



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:26 PM GMT

PDB ID : 4RXO
Title : The structure of GTP-bound SAMHD1
Authors : Zhu, C.F.; Wei, W.; Peng, X.; Dong, Y.H.; Gong, Y.; Yu, X.F.
Deposited on : 2014-12-11
Resolution : 2.60 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

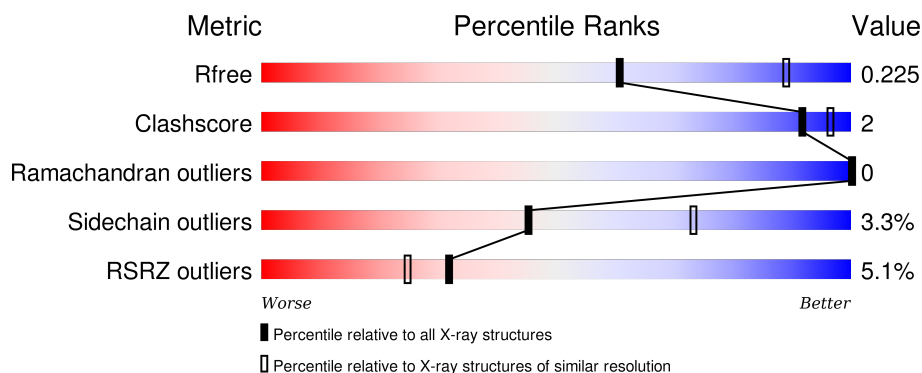
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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. 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	539	<div> <div>5%</div> <div>77%</div> <div>7%</div> <div>15%</div> </div>
1	B	539	<div> <div>2%</div> <div>76%</div> <div>• •</div> <div>20%</div> </div>
1	C	539	<div> <div>4%</div> <div>77%</div> <div>•</div> <div>19%</div> </div>
1	D	539	<div> <div>6%</div> <div>77%</div> <div>5% •</div> <div>18%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14977 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 Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	0	0
			3737	2395	649	674	19			
1	B	433	Total	C	N	O	S	0	0	0
			3555	2282	615	641	17			
1	C	434	Total	C	N	O	S	0	0	0
			3559	2282	616	643	18			
1	D	444	Total	C	N	O	S	0	0	0
			3642	2335	633	656	18			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	MET	-	EXPRESSION TAG	UNP Q9Y3Z3
A	89	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
A	90	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
A	91	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
A	92	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
A	93	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
A	94	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
A	95	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
A	96	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
A	97	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
A	98	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
A	99	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
A	100	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
A	101	GLU	-	EXPRESSION TAG	UNP Q9Y3Z3
A	102	ASN	-	EXPRESSION TAG	UNP Q9Y3Z3
A	103	LEU	-	EXPRESSION TAG	UNP Q9Y3Z3
A	104	TYR	-	EXPRESSION TAG	UNP Q9Y3Z3
A	105	PHE	-	EXPRESSION TAG	UNP Q9Y3Z3
A	106	GLN	-	EXPRESSION TAG	UNP Q9Y3Z3
A	107	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
A	108	SER	-	EXPRESSION TAG	UNP Q9Y3Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	266	TYR	CYS	CONFLICT	UNP Q9Y3Z3
B	88	MET	-	EXPRESSION TAG	UNP Q9Y3Z3
B	89	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
B	90	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
B	91	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
B	92	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
B	93	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
B	94	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
B	95	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
B	96	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
B	97	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
B	98	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
B	99	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
B	100	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
B	101	GLU	-	EXPRESSION TAG	UNP Q9Y3Z3
B	102	ASN	-	EXPRESSION TAG	UNP Q9Y3Z3
B	103	LEU	-	EXPRESSION TAG	UNP Q9Y3Z3
B	104	TYR	-	EXPRESSION TAG	UNP Q9Y3Z3
B	105	PHE	-	EXPRESSION TAG	UNP Q9Y3Z3
B	106	GLN	-	EXPRESSION TAG	UNP Q9Y3Z3
B	107	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
B	108	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
B	266	TYR	CYS	CONFLICT	UNP Q9Y3Z3
C	88	MET	-	EXPRESSION TAG	UNP Q9Y3Z3
C	89	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
C	90	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
C	91	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
C	92	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
C	93	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
C	94	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
C	95	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
C	96	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
C	97	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
C	98	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
C	99	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
C	100	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
C	101	GLU	-	EXPRESSION TAG	UNP Q9Y3Z3
C	102	ASN	-	EXPRESSION TAG	UNP Q9Y3Z3
C	103	LEU	-	EXPRESSION TAG	UNP Q9Y3Z3
C	104	TYR	-	EXPRESSION TAG	UNP Q9Y3Z3
C	105	PHE	-	EXPRESSION TAG	UNP Q9Y3Z3
C	106	GLN	-	EXPRESSION TAG	UNP Q9Y3Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	107	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
C	108	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
C	266	TYR	CYS	CONFLICT	UNP Q9Y3Z3
D	88	MET	-	EXPRESSION TAG	UNP Q9Y3Z3
D	89	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
D	90	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
D	91	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
D	92	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
D	93	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
D	94	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
D	95	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
D	96	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
D	97	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
D	98	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
D	99	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
D	100	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
D	101	GLU	-	EXPRESSION TAG	UNP Q9Y3Z3
D	102	ASN	-	EXPRESSION TAG	UNP Q9Y3Z3
D	103	LEU	-	EXPRESSION TAG	UNP Q9Y3Z3
D	104	TYR	-	EXPRESSION TAG	UNP Q9Y3Z3
D	105	PHE	-	EXPRESSION TAG	UNP Q9Y3Z3
D	106	GLN	-	EXPRESSION TAG	UNP Q9Y3Z3
D	107	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
D	108	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
D	266	TYR	CYS	CONFLICT	UNP Q9Y3Z3

