



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:48 PM UTC

PDB ID : 1OYY / pdb_00001oyy
Title : Structure of the RecQ Catalytic Core bound to ATP-gamma-S
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Deposited on : 2003-04-07
Resolution : 2.50 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

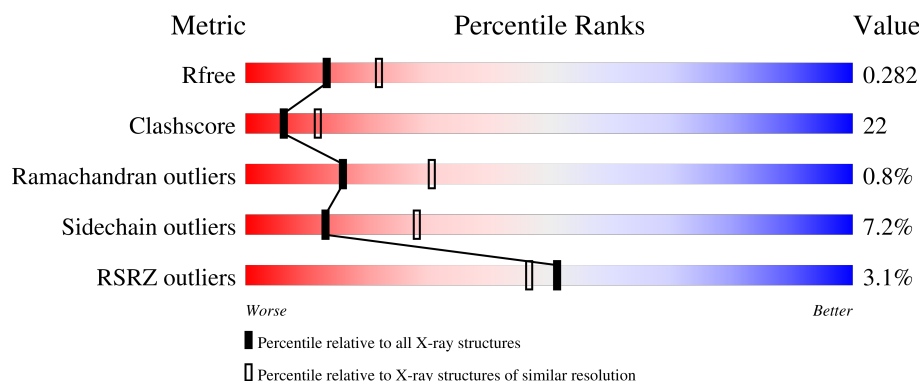
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 ≥ 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	523	

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
4	AGS	A	527	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4114 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	512	Total	C	N	O	S	0	0	0
			4037	2529	735	748	25			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P15043

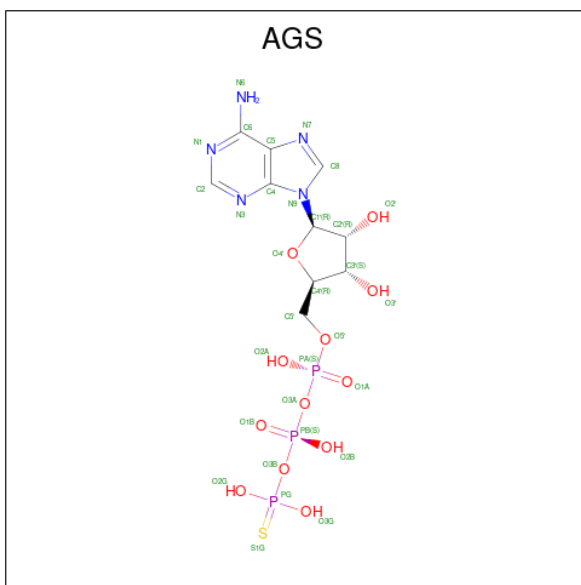
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mn	0	0
			2	2		

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



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

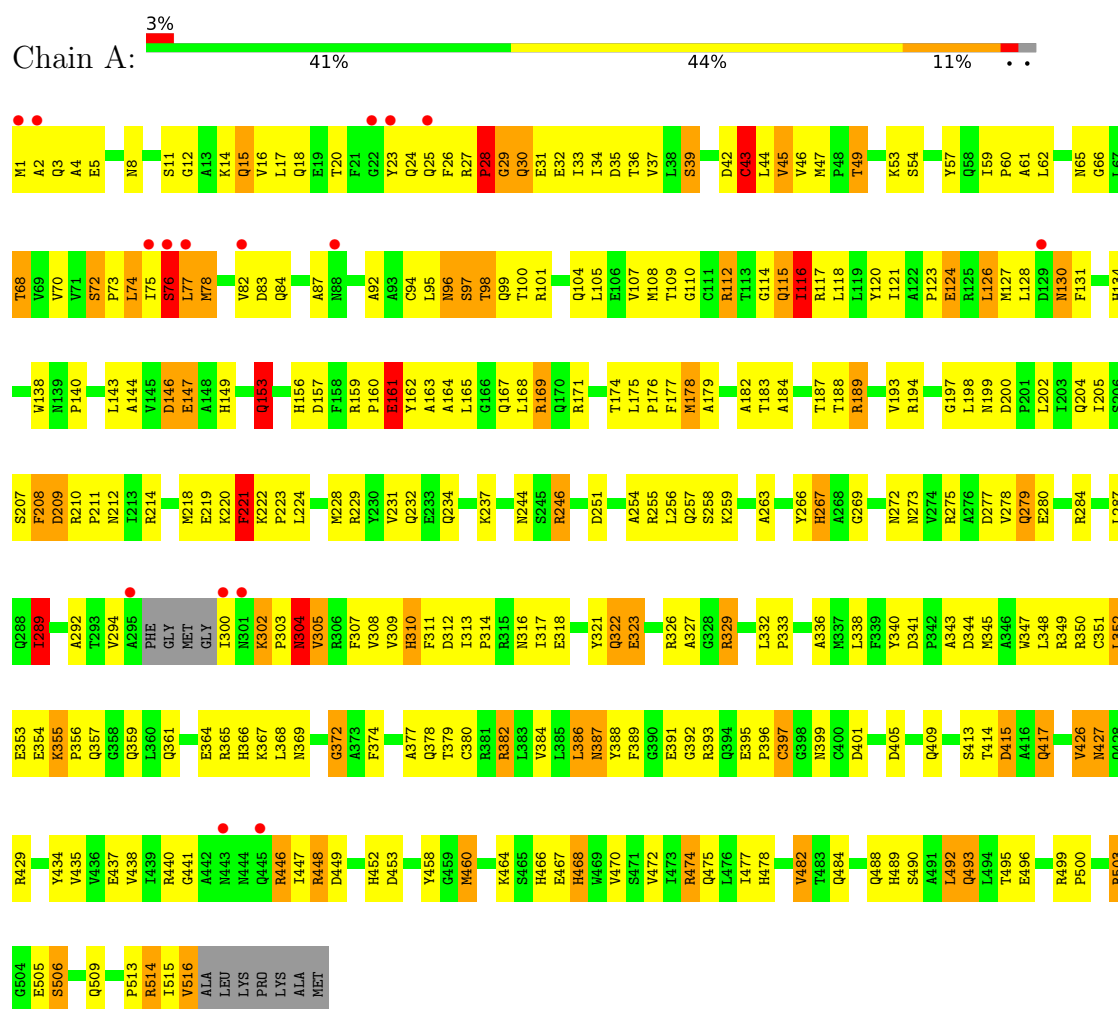
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	43	Total O 43 43	0	0

