



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:06 pm BST

PDB ID : 5DNY  
Title : Structure of the ATPPrS-Mre11/Rad50-DNA complex  
Authors : Liu, Y.  
Deposited on : 2015-09-10  
Resolution : 3.11 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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

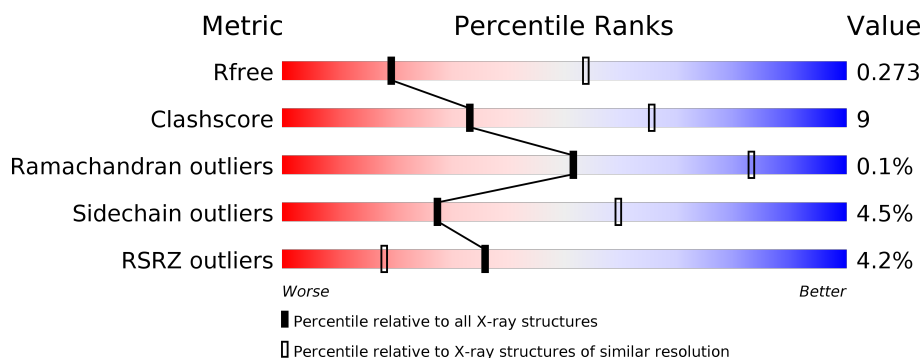
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.11 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))
$R_{free}$	130704	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	386	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	386	<div> <div>6%</div> <div> <div></div> <div>68%</div> <div>22%</div> <div>•</div> <div>9%</div> </div> </div>
2	B	371	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>22%</div> <div>•</div> <div>•</div> </div> </div>
2	D	371	<div> <div>5%</div> <div> <div></div> <div>72%</div> <div>22%</div> <div>•</div> <div>•</div> </div> </div>
3	E	27	<div> <div></div> <div> <div></div> <div>56%</div> <div>37%</div> <div>7%</div> </div> </div>
4	F	27	<div> <div></div> <div> <div></div> <div>44%</div> <div>41%</div> <div>15%</div> </div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12658 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 DNA double-strand break repair protein Mre11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2936	1895	493	538	10			
1	C	351	Total	C	N	O	S	0	0	0
			2919	1883	489	537	10			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q58719
A	-18	GLY	-	expression tag	UNP Q58719
A	-17	SER	-	expression tag	UNP Q58719
A	-16	SER	-	expression tag	UNP Q58719
A	-15	HIS	-	expression tag	UNP Q58719
A	-14	HIS	-	expression tag	UNP Q58719
A	-13	HIS	-	expression tag	UNP Q58719
A	-12	HIS	-	expression tag	UNP Q58719
A	-11	HIS	-	expression tag	UNP Q58719
A	-10	HIS	-	expression tag	UNP Q58719
A	-9	SER	-	expression tag	UNP Q58719
A	-8	SER	-	expression tag	UNP Q58719
A	-7	GLY	-	expression tag	UNP Q58719
A	-6	LEU	-	expression tag	UNP Q58719
A	-5	VAL	-	expression tag	UNP Q58719
A	-4	PRO	-	expression tag	UNP Q58719
A	-3	ARG	-	expression tag	UNP Q58719
A	-2	GLY	-	expression tag	UNP Q58719
A	-1	SER	-	expression tag	UNP Q58719
A	0	HIS	-	expression tag	UNP Q58719
C	-19	MET	-	expression tag	UNP Q58719
C	-18	GLY	-	expression tag	UNP Q58719
C	-17	SER	-	expression tag	UNP Q58719
C	-16	SER	-	expression tag	UNP Q58719
C	-15	HIS	-	expression tag	UNP Q58719

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	HIS	-	expression tag	UNP Q58719
C	-13	HIS	-	expression tag	UNP Q58719
C	-12	HIS	-	expression tag	UNP Q58719
C	-11	HIS	-	expression tag	UNP Q58719
C	-10	HIS	-	expression tag	UNP Q58719
C	-9	SER	-	expression tag	UNP Q58719
C	-8	SER	-	expression tag	UNP Q58719
C	-7	GLY	-	expression tag	UNP Q58719
C	-6	LEU	-	expression tag	UNP Q58719
C	-5	VAL	-	expression tag	UNP Q58719
C	-4	PRO	-	expression tag	UNP Q58719
C	-3	ARG	-	expression tag	UNP Q58719
C	-2	GLY	-	expression tag	UNP Q58719
C	-1	SER	-	expression tag	UNP Q58719
C	0	HIS	-	expression tag	UNP Q58719

- Molecule 2 is a protein called DNA double-strand break repair Rad50 ATPase, DNA double-strand break repair Rad50 ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	359	Total	C	N	O	S	0	0	0
			2877	1844	490	534	9			
2	D	358	Total	C	N	O	S	0	0	0
			2874	1845	488	533	8			

- Molecule 3 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	25	Total	C	N	O	P	0	0	0
			517	246	99	147	25			

- Molecule 4 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	23	Total	C	N	O	P	0	0	0
			467	223	83	138	23			

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

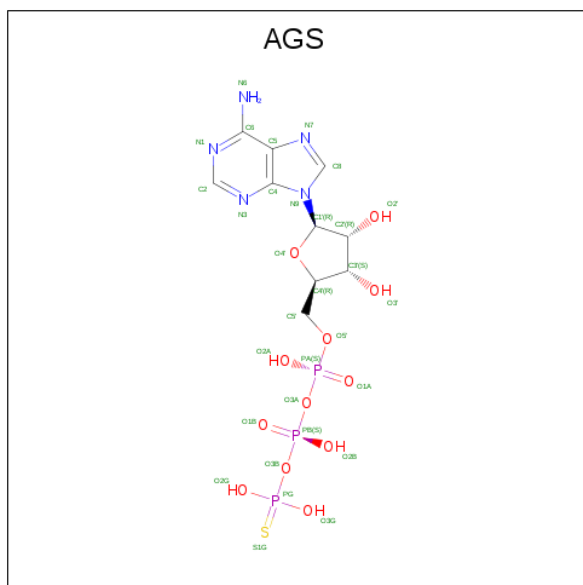
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	2	Total	Mg	0	0
			2	2		

- Molecule 6 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
6	D	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