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

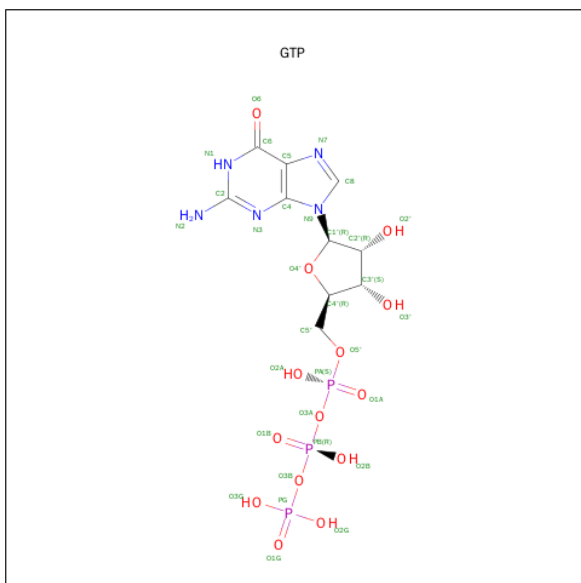
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

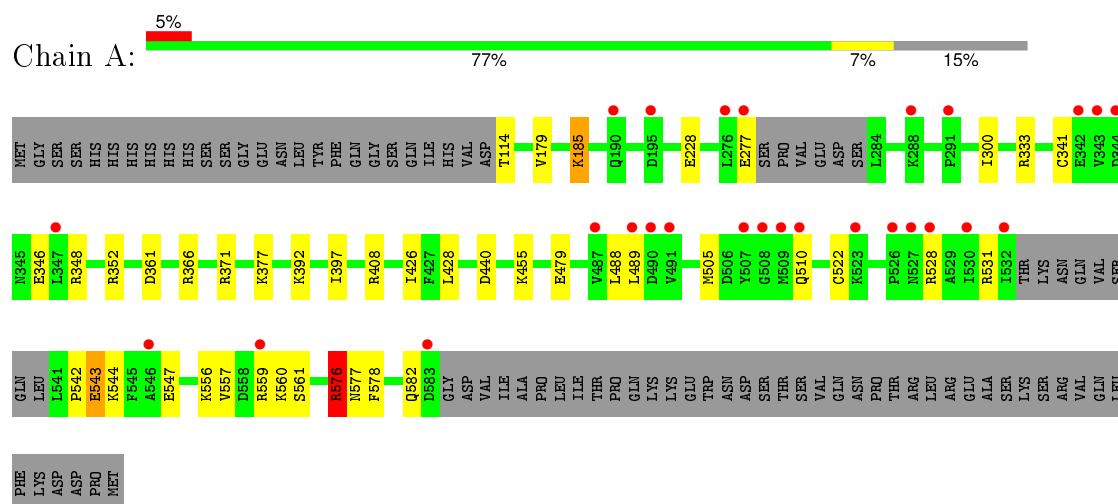
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	108	Total	O	0	0
			108	108		
5	B	89	Total	O	0	0
			89	89		
5	C	76	Total	O	0	0
			76	76		
5	D	59	Total	O	0	0
			59	59		

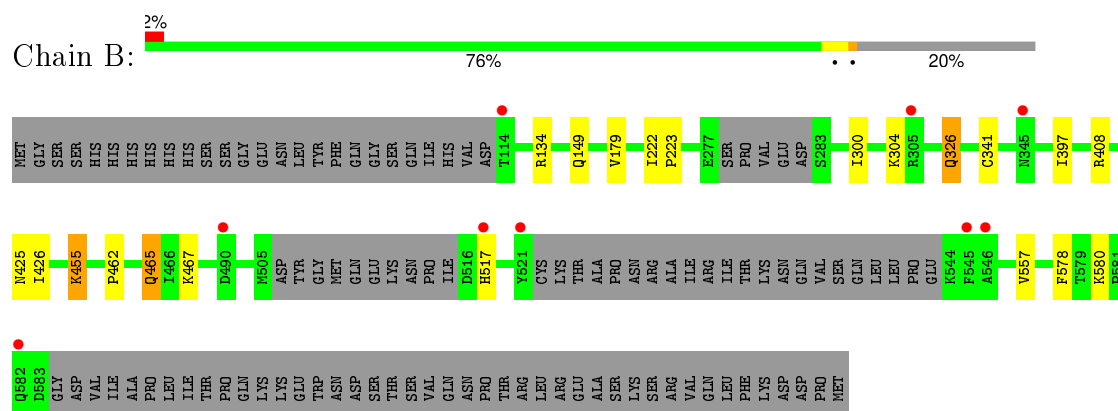
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

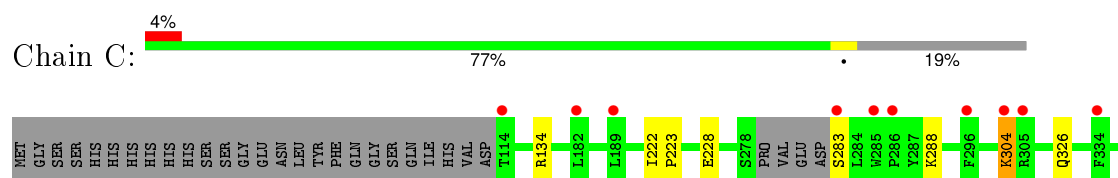
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

