



# Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2026 – 10:14 pm BST

PDB ID : 9S17 / pdb\_00009s17  
Title : WRN helicase in complex with molecule 81  
Authors : Fletcher, C.T.; Rucktooa, P.  
Deposited on : 2025-07-18  
Resolution : 1.91 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 : 1.8.4, CSD as541be (2020)  
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

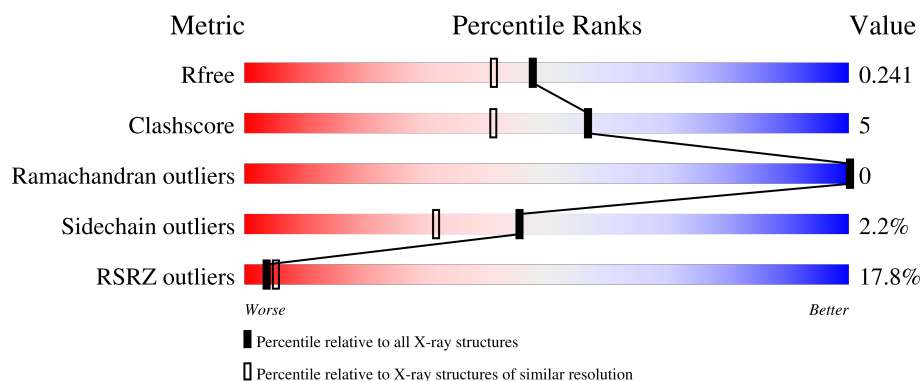
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.91 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	427	
1	B	427	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	DMS	B	1001	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6882 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 Bifunctional 3'-5' exonuclease/ATP-dependent helicase WRN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	0	7	0
			3247	2050	576	589	32			
1	B	402	Total	C	N	O	S	0	9	0
			3243	2047	574	591	31			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	515	GLY	-	expression tag	UNP Q14191
A	516	MET	-	expression tag	UNP Q14191
B	515	GLY	-	expression tag	UNP Q14191
B	516	MET	-	expression tag	UNP Q14191

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



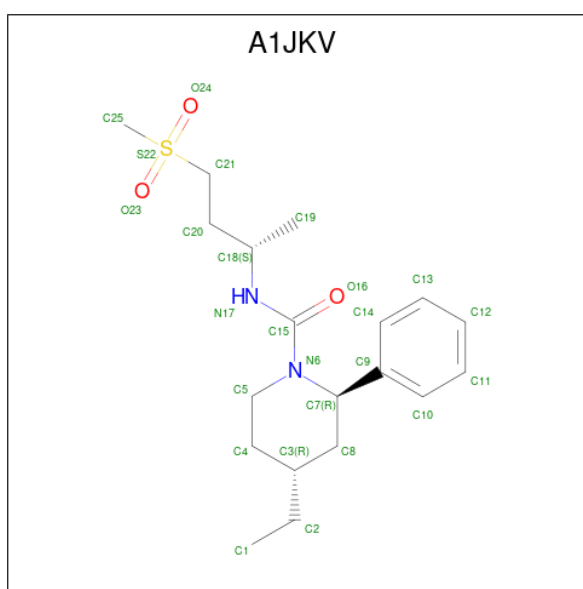
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is (2 {R},4 {R})-4-ethyl- {N}-[(2 {S})-4-methylsulfonylbutan-2-yl]-2-phenyl-piperidine-1-carboxamide (CCD ID: A1JKV) (formula: C<sub>19</sub>H<sub>30</sub>N<sub>2</sub>O<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



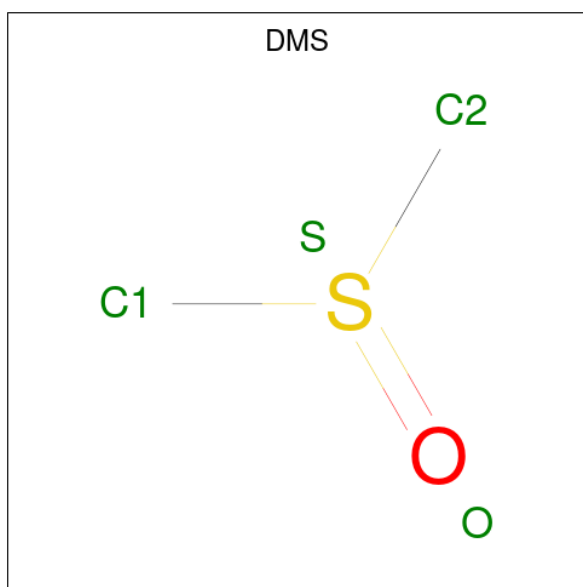
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			25	19	2	3	1		
4	B	1	Total	C	N	O	S	0	0
			25	19	2	3	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



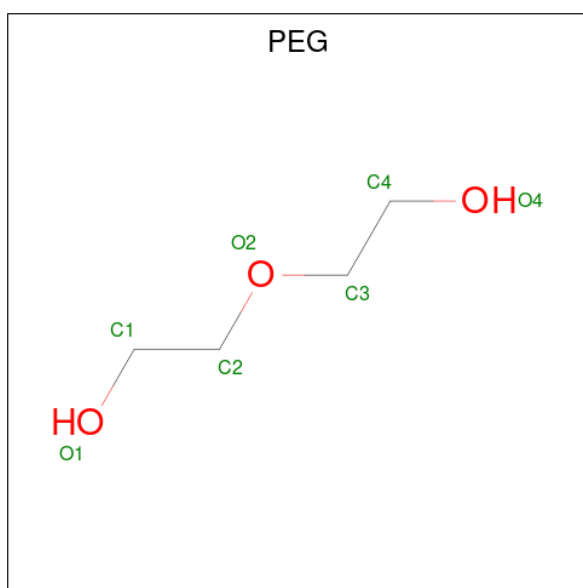
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	O	S	0	0
			4	2	1	1		
6	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O		
			7	4	3	0	0

- Molecule 8 is water.

