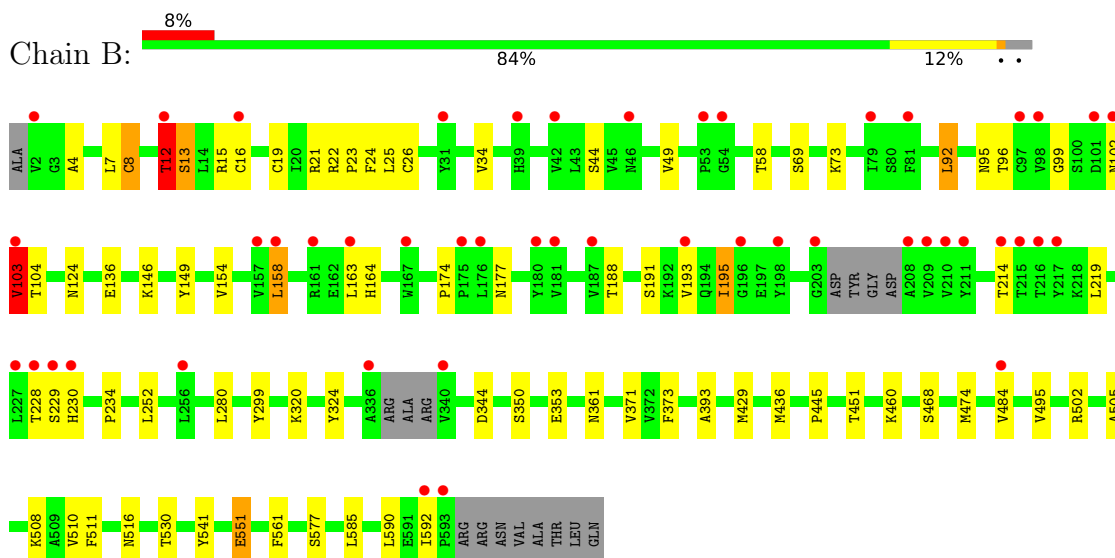
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	59.12Å 70.11Å 85.10Å 102.69° 95.96° 112.44°	Depositor
Resolution (Å)	81.20 – 1.97 81.20 – 1.97	Depositor EDS
% Data completeness (in resolution range)	95.8 (81.20-1.97) 95.8 (81.20-1.97)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 1.97Å)	Xtrriage
Refinement program	BUSTER 2.10.3 (20-MAY-2020)	Depositor
R, $R_{free}$	0.171 , 0.237 0.196 , 0.258	Depositor DCC
$R_{free}$ test set	4211 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.6	Xtrriage
Anisotropy	0.351	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 65.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9433	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PO4, S9S, 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	0.88	0/4517	1.13	9/6156 (0.1%)
1	B	0.90	1/4610 (0.0%)	1.13	15/6283 (0.2%)
All	All	0.89	1/9127 (0.0%)	1.13	24/12439 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	429	MET	SD-CE	-5.53	1.65	1.79

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	VAL	CA-C-N	7.02	129.69	120.28
1	B	103	VAL	C-N-CA	7.02	129.69	120.28
1	B	561	PHE	CA-CB-CG	-6.68	107.12	113.80
1	A	591	GLU	CA-C-N	6.31	133.06	121.70
1	A	591	GLU	C-N-CA	6.31	133.06	121.70
1	A	561	PHE	CA-CB-CG	-6.19	107.61	113.80
1	B	12	THR	N-CA-C	5.86	118.01	108.76
1	A	373	PHE	CA-CB-CG	5.81	119.61	113.80
1	B	373	PHE	CA-CB-CG	5.79	119.59	113.80
1	B	502	ARG	CA-C-N	5.75	128.97	122.59
1	B	502	ARG	C-N-CA	5.75	128.97	122.59
1	B	350	SER	CA-C-N	5.63	128.60	120.38
1	B	350	SER	C-N-CA	5.63	128.60	120.38
1	B	344	ASP	CA-CB-CG	5.41	118.00	112.60
1	B	214	THR	CA-C-N	5.37	131.80	121.54
1	B	214	THR	C-N-CA	5.37	131.80	121.54
1	B	361	ASN	CA-CB-CG	5.31	117.91	112.60
1	A	530	THR	N-CA-CB	-5.30	102.02	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	256	LEU	N-CA-C	-5.26	105.14	112.45
1	B	95	ASN	CA-CB-CG	5.15	117.75	112.60
1	A	179	ASN	CA-CB-CG	5.13	117.73	112.60
1	A	260	ASP	CA-C-N	5.01	127.25	120.38
1	A	260	ASP	C-N-CA	5.01	127.25	120.38
1	B	34	VAL	N-CA-CB	5.01	117.36	110.54

