Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:33 PM GMT

PDB ID	:	4TNR
Title	:	Structure basis of cellular dNTP regulation, SAMHD1-GTP-dATP-dATP complex
Authors	:	Ji, X.; Tang, C.; Zhao, Q.; Wang, W.; Xiong, Y.
Deposited on	:	2014-06-04
Resolution	:	2.75 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

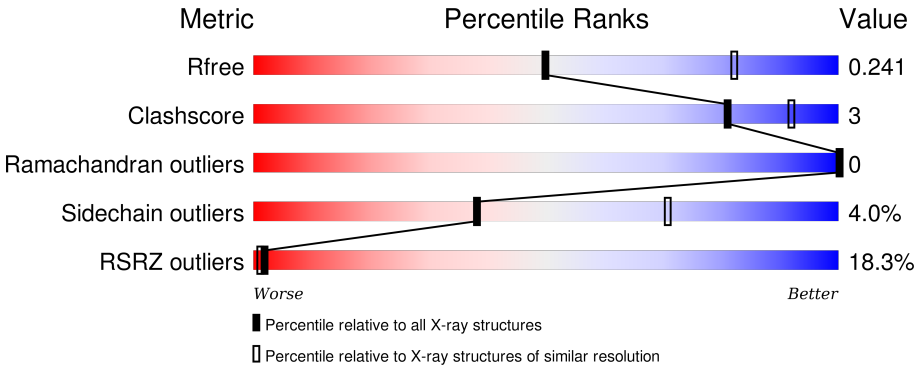
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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 <=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	514	26% 82% 11% 6%
1	B	514	19% 82% 11% 6%
1	C	514	18% 82% 11% 6%
1	D	514	6% 83% 11% 6%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DTP	B	704	-	-	-	X
2	DTP	C	701	-	-	-	X
2	DTP	D	701	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16156 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.

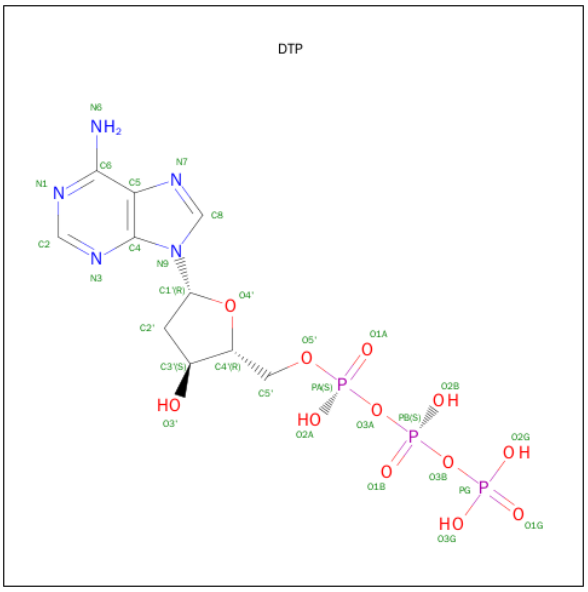
- Molecule 1 is a protein called Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	481	Total	C	N	O	S	0	2	0
			3948	2525	687	715	21			
1	C	481	Total	C	N	O	S	0	2	0
			3948	2525	687	715	21			
1	B	481	Total	C	N	O	S	0	2	0
			3948	2525	687	715	21			
1	A	481	Total	C	N	O	S	0	2	0
			3948	2525	687	715	21			

There are 8 discrepancies between the modelled and reference sequences:

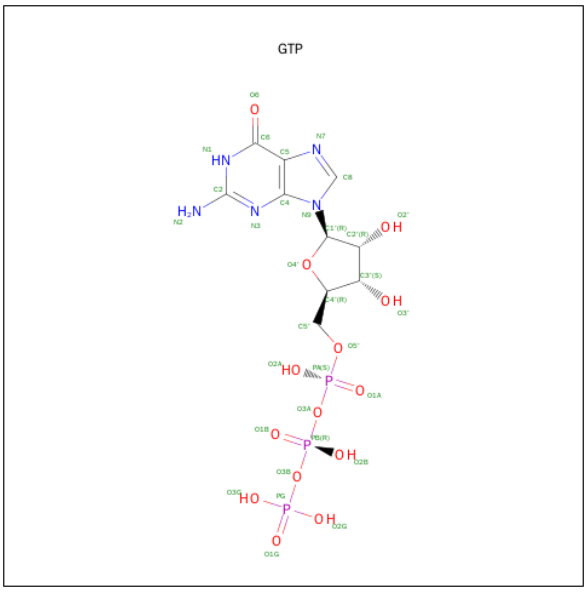
Chain	Residue	Modelled	Actual	Comment	Reference
D	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
D	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
C	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
C	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
B	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
B	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
A	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
A	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3

