



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:12 am BST

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

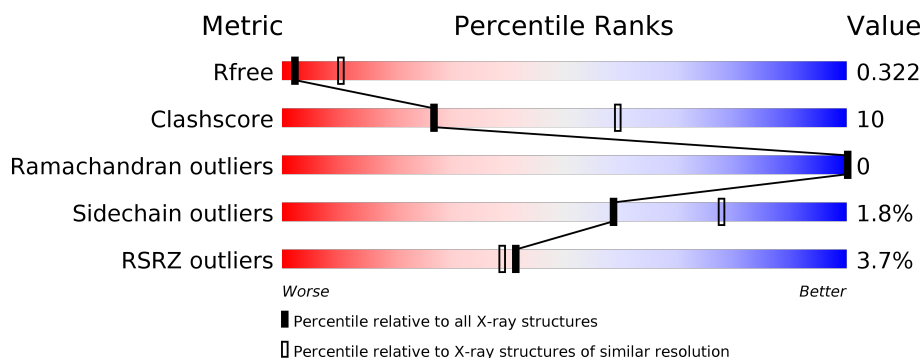
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.28 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}	130704	1177 (3.32-3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)
RSRZ outliers	127900	1141 (3.32-3.24)

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

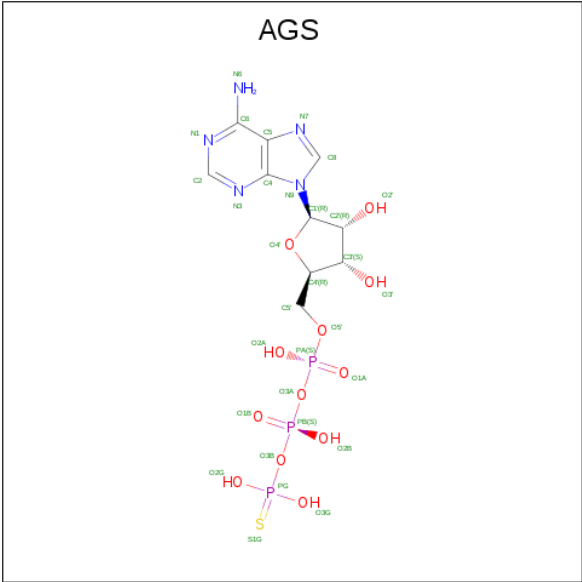
There are 2 discrepancies between the modelled and reference sequences:

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: C₁₀H₁₆N₅O₁₂P₃S).



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

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

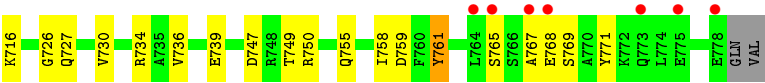
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

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.

- Chain A:
-
- 4% 73% 23%
- GLY L237 S238 K239 E240 Q241 I245 K246 L247 L248 E249 I254 F255 Y256 T257 G258 S259 K264 L267 M271 K276 Y279 G280 R281 G291 T301 F305 I308 G309 L310 G311 K312 D316 K317 L318 W332 I335 G336 A337 E342 I343 A348 F349 I350 L351 D352 K353 I357 A358 R359 R362 P367 F368 C376 F380 Q381 L382 V385 S386 K387 ASP PRO ASH ARG F392 F397 E398 S399 K400 A401 W402 G405 M408 T409 I410 M411 L412 R417 G420 D421 R430 M431 R432 L433 G434 D438 R442 K446 T464 R465 W466 E467 M472 L494 E495 D496 E497 E498 L499 L503 L504 S505 S506 F507 L508 K511 E512 L513 T530 N533 E541 Y551 L554 T555 K564 L565 L566 A569 E580 E581 E582 E583 SER ASP GLY GLU S589 A590 S596 B600 G601 F602 S605 K623 R624 VAL LYS THR ASP ASP GLU W631 K637 R638 K639 E640 E641 Q641 H647 Q648 N649 S650 A651 G652 K653 R654 R655 R669 I680 P687 S690 R691 L696 W697 L698 H705 K706 S707 V715 W716 W717 D718 L719 R720 R721 W722 F723 G726 Q727 A728 Y729 V730 R734 E739 H754 V757 I758 Y761 L762 T763 L764 S765 S766 A767 E768 S769 A770 Q773 E778 GLN VAL