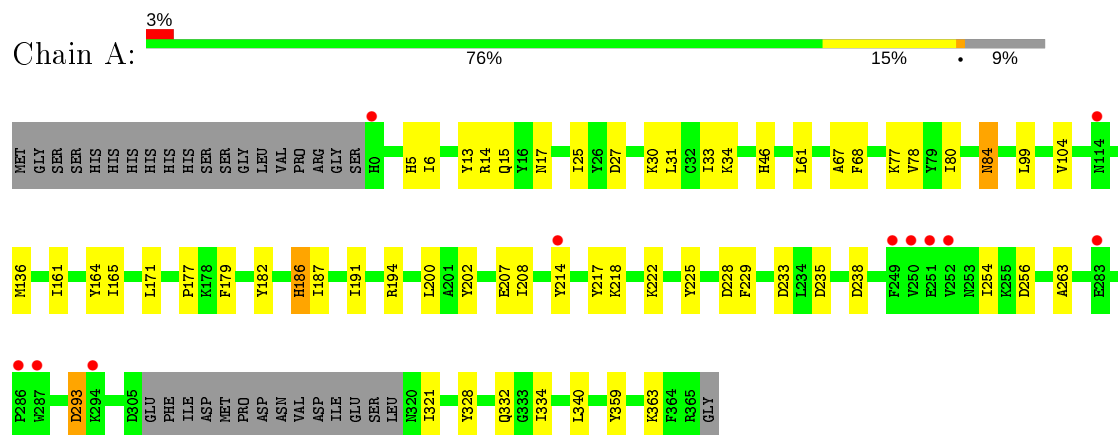
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O	0	0
			1	1		
7	C	1	Total	O	0	0
			1	1		

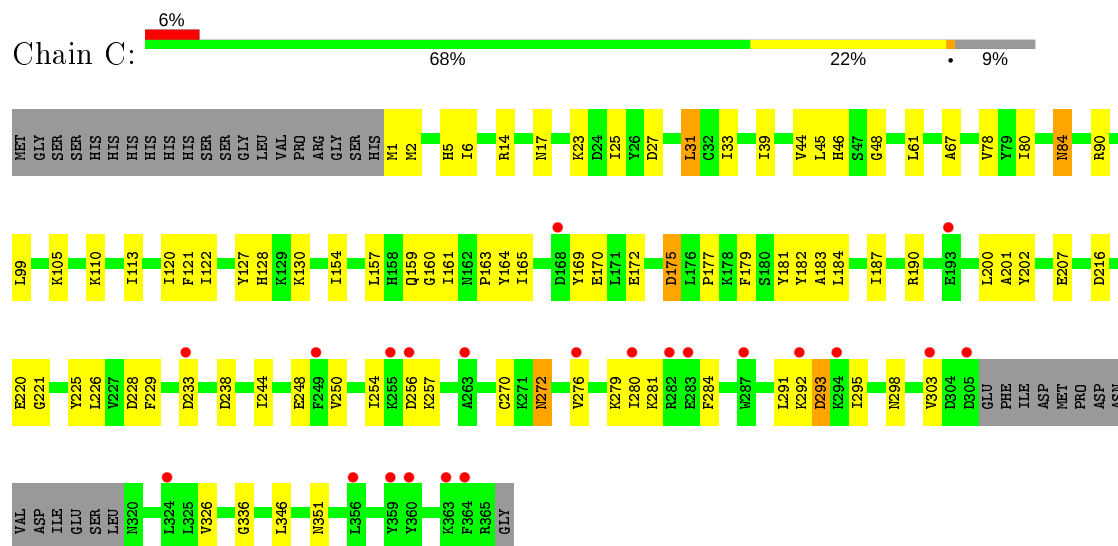
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: DNA double-strand break repair protein Mre11

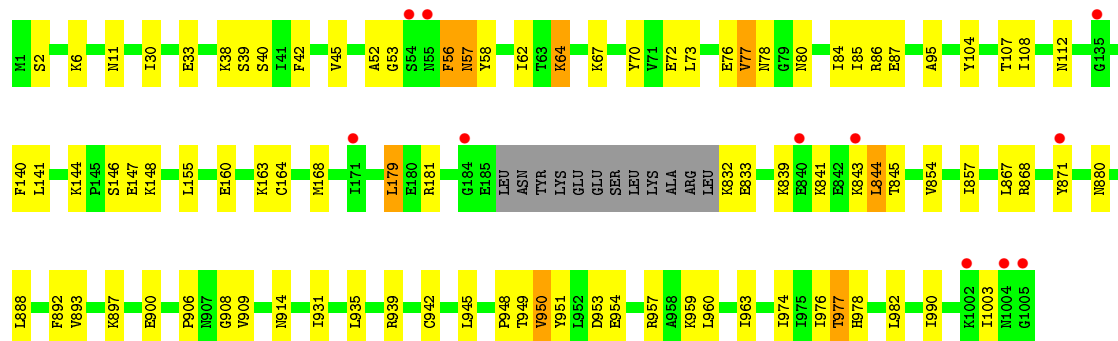


- Molecule 1: DNA double-strand break repair protein Mre11

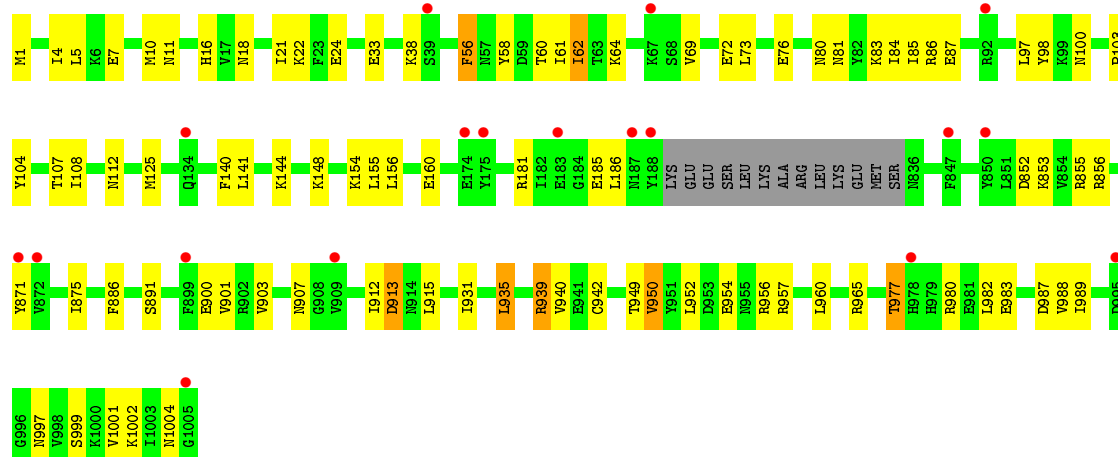


- Molecule 2: DNA double-strand break repair Rad50 ATPase, DNA double-strand break repair Rad50 ATPase

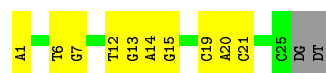




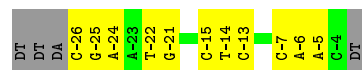
- Molecule 2: DNA double-strand break repair Rad50 ATPase, DNA double-strand break repair Rad50 ATPase