3 Residue-property plots

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: ATP-dependent DNA helicase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.59Å 54.53Å 78.69Å 90.00° 110.78° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.50) 90.8 (20.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.84 (at 2.49Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.210 , 0.298 0.198 , 0.282	Depositor DCC
R_{free} test set	826 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4114	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: AGS, MN, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.80	0/4108	2.11	152/5559 (2.7%)

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	17

There are no bond length outliers.

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	488	GLN	OE1-CD-NE2	11.77	134.37	122.60
1	A	284	ARG	CD-NE-CZ	10.41	138.98	124.40
1	A	112	ARG	CD-NE-CZ	10.32	138.84	124.40
1	A	344	ASP	CA-CB-CG	10.19	122.79	112.60
1	A	446	ARG	CD-NE-CZ	9.70	137.98	124.40
1	A	153	GLN	OE1-CD-NE2	-9.54	113.06	122.60
1	A	272	ASN	CA-C-O	-9.20	110.70	120.63
1	A	355	LYS	N-CA-C	-9.05	98.23	110.36
1	A	221	PHE	CA-CB-CG	-8.91	104.89	113.80
1	A	336	ALA	CA-C-O	-8.58	111.09	120.36
1	A	466	HIS	CA-CB-CG	-8.53	105.27	113.80
1	A	484	GLN	CA-C-O	-8.47	111.00	120.32
1	A	131	PHE	CA-CB-CG	-8.25	105.55	113.80
1	A	153	GLN	CB-CG-CD	8.04	126.26	112.60
1	A	322	GLN	N-CA-CB	7.93	121.90	110.16
1	A	237	LYS	CA-C-O	7.73	129.79	121.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	514	ARG	CD-NE-CZ	7.70	135.18	124.40
1	A	35	ASP	CA-CB-CG	-7.60	105.00	112.60
1	A	43	CYS	N-CA-C	7.44	120.67	108.99
1	A	405	ASP	CA-CB-CG	7.38	119.98	112.60
1	A	194	ARG	CD-NE-CZ	7.34	134.68	124.40
1	A	42	ASP	CA-CB-CG	7.29	119.89	112.60
1	A	384	VAL	N-CA-CB	7.24	118.51	110.62
1	A	382	ARG	NH1-CZ-NH2	7.21	128.67	119.30
1	A	493	GLN	CB-CG-CD	7.17	124.79	112.60
1	A	140	PRO	N-CA-CB	7.11	108.00	103.23
1	A	289	ILE	N-CA-C	7.05	118.27	108.12
1	A	393	ARG	NE-CZ-NH2	-7.03	112.88	119.20
1	A	144	ALA	CA-C-N	-6.92	113.87	122.93
1	A	144	ALA	C-N-CA	-6.92	113.87	122.93
1	A	316	ASN	OD1-CG-ND2	-6.90	115.70	122.60
1	A	177	PHE	CA-CB-CG	6.75	120.56	113.80
1	A	482	VAL	CA-C-O	-6.75	113.07	120.43
1	A	484	GLN	O-C-N	6.70	131.18	123.27
1	A	15	GLN	CB-CG-CD	6.69	123.98	112.60
1	A	388	TYR	CA-C-O	-6.69	112.82	120.24
1	A	179	ALA	CA-C-O	-6.67	113.16	120.30
1	A	8	ASN	CA-C-N	6.58	129.10	120.28
1	A	8	ASN	C-N-CA	6.58	129.10	120.28
1	A	382	ARG	NE-CZ-NH2	-6.58	113.28	119.20
1	A	208	PHE	CA-C-O	-6.53	111.71	119.35
1	A	130	ASN	CA-CB-CG	-6.49	106.11	112.60
1	A	323	GLU	O-C-N	-6.49	115.39	122.07
1	A	344	ASP	N-CA-CB	6.47	119.64	110.12
1	A	210	ARG	CA-C-N	6.45	126.14	119.56
1	A	210	ARG	C-N-CA	6.45	126.14	119.56
1	A	107	VAL	CA-C-O	-6.40	113.86	120.71
1	A	292	ALA	N-CA-C	6.34	118.71	109.07
1	A	97	SER	CA-C-N	6.34	132.23	121.14
1	A	97	SER	C-N-CA	6.34	132.23	121.14
1	A	45	VAL	CB-CA-C	-6.33	102.40	111.19
1	A	57	TYR	CA-C-O	-6.30	112.12	119.24
1	A	11	SER	CA-C-N	6.30	126.93	119.94
1	A	11	SER	C-N-CA	6.30	126.93	119.94
1	A	116	ILE	O-C-N	6.28	130.04	123.26
1	A	30	GLN	N-CA-C	6.24	118.60	111.11
1	A	209	ASP	CA-CB-CG	6.22	118.82	112.60
1	A	144	ALA	CA-C-O	-6.18	113.75	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	ARG	NE-CZ-NH1	6.15	127.65	121.50
1	A	57	TYR	N-CA-CB	6.14	118.76	110.59
1	A	72	SER	CA-C-O	6.13	125.26	119.13
1	A	44	LEU	CA-C-N	6.13	131.44	123.11
1	A	44	LEU	C-N-CA	6.13	131.44	123.11
1	A	267	HIS	CA-C-N	6.11	129.29	120.38
1	A	267	HIS	C-N-CA	6.11	129.29	120.38
1	A	304	ASN	CA-C-O	-6.07	111.83	120.51