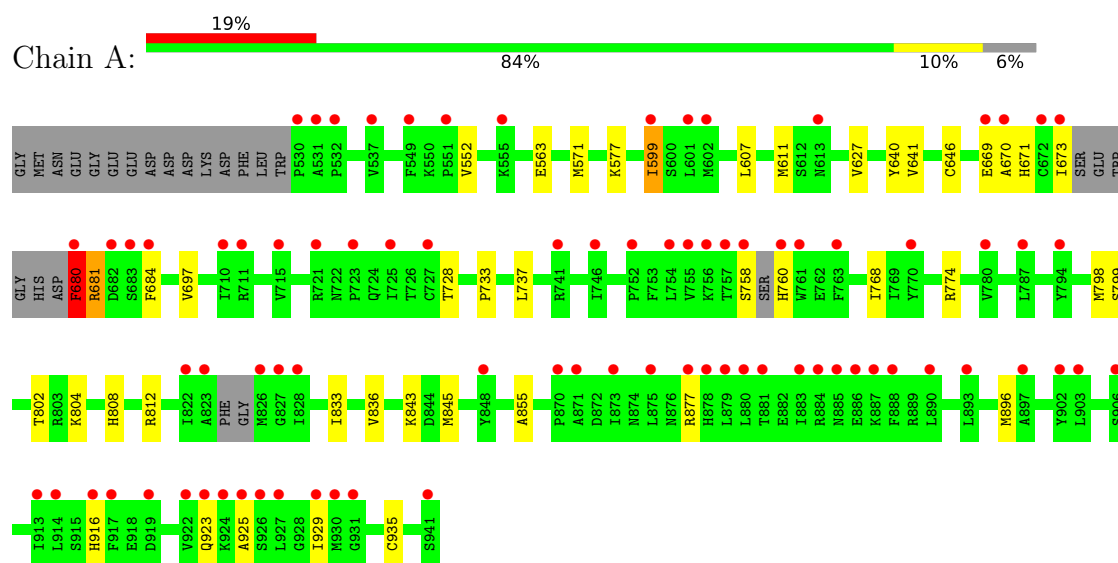


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	73	Total 73	O 73	0	0
8	B	154	Total 154	O 154	0	1

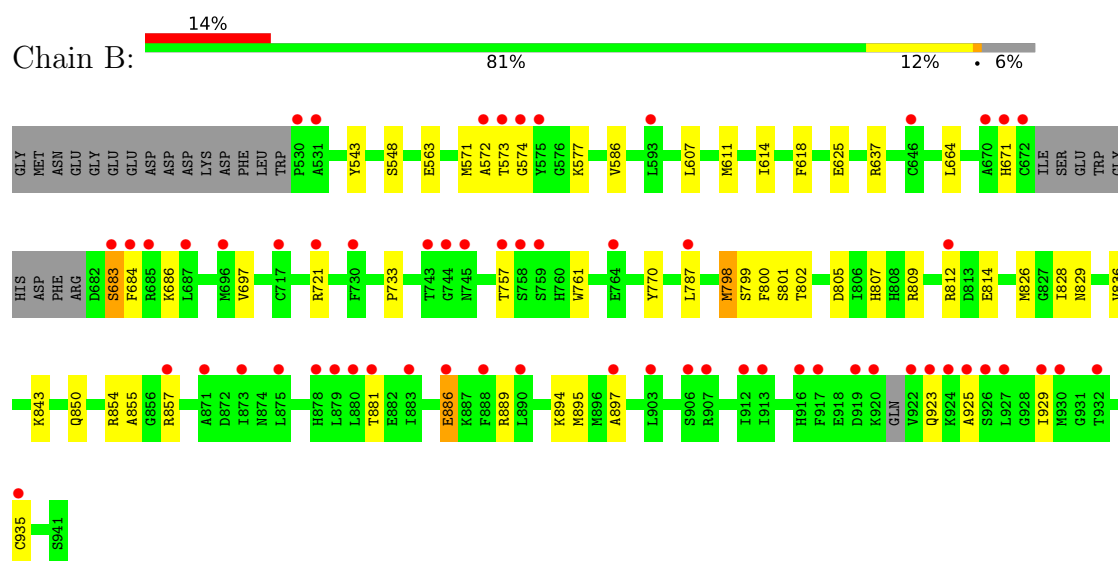
### 3 Residue-property plots [i](#)

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: Bifunctional 3'-5' exonuclease/ATP-dependent helicase WRN



- Molecule 1: Bifunctional 3'-5' exonuclease/ATP-dependent helicase WRN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.09Å 92.73Å 96.30Å 90.00° 105.57° 90.00°	Depositor
Resolution (Å)	92.77 – 1.91 92.76 – 1.91	Depositor EDS
% Data completeness (in resolution range)	65.0 (92.77-1.91) 65.0 (92.76-1.91)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 1.91Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, $R_{free}$	0.219 , 0.248 0.211 , 0.241	Depositor DCC
$R_{free}$ test set	2475 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.1	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6882	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.72% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, ZN, A1JKV, EDO, DMS, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.72	0/3312	1.06	4/4459 (0.1%)
1	B	0.79	3/3312 (0.1%)	1.07	5/4462 (0.1%)
All	All	0.76	3/6624 (0.0%)	1.07	9/8921 (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	A	0	1
1	B	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	571	MET	SD-CE	-6.04	1.64	1.79
1	B	895	MET	SD-CE	-5.15	1.66	1.79
1	B	798	MET	SD-CE	-5.05	1.67	1.79