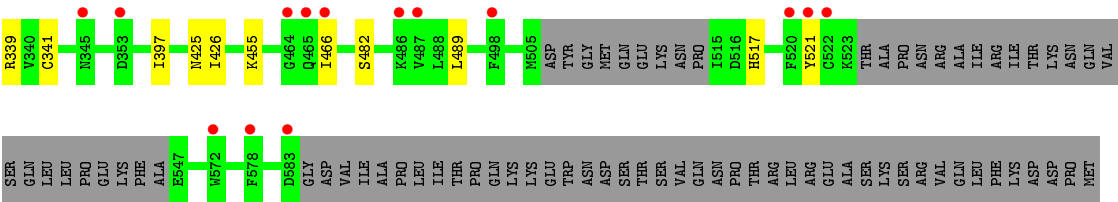


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

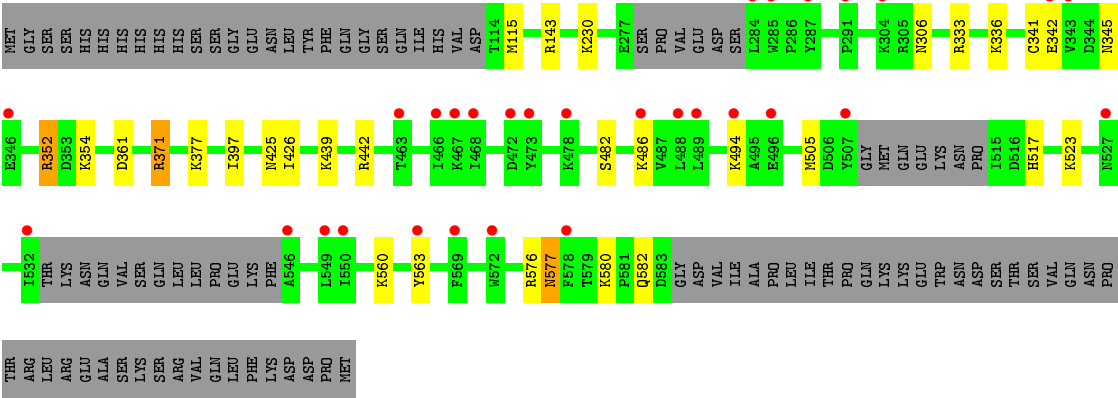
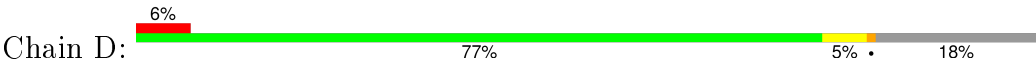


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





● Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.22Å 183.19Å 81.28Å 90.00° 100.62° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 48.74 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.6 (50.00-2.60) 96.7 (48.74-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.183 , 0.222 0.188 , 0.225	Depositor DCC
R_{free} test set	3257 reflections (5.21%)	DCC
Wilson B-factor (Å ²)	55.3	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.8	EDS
Estimated twinning fraction	0.021 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 65781 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14977	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GTP, ZN, PO4

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	0.46	0/3826	0.67	1/5161 (0.0%)
1	B	0.46	0/3639	0.65	0/4906
1	C	0.45	0/3642	0.64	0/4910
1	D	0.44	0/3727	0.64	0/5027
All	All	0.45	0/14834	0.65	1/20004 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	576	ARG	CG-CD-NE	-5.39	100.48	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3737	0	3703	22	0
1	B	3555	0	3520	14	0
1	C	3559	0	3527	8	0
1	D	3642	0	3613	21	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	B	64	0	24	0	0
4	C	32	0	12	0	0
4	D	32	0	12	0	0
5	A	108	0	0	2	0
5	B	89	0	0	2	0
5	C	76	0	0	0	0
5	D	59	0	0	2	0
All	All	14977	0	14411	60	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 2.

