



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2018 – 01:03 PM EST

PDB ID : 5O6D  
Title : Structure of ScPif1 in complex with polydT and ATPgS  
Authors : LU, K.Y.; CHEN, W.F.; RETY, S.; LIU, N.N.; XU, X.G.  
Deposited on : 2017-06-06  
Resolution : 3.28 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

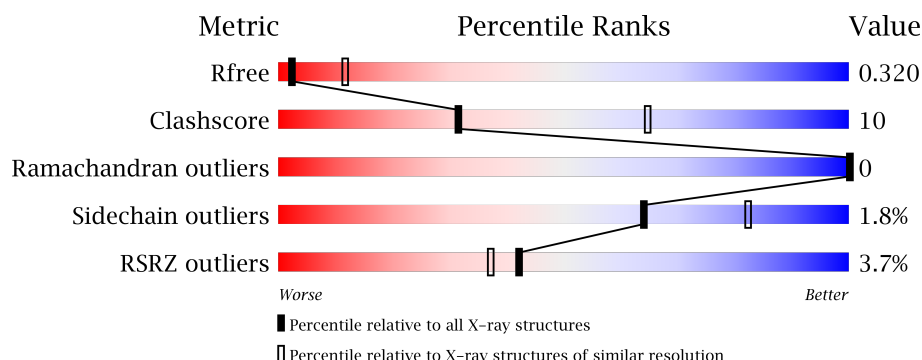
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.28 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))
$R_{free}$	100719	1006 (3.34-3.22)
Clashscore	112137	1070 (3.34-3.22)
Ramachandran outliers	110173	1050 (3.34-3.22)
Sidechain outliers	110143	1049 (3.34-3.22)
RSRZ outliers	101464	1011 (3.34-3.22)

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. 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	545	<div> <div>4%</div> <div>73%</div> <div>23%</div> <div>.</div> </div>
1	B	545	<div> <div>3%</div> <div>71%</div> <div>25%</div> <div>..</div> </div>
2	C	6	<div> <div>50%</div> <div>50%</div> </div>
2	D	6	<div> <div>83%</div> <div>17%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8658 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 ATP-dependent DNA helicase PIF1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	0	0
			4186	2652	739	775	20			
1	B	527	Total	C	N	O	S	0	0	0
			4186	2652	739	775	20			

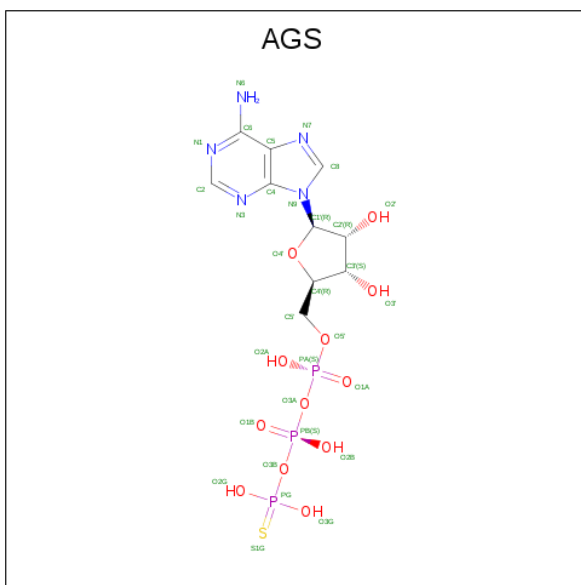
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	236	GLY	-	expression tag	UNP P07271
B	236	GLY	-	expression tag	UNP P07271

- Molecule 2 is a DNA chain called DNA (5'-D(P\*TP\*TP\*TP\*TP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	P	0	0	0
			111	55	10	40	6			
2	D	6	Total	C	N	O	P	0	0	0
			111	55	10	40	6			

- Molecule 3 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
3	A	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
3	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0