- Molecule 3: DNA (27-MER)



- Molecule 4: DNA (27-MER)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.30Å 130.11Å 166.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.87 – 3.11 40.86 – 3.11	Depositor EDS
% Data completeness (in resolution range)	95.8 (40.87-3.11) 95.8 (40.86-3.11)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.10-2152_1745)	Depositor
R, $R_{free}$	0.221 , 0.273 0.221 , 0.273	Depositor DCC
$R_{free}$ test set	1637 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	95.3	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 60.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12658	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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: MG, AGS

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	0.25	0/2997	0.42	0/4025
1	C	0.25	0/2979	0.43	0/4002
2	B	0.31	1/2920 (0.0%)	0.44	0/3913
2	D	0.26	0/2918	0.41	0/3913
3	E	0.55	0/581	0.91	0/895
4	F	0.56	0/522	0.91	0/802
All	All	0.30	1/12917 (0.0%)	0.49	0/17550

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	888	LEU	C-N	8.79	1.50	1.34

There are no bond angle outliers.

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	2936	0	2956	37	0
1	C	2919	0	2929	58	0
2	B	2877	0	2959	55	0
2	D	2874	0	2952	59	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	517	0	282	9	0
4	F	467	0	260	8	1
5	A	2	0	0	0	0
5	C	2	0	0	0	0
6	B	31	0	12	5	0
6	D	31	0	12	3	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
All	All	12658	0	12362	215	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (215) 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)
3:E:12:DT:H2"	3:E:13:DG:C8	2.20	0.77
1:C:14:ARG:NH1	1:C:17:ASN:OD1	2.19	0.75
2:D:84:ILE:HG12	2:D:97:LEU:HD13	1.72	0.71
3:E:19:DC:H2"	3:E:20:DA:H5"	1.72	0.71
3:E:6:DT:H2"	3:E:7:DG:C8	2.26	0.71
2:D:949:THR:HG21	2:D:982:LEU:HD11	1.73	0.70
2:D:901:VAL:HB	2:D:912:ILE:HD11	1.73	0.70
1:C:175:ASP:OD1	1:C:175:ASP:N	2.27	0.68
2:B:45:VAL:HG13	2:B:73:LEU:HD11	1.77	0.66
2:D:86:ARG:NH2	2:D:112:ASN:OD1	2.20	0.66
2:D:989:ILE:HG23	2:D:1004:ASN:HB2	1.78	0.66
2:D:977:THR:HG21	2:D:982:LEU:HD13	1.77	0.65
2:B:144:LYS:HZ3	2:B:146:SER:HG	1.44	0.65
2:D:1:MET:HE2	2:D:939:ARG:HE	1.61	0.65
1:C:122:ILE:HG12	1:C:154:ILE:HD11	1.78	0.65
1:C:2:MET:HG2	1:C:228:ASP:HA	1.79	0.65
1:A:165:ILE:HD11	1:A:187:ILE:HB	1.78	0.64
1:C:326:VAL:HG13	1:C:336:GLY:HA3	1.79	0.64
2:B:908:GLY:HA3	2:D:64:LYS:HB3	1.80	0.64
1:C:90:ARG:NH2	2:D:983:GLU:OE1	2.31	0.64
2:D:913:ASP:OD1	2:D:913:ASP:N	2.30	0.64
1:C:281:LYS:HB3	1:C:284:PHE:HD1	1.64	0.62
2:D:62:ILE:O	6:D:1101:AGS:N6	2.31	0.62
2:B:977:THR:HG21	2:B:982:LEU:HD13	1.83	0.60
1:C:154:ILE:HG22	1:C:181:TYR:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:ASP:O	1:C:220:GLU:N	2.27	0.60
1:A:25:ILE:HD13	1:A:207:GLU:HB3	1.83	0.60
2:D:141:LEU:HD13	2:D:912:ILE:HD13	1.84	0.60
2:B:155:LEU:HD13	2:B:931:ILE:HD13	1.84	0.59
2:D:148:LYS:NZ	2:D:900:GLU:OE1	2.22	0.59
2:D:98:TYR:HA	2:D:103:PRO:HA	1.85	0.59
2:D:125:MET:O	2:D:154:LYS:NZ	2.35	0.59
2:D:155:LEU:HD23	2:D:931:ILE:HD13	1.85	0.58
1:A:334:ILE:HG21	2:B:854:VAL:HG22	1.85	0.58
2:D:11:ASN:OD1	2:D:18:ASN:ND2	2.37	0.58
2:B:164:CYS:O	2:B:168:MET:HB2	2.04	0.58
1:C:177:PRO:HG2	1:C:179:PHE:HE1	1.68	0.57
1:C:127:TYR:HA	1:C:159:GLN:HE22	1.69	0.57
2:D:903:VAL:HG21	2:D:915:LEU:HD11	1.86	0.57
1:A:177:PRO:HG2	1:A:179:PHE:HE1	1.70	0.57
1:A:33:ILE:HG13	1:A:67:ALA:HB1	1.85	0.57
4:F:-22:DT:H2'	4:F:-21:DG:C8	2.41	0.56
2:B:62:ILE:O	6:B:1101:AGS:N6	2.38	0.56
2:D:72:GLU:HA	2:D:84:ILE:O	2.06	0.56
2:D:21:ILE:HG12	2:D:1001:VAL:HG11	1.88	0.56
1:A:14:ARG:HG2	1:A:17:ASN:HA	1.87	0.55