1	A	453	ASP	CA-CB-CG	6.04	118.64	112.60
1	A	409	GLN	OE1-CD-NE2	-6.02	116.58	122.60
1	A	159	ARG	CB-CA-C	5.99	117.50	109.42
1	A	157	ASP	CA-CB-CG	-5.98	106.62	112.60
1	A	279	GLN	OE1-CD-NE2	5.97	128.57	122.60
1	A	305	VAL	N-CA-CB	5.96	117.79	111.00
1	A	312	ASP	CA-C-O	-5.94	114.40	121.11
1	A	115	GLN	OE1-CD-NE2	-5.92	116.68	122.60
1	A	440	ARG	NE-CZ-NH1	-5.92	115.58	121.50
1	A	468	HIS	CA-C-O	5.88	127.00	120.82
1	A	384	VAL	CB-CA-C	-5.88	104.46	111.81
1	A	495	THR	CA-C-O	-5.85	113.83	121.73
1	A	171	ARG	NH1-CZ-NH2	5.85	126.91	119.30
1	A	401	ASP	CA-CB-CG	-5.84	106.76	112.60
1	A	426	VAL	O-C-N	-5.83	115.28	122.57
1	A	415	ASP	CA-CB-CG	-5.82	106.78	112.60
1	A	212	ASN	CA-C-N	-5.79	114.90	122.37
1	A	212	ASN	C-N-CA	-5.79	114.90	122.37
1	A	159	ARG	CA-CB-CG	5.78	125.66	114.10
1	A	267	HIS	O-C-N	-5.78	117.51	123.29
1	A	187	THR	CA-C-N	5.76	128.00	120.28
1	A	187	THR	C-N-CA	5.76	128.00	120.28
1	A	246	ARG	CA-C-O	-5.75	114.45	120.55
1	A	224	LEU	CA-C-O	-5.75	114.46	120.55
1	A	372	GLY	O-C-N	-5.75	116.02	122.28
1	A	207	SER	CA-C-O	-5.74	115.03	121.81
1	A	147	GLU	CA-C-O	-5.71	115.35	122.03
1	A	244	ASN	CB-CG-ND2	-5.70	107.85	116.40
1	A	317	ILE	CA-C-N	5.68	128.21	120.54
1	A	317	ILE	C-N-CA	5.68	128.21	120.54
1	A	231	VAL	O-C-N	-5.67	116.35	121.91
1	A	126	LEU	CA-C-O	-5.62	113.75	120.10
1	A	302	LYS	N-CA-C	-5.60	102.72	109.72
1	A	414	THR	CA-CB-OG1	-5.59	101.22	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	MET	O-C-N	-5.59	115.13	122.39
1	A	396	PRO	N-CA-CB	5.58	108.52	103.33
1	A	374	PHE	CA-CB-CG	5.57	119.37	113.80
1	A	470	VAL	N-CA-CB	5.57	117.06	110.55
1	A	211	PRO	N-CA-CB	5.56	109.04	103.48
1	A	39	SER	CA-C-O	-5.55	111.84	119.05
1	A	397	CYS	CA-C-O	-5.55	114.08	120.24
1	A	161	GLU	CB-CG-CD	5.54	122.02	112.60
1	A	43	CYS	CB-CA-C	-5.53	98.16	109.94
1	A	237	LYS	O-C-N	-5.52	115.75	122.82
1	A	310	HIS	CA-C-O	-5.52	114.45	120.36
1	A	389	PHE	CA-CB-CG	-5.50	108.30	113.80
1	A	340	TYR	CA-C-O	5.50	127.54	121.11
1	A	287	LEU	O-C-N	5.46	130.14	123.21
1	A	76	SER	CA-C-O	5.41	128.24	120.51
1	A	149	HIS	CA-CB-CG	-5.38	108.42	113.80
1	A	484	GLN	OE1-CD-NE2	5.38	127.98	122.60
1	A	509	GLN	OE1-CD-NE2	5.31	127.91	122.60
1	A	329	ARG	CD-NE-CZ	5.31	131.83	124.40
1	A	57	TYR	N-CA-C	-5.25	107.43	113.88
1	A	207	SER	N-CA-C	-5.24	103.47	110.55
1	A	503	ARG	CD-NE-CZ	5.23	131.72	124.40
1	A	466	HIS	N-CA-CB	-5.22	102.23	110.06
1	A	488	GLN	CG-CD-NE2	-5.20	108.60	116.40
1	A	287	LEU	N-CA-CB	5.19	119.05	110.69
1	A	302	LYS	CA-C-N	5.19	124.69	119.19
1	A	302	LYS	C-N-CA	5.19	124.69	119.19
1	A	438	VAL	O-C-N	-5.18	116.83	121.91
1	A	207	SER	CA-C-N	-5.17	114.01	122.54
1	A	207	SER	C-N-CA	-5.17	114.01	122.54
1	A	506	SER	CA-C-O	5.15	127.04	121.06
1	A	146	ASP	CA-CB-CG	-5.15	107.45	112.60
1	A	488	GLN	CA-C-O	-5.15	115.27	121.34
1	A	178	MET	CB-CA-C	5.13	119.50	109.35
1	A	352	LEU	N-CA-C	5.12	116.86	111.28
1	A	326	ARG	CA-CB-CG	-5.09	103.93	114.10
1	A	44	LEU	N-CA-CB	5.08	118.67	110.65
1	A	427	ASN	CA-CB-CG	-5.08	107.52	112.60
1	A	189	ARG	CB-CG-CD	5.08	122.97	111.30
1	A	377	ALA	N-CA-C	5.07	117.25	110.35
1	A	284	ARG	CA-C-O	-5.07	113.15	119.28
1	A	29	GLY	CA-C-N	5.06	127.37	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	GLY	C-N-CA	5.06	127.37	120.54
1	A	43	CYS	N-CA-CB	-5.05	102.13	111.52
1	A	474	ARG	CB-CG-CD	5.02	122.85	111.30
1	A	448	ARG	O-C-N	5.01	127.86	122.15
1	A	68	THR	O-C-N	-5.01	117.37	123.13
1	A	277	ASP	CA-C-N	5.01	126.87	120.56
1	A	277	ASP	C-N-CA	5.01	126.87	120.56
1	A	294	VAL	N-CA-C	5.00	119.75	109.34
1	A	256	LEU	CA-C-N	5.00	127.29	120.54
1	A	256	LEU	C-N-CA	5.00	127.29	120.54