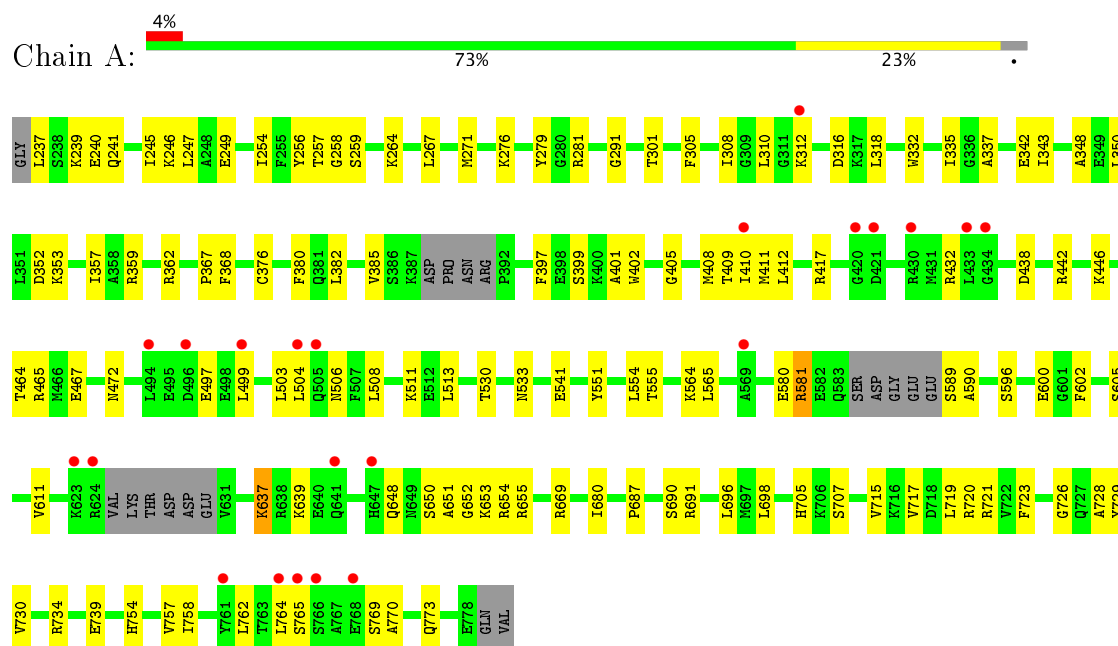
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0

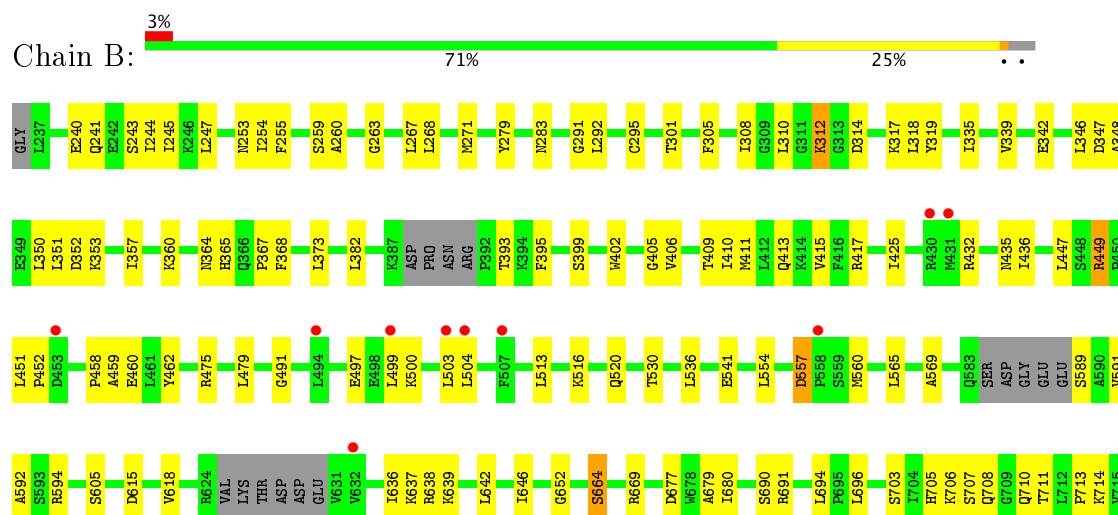
### 3 Residue-property plots

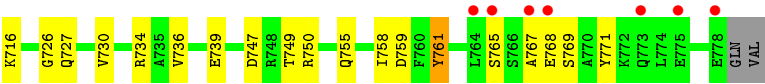
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: ATP-dependent DNA helicase PIF1