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	684	PHE	CA-CB-CG	-6.65	107.15	113.80
1	A	697	VAL	N-CA-C	5.81	113.63	107.76
1	B	618	PHE	CA-CB-CG	5.67	119.47	113.80
1	A	680	PHE	CA-CB-CG	5.62	119.42	113.80
1	B	571	MET	N-CA-C	5.39	118.18	109.40
1	A	577	LYS	CA-C-N	5.14	127.68	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	577	LYS	C-N-CA	5.14	127.68	120.28
1	B	828	ILE	CB-CA-C	5.13	117.34	110.42
1	B	697	VAL	N-CA-C	5.07	112.83	108.22

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	681	ARG	Sidechain
1	B	809	ARG	Sidechain

## 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	3247	0	3291	28	0
1	B	3243	0	3287	38	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	20	0	30	1	0
3	B	48	0	72	5	0
4	A	25	0	0	0	0
4	B	25	0	0	0	0
5	A	10	0	0	0	0
5	B	20	0	0	2	0
6	B	8	0	12	6	0
7	B	7	0	10	0	0
8	A	73	0	0	0	0
8	B	154	0	0	0	0
All	All	6882	0	6702	61	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 (61) 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:801:SER:HB3	6:B:1001:DMS:H22	1.44	0.98
1:A:669[B]:GLU:HA	1:A:671:HIS:CE1	2.24	0.73
1:A:599:ILE:HG22	6:B:1001:DMS:H21	1.72	0.71
1:A:669[A]:GLU:HA	1:A:671:HIS:CE1	2.25	0.71
1:A:877:ARG:HG2	1:A:896:MET:HE1	1.71	0.71
1:B:683:SER:HA	1:B:686:LYS:HD2	1.73	0.70
1:A:799:SER:HB2	3:A:1005:EDO:H11	1.72	0.69
1:B:798:MET:HE3	1:B:802:THR:HG22	1.73	0.69
1:B:829:ASN:HB3	1:B:857:ARG:CZ	2.24	0.67
1:A:680:PHE:HZ	1:B:805:ASP:HB3	1.61	0.65
1:B:573[B]:THR:HG21	1:B:854:ARG:NH2	2.12	0.64
1:B:886:GLU:H	1:B:886:GLU:CD	2.04	0.63
1:B:721:ARG:HD2	3:B:1014:EDO:H11	1.82	0.61
1:A:798:MET:HE3	1:A:802:THR:HG22	1.85	0.59
1:B:801:SER:CB	6:B:1001:DMS:H22	2.28	0.58
1:A:641:VAL:HG21	1:A:646[B]:CYS:SG	2.45	0.56
1:B:574:GLY:HA3	1:B:857:ARG:HH21	1.70	0.56
1:A:845:MET:HE2	1:A:916:HIS:CD2	2.42	0.54
1:A:680:PHE:CZ	1:B:805:ASP:HB3	2.43	0.54
1:B:637:ARG:HG3	3:B:1002:EDO:H12	1.89	0.53
1:B:671:HIS:H	1:B:671:HIS:CD2	2.26	0.53
1:A:680:PHE:CE1	1:B:802:THR:HG23	2.44	0.53
1:B:800:PHE:HB2	6:B:1001:DMS:H12	1.90	0.52
1:A:808:HIS:CE1	1:A:812:ARG:NE	2.77	0.52
1:B:761:TRP:CD1	1:B:787:LEU:HD22	2.45	0.51
1:A:552:VAL:CG2	1:A:571:MET:HE2	2.42	0.50
1:A:670:ALA:HA	1:A:684:PHE:HE1	1.77	0.50
1:B:897:ALA:HA	3:B:1012:EDO:H12	1.94	0.50
1:B:586:VAL:HG13	3:B:1002:EDO:H11	1.92	0.49
1:B:894:LYS:NZ	5:B:1019:SO4:O4	2.34	0.49
1:A:758:SER:HB2	1:A:760:HIS:N	2.28	0.49
1:B:573[B]:THR:HG21	1:B:854:ARG:CZ	2.42	0.49
1:A:808:HIS:CE1	1:A:812:ARG:CZ	2.96	0.49
1:B:573[B]:THR:HG23	5:B:1016:SO4:O1	2.13	0.49
1:B:881:THR:HA	1:B:889:ARG:HD3	1.94	0.49
1:A:571:MET:HG2	1:A:728:THR:HG23	1.95	0.49
1:A:836:VAL:HG23	1:A:855:ALA:HB2	1.95	0.48
1:A:599:ILE:HD11	1:A:640:TYR:HB3	1.95	0.48
1:A:627:VAL:HG21	1:B:625:GLU:HB3	1.95	0.48
1:B:807:HIS:CB	1:B:826:MET:HE1	2.45	0.47
1:A:552:VAL:HG22	1:A:571:MET:HE2	1.96	0.47
1:A:733:PRO:HG3	1:A:925:ALA:HB1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:799:SER:HB2	6:B:1001:DMS:O	2.16	0.46
1:B:800:PHE:HB2	6:B:1001:DMS:C1	2.45	0.46
1:A:680:PHE:CZ	1:B:802:THR:HA	2.52	0.45
1:A:680:PHE:N	1:A:680:PHE:CD2	2.85	0.45
1:B:577:LYS:HD3	3:B:1007:EDO:H21	1.99	0.44
1:B:733:PRO:HG3	1:B:925:ALA:HB1	1.98	0.44
1:B:543:TYR:HB3	1:B:614:ILE:HD11	2.00	0.44
1:A:673:ILE:HA	1:A:681:ARG:HG2	2.00	0.44
1:B:929:ILE:O	1:B:935:CYS:HB2	2.18	0.44
1:B:607:LEU:HG	1:B:611[B]:MET:HE2	2.00	0.43
1:B:836:VAL:HG23	1:B:855:ALA:HB2	2.00	0.43
1:B:854:ARG:HA	1:B:857:ARG:NH2	2.34	0.43
1:A:768:ILE:HD11	1:A:833:ILE:HD13	2.02	0.41
1:B:812[A]:ARG:NH2	1:B:814:GLU:OE2	2.53	0.41
1:A:929:ILE:O	1:A:935:CYS:HB2	2.20	0.41
1:B:770:TYR:OH	1:B:854:ARG:HD2	2.21	0.41
1:B:574:GLY:HA2	1:B:829:ASN:CG	2.46	0.41
1:B:572:ALA:HA	1:B:850[B]:GLN:OE1	2.22	0.40
1:A:607:LEU:HG	1:A:611[B]:MET:HE2	2.02	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	402/427 (94%)	391 (97%)	11 (3%)	0	100	100
1	B	405/427 (95%)	394 (97%)	11 (3%)	0	100	100
All	All	807/854 (94%)	785 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	364/377 (97%)	356 (98%)	8 (2%)	45	32
1	B	364/377 (97%)	356 (98%)	8 (2%)	45	32
All	All	728/754 (97%)	712 (98%)	16 (2%)	45	32