- Molecule 2 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	D	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	C	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	C	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- 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		
4	D	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	8	Total	O	0	0
			8	8		

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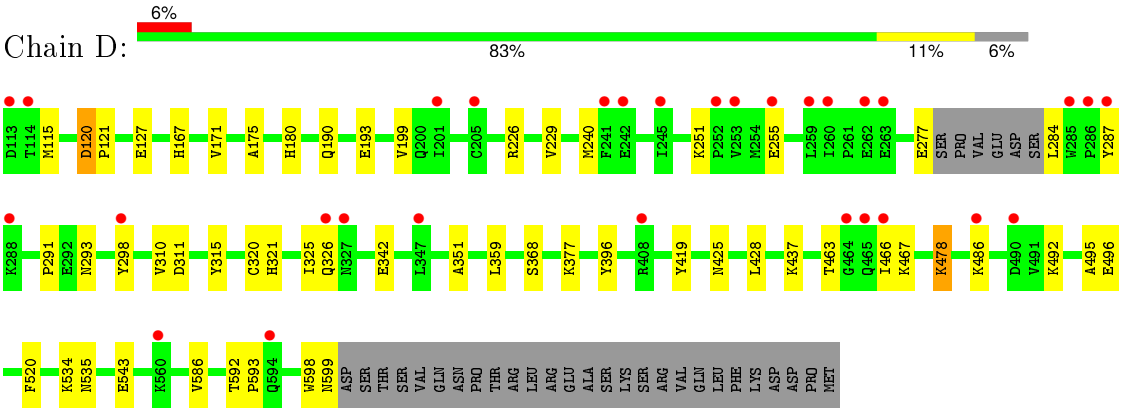
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	2	Total O 2 2	0	0
5	B	9	Total O 9 9	0	0
5	A	3	Total O 3 3	0	0

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.

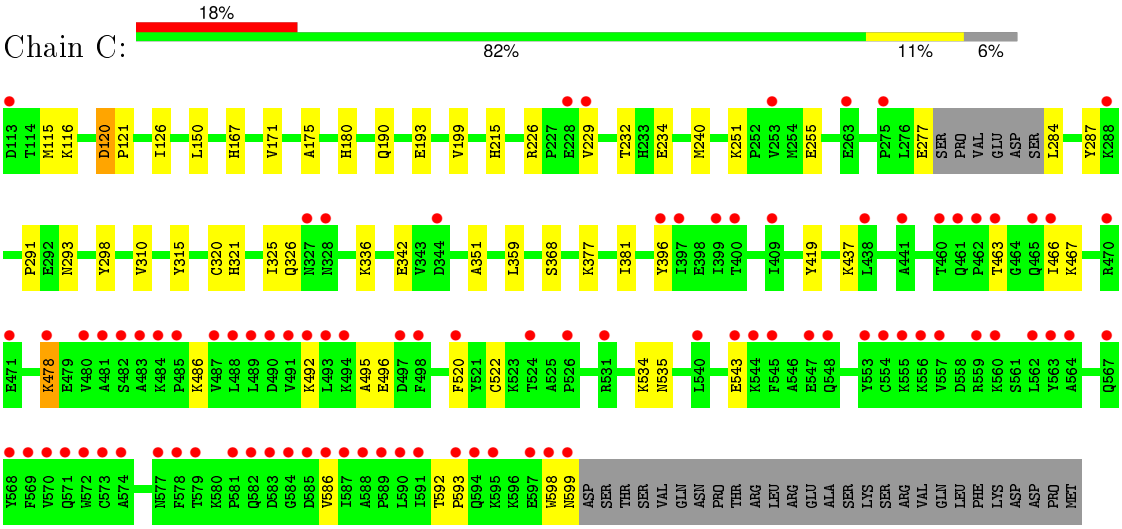
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain D:



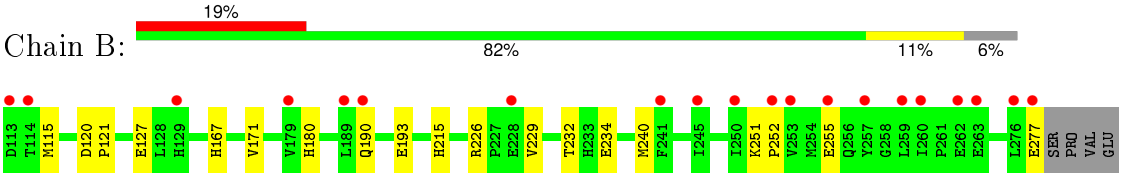
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

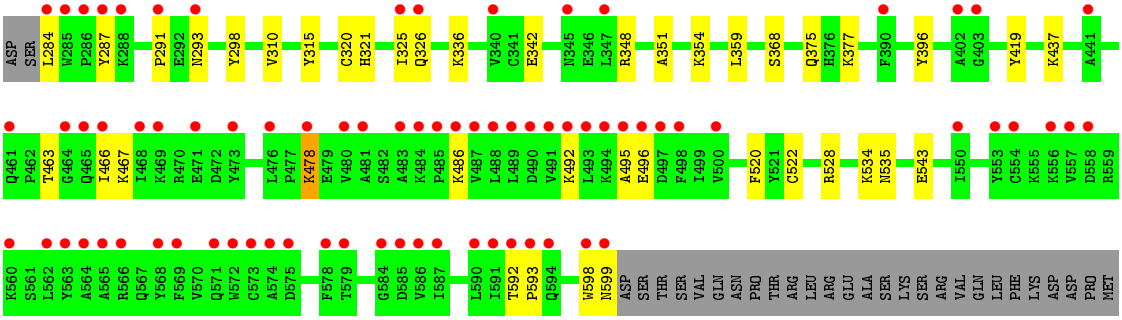
Chain C:



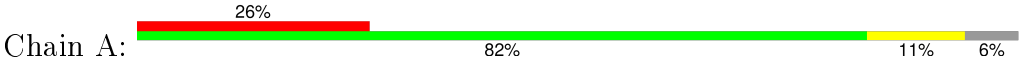
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

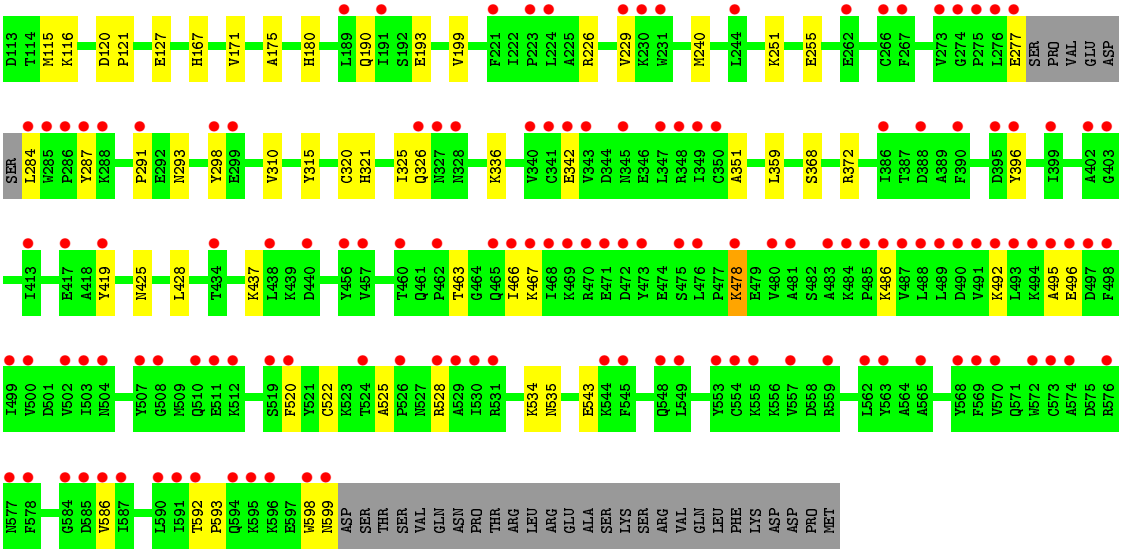
Chain B:





- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.92Å 141.70Å 97.52Å 90.00° 115.40° 90.00°	Depositor
Resolution (Å)	50.00 – 2.75 48.46 – 2.72	Depositor EDS
% Data completeness (in resolution range)	96.3 (50.00-2.75) 96.3 (48.46-2.72)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.224 , 0.242 0.222 , 0.241	Depositor DCC
R_{free} test set	2732 reflections (5.44%)	DCC
Wilson B-factor (Å^2)	65.3	Xtriage
Anisotropy	1.250	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 58.1	EDS
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	61 of 53664 reflections (0.114%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16156	wwPDB-VP
Average B, all atoms (Å^2)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GTP, MG, DTP

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	0.57	0/4040	0.71	0/5453
1	B	0.63	2/4040 (0.0%)	0.73	1/5453 (0.0%)
1	C	0.59	0/4040	0.72	1/5453 (0.0%)
1	D	0.64	0/4040	0.73	1/5453 (0.0%)
All	All	0.61	2/16160 (0.0%)	0.72	3/21812 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	528	ARG	CZ-NH2	10.12	1.46	1.33
1	B	528	ARG	CD-NE	5.14	1.55	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	528	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	D	120	ASP	CB-CG-OD1	5.23	123.00	118.30
1	C	120	ASP	CB-CG-OD1	5.20	122.98	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3948	0	3930	32	0
1	B	3948	0	3930	33	0
1	C	3948	0	3930	34	0
1	D	3948	0	3930	29	0
2	A	30	0	12	1	0
2	B	60	0	24	5	0
2	C	60	0	24	4	0
2	D	60	0	24	2	0
3	A	32	0	12	0	0
3	B	32	0	12	0	0
3	C	32	0	12	1	0
3	D	32	0	12	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	3	0	0	0	0
5	B	9	0	0	1	0
5	C	2	0	0	0	0
5	D	8	0	0	0	0
All	All	16156	0	15852	107	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 3.