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	THR	Mainchain
1	A	164	ALA	Mainchain
1	A	167	GLN	Mainchain
1	A	219	GLU	Mainchain
1	A	221	PHE	Mainchain
1	A	280	GLU	Mainchain
1	A	289	ILE	Mainchain
1	A	304	ASN	Mainchain
1	A	367	LYS	Mainchain
1	A	387	ASN	Mainchain
1	A	39	SER	Mainchain
1	A	397	CYS	Mainchain
1	A	429	ARG	Mainchain
1	A	449	ASP	Mainchain
1	A	460	MET	Mainchain
1	A	475	GLN	Mainchain
1	A	492	LEU	Mainchain

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	4037	0	4033	176	0
2	A	1	0	0	0	0
3	A	2	0	0	0	0
4	A	31	0	11	5	0
5	A	43	0	0	3	0
All	All	4114	0	4044	180	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 22.

All (180) 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)
4:A:527:AGS:S1G	4:A:527:AGS:PG	1.49	1.47
1:A:169:ARG:HD3	1:A:197:GLY:HA3	1.52	0.90
1:A:96:ASN:ND2	1:A:98:THR:HG22	1.87	0.90
1:A:366:HIS:HD2	1:A:490:SER:OG	1.55	0.88
1:A:514:ARG:HG3	1:A:516:VAL:HG22	1.58	0.86
1:A:228:MET:O	1:A:232:GLN:HG2	1.78	0.84
1:A:14:LYS:HE3	1:A:31:GLU:OE2	1.78	0.83
1:A:434:TYR:OH	1:A:452:HIS:HD2	1.61	0.82
1:A:112:ARG:HA	1:A:138:TRP:CD1	2.15	0.81
1:A:349:ARG:NH1	1:A:369:ASN:OD1	2.13	0.81
1:A:387:ASN:OD1	1:A:392:GLY:HA2	1.81	0.80
1:A:310:HIS:HE1	1:A:323:GLU:OE1	1.65	0.80
1:A:76:SER:O	1:A:77:LEU:HB2	1.80	0.80
4:A:527:AGS:S1G	4:A:527:AGS:O3G	2.42	0.77
4:A:527:AGS:S1G	4:A:527:AGS:O2G	2.40	0.77
1:A:118:LEU:HD21	1:A:120:TYR:CE1	2.19	0.76
1:A:434:TYR:OH	1:A:452:HIS:CD2	2.37	0.76
1:A:183:THR:HG22	1:A:183:THR:O	1.87	0.74
1:A:382:ARG:O	1:A:386:LEU:HD22	1.86	0.74
4:A:527:AGS:S1G	4:A:527:AGS:O3B	2.47	0.73
1:A:83:ASP:OD2	5:A:547:HOH:O	2.08	0.72
1:A:73:PRO:HD2	1:A:74:LEU:HD22	1.71	0.72
1:A:160:PRO:HG2	1:A:161:GLU:OE1	1.90	0.71
1:A:366:HIS:CD2	1:A:490:SER:OG	2.45	0.68
1:A:267:HIS:HD2	1:A:269:GLY:H	1.43	0.67
1:A:124:GLU:OE1	1:A:124:GLU:N	2.17	0.66
1:A:209:ASP:OD1	1:A:382:ARG:HD3	1.94	0.66
1:A:220:LYS:O	1:A:221:PHE:HB2	1.94	0.66
1:A:94:CYS:HA	1:A:120:TYR:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:ARG:HB3	1:A:500:PRO:HD3	1.78	0.65
1:A:126:LEU:HD23	1:A:127:MET:HE2	1.77	0.65
1:A:5:GLU:HG3	1:A:62:LEU:O	1.96	0.65
1:A:118:LEU:O	1:A:118:LEU:HD23	1.97	0.65
1:A:1:MET:HA	1:A:114:GLY:O	1.98	0.64
1:A:464:LYS:HD3	1:A:468:HIS:CE1	2.33	0.64
1:A:46:VAL:HG21	1:A:189:ARG:HD2	1.78	0.64
1:A:75:ILE:H	1:A:75:ILE:HD12	1.62	0.64
1:A:2:ALA:O	1:A:65:ASN:HA	1.97	0.63
1:A:95:LEU:HD23	1:A:121:ILE:HD12	1.78	0.63
1:A:310:HIS:HD2	5:A:540:HOH:O	1.80	0.63
1:A:30:GLN:O	1:A:34:ILE:HG13	1.98	0.63
1:A:341:ASP:OD1	1:A:343:ALA:N	2.31	0.63
1:A:267:HIS:CD2	1:A:269:GLY:H	2.17	0.62
1:A:160:PRO:CD	1:A:161:GLU:OE1	2.47	0.62
1:A:202:LEU:HD21	1:A:204:GLN:HB2	1.80	0.62
1:A:199:ASN:O	1:A:200:ASP:C	2.38	0.62
1:A:75:ILE:O	1:A:76:SER:CB	2.48	0.62
1:A:109:THR:OG1	1:A:112:ARG:NH2	2.33	0.62
1:A:169:ARG:CD	1:A:197:GLY:HA3	2.27	0.61
1:A:118:LEU:HD23	1:A:118:LEU:C	2.25	0.60