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	563	GLU
1	A	599	ILE
1	A	680	PHE
1	A	737	LEU
1	A	774	ARG
1	A	804	LYS
1	A	843	LYS
1	A	923	GLN
1	B	548	SER
1	B	563	GLU
1	B	664	LEU
1	B	683	SER
1	B	757	THR
1	B	843	LYS
1	B	886	GLU
1	B	923	GLN

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	567	ASN
1	A	605	GLN
1	A	626	ASN
1	A	724	GLN
1	A	808	HIS
1	A	876	ASN

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Mol	Chain	Res	Type
1	B	567	ASN
1	B	724	GLN
1	B	829	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 30 ligands modelled in this entry, 2 are monoatomic - leaving 28 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	$\# Z  > 2$
5	SO4	B	1017	-	4,4,4	0.21	0	6,6,6	0.36	0
5	SO4	B	1019	-	4,4,4	0.20	0	6,6,6	1.21	1 (16%)
3	EDO	A	1005	-	3,3,3	0.33	0	2,2,2	0.22	0
3	EDO	B	1006	-	3,3,3	0.36	0	2,2,2	0.18	0
3	EDO	B	1014	-	3,3,3	0.40	0	2,2,2	0.13	0
3	EDO	B	1005	-	3,3,3	0.31	0	2,2,2	0.15	0
6	DMS	B	1004	-	3,3,3	0.76	0	3,3,3	0.81	0
4	A1JKV	B	1015	1	26,26,26	0.73	1 (3%)	32,36,36	0.87	1 (3%)
3	EDO	A	1004	-	3,3,3	0.23	0	2,2,2	0.27	0
3	EDO	B	1013	-	3,3,3	0.18	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	A1JKV	A	1007	1	26,26,26	0.67	1 (3%)	32,36,36	0.85	2 (6%)
7	PEG	B	1010	-	6,6,6	0.25	0	5,5,5	0.13	0
3	EDO	A	1002	-	3,3,3	0.28	0	2,2,2	0.26	0
5	SO4	B	1018	-	4,4,4	0.15	0	6,6,6	0.15	0
3	EDO	B	1011	-	3,3,3	0.32	0	2,2,2	0.23	0
5	SO4	A	1009	-	4,4,4	0.17	0	6,6,6	0.25	0
3	EDO	B	1008	-	3,3,3	0.36	0	2,2,2	0.14	0
3	EDO	B	1007	-	3,3,3	0.26	0	2,2,2	0.21	0
6	DMS	B	1001	-	3,3,3	1.08	0	3,3,3	1.14	0
3	EDO	A	1003	-	3,3,3	0.32	0	2,2,2	0.20	0
3	EDO	B	1021	-	3,3,3	0.19	0	2,2,2	0.23	0
5	SO4	A	1008	-	4,4,4	0.13	0	6,6,6	0.39	0
3	EDO	B	1012	-	3,3,3	0.42	0	2,2,2	0.08	0
3	EDO	B	1002	-	3,3,3	0.33	0	2,2,2	0.10	0
3	EDO	B	1003	-	3,3,3	0.22	0	2,2,2	0.18	0
3	EDO	B	1009	-	3,3,3	0.40	0	2,2,2	0.06	0
5	SO4	B	1016	-	4,4,4	0.30	0	6,6,6	0.87	0
3	EDO	A	1006	-	3,3,3	0.20	0	2,2,2	0.21	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
3	EDO	A	1005	-	-	1/1/1/1	-
3	EDO	B	1006	-	-	1/1/1/1	-
3	EDO	B	1014	-	-	1/1/1/1	-
3	EDO	B	1005	-	-	1/1/1/1	-
4	A1JKV	B	1015	1	-	7/20/33/33	0/2/2/2
3	EDO	A	1004	-	-	1/1/1/1	-
3	EDO	B	1013	-	-	1/1/1/1	-
4	A1JKV	A	1007	1	-	4/20/33/33	0/2/2/2
7	PEG	B	1010	-	-	1/4/4/4	-
3	EDO	A	1002	-	-	0/1/1/1	-
3	EDO	B	1011	-	-	1/1/1/1	-
3	EDO	B	1008	-	-	1/1/1/1	-
3	EDO	B	1007	-	-	1/1/1/1	-
3	EDO	A	1003	-	-	1/1/1/1	-
3	EDO	B	1021	-	-	1/1/1/1	-
3	EDO	B	1012	-	-	0/1/1/1	-
3	EDO	B	1002	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	1003	-	-	0/1/1/1	-
3	EDO	B	1009	-	-	1/1/1/1	-
3	EDO	A	1006	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1015	A1JKV	C20-C21	-3.46	1.48	1.52
4	A	1007	A1JKV	C20-C21	-3.23	1.49	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1015	A1JKV	C3-C8-C7	3.43	121.72	110.11
4	A	1007	A1JKV	C8-C7-C9	3.09	120.78	112.14
4	A	1007	A1JKV	C3-C8-C7	2.63	119.01	110.11
5	B	1019	SO4	O3-S-O2	2.04	119.93	109.31