#### • Molecule 1: ATP-dependent DNA helicase PIF1

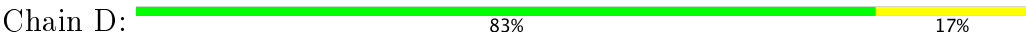




● Molecule 2: DNA (5'-D(P\*TP\*TP\*TP\*TP\*TP\*T)-3')



● Molecule 2: DNA (5'-D(P\*TP\*TP\*TP\*TP\*TP\*T)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.41Å 90.78Å 186.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.00 – 3.28 93.08 – 3.28	Depositor EDS
% Data completeness (in resolution range)	89.7 (65.00-3.28) 90.0 (93.08-3.28)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 3.26Å)	Xtriage
Refinement program	PHENIX (dev_2733: ???)	Depositor
R, $R_{free}$	0.252 , 0.322 0.249 , 0.320	Depositor DCC
$R_{free}$ test set	950 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	72.8	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 61.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8658	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.60 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.7228e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: 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	0/4254	0.47	0/5711
1	B	0.25	0/4254	0.47	0/5711
2	C	0.57	0/121	1.24	0/184
2	D	0.62	0/121	1.27	0/184
All	All	0.27	0/8750	0.51	0/11790

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	2
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	637	LYS	Peptide
1	B	557	ASP	Peptide
1	B	637	LYS	Peptide



## 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	4186	0	4288	90	0
1	B	4186	0	4290	95	0
2	C	111	0	67	6	0
2	D	111	0	67	1	0
3	A	31	0	12	1	0
3	B	31	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	8658	0	8736	177	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 10.