- Chain B:**

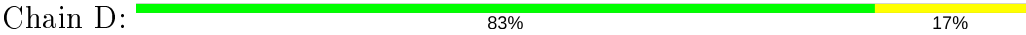
Category	Value	Color Group
A592	L451	Green
S593	E249	Red
R594	D453	Yellow
S605	P458	Green
D615	A459	Yellow
V618	E460	Green
R624	Y462	Yellow
VAL	R475	Yellow
LYS	H365	Green
THR	Q366	Yellow
ASP	P367	Yellow
GLU	G491	Yellow
W631	L494	Green
V632	L373	Green
I636	L382	Yellow
K637	K387	Green
R638	ASP	Yellow
K639	P80	Yellow
L642	ASN	Yellow
I646	ARG	Yellow
G652	P392	Yellow
S664	T393	Yellow
R669	K394	Yellow
D677	F395	Yellow
A679	S399	Yellow
I680	W402	Yellow
S690	G405	Yellow
R691	V406	Yellow
L694	T409	Yellow
P695	I410	Yellow
L696	M411	Yellow
S703	L412	Yellow
I704	Q413	Yellow
H705	K414	Yellow
K706	V415	Yellow
S707	F416	Yellow
Q708	R417	Yellow
G709	I425	Yellow
Q710	R430	Yellow
T711	M431	Yellow
L712	R432	Yellow
P713	M435	Yellow
K714	L436	Yellow
T715	L447	Yellow
L716	S448	Green
L717	G449	Yellow
L718	R449	Red
L719	A500	Yellow
L720	V501	Yellow
L721	ASP	Yellow
L722	GLY	Yellow
L723	GLU	Yellow
L724	S589	Yellow
L725	L589	Yellow
L726	L590	Yellow
L727	L591	Yellow
L728	L592	Yellow
L729	L593	Yellow
L730	L594	Yellow
L731	L595	Yellow
L732	L596	Yellow
L733	L597	Yellow
L734	L598	Yellow
L735	L599	Yellow
L736	L600	Yellow
L737	L601	Yellow
L738	L602	Yellow
L739	L603	Yellow
L740	L604	Yellow
L741	L605	Yellow
L742	L606	Yellow
L743	L607	Yellow
L744	L608	Yellow
L745	L609	Yellow
L746	L610	Yellow
L747	L611	Yellow
L748	L612	Yellow
L749	L613	Yellow
L750	L614	Yellow
L751	L615	Yellow
L752	L616	Yellow
L753	L617	Yellow
L754	L618	Yellow
L755	L619	Yellow
L756	L620	Yellow
L757	L621	Yellow
L758	L622	Yellow
L759	L623	Yellow
L760	L624	Yellow
L761	L625	Yellow
L762	L626	Yellow
L763	L627	Yellow
L764	L628	Yellow
L765	L629	Yellow
L766	L630	Yellow
L767	L631	Yellow
L768	L632	Yellow
L769	L633	Yellow
L770	L634	Yellow
L771	L635	Yellow
L772	L636	Yellow
L773	L637	Yellow
L774	L638	Yellow
L775	L639	Yellow
L776	L640	Yellow
L777	L641	Yellow
L778	L642	Yellow
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L780	L644	Yellow
L781	L645	Yellow
L782	L646	Yellow
L783	L647	Yellow
L784	L648	Yellow
L785	L649	Yellow
L786	L650	Yellow
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L788	L652	Yellow
L789	L653	Yellow
L790	L654	Yellow
L791	L655	Yellow
L792	L656	Yellow
L793	L657	Yellow
L794	L658	Yellow
L795	L659	Yellow
L796	L660	Yellow
L797	L661	Yellow
L798	L662	Yellow
L799	L663	Yellow
L800	L664	Yellow
L801	L665	Yellow
L802	L666	Yellow
L803	L667	Yellow
L804	L668	Yellow
L805	L669	Yellow
L806	L670	Yellow
L807	L671	Yellow
L808	L672	Yellow
L809	L673	Yellow
L810	L674	Yellow
L811	L675	Yellow
L812	L676	Yellow
L813	L677	Yellow
L814	L678	Yellow
L815	L679	Yellow
L816	L680	Yellow
L817	L681	Yellow
L818	L682	Yellow



● 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 3.26Å)	Xtriage
Refinement program	PHENIX (dev_2733: ???)	Depositor
R, R_{free}	0.252 , 0.322 0.251 , 0.322	Depositor DCC
R_{free} test set	950 reflections (5.29%)	wwPDB-VP
Wilson B-factor (Å ²)	72.8	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	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 ²)	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.*

¹ Intensities estimated from amplitudes.