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	4322	47	0
1	B	4508	0	4425	40	0
2	A	14	0	0	2	0
2	B	14	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	1	0
5	A	204	0	0	0	0
5	B	250	0	0	1	0
All	All	9433	0	8747	86	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 (86) 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:13:SER:HB3	1:B:92:LEU:HB2	1.43	1.00
1:A:129:ARG:HE	2:A:701:S9S:C5	1.86	0.88
1:B:21:ARG:HE	1:B:136:GLU:HG2	1.46	0.80
1:A:158:LEU:HD11	1:A:164:HIS:CE1	2.18	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:LEU:HD21	1:A:164:HIS:CE1	2.19	0.78
1:A:329:LYS:HZ3	1:A:355:TYR:HE2	1.33	0.74
1:B:12:THR:CG2	1:B:26:CYS:HA	2.18	0.73
1:A:326:PRO:HD2	1:A:329:LYS:NZ	2.04	0.73
1:B:21:ARG:NE	1:B:136:GLU:HG2	2.07	0.70
1:A:519:ASN:HB3	1:A:530:THR:CG2	2.26	0.65
2:B:701:S9S:N	4:B:705:PO4:O3	2.31	0.64
1:A:519:ASN:HB3	1:A:530:THR:HG23	1.80	0.64
1:B:228:THR:HG22	1:B:230:HIS:NE2	2.14	0.62
1:B:12:THR:HG21	1:B:26:CYS:HA	1.81	0.61
1:A:331:SER:HB2	1:A:353:GLU:HG3	1.83	0.61
1:A:215:THR:HG22	1:B:193:VAL:HG21	1.83	0.61
1:A:329:LYS:HE2	1:A:354:GLN:OE1	1.99	0.61
1:A:7:LEU:HD22	1:A:103:VAL:HG22	1.84	0.60
1:B:146:LYS:HD2	1:B:229:SER:HB3	1.83	0.59
1:B:511:PHE:HB3	1:B:530:THR:HG22	1.84	0.59
1:B:551:GLU:HG2	1:B:577:SER:HB3	1.84	0.59
1:A:326:PRO:HG2	1:A:329:LYS:NZ	2.18	0.58
1:A:352:LEU:HD11	1:B:234:PRO:HD3	1.86	0.57
1:A:158:LEU:HD21	1:A:164:HIS:ND1	2.19	0.57
1:B:474[B]:MET:HG2	1:B:590:LEU:HB2	1.87	0.56
1:B:510:VAL:HG21	1:B:541:TYR:CD1	2.42	0.55
1:A:326:PRO:CG	1:A:329:LYS:HZ2	2.20	0.55
1:A:551:GLU:HG2	1:A:577:SER:HB3	1.87	0.55
1:B:177:ASN:HB3	1:B:516:ASN:ND2	2.23	0.54
1:A:498:GLU:HG3	1:A:502:ARG:HH22	1.71	0.54
1:A:510:VAL:HG21	1:A:541:TYR:CD1	2.44	0.53
1:B:12:THR:HG21	1:B:25:LEU:O	2.09	0.53
1:A:13:SER:O	1:A:44:SER:HA	2.08	0.52
1:A:326:PRO:CD	1:A:329:LYS:NZ	2.72	0.52
1:B:12:THR:HG23	1:B:26:CYS:HA	1.90	0.52
1:A:326:PRO:HB2	1:A:329:LYS:HG3	1.92	0.52
1:A:326:PRO:HG2	1:A:329:LYS:HZ2	1.75	0.51
1:B:158:LEU:HD13	1:B:164:HIS:HB2	1.93	0.50
1:B:228:THR:CG2	1:B:230:HIS:NE2	2.75	0.50