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1015	A1JKV	C20-C21-S22-O24
4	B	1015	A1JKV	C20-C21-S22-O23
4	B	1015	A1JKV	C1-C2-C3-C4
4	B	1015	A1JKV	C1-C2-C3-C8
4	B	1015	A1JKV	C18-C20-C21-S22
4	A	1007	A1JKV	C18-C20-C21-S22
3	B	1006	EDO	O1-C1-C2-O2
3	A	1003	EDO	O1-C1-C2-O2
3	A	1005	EDO	O1-C1-C2-O2
3	B	1008	EDO	O1-C1-C2-O2
3	B	1011	EDO	O1-C1-C2-O2
3	B	1014	EDO	O1-C1-C2-O2
4	A	1007	A1JKV	C19-C18-N17-C15
4	B	1015	A1JKV	C19-C18-N17-C15
3	B	1005	EDO	O1-C1-C2-O2
3	B	1013	EDO	O1-C1-C2-O2
4	A	1007	A1JKV	C20-C21-S22-O23
3	B	1009	EDO	O1-C1-C2-O2
3	B	1021	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
7	B	1010	PEG	O1-C1-C2-O2
3	A	1004	EDO	O1-C1-C2-O2
3	B	1007	EDO	O1-C1-C2-O2
4	A	1007	A1JKV	C20-C21-S22-O24
4	B	1015	A1JKV	C20-C21-S22-C25

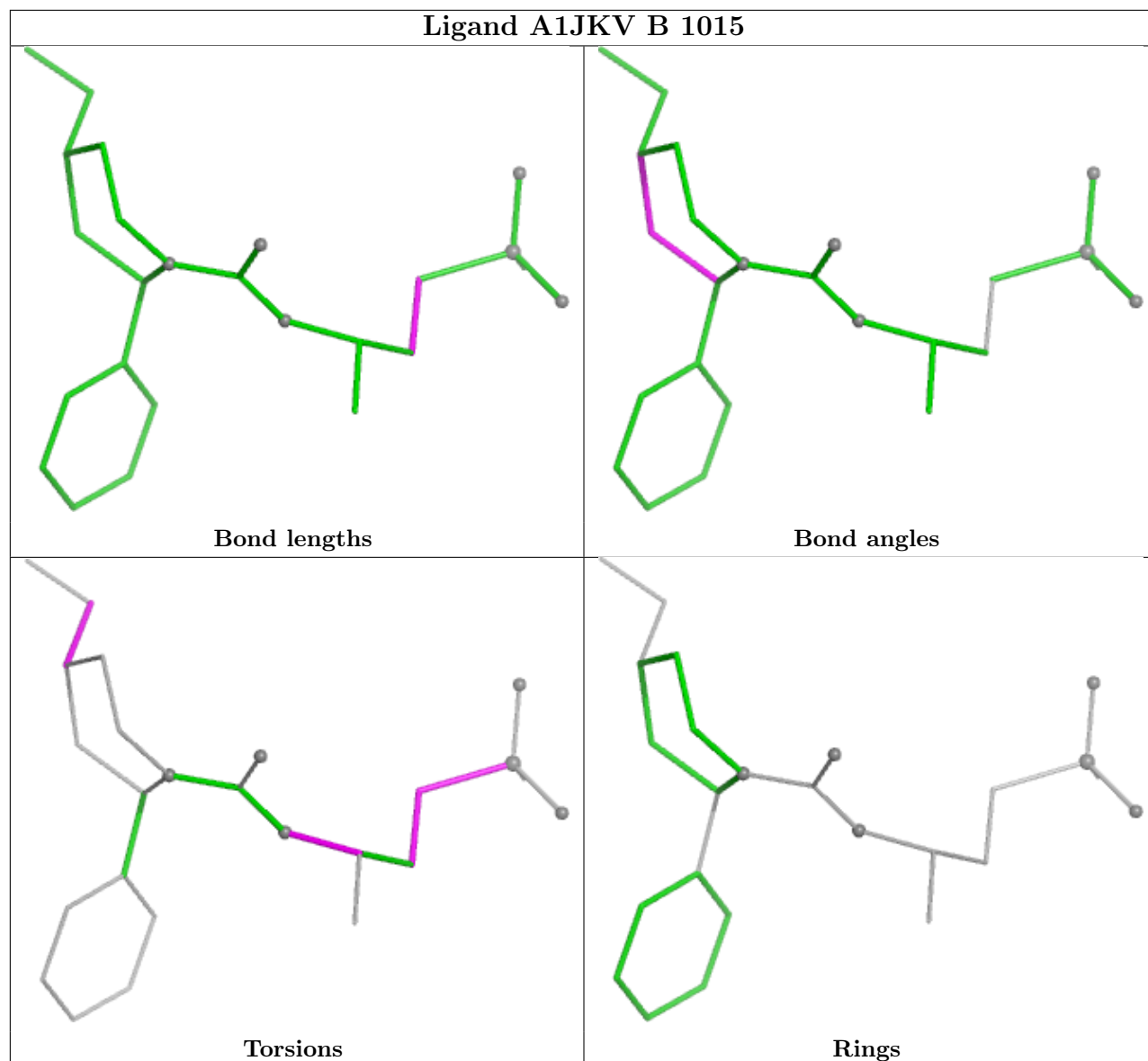
There are no ring outliers.