All (60) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:VAL:HG22	1:A:300:ILE:HD13	1.76	0.67
1:D:439:LYS:HE3	1:D:442:ARG:HH21	1.61	0.66
1:B:179:VAL:HG22	1:B:300:ILE:HD13	1.77	0.64
1:D:371:ARG:HH11	1:D:505:MET:HE2	1.62	0.64
1:D:371:ARG:NH1	1:D:505:MET:HE2	2.11	0.64
1:A:576:ARG:HG2	1:A:578:PHE:CE2	2.34	0.62
1:D:371:ARG:NH1	1:D:505:MET:CE	2.63	0.61
1:D:306:ASN:HB3	1:D:517:HIS:HB3	1.83	0.60
1:A:576:ARG:HG2	1:A:578:PHE:CZ	2.37	0.60
1:A:366:ARG:HH12	1:A:505:MET:HE1	1.67	0.60
1:D:560:LYS:HD2	1:D:560:LYS:N	2.19	0.57
1:B:179:VAL:CG2	1:B:300:ILE:HD13	2.34	0.57
1:A:179:VAL:CG2	1:A:300:ILE:HD13	2.34	0.57
1:A:505:MET:HB2	1:A:547:GLU:OE1	2.05	0.56
1:C:304:LYS:HE2	1:C:304:LYS:HA	1.87	0.55
1:A:346:GLU:OE1	1:A:348:ARG:NH2	2.39	0.55
1:A:366:ARG:NH1	1:A:505:MET:HE1	2.22	0.55
1:A:542:PRO:HB3	1:A:543:GLU:OE1	2.08	0.54
1:B:326:GLN:HB2	5:B:973:HOH:O	2.09	0.51
1:A:333:ARG:NH2	1:D:361:ASP:OD1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:560:LYS:HD2	1:D:560:LYS:H	1.76	0.50
1:D:371:ARG:HH11	1:D:505:MET:CE	2.23	0.49
1:A:582:GLN:NE2	5:A:851:HOH:O	2.35	0.47
1:D:560:LYS:H	1:D:560:LYS:CD	2.28	0.47
1:A:455:LYS:HG2	1:A:557:VAL:HG12	1.95	0.47
1:D:352:ARG:HG2	1:D:354:LYS:HG2	1.96	0.47
1:B:465:GLN:HA	1:B:465:GLN:OE1	2.15	0.46
1:A:543:GLU:CD	1:A:543:GLU:N	2.70	0.46
1:C:339:ARG:HD3	1:C:521:TYR:CZ	2.50	0.45
1:A:556:LYS:NZ	5:A:850:HOH:O	2.43	0.45
1:B:397:ILE:HG21	1:B:426:ILE:HD11	1.99	0.45
1:B:455:LYS:HD3	1:B:557:VAL:HG13	1.99	0.44
1:D:143:ARG:HD3	5:D:803:HOH:O	2.17	0.44
1:C:397:ILE:HG21	1:C:426:ILE:HD11	2.00	0.43
1:B:557:VAL:HG12	1:B:557:VAL:O	2.18	0.43