1:C:248:GLU:H	1:C:272:ASN:HD21	1.54	0.55
2:B:954:GLU:HG3	2:B:957:ARG:NH1	2.21	0.55
2:B:949:THR:HG21	2:B:982:LEU:HD11	1.88	0.55
1:C:182:TYR:HB2	1:C:200:LEU:HA	1.89	0.55
2:D:5:LEU:HD22	2:D:73:LEU:HD11	1.90	0.54
1:C:161:ILE:HB	1:C:164:TYR:HD1	1.72	0.54
2:B:144:LYS:HZ2	2:B:147:GLU:HG3	1.73	0.53
1:C:23:LYS:NZ	1:C:27:ASP:OD2	2.36	0.53
2:D:7:GLU:HB3	2:D:22:LYS:HD2	1.90	0.53
1:C:110:LYS:HB2	1:C:121:PHE:HE1	1.74	0.53
4:F:-26:DC:H2''	4:F:-25:DG:C8	2.43	0.53
2:B:950:VAL:HG22	2:D:950:VAL:HG22	1.90	0.53
2:B:77:VAL:HG22	2:B:78:ASN:ND2	2.24	0.52
2:B:6:LYS:HD2	2:B:76:GLU:HG3	1.89	0.52
2:D:156:LEU:HD21	2:D:875:ILE:HD11	1.92	0.52
2:D:886:PHE:HD1	2:D:956:ARG:HD2	1.74	0.52
2:B:160:GLU:HA	2:B:163:LYS:HD2	1.91	0.52
2:D:33:GLU:O	2:D:38:LYS:NZ	2.42	0.52
4:F:-25:DG:H2''	4:F:-24:DA:C8	2.45	0.52
2:B:86:ARG:NH2	2:B:112:ASN:OD1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:ILE:HB	1:C:280:ILE:HA	1.91	0.52
2:D:24:GLU:HG3	2:D:988:VAL:HG21	1.91	0.51
2:B:72:GLU:HA	2:B:84:ILE:O	2.11	0.51
2:B:141:LEU:O	2:B:148:LYS:NZ	2.36	0.50
2:B:978:HIS:CD2	2:B:978:HIS:H	2.29	0.50
2:D:954:GLU:HG3	2:D:957:ARG:HH11	1.76	0.50
2:D:144:LYS:O	2:D:148:LYS:N	2.38	0.50
1:A:182:TYR:HB2	1:A:200:LEU:HA	1.94	0.50
2:B:95:ALA:HB3	2:B:108:ILE:HA	1.93	0.50
2:D:81:ASN:HD22	2:D:100:ASN:ND2	2.09	0.50
1:A:191:ILE:HB	1:A:202:TYR:HB2	1.93	0.50
4:F:-14:DT:H2'	4:F:-13:DC:C6	2.47	0.50
1:A:228:ASP:HB3	1:A:238:ASP:HB2	1.94	0.49
2:B:33:GLU:O	2:B:38:LYS:NZ	2.45	0.49
1:C:46:HIS:O	1:C:80:ILE:HA	2.12	0.49
2:D:852:ASP:OD1	2:D:855:ARG:NH1	2.41	0.49
2:B:72:GLU:HB3	2:B:85:ILE:HG12	1.95	0.49
1:C:254:ILE:HD12	1:C:280:ILE:HG12	1.94	0.49
2:B:30:ILE:HB	2:B:976:ILE:HG12	1.94	0.48
1:A:254:ILE:HD11	1:A:263:ALA:HB2	1.95	0.48
1:A:27:ASP:O	1:A:31:LEU:HG	2.13	0.48
2:B:38:LYS:N	6:B:1101:AGS:O1B	2.39	0.48
2:D:853:LYS:HA	2:D:856:ARG:HD3	1.95	0.48
2:B:949:THR:HB	2:B:957:ARG:HG2	1.95	0.48
2:D:954:GLU:HG3	2:D:957:ARG:NH1	2.28	0.48
2:D:965:ARG:NH2	2:D:987:ASP:OD1	2.42	0.48
2:B:841:LYS:O	2:B:845:THR:OG1	2.23	0.48
1:C:276:VAL:HB	1:C:295:ILE:HD11	1.95	0.48
2:D:181:ARG:NH1	2:D:185:GLU:OE2	2.46	0.48
2:B:179:LEU:HG	2:B:844:LEU:HD13	1.96	0.48
2:D:10:MET:HE2	2:D:16:HIS:HB2	1.94	0.48
1:A:186:HIS:O	1:A:186:HIS:ND1	2.46	0.48
1:C:130:LYS:HD3	1:C:169:TYR:O	2.13	0.48
2:D:949:THR:HG22	2:D:960:LEU:HD23	1.96	0.48
2:D:86:ARG:HH12	2:D:108:ILE:HG23	1.78	0.47
2:B:57:ASN:HD22	2:B:58:TYR:N	2.10	0.47
1:C:187:ILE:HG22	1:C:202:TYR:CD1	2.50	0.47
2:B:990:ILE:HG12	2:B:1003:ILE:HG23	1.96	0.47
2:B:945:LEU:HB3	2:B:948:PRO:HG3	1.95	0.47
1:C:113:ILE:HD13	1:C:122:ILE:HD11	1.96	0.47
3:E:13:DG:H2'	3:E:14:DA:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:ILE:HG13	1:C:67:ALA:HB1	1.96	0.47
1:C:84:ASN:HD22	1:C:84:ASN:H	1.62	0.47
1:C:25:ILE:HD13	1:C:207:GLU:HB3	1.96	0.46
1:C:279:LYS:HD2	1:C:303:VAL:HG21	1.96	0.46
2:B:40:SER:OG	6:B:1101:AGS:O1A	2.26	0.46
1:A:321:ILE:HG22	2:B:867:LEU:HD11	1.97	0.46
2:B:906:PRO:HD2	2:D:997:ASN:HD21	1.81	0.46
1:C:256:ASP:OD1	1:C:256:ASP:N	2.48	0.46
2:B:839:LYS:O	2:B:843:LYS:HB2	2.15	0.46
2:B:949:THR:HG22	2:B:960:LEU:HD23	1.97	0.46
2:D:160:GLU:OE2	2:D:939:ARG:NH1	2.43	0.46
1:A:136:MET:HG2	1:A:171:LEU:HD11	1.98	0.46
1:A:161:ILE:HB	1:A:164:TYR:HD1	1.81	0.46
1:C:39:ILE:HD13	1:C:226:LEU:HD22	1.97	0.46
2:B:76:GLU:HA	2:B:80:ASN:O	2.17	0.45
1:C:46:HIS:HD1	1:C:48:GLY:H	1.64	0.45
1:A:61:LEU:HD22	1:A:99:LEU:HD12	1.98	0.45
1:C:6:ILE:O	1:C:46:HIS:HA	2.16	0.45
1:A:194:ARG:NH1	1:A:235:ASP:OD1	2.49	0.45
2:B:11:ASN:HB2	2:B:70:TYR:HB3	1.99	0.45
1:C:257:LYS:HA	1:C:284:PHE:CZ	2.52	0.45
1:C:31:LEU:HB3	1:C:244:ILE:HD11	1.97	0.45
4:F:-7:DC:H2"	4:F:-6:DA:C8	2.52	0.45
1:A:334:ILE:HD12	2:B:857:ILE:HD11	1.98	0.45