All (177) 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:B:1001:AGS:S1G	3:B:1001:AGS:O2B	2.40	0.80
1:A:503:LEU:HG	1:B:499:LEU:HD22	1.69	0.73
1:A:506:ASN:HD21	1:B:499:LEU:HD11	1.55	0.71
1:A:499:LEU:HD11	1:B:503:LEU:HB2	1.77	0.66
1:A:497:GLU:OE2	1:B:312:LYS:NZ	2.28	0.66
1:B:554:LEU:HD11	1:B:639:LYS:HD3	1.78	0.65
1:B:713:PRO:HA	1:B:736:VAL:CG1	2.27	0.64
1:B:497:GLU:HA	1:B:500:LYS:HB3	1.79	0.64
3:A:1001:AGS:O1A	3:A:1001:AGS:O2B	2.12	0.64
1:A:312:LYS:HE2	1:B:497:GLU:HB2	1.80	0.64
1:A:308:ILE:HB	1:A:318:LEU:HD22	1.80	0.64
1:A:359:ARG:HH21	1:A:367:PRO:HA	1.63	0.63
1:B:513:LEU:HD21	1:B:696:LEU:HB2	1.81	0.62
1:A:367:PRO:HB3	1:A:405:GLY:HA2	1.82	0.62
1:B:382:LEU:HD13	1:B:705:HIS:HA	1.82	0.61
1:A:305:PHE:HZ	1:A:335:ILE:HD13	1.65	0.61
1:A:499:LEU:HD22	1:B:499:LEU:HD23	1.83	0.59
1:A:246:LYS:HA	1:A:249:GLU:HB2	1.83	0.59
1:B:768:GLU:HG3	1:B:771:TYR:CD2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:LEU:HD12	1:B:503:LEU:HD12	1.85	0.58
1:A:259:SER:OG	1:A:432:ARG:NH1	2.37	0.58
1:A:611:VAL:O	1:A:648:GLN:NE2	2.37	0.58
1:A:769:SER:O	1:A:773:GLN:NE2	2.37	0.57
1:B:458:PRO:HB3	1:B:714:LYS:HE2	1.87	0.56
1:B:353:LYS:O	1:B:357:ILE:HG13	2.05	0.56
1:B:350:LEU:HA	1:B:353:LYS:HD2	1.87	0.56
1:A:506:ASN:ND2	1:B:499:LEU:HD11	2.20	0.56
1:A:465:ARG:HH22	1:A:506:ASN:HA	1.71	0.55
1:B:253:ASN:HD22	1:B:373:LEU:HG	1.72	0.55
1:A:739:GLU:OE1	1:A:739:GLU:N	2.38	0.55
1:A:720:ARG:HG3	1:B:750:ARG:HH22	1.72	0.55
1:B:565:LEU:HB3	1:B:642:LEU:HD13	1.89	0.54
1:A:596:SER:O	1:A:600:GLU:N	2.38	0.54
1:A:730:VAL:O	1:A:734:ARG:HG2	2.06	0.54
1:B:479:LEU:O	1:B:516:LYS:NZ	2.34	0.54
1:B:240:GLU:OE2	1:B:240:GLU:N	2.38	0.54
1:A:350:LEU:HA	1:A:353:LYS:HD2	1.89	0.53
1:A:503:LEU:HD11	1:A:680:ILE:HD13	1.90	0.53
1:B:520:GLN:HE21	1:B:536:LEU:HD22	1.72	0.53
1:A:240:GLU:OE2	1:A:240:GLU:N	2.41	0.53
1:A:254:ILE:HG22	1:A:408:MET:HB3	1.90	0.53
1:A:241:GLN:HG2	1:A:267:LEU:HD12	1.91	0.52
1:A:467:GLU:HG3	1:A:721:ARG:NH2	2.25	0.52
1:A:245:ILE:HG12	1:A:271:MET:HB2	1.92	0.52
1:A:650:SER:HA	1:A:653:LYS:HD2	1.91	0.52
1:B:291:GLY:HA2	1:B:301:THR:HG22	1.91	0.52
1:A:257:THR:OG1	1:A:258:GLY:N	2.42	0.51
1:B:259:SER:OG	1:B:432:ARG:NH1	2.43	0.51
1:B:513:LEU:HD23	1:B:694:LEU:HB2	1.92	0.51
1:B:497:GLU:HG3	1:B:500:LYS:HD2	1.93	0.51
1:A:530:THR:OG1	1:A:669:ARG:NH1	2.43	0.51
1:B:730:VAL:O	1:B:734:ARG:HG2	2.10	0.51
1:A:773:GLN:N	1:A:773:GLN:OE1	2.43	0.50
1:B:726:GLY:O	1:B:730:VAL:HG23	2.11	0.50
1:B:382:LEU:HD21	1:B:727:GLN:HB2	1.92	0.50
1:B:768:GLU:HG3	1:B:771:TYR:CE2	2.46	0.50
1:B:241:GLN:HE21	1:B:263:GLY:HA3	1.75	0.50
1:B:530:THR:OG1	1:B:669:ARG:NH1	2.45	0.50
1:B:292:LEU:HD23	1:B:706:LYS:O	2.12	0.50
1:A:504:LEU:HD22	1:A:691:ARG:HE	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:723:PHE:HB3	2:C:3:DT:H72	1.93	0.49