1:C:228:GLU:CD	1:C:228:GLU:H	2.22	0.43
1:C:455:LYS:HD3	1:C:455:LYS:HA	1.72	0.43
1:D:560:LYS:N	1:D:560:LYS:CD	2.82	0.43
1:D:580:LYS:HB2	1:D:580:LYS:HE2	1.88	0.42
1:B:179:VAL:HG22	1:B:300:ILE:CD1	2.48	0.42
1:B:326:GLN:NE2	1:C:326:GLN:HG2	2.35	0.42
1:C:425:ASN:OD1	1:D:425:ASN:OD1	2.38	0.42
1:D:115:MET:HA	5:D:833:HOH:O	2.20	0.42
1:D:397:ILE:HG21	1:D:426:ILE:HD11	2.01	0.42
1:A:185:LYS:HA	1:A:185:LYS:HD2	1.86	0.42
1:A:560:LYS:HG3	1:A:561:SER:N	2.35	0.41
1:B:462:PRO:HA	1:B:578:PHE:CD1	2.55	0.41
1:B:222:ILE:HB	1:B:223:PRO:HD3	2.02	0.41
1:D:576:ARG:O	1:D:577:ASN:OD1	2.38	0.41
1:A:479:GLU:OE1	1:A:576:ARG:NH1	2.53	0.41
1:A:361:ASP:OD1	1:D:333:ARG:NH2	2.52	0.41
1:B:467:LYS:O	1:B:467:LYS:HG3	2.20	0.41
1:C:222:ILE:HB	1:C:223:PRO:HD3	2.02	0.41
1:A:428:LEU:HD13	1:B:425:ASN:HB2	2.02	0.41
1:D:352:ARG:CZ	1:D:523:LYS:HD3	2.51	0.41
1:A:377:LYS:HB2	1:A:377:LYS:HE3	1.81	0.41
1:D:439:LYS:HE3	1:D:442:ARG:NH2	2.31	0.41
1:A:392:LYS:HD3	1:A:440:ASP:HB3	2.03	0.40
1:B:408:ARG:NH1	5:B:967:HOH:O	2.54	0.40
1:A:397:ILE:HG21	1:A:426:ILE:HD11	2.02	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	450/539 (84%)	445 (99%)	5 (1%)	0	100	100
1	B	425/539 (79%)	417 (98%)	8 (2%)	0	100	100
1	C	426/539 (79%)	419 (98%)	7 (2%)	0	100	100
1	D	436/539 (81%)	429 (98%)	7 (2%)	0	100	100
All	All	1737/2156 (81%)	1710 (98%)	27 (2%)	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	403/481 (84%)	384 (95%)	19 (5%)	32	59
1	B	384/481 (80%)	375 (98%)	9 (2%)	58	83
1	C	386/481 (80%)	377 (98%)	9 (2%)	58	83
1	D	393/481 (82%)	379 (96%)	14 (4%)	42	71
All	All	1566/1924 (81%)	1515 (97%)	51 (3%)	45	73