1:A:101:ARG:O	1:A:105:LEU:HG	2.01	0.60
1:A:33:ILE:HD12	1:A:45:VAL:HG22	1.83	0.60
1:A:160:PRO:CG	1:A:161:GLU:OE1	2.51	0.59
1:A:214:ARG:HB2	1:A:399:ASN:OD1	2.03	0.58
1:A:345:MET:O	1:A:349:ARG:HG3	2.03	0.58
1:A:1:MET:O	1:A:2:ALA:HB3	2.01	0.58
1:A:160:PRO:HD2	1:A:161:GLU:OE1	2.04	0.58
1:A:193:VAL:HG22	1:A:198:LEU:HD12	1.86	0.57
1:A:109:THR:O	1:A:109:THR:HG22	2.02	0.57
1:A:303:PRO:HA	1:A:329:ARG:HB2	1.87	0.57
1:A:127:MET:HE3	1:A:165:LEU:HD23	1.85	0.57
1:A:202:LEU:C	1:A:202:LEU:HD23	2.30	0.56
1:A:174:THR:O	1:A:176:PRO:HD3	2.05	0.56
1:A:127:MET:CE	1:A:165:LEU:HD23	2.36	0.56
1:A:53:LYS:NZ	1:A:182:ALA:HB2	2.20	0.56
1:A:96:ASN:HD21	1:A:99:GLN:HG3	1.71	0.56
1:A:109:THR:O	1:A:109:THR:CG2	2.53	0.56
1:A:161:GLU:OE1	1:A:161:GLU:N	2.32	0.56
1:A:220:LYS:HG2	1:A:223:PRO:HB3	1.87	0.55
1:A:1:MET:CA	1:A:114:GLY:O	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ILE:O	1:A:37:VAL:HG23	2.07	0.55
1:A:96:ASN:C	1:A:96:ASN:HD22	2.15	0.55
1:A:345:MET:HE1	1:A:368:LEU:HG	1.89	0.54
1:A:47:MET:HB2	1:A:53:LYS:HG3	1.89	0.54
1:A:352:LEU:HD12	1:A:352:LEU:O	2.06	0.54
1:A:32:GLU:O	1:A:36:THR:OG1	2.16	0.54
1:A:75:ILE:O	1:A:76:SER:HB2	2.07	0.54
1:A:413:SER:O	1:A:417:GLN:HG3	2.08	0.54
1:A:53:LYS:HB2	4:A:527:AGS:O2B	2.07	0.54
1:A:308:VAL:HG23	1:A:327:ALA:HB2	1.90	0.54
1:A:20:THR:HG21	1:A:62:LEU:HD11	1.90	0.53
1:A:208:PHE:N	1:A:391:GLU:OE1	2.38	0.53
1:A:130:ASN:O	1:A:134:HIS:HD2	1.92	0.53
1:A:223:PRO:HB2	1:A:311:PHE:CZ	2.44	0.53
1:A:234:GLN:HG3	1:A:307:PHE:CD1	2.44	0.53
1:A:169:ARG:HD3	1:A:197:GLY:CA	2.34	0.52
1:A:352:LEU:HD11	1:A:361:GLN:HG3	1.91	0.52
1:A:175:LEU:HD12	1:A:176:PRO:HD2	1.92	0.52
1:A:12:GLY:O	1:A:16:VAL:HG23	2.11	0.51
1:A:27:ARG:O	1:A:28:PRO:C	2.53	0.51
1:A:161:GLU:H	1:A:161:GLU:CD	2.18	0.51
1:A:2:ALA:HB1	1:A:66:GLY:H	1.76	0.51
1:A:183:THR:HG21	1:A:318:GLU:HB3	1.93	0.50
1:A:17:LEU:HD13	1:A:26:PHE:CE1	2.46	0.50
1:A:96:ASN:HD21	1:A:98:THR:HG22	1.74	0.50
1:A:1:MET:SD	1:A:115:GLN:OE1	2.70	0.50
1:A:229:ARG:O	1:A:229:ARG:HG2	2.12	0.50
1:A:246:ARG:NH1	1:A:269:GLY:HA3	2.26	0.49
1:A:266:TYR:HD2	1:A:278:VAL:HG11	1.76	0.49
1:A:110:GLY:HA3	1:A:116:ILE:HD12	1.95	0.49
1:A:47:MET:O	1:A:182:ALA:HA	2.13	0.49
1:A:378:GLN:HE22	1:A:513:PRO:HA	1.76	0.49
1:A:313:ILE:HG13	1:A:338:LEU:HD11	1.95	0.49
1:A:310:HIS:CE1	1:A:323:GLU:OE1	2.55	0.48
1:A:435:VAL:HG21	1:A:492:LEU:HD12	1.95	0.48
1:A:59:ILE:N	1:A:60:PRO:HD2	2.28	0.48
1:A:222:LYS:N	1:A:223:PRO:CD	2.76	0.48
1:A:468:HIS:O	1:A:472:VAL:HG23	2.14	0.48
1:A:302:LYS:HE2	1:A:304:ASN:OD1	2.13	0.47
1:A:4:ALA:N	1:A:65:ASN:OD1	2.32	0.47
1:A:156:HIS:H	1:A:156:HIS:HD1	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:ARG:O	1:A:351:CYS:C	2.56	0.47
1:A:14:LYS:HG2	1:A:26:PHE:CE2	2.49	0.47
1:A:153:GLN:HG3	1:A:359:GLN:HE22	1.79	0.47
1:A:275:ARG:O	1:A:278:VAL:HB	2.14	0.47
1:A:3:GLN:HA	1:A:65:ASN:OD1	2.14	0.47
1:A:332:LEU:HB3	1:A:333:PRO:CD	2.45	0.47