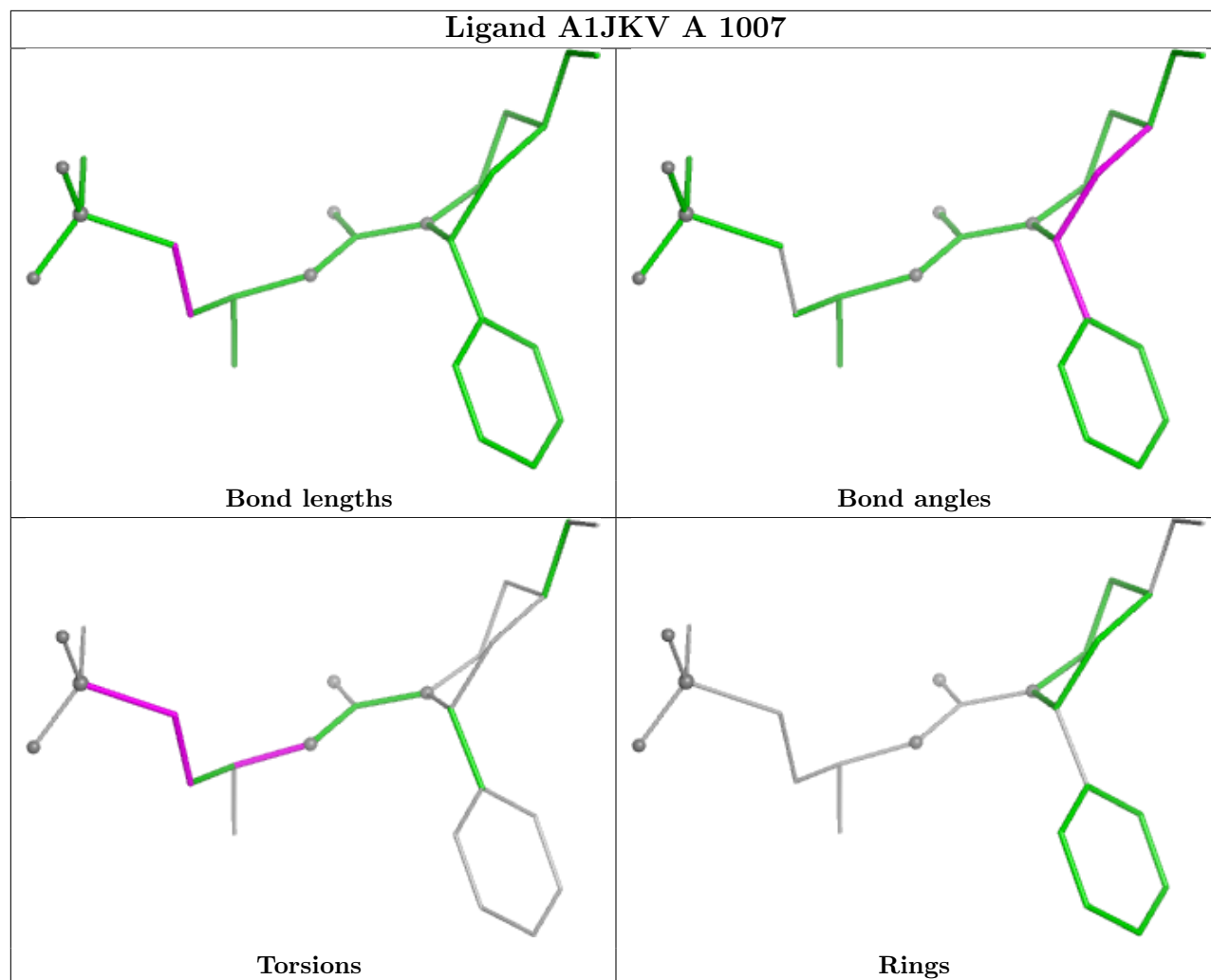
8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1019	SO4	1	0
3	A	1005	EDO	1	0
3	B	1014	EDO	1	0
3	B	1007	EDO	1	0
6	B	1001	DMS	6	0
3	B	1012	EDO	1	0
3	B	1002	EDO	2	0
5	B	1016	SO4	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.

## Ligand A1JKV B 1015





## 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, 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	403/427 (94%)	1.21	83 (20%) <b>2</b> <b>3</b>	16, 54, 93, 109	7 (1%)
1	B	402/427 (94%)	0.82	60 (14%) <b>5</b> <b>7</b>	16, 42, 83, 106	10 (2%)
All	All	805/854 (94%)	1.01	143 (17%) <b>4</b> <b>5</b>	16, 48, 91, 109	17 (2%)