6:B:1101:AGS:O2G	6:B:1101:AGS:O2A	2.35	0.44
4:F:-25:DG:H2"	4:F:-24:DA:N7	2.32	0.44
2:B:868:ARG:NH1	2:B:897:LYS:O	2.50	0.44
3:E:14:DA:H2"	3:E:15:DG:H8	1.81	0.44
6:D:1101:AGS:O2B	6:D:1101:AGS:O2A	2.36	0.44
1:A:293:ASP:OD2	1:A:293:ASP:N	2.51	0.44
2:B:42:PHE:HZ	2:B:974:ILE:HG21	1.82	0.44
1:C:190:ARG:NH2	1:C:221:GLY:O	2.40	0.44
1:C:293:ASP:N	1:C:293:ASP:OD2	2.51	0.44
1:C:46:HIS:HB3	1:C:80:ILE:HG13	2.00	0.44
3:E:13:DG:C2'	3:E:14:DA:C8	3.00	0.44
1:A:217:TYR:HD1	1:A:222:LYS:HG3	1.83	0.44
2:D:56:PHE:HD1	2:D:56:PHE:HA	1.70	0.44
1:A:13:TYR:CE2	1:A:15:GLN:HB2	2.53	0.44
1:C:201:ALA:HB1	1:C:225:TYR:HE2	1.83	0.44
1:C:228:ASP:HB3	1:C:238:ASP:HB2	1.98	0.44
2:D:58:TYR:HA	2:D:61:ILE:HG12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:HIS:H	1:C:159:GLN:HE22	1.64	0.44
1:A:84:ASN:HD22	1:A:84:ASN:H	1.66	0.44
2:B:914:ASN:HD22	2:D:60:THR:HG23	1.83	0.43
2:D:72:GLU:HB3	2:D:85:ILE:HG12	1.99	0.43
2:D:69:VAL:O	2:D:87:GLU:HA	2.18	0.43
1:C:45:LEU:HD11	1:C:154:ILE:HD12	1.99	0.43
1:C:172:GLU:HB2	1:C:175:ASP:OD1	2.19	0.43
1:A:256:ASP:OD1	1:A:256:ASP:N	2.51	0.43
1:C:5:HIS:CE1	1:C:183:ALA:HA	2.53	0.43
2:D:154:LYS:HB3	2:D:154:LYS:HE2	1.74	0.43
2:B:53:GLY:H	2:B:56:PHE:HB3	1.83	0.43
2:B:950:VAL:O	2:B:951:TYR:HB2	2.18	0.43
2:B:914:ASN:ND2	2:D:60:THR:HG23	2.34	0.43
2:B:909:VAL:O	2:D:64:LYS:HE2	2.17	0.43
2:D:952:LEU:O	2:D:957:ARG:NH2	2.51	0.43
2:B:39:SER:OG	6:B:1101:AGS:O3G	2.36	0.43
1:C:250:VAL:HB	1:C:276:VAL:HG22	2.01	0.43
1:A:187:ILE:HA	1:A:187:ILE:HD12	1.86	0.43
1:A:46:HIS:O	1:A:80:ILE:HA	2.18	0.43
4:F:-6:DA:H2"	4:F:-5:DA:H8	1.84	0.43
1:C:127:TYR:HA	1:C:159:GLN:NE2	2.33	0.43
3:E:1:DA:C8	3:E:1:DA:P	3.12	0.43
2:B:959:LYS:O	2:B:963:ILE:HG13	2.19	0.42
1:C:61:LEU:HD22	1:C:99:LEU:HD12	2.00	0.42
2:D:148:LYS:HE3	2:D:148:LYS:HB2	1.81	0.42
1:A:68:PHE:CE1	1:A:78:VAL:HG11	2.54	0.42
2:B:64:LYS:HA	2:B:64:LYS:HD2	1.74	0.42
2:D:38:LYS:NZ	6:D:1101:AGS:O1B	2.48	0.42
1:A:6:ILE:O	1:A:46:HIS:HA	2.19	0.42
1:C:161:ILE:HG22	1:C:163:PRO:HD2	2.00	0.42
1:C:44:VAL:HB	1:C:78:VAL:HG22	2.01	0.42
1:C:160:GLY:H	1:C:170:GLU:HG2	1.85	0.42
1:C:298:ASN:OD1	1:C:298:ASN:N	2.53	0.42
2:B:2:SER:HB3	2:B:78:ASN:HA	2.02	0.42
2:B:880:ASN:ND2	2:B:893:VAL:O	2.47	0.42
2:D:64:LYS:HA	2:D:64:LYS:HD3	1.85	0.42
1:A:359:TYR:HA	1:A:363:LYS:HG3	2.01	0.41
1:C:110:LYS:HB2	1:C:121:PHE:CE1	2.54	0.41
1:C:157:LEU:O	1:C:184:LEU:HA	2.20	0.41
1:A:187:ILE:HG22	1:A:202:TYR:CD1	2.55	0.41
1:A:208:ILE:HD13	1:A:214:TYR:HD1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:HIS:HB3	1:A:225:TYR:HB2	2.00	0.41
2:B:906:PRO:HD2	2:D:997:ASN:ND2	2.34	0.41
1:C:165:ILE:HD12	1:C:187:ILE:HD13	2.01	0.41
2:D:72:GLU:OE1	2:D:83:LYS:NZ	2.53	0.41
1:C:90:ARG:NH2	2:D:980:ARG:HG2	2.35	0.41
1:A:161:ILE:HB	1:A:164:TYR:CD1	2.56	0.41
1:A:77:LYS:HD2	1:A:77:LYS:HA	1.79	0.41
2:D:156:LEU:HA	2:D:935:LEU:HD21	2.02	0.41
1:A:218:LYS:HA	1:A:218:LYS:HD3	1.84	0.41
2:B:141:LEU:HA	2:B:141:LEU:HD23	1.88	0.41
1:C:248:GLU:HG3	1:C:270:CYS:HB2	2.03	0.41
1:A:328:TYR:O	1:A:332:GLN:HG2	2.21	0.41
2:D:76:GLU:HA	2:D:80:ASN:O	2.20	0.41
2:D:1:MET:HG3	2:D:939:ARG:NH2	2.36	0.41
1:A:78:VAL:HB	1:A:104:VAL:HG22	2.03	0.40
2:B:953:ASP:O	2:B:957:ARG:HG3	2.21	0.40
2:B:960:LEU:HA	2:B:963:ILE:HD12	2.03	0.40
1:C:292:LYS:HA	1:C:295:ILE:HG22	2.04	0.40
2:D:144:LYS:HG2	3:E:14:DA:OP1	2.21	0.40
3:E:20:DA:H2"	3:E:21:DC:C6	2.56	0.40
1:C:201:ALA:HB1	1:C:225:TYR:CE2	2.57	0.40
1:A:30:LYS:O	1:A:34:LYS:HG3	2.22	0.40
4:F:-15:DC:H2"	4:F:-14:DT:O4'	2.22	0.40
2:B:52:ALA:HB1	2:B:56:PHE:O	2.21	0.40
1:C:113:ILE:HG13	1:C:120:ILE:HB	2.04	0.40
1:C:5:HIS:HB3	1:C:225:TYR:HB2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1002:LYS:NZ	4:F:-13:DC:OP1[3_554]	2.15	0.05