1:A:234:GLN:HG3	1:A:307:PHE:CE1	2.50	0.46
1:A:415:ASP:OD2	1:A:468:HIS:HE1	1.98	0.46
1:A:117:ARG:HG3	1:A:117:ARG:HH11	1.81	0.46
1:A:146:ASP:O	1:A:147:GLU:C	2.59	0.46
1:A:78:MET:O	1:A:82:VAL:HG23	2.16	0.46
1:A:143:LEU:HD13	1:A:168:LEU:HD13	1.97	0.45
1:A:434:TYR:CZ	1:A:452:HIS:HD2	2.34	0.45
1:A:20:THR:HG21	1:A:62:LEU:CD1	2.47	0.45
1:A:162:TYR:O	1:A:163:ALA:C	2.59	0.45
1:A:279:GLN:HG3	1:A:300:ILE:HB	1.98	0.45
1:A:467:GLU:OE2	1:A:515:ILE:HA	2.17	0.44
1:A:496:GLU:OE1	1:A:499:ARG:NH1	2.35	0.44
1:A:251:ASP:O	1:A:255:ARG:HG3	2.17	0.44
1:A:263:ALA:HA	1:A:289:ILE:O	2.18	0.44
1:A:184:ALA:HB1	1:A:188:THR:CG2	2.47	0.44
1:A:156:HIS:NE2	1:A:322:GLN:NE2	2.65	0.44
1:A:345:MET:HE2	1:A:372:GLY:HA3	1.98	0.44
1:A:46:VAL:HB	1:A:205:ILE:HA	2.00	0.43
1:A:46:VAL:HG21	1:A:189:ARG:CD	2.47	0.43
1:A:1:MET:HB3	1:A:3:GLN:HE21	1.84	0.43
1:A:78:MET:SD	1:A:94:CYS:HB2	2.58	0.43
1:A:84:GLN:O	1:A:87:ALA:HB3	2.19	0.43
1:A:254:ALA:O	1:A:257:GLN:HB2	2.18	0.43
1:A:307:PHE:CD2	1:A:309:VAL:HG23	2.54	0.43
1:A:25:GLN:HG2	1:A:26:PHE:N	2.34	0.43
1:A:353:GLU:OE1	1:A:365:ARG:NE	2.47	0.43
1:A:492:LEU:O	1:A:493:GLN:HG2	2.19	0.43
1:A:313:ILE:HA	1:A:314:PRO:HD3	1.75	0.43
1:A:223:PRO:HB2	1:A:311:PHE:HZ	1.84	0.42
1:A:441:GLY:HA2	1:A:458:TYR:CE1	2.54	0.42
1:A:332:LEU:HB3	1:A:333:PRO:HD2	2.00	0.42
1:A:379:THR:HG22	1:A:380:CYS:N	2.33	0.42
1:A:104:GLN:O	1:A:108:MET:HG2	2.19	0.42
1:A:347:TRP:O	1:A:348:LEU:C	2.62	0.42
1:A:29:GLY:CA	1:A:204:GLN:OE1	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:GLU:OE2	1:A:117:ARG:NH2	2.53	0.42
1:A:354:GLU:O	1:A:354:GLU:HG3	2.19	0.42
1:A:503:ARG:HB3	1:A:505:GLU:HG3	2.01	0.42
1:A:43:CYS:O	1:A:178:MET:HA	2.19	0.42
1:A:426:VAL:O	1:A:427:ASN:HB2	2.20	0.42
1:A:478:HIS:HD2	5:A:533:HOH:O	2.01	0.42
1:A:73:PRO:CD	1:A:74:LEU:HD22	2.46	0.41
1:A:446:ARG:O	1:A:447:ILE:C	2.62	0.41
1:A:477:ILE:HA	1:A:482:VAL:O	2.20	0.41
1:A:14:LYS:O	1:A:15:GLN:C	2.63	0.41
1:A:355:LYS:HB3	1:A:356:PRO:HD2	2.02	0.41
1:A:49:THR:HG23	1:A:321:TYR:CE2	2.55	0.41
1:A:127:MET:HE3	1:A:165:LEU:HA	2.02	0.41
1:A:218:MET:HE3	1:A:218:MET:HB2	1.77	0.41
1:A:415:ASP:OD2	1:A:468:HIS:CE1	2.74	0.41
1:A:123:PRO:HG3	1:A:162:TYR:CE2	2.55	0.41
1:A:352:LEU:O	1:A:361:GLN:NE2	2.54	0.41
1:A:489:HIS:O	1:A:490:SER:HB2	2.20	0.41
1:A:305:VAL:HB	1:A:327:ALA:HA	2.03	0.41
1:A:18:GLN:HA	1:A:23:TYR:O	2.21	0.40
1:A:92:ALA:HA	1:A:118:LEU:O	2.21	0.40
1:A:109:THR:HA	1:A:112:ARG:NH2	2.36	0.40
1:A:202:LEU:CD2	1:A:204:GLN:HB2	2.50	0.40
1:A:59:ILE:N	1:A:60:PRO:CD	2.84	0.40
1:A:162:TYR:O	1:A:165:LEU:HB2	2.21	0.40
1:A:184:ALA:O	1:A:189:ARG:NH1	2.51	0.40
1:A:70:VAL:O	1:A:120:TYR:HA	2.21	0.40
1:A:61:ALA:HB2	1:A:68:THR:HG21	2.04	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	508/523 (97%)	476 (94%)	28 (6%)	4 (1%)	16	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	SER
1	A	221	PHE
1	A	77	LEU
1	A	28	PRO