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	THR
1	A	185	LYS

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Mol	Chain	Res	Type
1	A	228	GLU
1	A	277	GLU
1	A	341	CYS
1	A	352	ARG
1	A	371	ARG
1	A	408	ARG
1	A	488	LEU
1	A	489	LEU
1	A	510	GLN
1	A	522	CYS
1	A	528	ARG
1	A	531	ARG
1	A	543	GLU
1	A	544	LYS
1	A	559	ARG
1	A	576	ARG
1	A	577	ASN
1	B	134	ARG
1	B	149	GLN
1	B	304	LYS
1	B	326	GLN
1	B	341	CYS
1	B	455	LYS
1	B	465	GLN
1	B	517	HIS
1	B	580	LYS
1	C	134	ARG
1	C	283	SER
1	C	288	LYS
1	C	304	LYS
1	C	341	CYS
1	C	466	ILE
1	C	482	SER
1	C	489	LEU
1	C	517	HIS
1	D	230	LYS
1	D	336	LYS
1	D	341	CYS
1	D	342	GLU
1	D	345	ASN
1	D	352	ARG
1	D	371	ARG

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Mol	Chain	Res	Type
1	D	377	LYS
1	D	482	SER
1	D	486	LYS
1	D	494	LYS
1	D	563	TYR
1	D	577	ASN
1	D	582	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	577	ASN
1	B	326	GLN
1	B	345	ASN
1	D	210	HIS
1	D	577	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	PO4	A	702	2	4,4,4	0.64	0	6,6,6	0.26	0
4	GTP	B	801	-	25,34,34	1.08	3 (12%)	34,54,54	1.71	7 (20%)
4	GTP	B	803	-	25,34,34	1.07	2 (8%)	34,54,54	1.79	7 (20%)
3	PO4	B	804	2	4,4,4	0.57	0	6,6,6	0.25	0
4	GTP	C	702	-	25,34,34	1.12	3 (12%)	34,54,54	1.72	9 (26%)
3	PO4	C	703	2	4,4,4	0.72	0	6,6,6	0.25	0
4	GTP	D	702	-	25,34,34	1.07	2 (8%)	34,54,54	1.82	8 (23%)
3	PO4	D	703	2	4,4,4	0.57	0	6,6,6	0.25	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	A	702	2	-	0/0/0/0	0/0/0/0
4	GTP	B	801	-	-	0/18/38/38	0/3/3/3
4	GTP	B	803	-	-	0/18/38/38	0/3/3/3
3	PO4	B	804	2	-	0/0/0/0	0/0/0/0
4	GTP	C	702	-	-	0/18/38/38	0/3/3/3
3	PO4	C	703	2	-	0/0/0/0	0/0/0/0
4	GTP	D	702	-	-	0/18/38/38	0/3/3/3
3	PO4	D	703	2	-	0/0/0/0	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	801	GTP	O4'-C1'	2.08	1.43	1.41
4	C	702	GTP	O4'-C1'	2.57	1.44	1.41
4	B	801	GTP	C5-C4	2.71	1.46	1.40
4	B	803	GTP	C5-C4	2.76	1.46	1.40
4	C	702	GTP	C6-C5	3.02	1.47	1.41
4	D	702	GTP	C5-C4	3.05	1.47	1.40
4	D	702	GTP	C6-C5	3.13	1.47	1.41
4	C	702	GTP	C5-C4	3.26	1.47	1.40
4	B	801	GTP	C6-C5	3.48	1.48	1.41
4	B	803	GTP	C6-C5	3.71	1.48	1.41