## 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	348/386 (90%)	325 (93%)	23 (7%)	0	100	100
1	C	347/386 (90%)	325 (94%)	22 (6%)	0	100	100
2	B	355/371 (96%)	333 (94%)	22 (6%)	0	100	100
2	D	354/371 (95%)	330 (93%)	23 (6%)	1 (0%)	41	73
All	All	1404/1514 (93%)	1313 (94%)	90 (6%)	1 (0%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	891	SER

### 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	322/352 (92%)	316 (98%)	6 (2%)	57	80
1	C	319/352 (91%)	307 (96%)	12 (4%)	33	65
2	B	312/324 (96%)	290 (93%)	22 (7%)	14	44
2	D	311/324 (96%)	294 (94%)	17 (6%)	21	52
All	All	1264/1352 (94%)	1207 (96%)	57 (4%)	27	59

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	186	HIS
1	A	229	PHE
1	A	233	ASP
1	A	293	ASP
1	A	340	LEU
2	B	56	PHE

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Mol	Chain	Res	Type
2	B	57	ASN
2	B	64	LYS
2	B	67	LYS
2	B	77	VAL
2	B	87	GLU
2	B	104	TYR
2	B	107	THR
2	B	140	PHE
2	B	179	LEU
2	B	181	ARG
2	B	832	LYS
2	B	833	GLU
2	B	844	LEU
2	B	871	TYR
2	B	892	PHE
2	B	900	GLU
2	B	935	LEU
2	B	939	ARG
2	B	942	CYS
2	B	950	VAL
2	B	977	THR
1	C	1	MET
1	C	31	LEU
1	C	84	ASN
1	C	105	LYS
1	C	175	ASP
1	C	229	PHE
1	C	233	ASP
1	C	272	ASN
1	C	291	LEU
1	C	293	ASP
1	C	346	LEU
1	C	351	ASN
2	D	4	ILE
2	D	56	PHE
2	D	62	ILE
2	D	104	TYR
2	D	107	THR
2	D	140	PHE
2	D	186	LEU
2	D	871	TYR
2	D	907	ASN

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Mol	Chain	Res	Type
2	D	913	ASP
2	D	935	LEU
2	D	939	ARG
2	D	940	VAL
2	D	942	CYS
2	D	950	VAL
2	D	977	THR
2	D	999	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	128	HIS
2	B	57	ASN
2	B	78	ASN
2	B	81	ASN
2	B	997	ASN
1	C	9	ASN
1	C	84	ASN
1	C	186	HIS
1	C	261	ASN
1	C	272	ASN
1	C	330	ASN
1	C	348	ASN
2	D	81	ASN
2	D	880	ASN
2	D	978	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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
6	AGS	B	1101	-	26,33,33	0.75	1 (3%)	26,52,52	1.09	2 (7%)
6	AGS	D	1101	-	26,33,33	0.77	1 (3%)	26,52,52	1.12	2 (7%)

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
6	AGS	B	1101	-	-	7/17/38/38	0/3/3/3
6	AGS	D	1101	-	-	4/17/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1101	AGS	PG-S1G	2.11	1.95	1.90
6	D	1101	AGS	PG-S1G	2.09	1.95	1.90

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1101	AGS	PA-O3A-PB	-4.07	118.85	132.83
6	B	1101	AGS	PA-O3A-PB	-3.30	121.49	132.83
6	D	1101	AGS	C5-C6-N6	2.37	123.96	120.35
6	B	1101	AGS	C5-C6-N6	2.33	123.89	120.35

There are no chirality outliers.

All (11) torsion outliers are listed below:

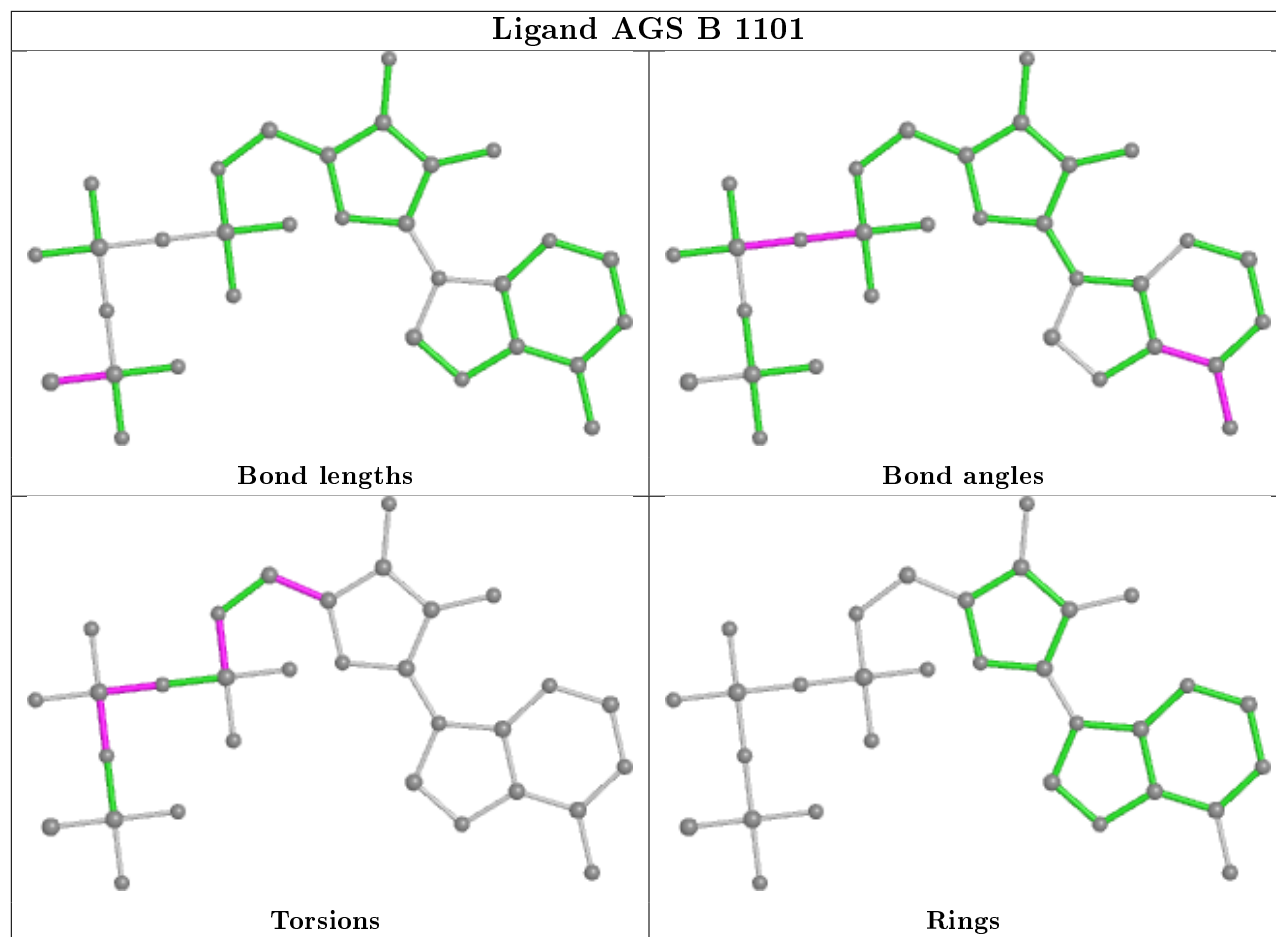
Mol	Chain	Res	Type	Atoms
6	D	1101	AGS	C3'-C4'-C5'-O5'
6	B	1101	AGS	C5'-O5'-PA-O1A
6	B	1101	AGS	O4'-C4'-C5'-O5'
6	D	1101	AGS	PG-O3B-PB-O1B
6	D	1101	AGS	O4'-C4'-C5'-O5'
6	B	1101	AGS	C5'-O5'-PA-O3A
6	B	1101	AGS	C3'-C4'-C5'-O5'
6	B	1101	AGS	C5'-O5'-PA-O2A
6	B	1101	AGS	PG-O3B-PB-O1B
6	D	1101	AGS	PA-O3A-PB-O2B
6	B	1101	AGS	PA-O3A-PB-O1B