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	432/439 (98%)	401 (93%)	31 (7%)	13	28

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	28	PRO
1	A	43	CYS
1	A	49	THR
1	A	54	SER
1	A	72	SER
1	A	74	LEU
1	A	76	SER
1	A	78	MET
1	A	96	ASN
1	A	97	SER
1	A	98	THR
1	A	116	ILE
1	A	124	GLU
1	A	128	LEU
1	A	153	GLN
1	A	161	GLU

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Mol	Chain	Res	Type
1	A	169	ARG
1	A	258	SER
1	A	259	LYS
1	A	273	ASN
1	A	357	GLN
1	A	364	GLU
1	A	386	LEU
1	A	395	GLU
1	A	417	GLN
1	A	437	GLU
1	A	448	ARG
1	A	474	ARG
1	A	506	SER
1	A	516	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	15	GLN
1	A	96	ASN
1	A	115	GLN
1	A	134	HIS
1	A	153	GLN
1	A	232	GLN
1	A	234	GLN
1	A	257	GLN
1	A	267	HIS
1	A	310	HIS
1	A	322	GLN
1	A	357	GLN
1	A	359	GLN
1	A	366	HIS
1	A	378	GLN
1	A	394	GLN
1	A	427	ASN
1	A	452	HIS
1	A	468	HIS
1	A	478	HIS
1	A	488	GLN
1	A	509	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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
4	AGS	A	527	3	32,33,33	3.67	7 (21%)	45,52,52	2.00	10 (22%)

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
4	AGS	A	527	3	1/1/7/7	4/21/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	527	AGS	PG-S1G	-19.00	1.49	1.90
4	A	527	AGS	C5-N7	-4.08	1.31	1.39
4	A	527	AGS	PA-O3A	3.29	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	527	AGS	C8-N7	-2.45	1.27	1.31
4	A	527	AGS	C2-N1	2.44	1.38	1.33
4	A	527	AGS	PB-O3A	2.14	1.61	1.59
4	A	527	AGS	PG-O2G	-2.02	1.48	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	527	AGS	O2'-C2'-C3'	5.95	130.90	111.82
4	A	527	AGS	O2B-PB-O3B	5.17	121.24	107.27
4	A	527	AGS	O2G-PG-O3B	4.11	118.36	104.64
4	A	527	AGS	O4'-C1'-N9	3.76	115.32	108.09
4	A	527	AGS	O2'-C2'-C1'	3.69	122.82	110.10
4	A	527	AGS	PB-O3B-PG	3.67	146.61	133.17
4	A	527	AGS	C4-N9-C8	-3.48	102.09	105.74
4	A	527	AGS	O3'-C3'-C4'	-2.68	103.37	111.08
4	A	527	AGS	O5'-C5'-C4'	2.15	116.33	108.99
4	A	527	AGS	C5-C6-N6	2.15	128.62	123.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	527	AGS	C2'

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	527	AGS	C3'-C4'-C5'-O5'
4	A	527	AGS	PB-O3A-PA-O1A
4	A	527	AGS	O4'-C4'-C5'-O5'
4	A	527	AGS	PB-O3A-PA-O2A

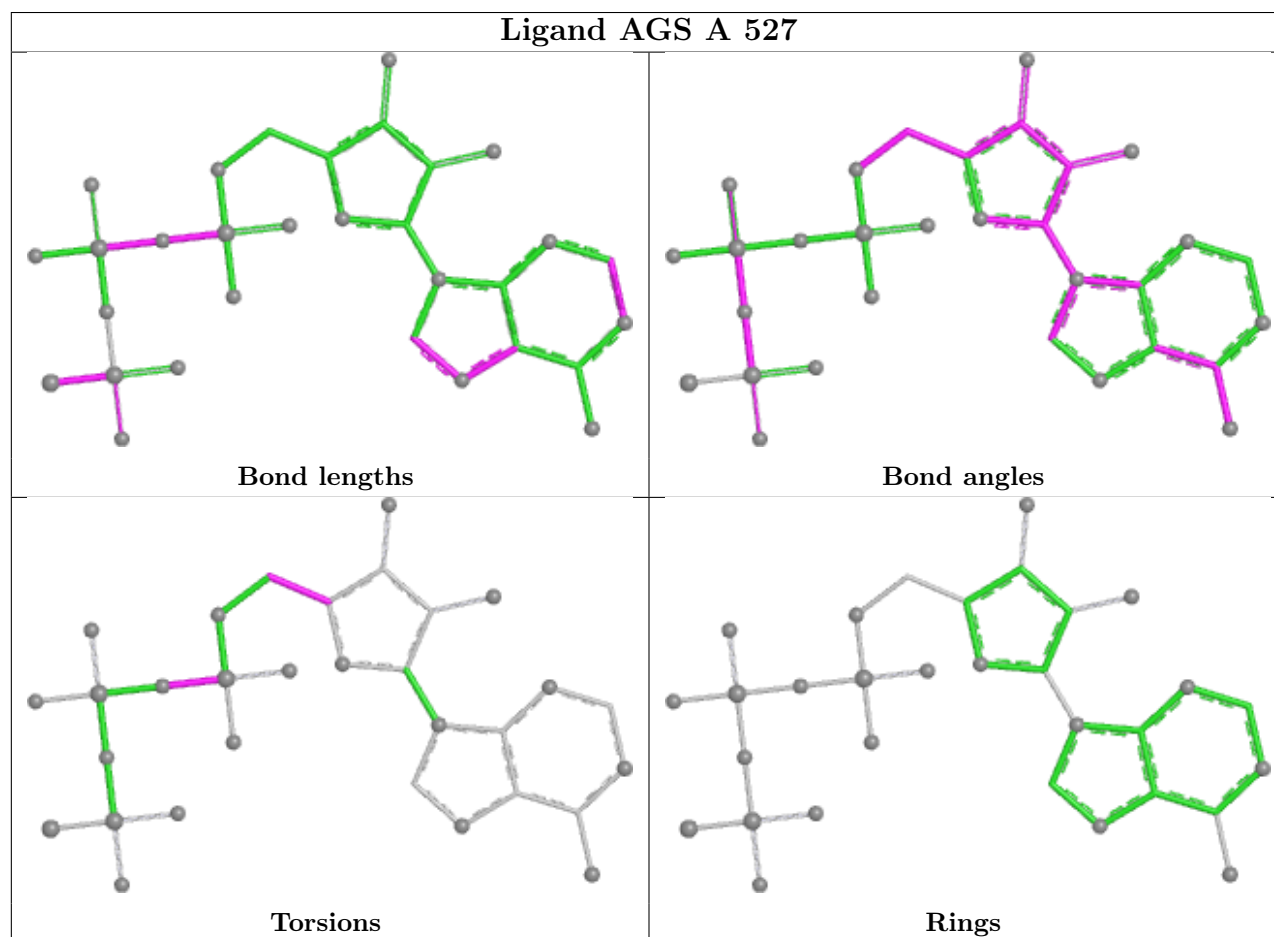
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	527	AGS	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	512/523 (97%)	-0.05	16 (3%) 51 47	27, 50, 95, 128	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	300	ILE	4.1
1	A	2	ALA	3.1
1	A	22	GLY	2.9
1	A	76	SER	2.9
1	A	295	ALA	2.8
1	A	77	LEU	2.8
1	A	1	MET	2.7
1	A	25	GLN	2.7
1	A	23	TYR	2.7
1	A	301	ASN	2.5
1	A	75	ILE	2.5
1	A	88	ASN	2.2
1	A	443	ASN	2.2
1	A	129	ASP	2.2
1	A	82	VAL	2.2
1	A	445	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](#)