² 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:B:642:LEU:O	1:B:646:ILE:HG13	2.13	0.49
1:A:723:PHE:HB3	2:C:3:DT:H72	1.93	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:385:VAL:HG13	2:C:4:DT:C2	2.54	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: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: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:A:511:LYS:HA	1:A:691:ARG:HH12	1.85	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%)	59	78
1	B	457/473 (97%)	449 (98%)	8 (2%)	59	78
All	All	914/946 (97%)	898 (98%)	16 (2%)	59	78

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 ⓘ

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 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	0.87	1 (3%)	26,52,52	1.37	2 (7%)
3	AGS	B	1001	-	26,33,33	0.74	1 (3%)	26,52,52	1.11	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
3	AGS	A	1001	1,4	-	1/17/38/38	0/3/3/3
3	AGS	B	1001	-	-	5/17/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	AGS	PG-S1G	2.46	1.96	1.90
3	B	1001	AGS	PG-S1G	2.38	1.95	1.90

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	AGS	PA-O3A-PB	-5.98	112.30	132.83
3	B	1001	AGS	PA-O3A-PB	-4.27	118.17	132.83
3	B	1001	AGS	C5-C6-N6	2.28	123.81	120.35
3	A	1001	AGS	C5-C6-N6	2.26	123.79	120.35

There are no chirality outliers.

All (6) torsion outliers are listed below:

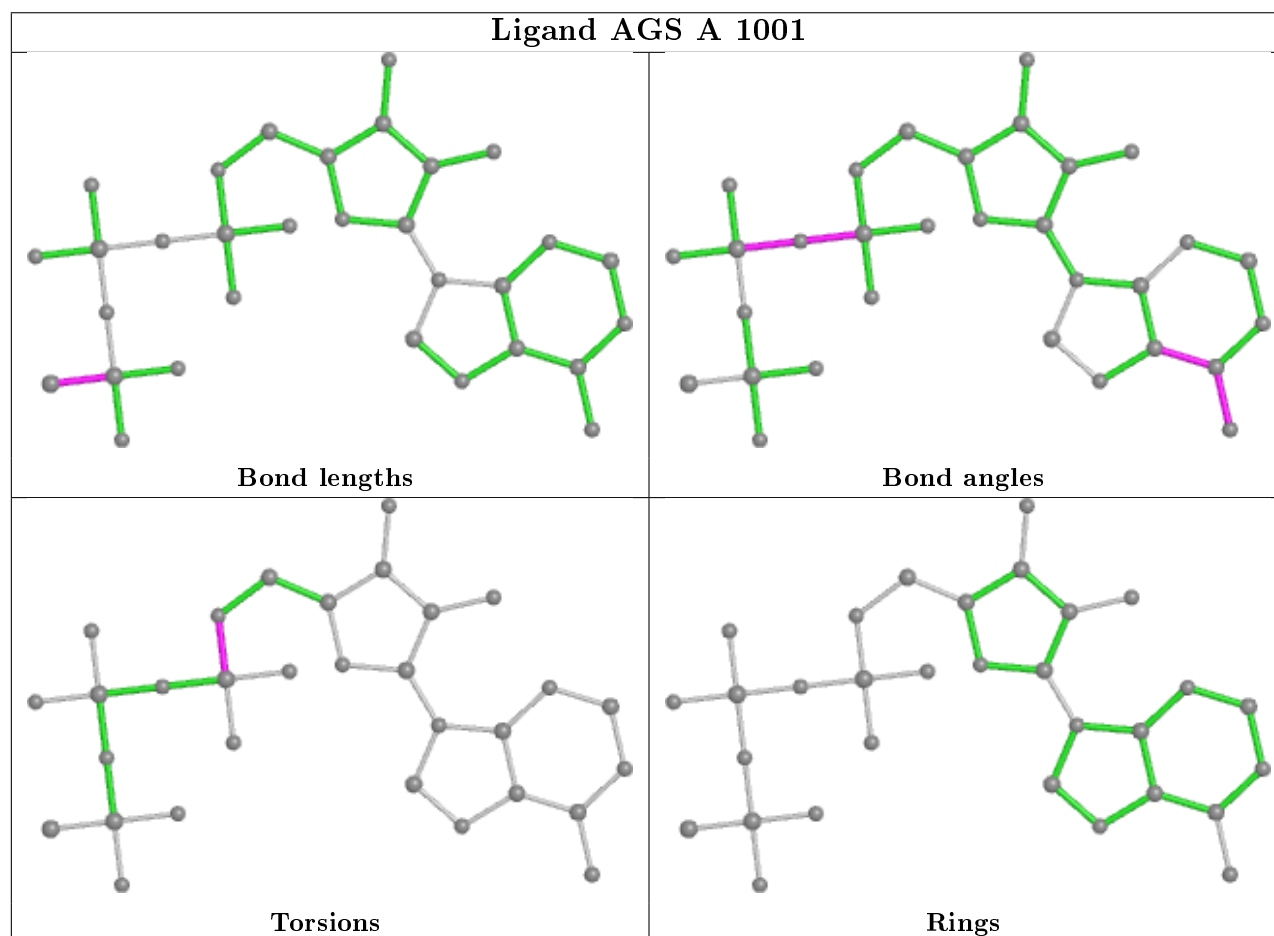
Mol	Chain	Res	Type	Atoms
3	B	1001	AGS	PB-O3B-PG-O2G
3	B	1001	AGS	PB-O3B-PG-O3G
3	B	1001	AGS	O4'-C4'-C5'-O5'
3	B	1001	AGS	C3'-C4'-C5'-O5'
3	B	1001	AGS	PG-O3B-PB-O2B
3	A	1001	AGS	C5'-O5'-PA-O3A