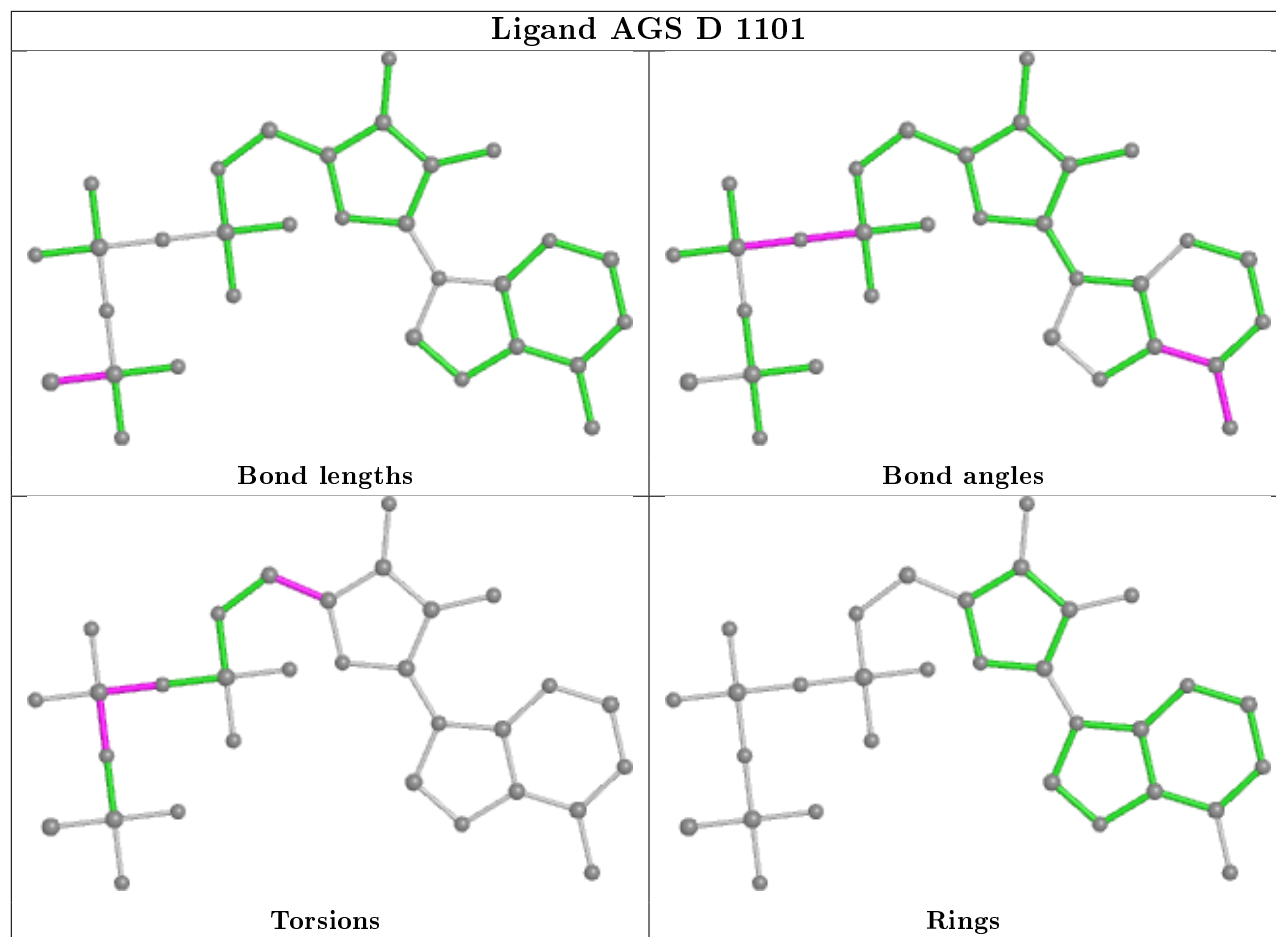
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1101	AGS	5	0
6	D	1101	AGS	3	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, 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	352/386 (91%)	0.16	11 (3%) 49 26	54, 105, 169, 195	0
1	C	351/386 (90%)	0.25	22 (6%) 20 8	52, 99, 170, 207	0
2	B	359/371 (96%)	0.07	11 (3%) 49 26	52, 93, 142, 173	0
2	D	358/371 (96%)	0.33	18 (5%) 28 13	63, 109, 155, 193	0
3	E	25/27 (92%)	0.30	0 100 100	120, 147, 181, 184	0
4	F	23/27 (85%)	-0.03	0 100 100	88, 150, 182, 192	0
All	All	1468/1568 (93%)	0.20	62 (4%) 36 18	52, 102, 165, 207	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	188	TYR	8.5
1	C	287	TRP	5.0
1	A	283	GLU	4.8
1	A	252	VAL	4.6
1	C	359	TYR	4.5
1	A	287	TRP	4.1
2	D	134	GLN	4.1
1	C	283	GLU	4.0
2	B	54	SER	3.9
2	D	899	PHE	3.9
2	D	871	TYR	3.6
2	B	184	GLY	3.6
1	C	303	VAL	3.4
2	D	187	ASN	3.4
1	A	249	PHE	3.3
2	B	135	GLY	3.1
1	C	193	GLU	3.0
1	C	255	LYS	3.0
1	A	214	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	256	ASP	3.0
1	C	280	ILE	2.9
2	D	850	TYR	2.8
1	A	0	HIS	2.8
1	C	324	LEU	2.8
1	C	233	ASP	2.8
1	A	114	ASN	2.8
2	D	872	VAL	2.8
1	A	250	VAL	2.6
1	C	363	LYS	2.6
1	C	364	PHE	2.6
2	B	1004	ASN	2.5
2	B	1005	GLY	2.5
1	A	294	LYS	2.5
2	D	978	HIS	2.5
2	D	183	GLU	2.5
1	A	251	GLU	2.4
2	B	843	LYS	2.4
2	D	1005	GLY	2.4
2	D	909	VAL	2.4
2	D	847	PHE	2.4
1	C	292	LYS	2.3
2	B	1002	LYS	2.3
2	B	171	ILE	2.3
2	B	840	GLU	2.2
2	D	175	TYR	2.2
2	B	55	ASN	2.2
1	C	356	LEU	2.2
1	C	305	ASP	2.2
2	D	67	LYS	2.2
1	A	286	PRO	2.1
1	C	168	ASP	2.1
1	C	276	VAL	2.1
1	C	360	TYR	2.1
2	B	871	TYR	2.1
2	D	39	SER	2.1
1	C	249	PHE	2.1
2	D	174	GLU	2.1
2	D	995	ASP	2.1
1	C	263	ALA	2.0
2	D	92	ARG	2.0
1	C	294	LYS	2.0