1:B:280:LEU:HB2	1:B:436:MET:HE3	1.95	0.49
1:A:326:PRO:CG	1:A:329:LYS:NZ	2.77	0.48
1:B:149:TYR:HB3	1:B:174:PRO:HD3	1.95	0.48
1:B:19:CYS:HB2	1:B:23:PRO:HD2	1.95	0.48
1:A:12:THR:HG21	1:A:26:CYS:HA	1.95	0.48
1:A:505:ALA:O	1:A:508:LYS:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:PRO:HB3	1:A:468:SER:HB3	1.96	0.47
1:A:519:ASN:HB3	1:A:530:THR:HG21	1.96	0.47
1:A:136:GLU:OE1	2:A:701:S9S:N	2.48	0.47
1:B:228:THR:CG2	1:B:230:HIS:CE1	2.97	0.47
1:A:158:LEU:HD21	1:A:164:HIS:HE1	1.78	0.47
1:B:16:CYS:O	1:B:22:ARG:HA	2.15	0.47
1:B:505:ALA:O	1:B:508:LYS:HG2	2.15	0.46
1:B:445:PRO:HB3	1:B:468:SER:HB3	1.97	0.45
1:A:149:TYR:HB3	1:A:174:PRO:HD3	1.98	0.45
1:B:4:ALA:O	1:B:24:PHE:HB2	2.16	0.45
1:B:8:CYS:SG	1:B:99:GLY:N	2.88	0.45
1:B:460:LYS:NZ	5:B:811:HOH:O	2.50	0.45
1:A:140:ALA:O	1:A:144:THR:HG23	2.17	0.45
1:B:102:ASN:C	1:B:104:THR:H	2.26	0.44
1:A:524:LYS:HA	1:A:524:LYS:HD2	1.85	0.44
1:A:531:GLN:HG2	1:A:536:SER:HB3	1.98	0.44
1:A:498:GLU:HG3	1:A:502:ARG:NH2	2.32	0.44
1:B:7:LEU:HD13	1:B:103:VAL:HG22	1.98	0.43
1:A:280:LEU:HB2	1:A:436:MET:HE3	1.99	0.43
1:A:451:THR:HG21	1:A:585:LEU:HD23	2.01	0.43
1:B:19:CYS:CB	1:B:23:PRO:HD2	2.49	0.43
1:A:19:CYS:HB2	1:A:23:PRO:HD2	2.01	0.43
1:A:158:LEU:HD12	1:A:162:GLU:HB3	2.00	0.43
1:B:195:ILE:HG23	1:B:195:ILE:O	2.19	0.43
1:B:371:VAL:HG23	1:B:393:ALA:HB2	2.01	0.42
1:B:451:THR:HG21	1:B:585:LEU:HD23	2.00	0.42
1:A:320:LYS:HE3	1:A:324:TYR:HE1	1.84	0.42
1:A:409:ARG:NH2	1:A:422:PHE:O	2.52	0.42
1:B:15:ARG:HG3	1:B:24:PHE:CD2	2.55	0.41
1:B:252:LEU:HB3	1:B:299:TYR:CD1	2.55	0.41
1:B:320:LYS:HE3	1:B:324:TYR:HE1	1.85	0.41
1:A:376:ILE:HD12	1:A:376:ILE:HA	1.97	0.41
1:A:329:LYS:NZ	1:A:355:TYR:HE2	2.11	0.41
1:B:49:VAL:HG23	1:B:58:THR:HG22	2.02	0.41
1:A:158:LEU:HD21	1:A:164:HIS:HD1	1.86	0.41
1:A:7:LEU:HD21	1:A:106:PHE:HB2	2.03	0.41
1:A:49:VAL:HG23	1:A:58:THR:HG22	2.03	0.41
1:B:13:SER:O	1:B:44:SER:HA	2.20	0.41
1:A:31:TYR:CZ	1:A:35:ILE:HD12	2.56	0.40
1:A:512:ILE:O	1:A:546:PHE:HA	2.21	0.40
1:B:154:VAL:HG13	1:B:163:LEU:HD22	2.03	0.40