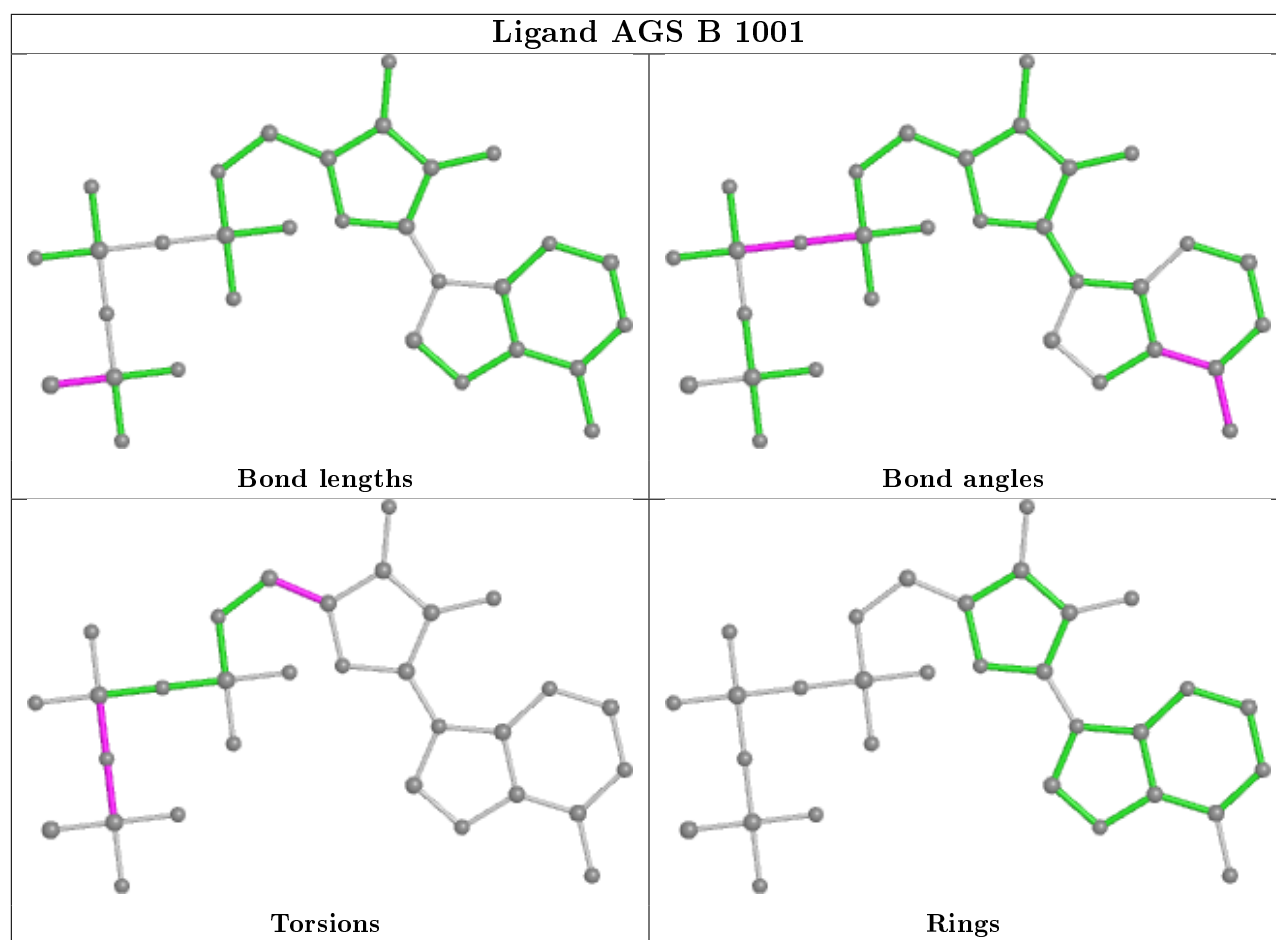
There are no ring outliers.