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	680	PHE	8.1
1	B	684	PHE	6.2
1	B	922	VAL	6.2
1	A	684	PHE	5.1
1	A	673	ILE	5.0
1	A	823	ALA	5.0
1	A	530	PRO	4.8
1	A	828	ILE	4.8
1	A	879	LEU	4.8
1	B	925	ALA	4.6
1	B	927	LEU	4.5
1	A	875	LEU	4.5
1	B	875	LEU	4.5
1	B	920	LYS	4.2
1	A	880	LEU	4.2
1	A	927	LEU	4.2
1	A	883	ILE	4.1
1	A	922	VAL	4.1
1	A	758	SER	4.1
1	A	672	CYS	4.1
1	B	575	TYR	4.1
1	A	917	PHE	4.0
1	B	573[A]	THR	3.9
1	B	670	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	530	PRO	3.7
1	B	883	ILE	3.7
1	A	878	HIS	3.6
1	B	924	LYS	3.6
1	B	926	SER	3.6
1	A	826	MET	3.5
1	B	721	ARG	3.5
1	A	549	PHE	3.5
1	A	721	ARG	3.5
1	A	881	THR	3.5
1	A	888	PHE	3.5
1	B	890	LEU	3.2
1	A	763	PHE	3.2
1	A	787	LEU	3.2
1	A	913	ILE	3.1
1	A	770	TYR	3.1
1	B	873	ILE	3.1
1	B	879	LEU	3.1
1	B	917	PHE	3.1
1	B	593	LEU	3.1
1	B	880	LEU	3.1
1	A	941	SER	3.0
1	A	532	PRO	3.0
1	B	929	ILE	3.0
1	A	602	MET	3.0
1	B	672	CYS	3.0
1	A	683	SER	2.9
1	A	682	ASP	2.9
1	A	871	ALA	2.9
1	A	925	ALA	2.9
1	A	822	ILE	2.9
1	B	903	LEU	2.9
1	A	754	LEU	2.8
1	B	881	THR	2.8
1	A	926	SER	2.8
1	B	683	SER	2.8
1	A	670	ALA	2.8
1	B	764	GLU	2.8
1	B	886	GLU	2.8
1	A	887	LYS	2.7
1	A	715	VAL	2.7
1	A	902	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	932	THR	2.7
1	A	755	VAL	2.7
1	A	906	SER	2.6
1	A	725	ILE	2.6
1	A	929	ILE	2.6
1	B	878	HIS	2.6
1	A	897	ALA	2.6
1	A	890	LEU	2.6
1	A	599	ILE	2.6
1	B	696[A]	MET	2.5
1	B	730	PHE	2.5
1	B	687	LEU	2.5
1	A	756	LYS	2.5
1	A	827	GLY	2.5
1	A	885	ASN	2.5
1	B	888	PHE	2.5
1	B	916	HIS	2.5
1	B	757	THR	2.5
1	A	848	TYR	2.5
1	A	741	ARG	2.5
1	B	671	HIS	2.5
1	A	669[A]	GLU	2.5
1	A	780	VAL	2.5
1	B	935	CYS	2.4
1	B	897	ALA	2.4
1	B	906	SER	2.4
1	A	761	TRP	2.4
1	A	555	LYS	2.4
1	A	919	ASP	2.3
1	B	812[A]	ARG	2.3
1	A	710	ILE	2.3
1	A	760	HIS	2.3
1	A	537	VAL	2.3
1	A	711[A]	ARG	2.3
1	B	717	CYS	2.3
1	B	787	LEU	2.3
1	B	913	ILE	2.3
1	B	919	ASP	2.3
1	B	857	ARG	2.3
1	A	601	LEU	2.3
1	A	903	LEU	2.3
1	A	870	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	574	GLY	2.2
1	A	924	LYS	2.2
1	B	930	MET	2.2
1	A	723	PRO	2.2
1	A	752	PRO	2.2
1	B	758	SER	2.2
1	B	531	ALA	2.2
1	B	745	ASN	2.2
1	A	914	LEU	2.2
1	B	871	ALA	2.2
1	A	551	PRO	2.2
1	A	531	ALA	2.2
1	A	613	ASN	2.1
1	A	794	TYR	2.1
1	A	873	ILE	2.1
1	B	923	GLN	2.1
1	A	931	GLY	2.1
1	A	727	CYS	2.1
1	A	916	HIS	2.1
1	A	757	THR	2.1
1	B	759	SER	2.1
1	B	744	GLY	2.1
1	A	923	GLN	2.1
1	B	572	ALA	2.1
1	B	912	ILE	2.1
1	A	884	ARG	2.1
1	B	743	THR	2.1
1	A	893	LEU	2.1
1	B	685	ARG	2.1
1	A	746	ILE	2.0
1	B	646	CYS	2.0
1	A	877	ARG	2.0
1	A	886	GLU	2.0
1	A	930	MET	2.0
1	B	907	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no 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, 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.