There are no symmetry-related clashes.

## 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%)	542 (96%)	20 (4%)	2 (0%)	30	20
1	B	580/601 (96%)	551 (95%)	29 (5%)	0	100	100
All	All	1144/1202 (95%)	1093 (96%)	49 (4%)	2 (0%)	43	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	484	VAL
1	A	195	ILE

### 5.3.2 Protein sidechains [i](#)

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%)	464 (96%)	21 (4%)	26	14
1	B	498/523 (95%)	479 (96%)	19 (4%)	29	19
All	All	983/1046 (94%)	943 (96%)	40 (4%)	27	16

All (40) 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	35	ILE
1	A	44	SER
1	A	46	ASN
1	A	69	SER
1	A	81	PHE
1	A	162	GLU
1	A	173	ARG
1	A	179	ASN
1	A	201	GLU
1	A	209	VAL
1	A	217	TYR
1	A	255	THR
1	A	337	ARG
1	A	416	THR
1	A	495	VAL
1	A	502	ARG
1	A	530	THR
1	A	531	GLN
1	A	551	GLU
1	B	8	CYS
1	B	12	THR
1	B	13	SER
1	B	69	SER
1	B	73	LYS
1	B	92	LEU
1	B	96	THR
1	B	103	VAL
1	B	124	ASN
1	B	158	LEU
1	B	188	THR
1	B	191	SER
1	B	195	ILE
1	B	219	LEU
1	B	353	GLU
1	B	484	VAL
1	B	495	VAL
1	B	551	GLU
1	B	592	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	116	ASN
1	A	164	HIS
1	A	230	HIS
1	A	245	HIS
1	A	275	GLN
1	A	404	GLN
1	B	116	ASN
1	B	179	ASN
1	B	245	HIS
1	B	268	ASN
1	B	404	GLN
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	$\# Z  > 2$
2	S9S	B	701	-	14,14,14	0.32	0	18,19,19	0.49	0
4	PO4	B	706	-	4,4,4	2.54	1 (25%)	6,6,6	1.41	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PO4	A	706	-	4,4,4	2.68	3 (75%)	6,6,6	0.65	0
4	PO4	A	705	-	4,4,4	2.57	2 (50%)	6,6,6	0.45	0
4	PO4	B	705	-	4,4,4	2.52	1 (25%)	6,6,6	0.52	0
2	S9S	A	701	-	14,14,14	0.26	0	18,19,19	0.43	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	S9S	B	701	-	-	2/7/7/7	0/1/1/1
2	S9S	A	701	-	-	0/7/7/7	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	706	PO4	P-O1	4.48	1.61	1.50
4	A	706	PO4	P-O1	4.42	1.60	1.50
4	B	705	PO4	P-O1	4.31	1.60	1.50
4	A	705	PO4	P-O1	4.26	1.60	1.50
4	A	706	PO4	P-O3	2.10	1.60	1.54
4	A	705	PO4	P-O4	2.07	1.60	1.54
4	A	706	PO4	P-O4	2.01	1.60	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	706	PO4	O3-P-O1	2.54	119.92	110.95

There are no chirality outliers.

All (2) torsion outliers are listed below:

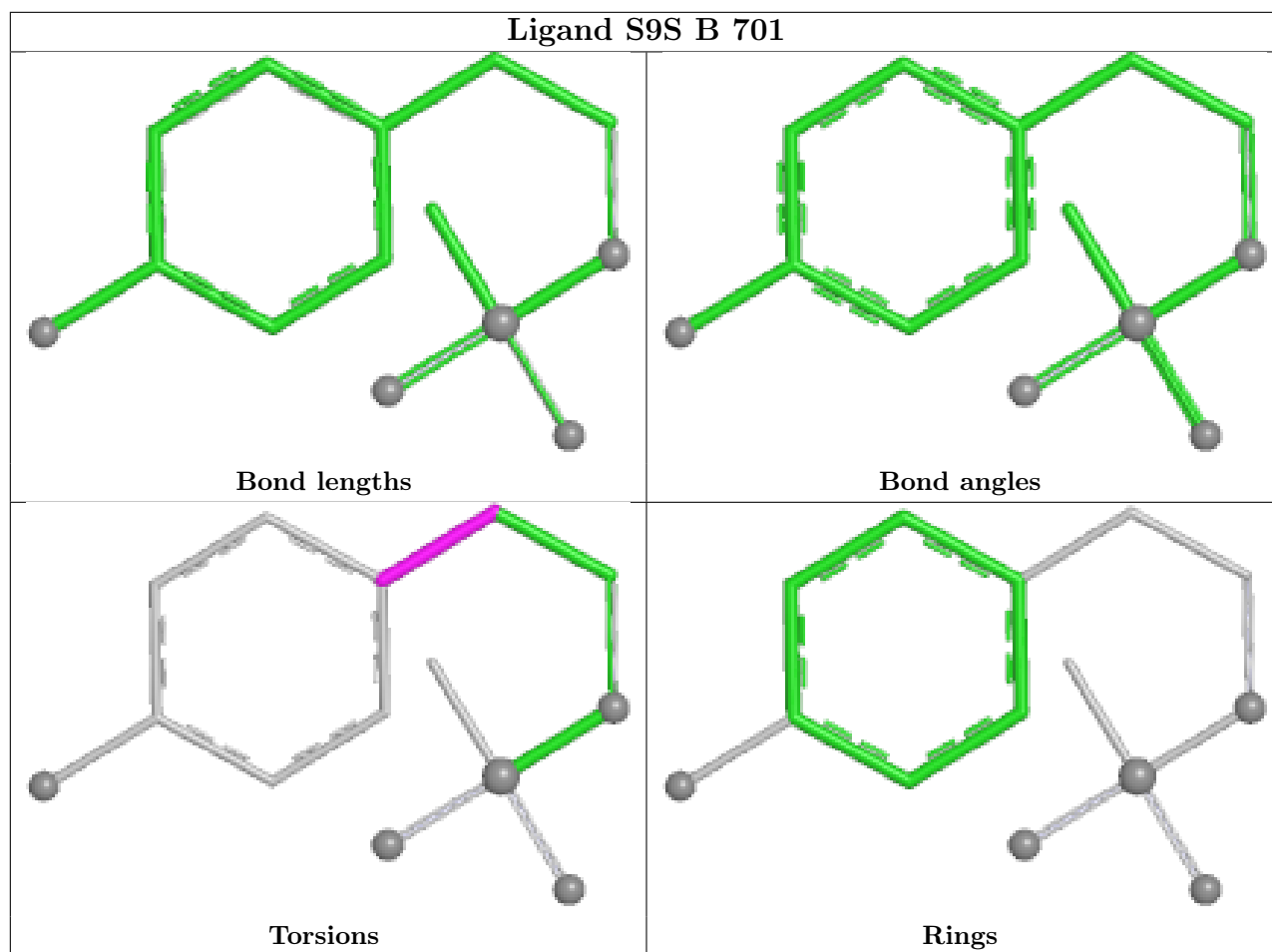
Mol	Chain	Res	Type	Atoms
2	B	701	S9S	C1-C2-C3-C8
2	B	701	S9S	C1-C2-C3-C4