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	527/545 (96%)	0.25	22 (4%) 36 34	31, 86, 158, 193	0
1	B	527/545 (96%)	0.05	17 (3%) 47 46	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%) 41 39	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	764	LEU	3.1
1	B	775	GLU	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	2.7
1	B	632	VAL	2.6
1	A	504	LEU	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](#)

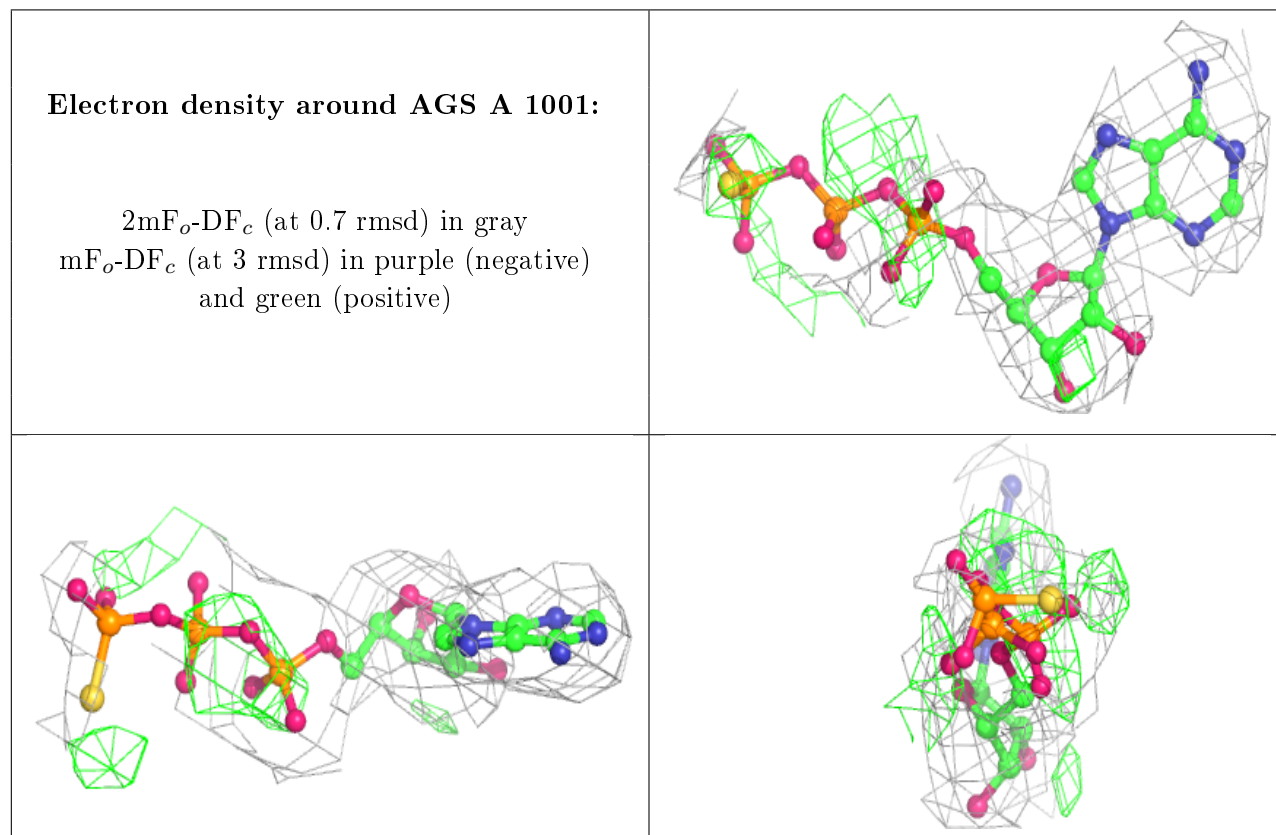
There are no carbohydrates in this entry.