1:B:642:LEU:O	1:B:646:ILE:HG13	2.13	0.49
1:B:308:ILE:HB	1:B:318:LEU:HD22	1.95	0.49
1:A:438:ASP:HB3	1:A:442:ARG:HH12	1.77	0.49
1:B:747:ASP:OD2	1:B:749:THR:OG1	2.31	0.49
1:A:256:TYR:OH	1:A:264:LYS:O	2.29	0.48
1:A:382:LEU:HD13	1:A:705:HIS:HA	1.95	0.48
1:B:713:PRO:HA	1:B:736:VAL:HG12	1.95	0.48
1:A:758:ILE:O	1:A:762:LEU:HD23	2.14	0.48
1:B:319:TYR:CE2	1:B:360:LYS:HB3	2.48	0.48
1:B:417:ARG:HG3	1:B:711:THR:HG23	1.95	0.48
1:A:353:LYS:O	1:A:357:ILE:HG12	2.14	0.48
1:B:460:GLU:OE2	1:B:475:ARG:NH2	2.44	0.48
1:B:758:ILE:HG23	1:B:761:TYR:HE2	1.78	0.48
1:A:551:TYR:O	1:A:555:THR:HG23	2.14	0.48
1:B:255:PHE:O	1:B:409:THR:HA	2.14	0.48
1:B:260:ALA:HB1	1:B:417:ARG:HH12	1.79	0.47
1:A:726:GLY:O	1:A:730:VAL:HG23	2.14	0.47
1:A:432:ARG:HB2	1:A:729:TYR:CE2	2.50	0.47
1:B:241:GLN:NE2	1:B:263:GLY:HA3	2.30	0.47
1:B:679:ALA:O	1:B:680:ILE:HD12	2.15	0.47
1:B:295:CYS:O	1:B:664:SER:HB3	2.14	0.47
1:A:499:LEU:CD1	1:B:503:LEU:HD12	2.45	0.47
1:B:569:ALA:HA	1:B:646:ILE:HG12	1.97	0.47
1:A:580:GLU:OE1	1:A:580:GLU:N	2.47	0.47
1:A:305:PHE:CZ	1:A:335:ILE:HD13	2.48	0.46
1:A:513:LEU:HD21	1:A:696:LEU:HB2	1.97	0.46
1:B:305:PHE:HZ	1:B:335:ILE:HD13	1.79	0.46
1:A:291:GLY:HA2	1:A:301:THR:HG22	1.97	0.46
1:B:605:SER:HB2	1:B:652:GLY:C	2.36	0.46
1:B:459:ALA:O	1:B:716:LYS:N	2.32	0.46
1:B:739:GLU:OE1	1:B:739:GLU:N	2.48	0.46
1:A:464:THR:HG22	2:C:3:DT:H2"	1.98	0.46
1:A:276:LYS:HB3	1:A:281:ARG:HA	1.98	0.46
1:B:347:ASP:HB2	1:B:393:THR:HB	1.98	0.46
1:A:409:THR:HG21	1:A:764:LEU:HD22	1.98	0.46
1:A:719:LEU:HD21	1:A:728:ALA:HB1	1.98	0.46
1:B:458:PRO:HG2	1:B:475:ARG:HH22	1.80	0.46
1:A:723:PHE:CD2	2:C:3:DT:H73	2.52	0.45
1:A:754:HIS:HB3	1:A:757:VAL:HG23	1.97	0.45
1:B:589:SER:HB3	1:B:592:ALA:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:ASP:HB2	1:B:560:MET:HB2	1.99	0.45
1:A:687:PRO:HB2	1:A:690:SER:HB3	1.98	0.45
1:B:554:LEU:HD13	1:B:565:LEU:HD11	1.99	0.45
1:B:342:GLU:OE1	1:B:708:GLN:NE2	2.49	0.45
1:B:410:ILE:HG22	1:B:411:MET:H	1.82	0.45
1:B:411:MET:O	1:B:767:ALA:HB2	2.17	0.44
1:B:243:SER:O	1:B:247:LEU:HD13	2.18	0.44
1:B:314:ASP:HB3	1:B:317:LYS:HG3	1.99	0.44
1:B:758:ILE:HA	1:B:761:TYR:HD2	1.83	0.44
1:A:564:LYS:HB3	1:A:564:LYS:HE2	1.72	0.44
1:A:589:SER:OG	1:A:590:ALA:N	2.50	0.44
1:B:351:LEU:HD12	1:B:351:LEU:HA	1.86	0.44
1:A:279:TYR:HE2	1:A:337:ALA:HB2	1.83	0.44
1:A:410:ILE:HG22	1:A:411:MET:N	2.32	0.44
1:A:554:LEU:HD13	1:A:565:LEU:HD11	1.99	0.44
1:A:410:ILE:HG22	1:A:411:MET:H	1.83	0.44
1:B:367:PRO:HB3	1:B:405:GLY:HA2	1.99	0.44
1:A:410:ILE:HG23	1:A:770:ALA:HB2	2.00	0.44
1:B:348:ALA:HB2	1:B:395:PHE:O	2.18	0.44
1:A:397:PHE:HA	1:A:402:TRP:CG	2.53	0.43
1:A:352:ASP:HA	1:A:401:ALA:HB2	2.00	0.43