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	702	GTP	C5-C6-N1	-4.56	117.35	123.59
4	B	803	GTP	C5-C6-N1	-4.31	117.69	123.59
4	B	801	GTP	C5-C6-N1	-4.26	117.77	123.59
4	C	702	GTP	C5-C6-N1	-4.22	117.82	123.59
4	D	702	GTP	PB-O3B-PG	-3.71	120.22	132.67
4	B	803	GTP	C4-C5-N7	-3.48	106.28	109.48
4	B	803	GTP	N3-C2-N1	-3.34	122.35	127.44
4	B	803	GTP	C6-C5-C4	-3.13	117.15	120.90
4	B	801	GTP	C6-C5-C4	-2.94	117.38	120.90
4	C	702	GTP	C6-C5-C4	-2.93	117.39	120.90
4	B	801	GTP	O3A-PA-O5'	-2.93	95.17	102.94
4	D	702	GTP	N3-C2-N1	-2.87	123.07	127.44
4	D	702	GTP	C2'-C1'-N9	-2.86	109.93	114.29
4	B	801	GTP	N3-C2-N1	-2.84	123.12	127.44
4	B	801	GTP	C4-C5-N7	-2.80	106.90	109.48
4	C	702	GTP	N3-C2-N1	-2.80	123.18	127.44
4	D	702	GTP	C6-C5-C4	-2.42	118.01	120.90
4	C	702	GTP	PB-O3B-PG	-2.36	124.76	132.67
4	C	702	GTP	O3A-PA-O5'	-2.30	96.83	102.94
4	B	801	GTP	PB-O3B-PG	-2.27	125.04	132.67
4	C	702	GTP	C4-C5-N7	-2.23	107.42	109.48
4	B	803	GTP	PB-O3B-PG	-2.06	125.75	132.67
4	B	803	GTP	PA-O3A-PB	-2.03	127.03	132.73
4	D	702	GTP	C4-C5-N7	-2.01	107.63	109.48
4	C	702	GTP	PA-O3A-PB	-2.01	127.09	132.73
4	C	702	GTP	O3G-PG-O2G	2.09	115.33	107.38
4	D	702	GTP	O2A-PA-O3A	2.16	114.88	105.09
4	B	801	GTP	C6-N1-C2	4.55	122.26	115.94
4	B	803	GTP	C6-N1-C2	4.83	122.64	115.94
4	C	702	GTP	C6-N1-C2	4.86	122.69	115.94
4	D	702	GTP	C6-N1-C2	4.90	122.75	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	456/539 (84%)	0.23	27 (5%) 26 19	33, 59, 115, 143	0
1	B	433/539 (80%)	0.08	9 (2%) 67 61	30, 55, 112, 150	0
1	C	434/539 (80%)	0.21	24 (5%) 29 21	33, 60, 117, 143	0
1	D	444/539 (82%)	0.35	30 (6%) 20 15	36, 63, 119, 145	0
All	All	1767/2156 (81%)	0.22	90 (5%) 32 25	30, 59, 117, 150	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	488	LEU	5.2
1	A	532	ILE	4.8
1	C	114	THR	4.8
1	D	346	GLU	4.7
1	A	487	VAL	4.6
1	D	489	LEU	4.5
1	A	508	GLY	4.3
1	B	490	ASP	4.2
1	C	521	TYR	4.1
1	A	276	LEU	3.9
1	C	465	GLN	3.8
1	B	521	TYR	3.8
1	D	549	LEU	3.5
1	C	304	LYS	3.5
1	D	494	LYS	3.5
1	D	578	PHE	3.5