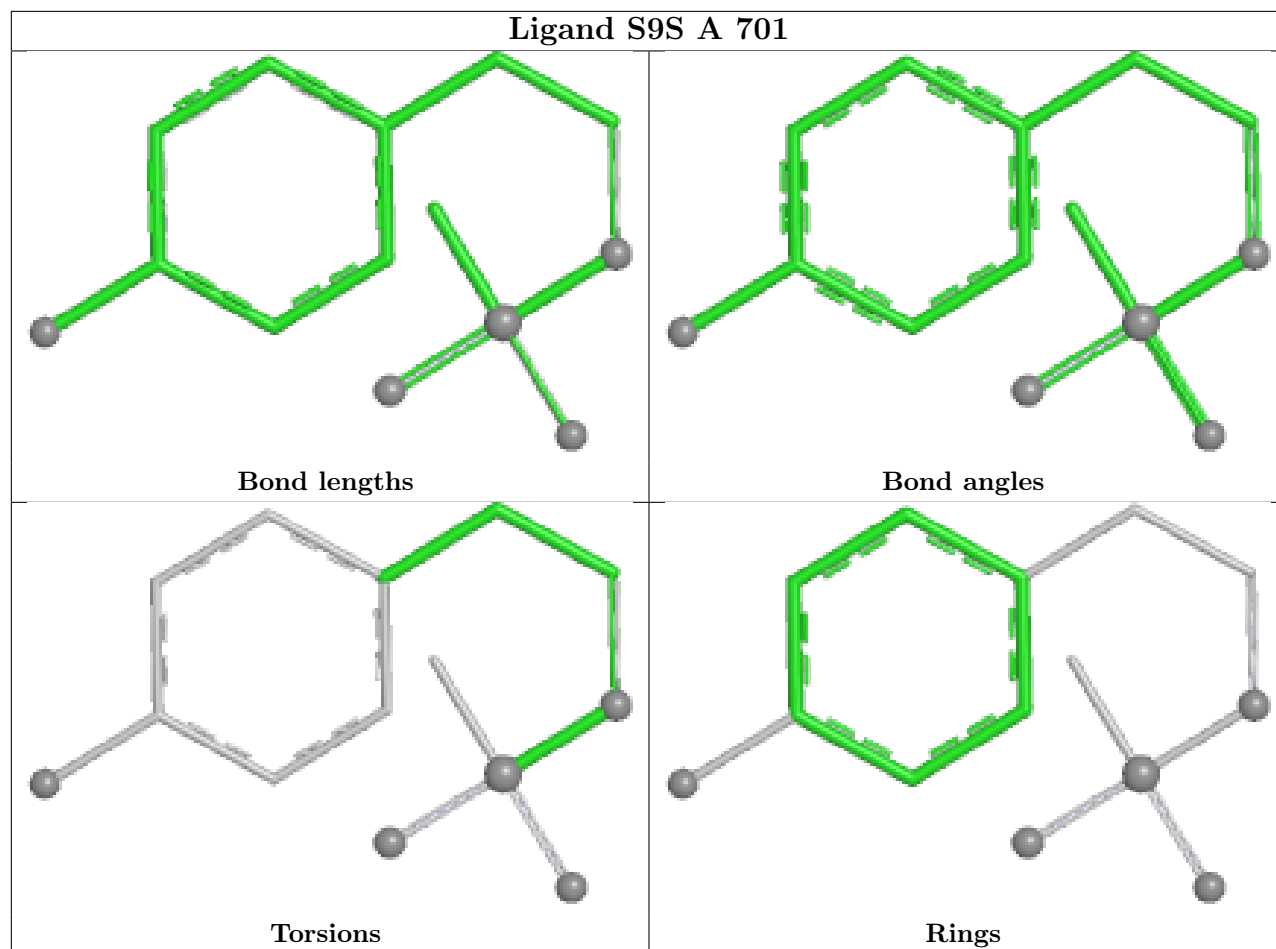
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	S9S	1	0
4	B	705	PO4	1	0
2	A	701	S9S	2	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	572/601 (95%)	1.09	116 (20%) <b>3</b> <b>3</b>	32, 65, 131, 162	0
1	B	585/601 (97%)	0.51	48 (8%) <b>17</b> <b>24</b>	21, 49, 100, 138	1 (0%)
All	All	1157/1202 (96%)	0.80	164 (14%) <b>6</b> <b>8</b>	21, 56, 118, 162	1 (0%)