1:B:435:ASN:C	1:B:436:ILE:HD12	2.39	0.43
1:B:504:LEU:O	1:B:691:ARG:NH1	2.50	0.43
1:A:554:LEU:HD11	1:A:639:LYS:HD3	2.01	0.43
1:A:605:SER:HB2	1:A:652:GLY:C	2.38	0.43
1:B:254:ILE:HD12	1:B:410:ILE:HD13	1.99	0.43
1:B:413:GLN:N	1:B:413:GLN:OE1	2.52	0.43
1:A:465:ARG:HH21	1:A:508:LEU:HD23	1.84	0.43
1:A:715:VAL:HG22	1:A:717:VAL:HG23	2.01	0.43
1:A:343:ILE:HD13	1:A:402:TRP:HZ3	1.84	0.42
1:A:602:PHE:O	1:A:654:ARG:HD3	2.19	0.42
1:B:402:TRP:CE2	1:B:406:VAL:HG21	2.54	0.42
1:B:615:ASP:O	1:B:618:VAL:HG22	2.19	0.42
1:A:765:SER:HB3	1:A:769:SER:HB2	1.99	0.42
1:A:237:LEU:HD23	1:A:237:LEU:HA	1.86	0.42
1:A:241:GLN:HG2	1:A:412:LEU:HD21	2.00	0.42
1:B:352:ASP:OD1	1:B:399:SER:HB2	2.18	0.42
1:A:385:VAL:HG13	2:C:4:DT:C2	2.54	0.42
1:B:268:LEU:HD11	1:B:339:VAL:HG11	2.02	0.42
1:B:346:LEU:HD12	1:B:351:LEU:HD13	2.01	0.42
1:A:442:ARG:O	1:A:446:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:VAL:HB	1:B:425:ILE:HD13	2.02	0.42
1:B:491:GLY:N	1:B:690:SER:O	2.52	0.42
1:A:511:LYS:HA	1:A:691:ARG:HH12	1.85	0.42
1:A:581:ARG:HG3	1:A:581:ARG:O	2.18	0.42
1:A:651:ALA:HA	1:A:655:ARG:HH21	1.84	0.42
1:B:348:ALA:HB1	1:B:399:SER:HB3	2.01	0.42
1:A:247:LEU:HA	1:A:247:LEU:HD23	1.87	0.41
1:B:279:TYR:O	1:B:283:ASN:ND2	2.52	0.41
1:A:438:ASP:HB3	1:A:442:ARG:NH1	2.35	0.41
1:A:503:LEU:HD13	1:A:680:ILE:HG21	2.01	0.41
1:A:432:ARG:HD2	1:A:729:TYR:CZ	2.56	0.41
1:B:462:TYR:O	1:B:703:SER:HA	2.20	0.41
1:B:758:ILE:HA	1:B:761:TYR:CD2	2.56	0.41
1:B:755:GLN:HG3	1:B:759:ASP:OD1	2.20	0.41
1:A:417:ARG:HH12	1:A:734:ARG:CZ	2.34	0.41
1:B:244:ILE:HD12	1:B:267:LEU:HD11	2.03	0.41
1:B:710:GLN:O	1:B:734:ARG:HD3	2.20	0.41
1:B:765:SER:HB3	1:B:769:SER:HB2	2.02	0.41
1:A:472:ASN:HB3	1:A:698:LEU:HB2	2.01	0.41
1:B:504:LEU:HB3	1:B:691:ARG:NH2	2.36	0.41
1:B:245:ILE:HG12	1:B:271:MET:HB2	2.03	0.41
1:B:364:ASN:OD1	1:B:365:HIS:N	2.54	0.41
1:B:503:LEU:HD21	1:B:680:ILE:HD13	2.01	0.41
1:A:721:ARG:HD3	2:D:3:DT:H72	2.03	0.41
1:B:591:VAL:O	1:B:594:ARG:HB3	2.21	0.40
1:A:723:PHE:HD2	2:C:3:DT:H73	1.87	0.40
1:B:451:LEU:HB3	1:B:452:PRO:HD2	2.02	0.40
1:A:533:ASN:ND2	2:C:7:DT:OP2	2.51	0.40
1:A:332:TRP:O	1:A:362:ARG:NH1	2.52	0.40
1:A:342:GLU:N	1:A:376:CYS:O	2.55	0.40
1:A:348:ALA:HB1	1:A:399:SER:HB3	2.04	0.40
1:B:310:LEU:HD23	1:B:310:LEU:HA	1.80	0.40
1:A:380:PHE:HB2	1:A:432:ARG:HE	1.87	0.40
1:B:447:LEU:O	1:B:449:ARG:NH1	2.55	0.40
1:B:636:ILE:O	1:B:638:ARG:N	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	519/545 (95%)	511 (98%)	8 (2%)	0	100	100
1	B	519/545 (95%)	512 (99%)	7 (1%)	0	100	100
All	All	1038/1090 (95%)	1023 (99%)	15 (1%)	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	457/473 (97%)	449 (98%)	8 (2%)	64	82
1	B	457/473 (97%)	449 (98%)	8 (2%)	64	82
All	All	914/946 (97%)	898 (98%)	16 (2%)	64	82