*Continued on next page...*



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Mol	Chain	Res	Type	RSRZ
1	C	282	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

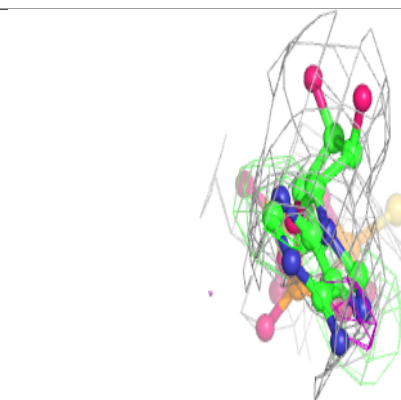
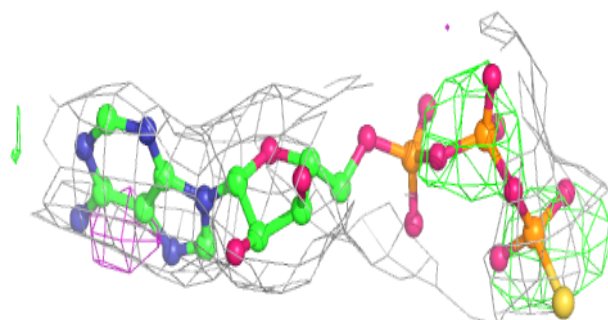
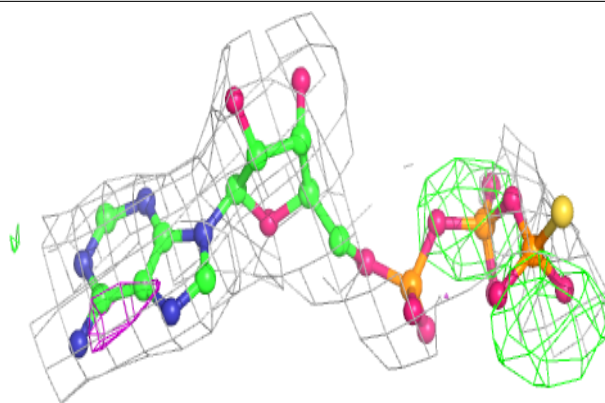
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	AGS	D	1101	31/31	0.73	0.35	50,75,294,338	0
5	MG	A	401	1/1	0.74	0.31	92,92,92,92	1
6	AGS	B	1101	31/31	0.81	0.26	29,86,180,215	0
5	MG	A	402	1/1	0.89	0.26	75,75,75,75	0
5	MG	C	401	1/1	0.91	0.29	83,83,83,83	0
5	MG	C	402	1/1	0.96	0.40	79,79,79,79	0

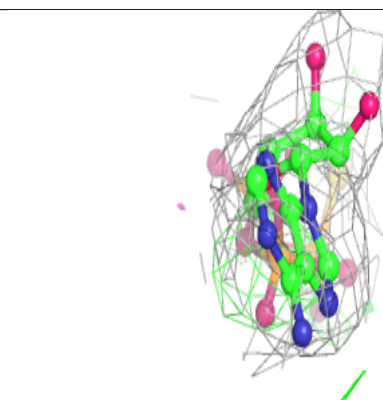
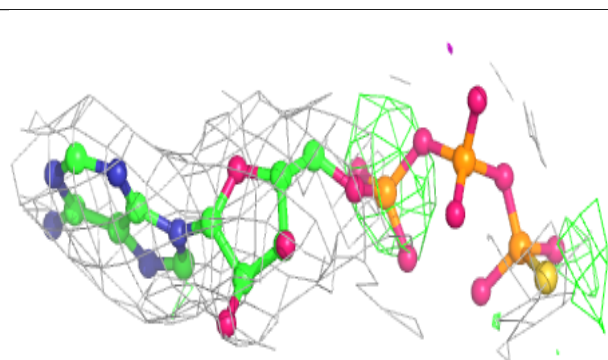
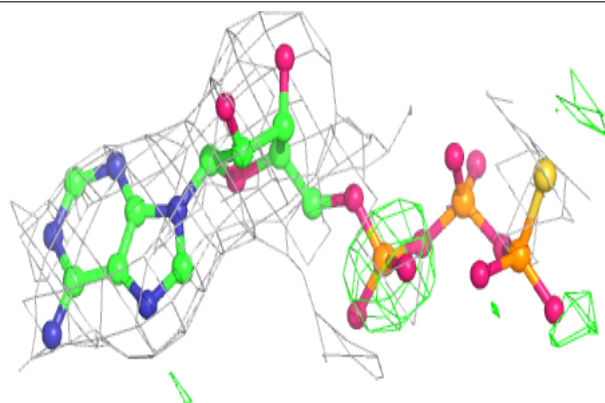
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around AGS D 1101:**

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

**Electron density around AGS B 1101:**

$2mF_o-DF_c$  (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.