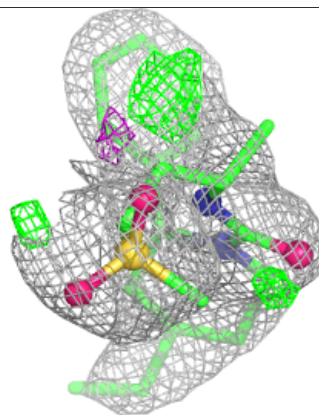
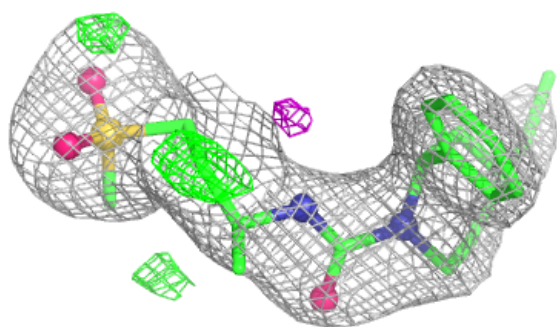
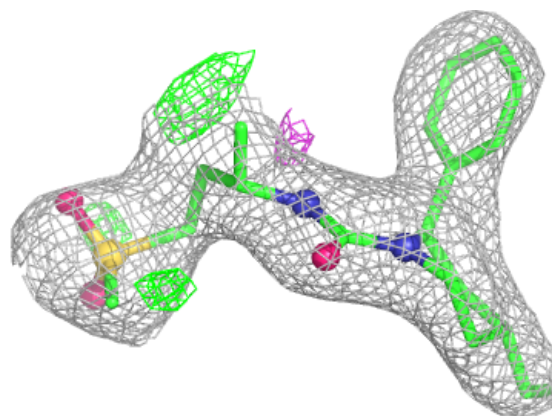
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	EDO	A	1002	4/4	0.53	0.28	84,85,85,86	0
7	PEG	B	1010	7/7	0.61	0.24	84,84,84,85	0
3	EDO	B	1011	4/4	0.70	0.19	63,64,64,65	0
3	EDO	B	1014	4/4	0.77	0.18	61,62,62,63	0
3	EDO	B	1008	4/4	0.79	0.17	64,65,65,65	0
5	SO4	B	1018	5/5	0.80	0.10	112,112,112,112	0
3	EDO	B	1009	4/4	0.81	0.34	49,50,50,51	0
3	EDO	A	1003	4/4	0.83	0.16	67,67,67,67	0
5	SO4	B	1017	5/5	0.84	0.10	77,78,78,78	0
3	EDO	B	1005	4/4	0.85	0.15	54,55,56,57	0
3	EDO	A	1005	4/4	0.85	0.17	59,60,61,62	0
3	EDO	B	1012	4/4	0.85	0.20	81,82,82,84	0
3	EDO	B	1013	4/4	0.85	0.19	71,71,71,72	0
6	DMS	B	1004	4/4	0.86	0.20	63,64,64,64	0
3	EDO	B	1006	4/4	0.87	0.16	65,66,66,66	0
5	SO4	A	1009	5/5	0.87	0.09	92,92,92,92	0
3	EDO	B	1003	4/4	0.87	0.21	63,65,65,66	0
3	EDO	A	1004	4/4	0.88	0.15	64,64,65,65	0
4	A1JKV	A	1007	25/25	0.89	0.14	56,61,76,77	0
5	SO4	B	1019	5/5	0.89	0.11	54,54,54,55	0
4	A1JKV	B	1015	25/25	0.90	0.12	33,45,61,63	0
6	DMS	B	1001	4/4	0.90	0.27	48,49,49,49	0
3	EDO	B	1021	4/4	0.91	0.12	64,64,64,64	0
3	EDO	B	1007	4/4	0.91	0.10	53,53,54,54	0
3	EDO	A	1006	4/4	0.93	0.10	54,54,54,56	0
5	SO4	A	1008	5/5	0.96	0.07	54,54,54,54	0
3	EDO	B	1002	4/4	0.96	0.10	57,58,58,58	0
5	SO4	B	1016	5/5	0.97	0.07	37,37,38,38	0
2	ZN	B	1020	1/1	0.98	0.04	57,57,57,57	0
2	ZN	A	1001	1/1	0.99	0.07	72,72,72,72	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.

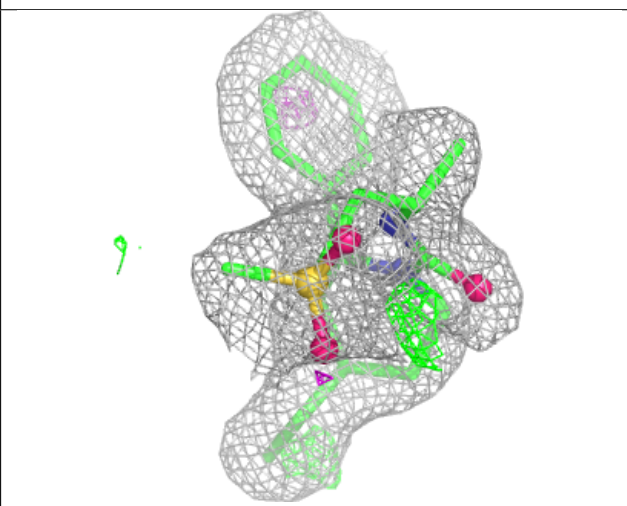
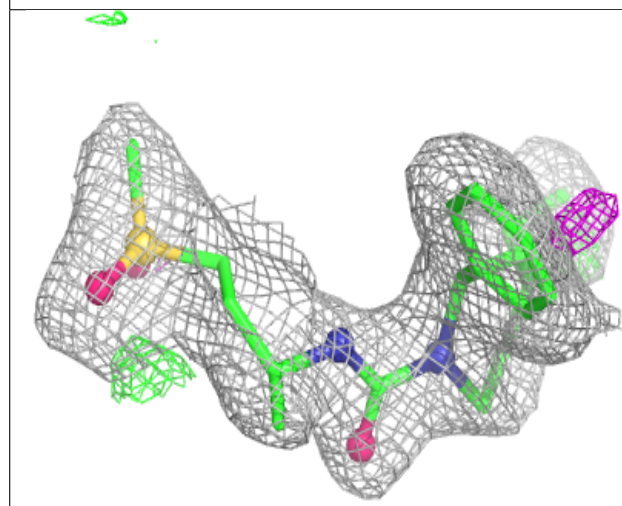
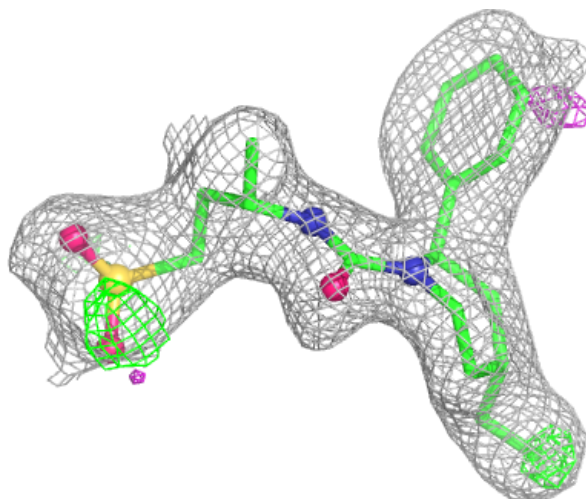
**Electron density around A1JKV A 1007:**

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



**Electron density around A1JKV B 1015:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.