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	225	PHE	5.9
1	A	169	VAL	5.0
1	A	209	VAL	5.0
1	A	340	VAL	4.9
1	A	592	ILE	4.7
1	A	151	ILE	4.7
1	A	210	VAL	4.6
1	A	226	VAL	4.4
1	A	81	PHE	4.3
1	A	221	VAL	4.2
1	A	247	VAL	4.2
1	B	176	LEU	4.2
1	A	182	PHE	4.1
1	A	152	ALA	4.1
1	A	6	VAL	4.0
1	A	167	TRP	3.9
1	A	185	TYR	3.9
1	B	208	ALA	3.8
1	A	92	LEU	3.8
1	A	195	ILE	3.8
1	B	2	VAL	3.8
1	A	145	PHE	3.7
1	B	217	TYR	3.6
1	B	16	CYS	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	336	ALA	3.6
1	A	258	ILE	3.6
1	B	98	VAL	3.6
1	A	336	ALA	3.6
1	A	149	TYR	3.5
1	A	222	GLY	3.5
1	A	202	LYS	3.5
1	A	227	LEU	3.5
1	A	200	PHE	3.5
1	B	340	VAL	3.5
1	A	165	LEU	3.5
1	A	224	TYR	3.4
1	A	157	VAL	3.4
1	A	208	ALA	3.4
1	A	219	LEU	3.4
1	A	94	LYS	3.3
1	A	214	THR	3.3
1	A	352	LEU	3.2
1	B	196	GLY	3.2
1	A	153	THR	3.2
1	A	45	VAL	3.2
1	A	176	LEU	3.2
1	B	203	GLY	3.2
1	A	1	ALA	3.1
1	B	198	TYR	3.0
1	A	43	LEU	3.0
1	A	217	TYR	3.0
1	B	193	VAL	3.0
1	A	2	VAL	2.9
1	A	229	SER	2.9
1	B	209	VAL	2.9
1	A	154	VAL	2.9
1	B	12	THR	2.9
1	A	254	PRO	2.9
1	A	25	LEU	2.9
1	A	256	LEU	2.9
1	B	210	VAL	2.9
1	B	227	LEU	2.9
1	A	179	ASN	2.8
1	B	228	THR	2.8
1	A	150	GLY	2.8
1	B	592	ILE	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	155	ARG	2.7
1	B	229	SER	2.7
1	A	103	VAL	2.7
1	A	7	LEU	2.7
1	B	256	LEU	2.7
1	A	48	TYR	2.7
1	A	170	GLY	2.7
1	B	81	PHE	2.7
1	A	216	THR	2.7
1	B	53	PRO	2.7
1	A	24	PHE	2.6
1	B	214	THR	2.6
1	A	65	LEU	2.6
1	A	348	VAL	2.6
1	A	253	TYR	2.6
1	B	211	TYR	2.6
1	A	215	THR	2.6
1	A	228	THR	2.6
1	A	339	ARG	2.6
1	A	181	VAL	2.6
1	A	90	PHE	2.5
1	B	163	LEU	2.5
1	A	230	HIS	2.5
1	A	266	VAL	2.5
1	A	27	CYS	2.5
1	B	97	CYS	2.5
1	A	93	TYR	2.5
1	A	163	LEU	2.5
1	A	54	GLY	2.5
1	A	67	GLY	2.5
1	A	338	ALA	2.5
1	A	393	ALA	2.5
1	A	343	PHE	2.5
1	B	593	PRO	2.5
1	A	180	TYR	2.4
1	B	101	ASP	2.4
1	B	216	THR	2.4
1	A	91	GLY	2.4
1	A	249	ILE	2.4
1	A	174	PRO	2.4
1	A	371	VAL	2.4
1	B	157	VAL	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	12	THR	2.3
1	B	215	THR	2.3
1	B	54	GLY	2.3
1	B	42	VAL	2.3
1	A	255	THR	2.3
1	B	102	ASN	2.3
1	A	18	ALA	2.3
1	A	178	ARG	2.3
1	A	484	VAL	2.3
1	B	175	PRO	2.3
1	A	184	GLY	2.3
1	A	166	SER	2.3
1	B	46	ASN	2.3
1	A	83	LEU	2.3
1	A	104	THR	2.3
1	A	351	THR	2.3
1	B	167	TRP	2.2
1	A	396	TYR	2.2
1	B	31	TYR	2.2
1	A	44	SER	2.2
1	A	164	HIS	2.2
1	A	231	THR	2.2
1	B	180	TYR	2.2
1	A	333	ILE	2.2
1	A	305	VAL	2.2
1	A	20	ILE	2.2
1	A	82	PRO	2.2
1	A	175	PRO	2.2
1	B	39	HIS	2.1
1	B	230	HIS	2.1
1	B	79	ILE	2.1
1	A	144	THR	2.1
1	A	416	THR	2.1
1	B	187	VAL	2.1
1	A	196	GLY	2.1
1	B	158	LEU	2.1
1	A	198	TYR	2.1
1	A	211	TYR	2.1
1	A	49	VAL	2.1
1	B	103	VAL	2.1
1	B	161	ARG	2.1
1	B	484	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	245	HIS	2.1
1	A	158	LEU	2.1
1	A	504	PRO	2.1
1	A	346	PHE	2.1
1	A	334	ILE	2.1
1	A	57	VAL	2.1
1	A	199	THR	2.0
1	A	78	PRO	2.0
1	B	181	VAL	2.0
1	A	168	GLU	2.0
1	A	35	ILE	2.0
1	A	31	TYR	2.0
1	A	70	TYR	2.0
1	A	241	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, 95<sup>th</sup> 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.