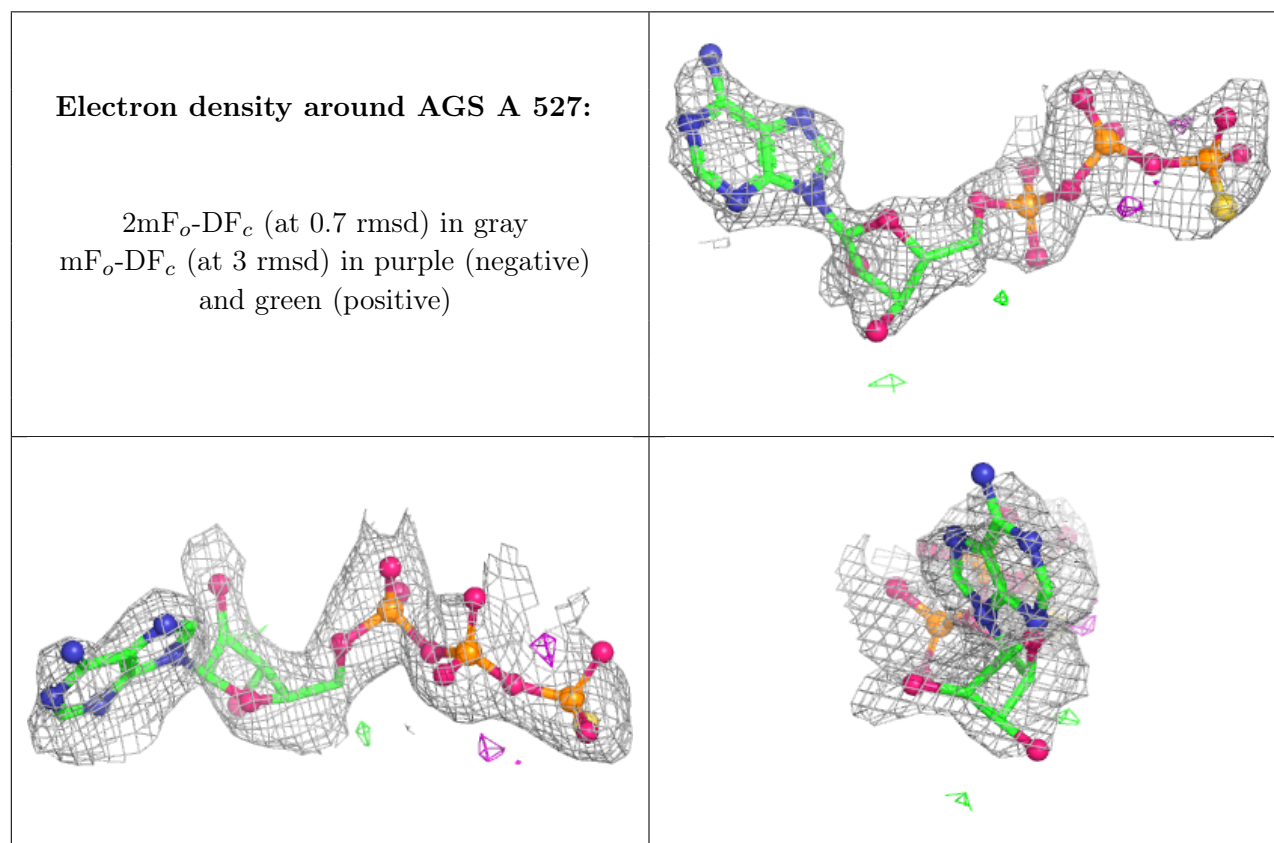
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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($\text{\AA}^2$)	Q<0.9
4	AGS	A	527	31/31	0.90	0.11	51,66,94,98	0
3	MN	A	526	1/1	0.96	0.06	69,69,69,69	0
3	MN	A	525	1/1	0.97	0.04	83,83,83,83	0
2	ZN	A	524	1/1	0.99	0.03	32,32,32,32	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.