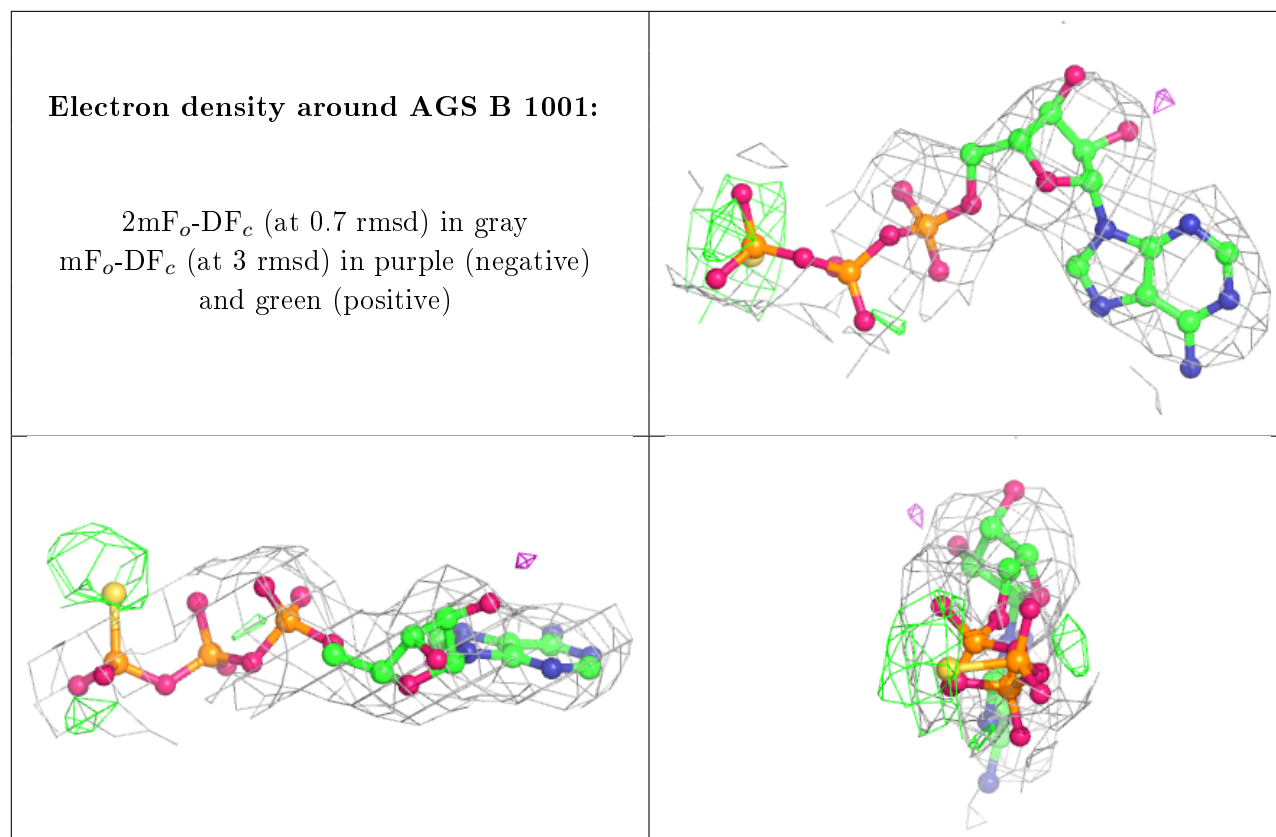
6.4 Ligands [i](#)

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	B	1002	1/1	0.80	0.22	49,49,49,49	0
3	AGS	A	1001	31/31	0.90	0.20	68,76,144,150	0
3	AGS	B	1001	31/31	0.94	0.20	32,70,128,139	0
4	MG	A	1002	1/1	0.94	0.10	19,19,19,19	0

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





6.5 Other polymers [i](#)

There are no such residues in this entry.