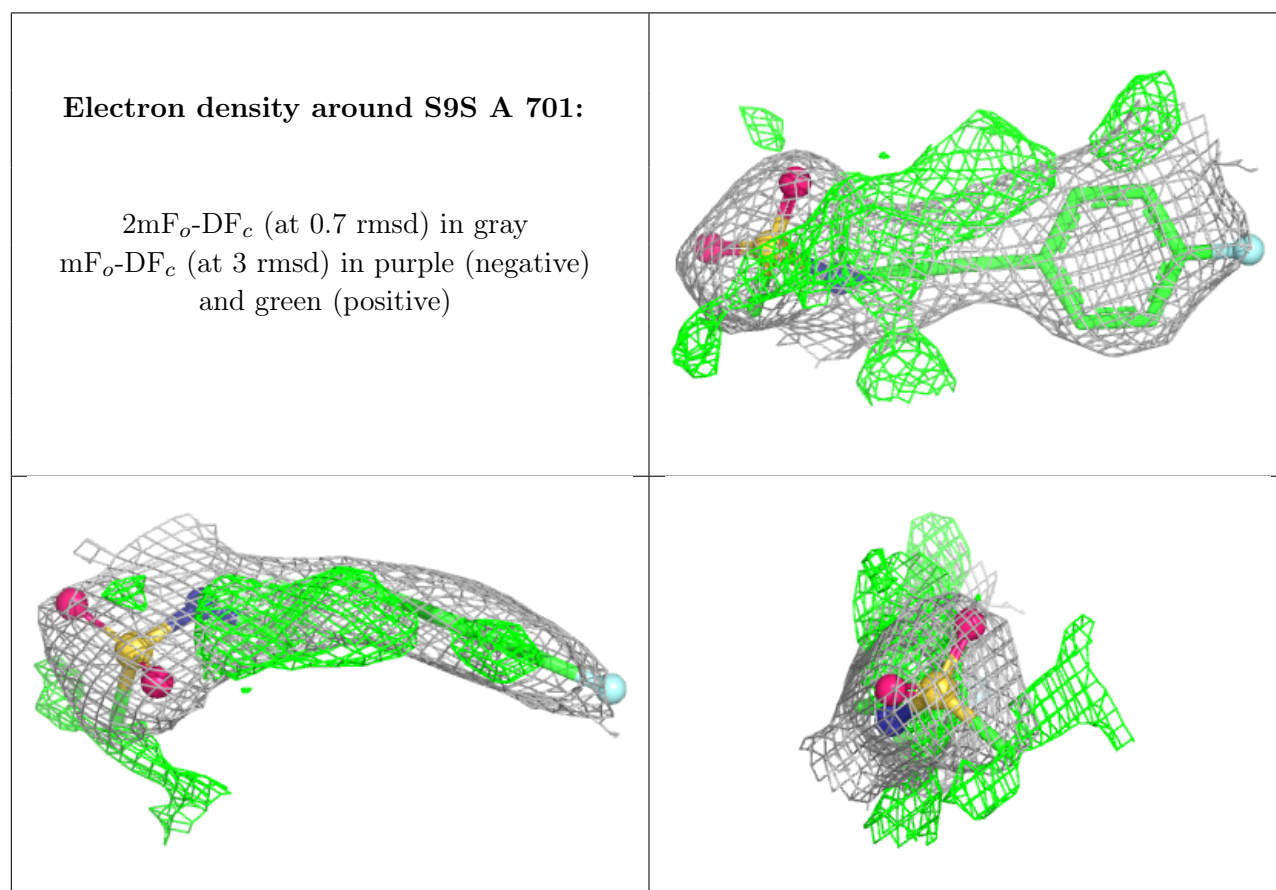
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	S9S	A	701	14/14	0.88	0.20	39,40,43,43	14
2	S9S	B	701	14/14	0.88	0.20	34,36,37,37	14
4	PO4	A	705	5/5	0.97	0.06	49,50,52,54	0
4	PO4	B	705	5/5	0.97	0.07	45,47,50,50	0
4	PO4	B	706	5/5	0.97	0.07	39,40,42,44	0
3	ZN	A	704	1/1	0.98	0.04	94,94,94,94	0
4	PO4	A	706	5/5	0.98	0.06	45,45,48,50	0
3	ZN	A	703	1/1	0.99	0.04	66,66,66,66	0
3	ZN	A	702	1/1	0.99	0.04	66,66,66,66	0