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

Mol	Chain	Res	Type
1	A	239	LYS
1	A	310	LEU
1	A	316	ASP
1	A	368	PHE
1	A	541	GLU
1	A	581	ARG
1	A	637	LYS
1	A	707	SER

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Mol	Chain	Res	Type
1	B	312	LYS
1	B	368	PHE
1	B	449	ARG
1	B	541	GLU
1	B	664	SER
1	B	677	ASP
1	B	707	SER
1	B	761	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	520	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 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
3	AGS	A	1001	1,4	26,33,33	0.86	1 (3%)	22,52,52	1.26	1 (4%)
3	AGS	B	1001	-	26,33,33	0.74	1 (3%)	22,52,52	0.80	1 (4%)

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	AGS	A	1001	1,4	-	0/17/38/38	0/3/3/3
3	AGS	B	1001	-	-	0/17/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1001	AGS	PG-S1G	2.74	1.95	1.90
3	A	1001	AGS	PG-S1G	2.83	1.96	1.90

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	AGS	PB-O3B-PG	-5.37	115.00	132.35
3	B	1001	AGS	PB-O3B-PG	-2.60	123.93	132.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	AGS	1	0
3	B	1001	AGS	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

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	527/545 (96%)	0.25	22 (4%) 37 34	31, 86, 158, 193	0
1	B	527/545 (96%)	0.05	17 (3%) 48 45	24, 64, 148, 209	0
2	C	6/6 (100%)	-0.06	0 100 100	76, 78, 87, 89	0
2	D	6/6 (100%)	-0.18	0 100 100	55, 66, 93, 103	0
All	All	1066/1102 (96%)	0.15	39 (3%) 42 37	24, 76, 154, 209	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	765	SER	8.9
1	B	504	LEU	5.9
1	A	764	LEU	5.3
1	A	569	ALA	4.2
1	B	765	SER	4.1
1	A	623	LYS	3.9
1	A	499	LEU	3.9
1	A	421	ASP	3.9
1	B	558	PRO	3.8
1	A	420	GLY	3.7
1	A	496	ASP	3.6
1	A	766	SER	3.6
1	A	761	TYR	3.5
1	A	410	ILE	3.5
1	B	775	GLU	3.1
1	B	764	LEU	3.1
1	A	505	GLN	2.9
1	B	503	LEU	2.9
1	B	453	ASP	2.8
1	A	433	LEU	2.8
1	A	430	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	647	HIS	2.7
1	B	430	ARG	2.6
1	A	504	LEU	2.6
1	B	632	VAL	2.6
1	B	507	PHE	2.6
1	A	434	GLY	2.4
1	B	768	GLU	2.4
1	A	312	LYS	2.4
1	A	494	LEU	2.3
1	A	768	GLU	2.2
1	B	767	ALA	2.2
1	A	624	ARG	2.2
1	B	431	MET	2.2
1	B	773	GLN	2.1
1	B	499	LEU	2.1
1	B	778	GLU	2.1
1	B	494	LEU	2.1
1	A	641	GLN	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	AGS	A	1001	31/31	0.90	0.20	-0.45	68,76,144,150	0
3	AGS	B	1001	31/31	0.94	0.20	-0.49	32,70,128,139	0
4	MG	B	1002	1/1	0.80	0.22	-	49,49,49,49	0
4	MG	A	1002	1/1	0.94	0.10	-	19,19,19,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.