1	A	347	LEU	3.4
1	B	517	HIS	3.4
1	C	498	PHE	3.4
1	C	283	SER	3.3
1	A	490	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	489	LEU	3.3
1	A	190	GLN	3.2
1	A	527	ASN	3.2
1	A	546	ALA	3.1
1	D	546	ALA	3.1
1	B	545	PHE	3.1
1	C	345	ASN	3.1
1	B	345	ASN	3.1
1	A	526	PRO	3.0
1	A	507	TYR	3.0
1	D	304	LYS	2.9
1	A	277	GLU	2.9
1	C	466	ILE	2.9
1	D	472	ASP	2.9
1	A	342	GLU	2.9
1	C	464	GLY	2.8
1	C	305	ARG	2.8
1	C	522	CYS	2.8
1	D	342	GLU	2.7
1	D	527	ASN	2.7
1	B	305	ARG	2.7
1	A	509	MET	2.7
1	B	546	ALA	2.7
1	D	284	LEU	2.6
1	D	291	PRO	2.6
1	C	520	PHE	2.6
1	B	114	THR	2.6
1	B	582	GLN	2.5
1	D	466	ILE	2.5
1	A	510	GLN	2.5
1	D	463	THR	2.5
1	C	487	VAL	2.5
1	C	583	ASP	2.5
1	A	559	ARG	2.5
1	D	467	LYS	2.5
1	C	334	PHE	2.5
1	D	285	TRP	2.5
1	C	353	ASP	2.4
1	D	343	VAL	2.4
1	D	532	ILE	2.4
1	C	285	TRP	2.4
1	C	572	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	528	ARG	2.4
1	D	507	TYR	2.4
1	A	491	VAL	2.3
1	D	478	LYS	2.3
1	C	578	PHE	2.3
1	A	344	ASP	2.3
1	C	296	PHE	2.3
1	D	496	GLU	2.3
1	D	572	TRP	2.2
1	D	287	TYR	2.2
1	A	195	ASP	2.2
1	A	343	VAL	2.2
1	A	583	ASP	2.2
1	C	189	LEU	2.2
1	D	569	PHE	2.2
1	C	182	LEU	2.1
1	D	486	LYS	2.1
1	C	486	LYS	2.1
1	D	468	ILE	2.1
1	A	523	LYS	2.1
1	D	550	ILE	2.1
1	D	563	TYR	2.1
1	A	288	LYS	2.1
1	A	530	ILE	2.1
1	D	473	TYR	2.1
1	A	291	PRO	2.0
1	C	286	PRO	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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	PO4	A	702	5/5	0.97	0.16	-0.28	53,57,63,63	0
3	PO4	B	804	5/5	0.97	0.13	-0.83	63,65,67,72	0
3	PO4	C	703	5/5	0.98	0.11	-1.32	62,66,75,81	0
4	GTP	B	801	32/32	0.95	0.13	-1.85	47,63,103,104	0
3	PO4	D	703	5/5	0.95	0.12	-1.88	65,69,75,75	0
2	ZN	A	701	1/1	0.98	0.12	-1.94	58,58,58,58	0
4	GTP	D	702	32/32	0.94	0.13	-2.03	52,66,102,110	0
4	GTP	C	702	32/32	0.97	0.11	-2.03	46,54,109,116	0
2	ZN	C	701	1/1	0.96	0.10	-2.04	62,62,62,62	0
4	GTP	B	803	32/32	0.95	0.13	-2.16	50,55,92,97	0
2	ZN	B	802	1/1	1.00	0.08	-2.55	56,56,56,56	0
2	ZN	D	701	1/1	0.99	0.07	-8.04	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.