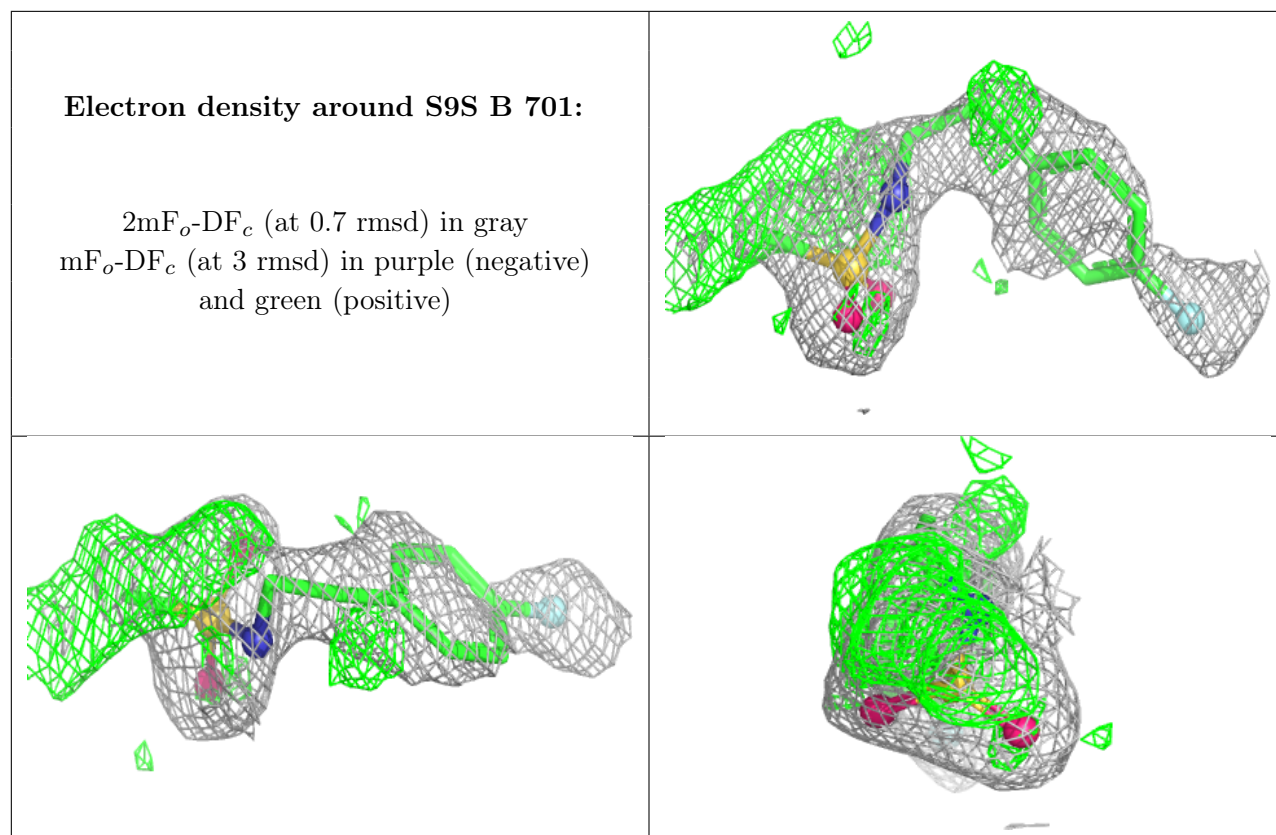
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	B	702	1/1	0.99	0.03	35,35,35,35	0
3	ZN	B	704	1/1	0.99	0.03	79,79,79,79	0
3	ZN	B	703	1/1	1.00	0.04	63,63,63,63	0

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 [i](#)

There are no such residues in this entry.