All (107) 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:C:377:LYS:NZ	2:A:702:DTP:O2B	1.97	0.96
1:C:326:GLN:HG2	1:A:326:GLN:HG2	1.62	0.81
1:D:326:GLN:HG2	1:B:326:GLN:HG2	1.66	0.76
1:C:215:HIS:CD2	2:C:701:DTP:C8	2.70	0.75
1:A:291:PRO:HG2	1:A:293:ASN:OD1	1.90	0.72
1:C:291:PRO:HG2	1:C:293:ASN:OD1	1.90	0.71
1:B:291:PRO:HG2	1:B:293:ASN:OD1	1.91	0.70
1:D:291:PRO:HG2	1:D:293:ASN:OD1	1.92	0.69
1:B:375:GLN:HE22	2:B:704:DTP:HN61	1.44	0.65
1:D:311:ASP:OD2	2:D:701:DTP:O1A	2.15	0.64
2:D:703:DTP:O2B	1:B:377:LYS:NZ	2.31	0.63
1:B:127:GLU:HG3	1:A:336:LYS:HE3	1.82	0.62
1:B:348:ARG:HD3	5:B:809:HOH:O	1.98	0.62
1:D:543:GLU:HG3	1:B:543:GLU:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:ASP:OD1	1:D:121:PRO:HD2	2.02	0.58
1:B:226:ARG:O	1:B:229:VAL:HG12	2.05	0.57
1:B:375:GLN:NE2	2:B:704:DTP:N6	2.49	0.57
1:D:586:VAL:HG11	1:B:522[A]:CYS:SG	2.45	0.56
1:A:287:TYR:CD1	1:A:298:TYR:CE1	2.93	0.56
1:B:287:TYR:CD1	1:B:298:TYR:CE1	2.93	0.56
1:D:287:TYR:CD1	1:D:298:TYR:CE1	2.94	0.56
1:A:226:ARG:O	1:A:229:VAL:HG12	2.05	0.56
1:D:226:ARG:O	1:D:229:VAL:HG12	2.06	0.55
1:C:226:ARG:O	1:C:229:VAL:HG12	2.05	0.55
1:B:120:ASP:OD1	1:B:121:PRO:HD2	2.05	0.55
1:A:120:ASP:OD1	1:A:121:PRO:HD2	2.07	0.55
1:C:120:ASP:OD1	1:C:121:PRO:HD2	2.06	0.54
1:D:321:HIS:CE1	1:A:321:HIS:CE1	2.96	0.54
1:C:586:VAL:HG22	1:A:528:ARG:HD3	1.91	0.52
1:C:287:TYR:CD1	1:C:298:TYR:CE1	2.96	0.52
1:D:377:LYS:NZ	2:B:701:DTP:O2B	2.43	0.52
2:C:704:DTP:N6	1:A:372:ARG:HG2	2.26	0.51
1:A:167:HIS:O	1:A:171:VAL:HG23	2.10	0.51
1:C:586:VAL:HG11	1:A:522[A]:CYS:SG	2.50	0.51
1:A:463:THR:O	1:A:466:ILE:HG12	2.11	0.51
1:D:127:GLU:HG3	1:C:336:LYS:HE3	1.93	0.50
1:B:167:HIS:O	1:B:171:VAL:HG23	2.11	0.50
1:C:167:HIS:O	1:C:171:VAL:HG23	2.10	0.50
1:C:543:GLU:HG3	1:A:543:GLU:HG3	1.93	0.50
1:C:326:GLN:HG2	1:A:326:GLN:CG	2.39	0.50
1:B:463:THR:O	1:B:466:ILE:HG12	2.12	0.50
1:D:463:THR:O	1:D:466:ILE:HG12	2.11	0.49
1:C:326:GLN:CG	1:A:326:GLN:HG2	2.39	0.49
1:C:463:THR:O	1:C:466:ILE:HG12	2.12	0.49
1:D:167:HIS:O	1:D:171:VAL:HG23	2.13	0.48
1:C:116:LYS:HE3	3:C:703:GTP:O1A	2.14	0.48
1:C:592:THR:N	1:C:593:PRO:CD	2.77	0.48
1:B:336:LYS:HE3	1:A:127:GLU:HG3	1.97	0.47
1:C:251:LYS:O	1:C:255:GLU:HG3	2.14	0.47
1:D:592:THR:N	1:D:593:PRO:CD	2.78	0.47
1:A:592:THR:N	1:A:593:PRO:CD	2.78	0.47
1:B:592:THR:N	1:B:593:PRO:CD	2.78	0.47
1:D:320:CYS:HB3	1:D:325:ILE:O	2.15	0.47
1:D:251:LYS:O	1:D:255:GLU:HG3	2.14	0.47
1:A:251:LYS:O	1:A:255:GLU:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:ALA:O	1:C:520:PHE:HA	2.16	0.46
1:B:232:THR:HB	1:B:234:GLU:OE1	2.16	0.46
1:D:326:GLN:HG2	1:B:326:GLN:CG	2.42	0.46
1:D:478:LYS:HE2	1:D:495:ALA:HB1	1.98	0.46
1:B:240:MET:CE	1:B:419:TYR:HD2	2.28	0.46
1:A:478:LYS:HE2	1:A:495:ALA:HB1	1.98	0.46
1:B:251:LYS:O	1:B:255:GLU:HG3	2.16	0.45
1:A:396:TYR:CD1	1:A:437:LYS:HD2	2.50	0.45
1:B:396:TYR:CD1	1:B:437:LYS:HD2	2.52	0.45
1:C:478:LYS:HE2	1:C:495:ALA:HB1	1.98	0.45
1:C:522[A]:CYS:SG	1:A:586:VAL:HG11	2.56	0.45
3:D:702:GTP:O2G	1:A:116:LYS:NZ	2.29	0.45
1:D:396:TYR:CD1	1:D:437:LYS:HD2	2.52	0.45
1:D:543:GLU:CG	1:B:543:GLU:CG	2.95	0.44
1:A:351:ALA:O	1:A:520:PHE:HA	2.17	0.44
1:C:240:MET:CE	1:C:419:TYR:HD2	2.31	0.44
1:C:320:CYS:HB3	1:C:325:ILE:O	2.17	0.44
1:D:171:VAL:HG13	1:D:310:VAL:HG23	2.00	0.44
1:B:478:LYS:HE2	1:B:495:ALA:HB1	1.98	0.44
1:D:543:GLU:HG2	1:B:543:GLU:HG2	2.00	0.44
1:C:396:TYR:CD1	1:C:437:LYS:HD2	2.53	0.44
1:D:240:MET:CE	1:D:419:TYR:HD2	2.30	0.44
1:A:240:MET:CE	1:A:419:TYR:HD2	2.30	0.43
1:D:351:ALA:O	1:D:520:PHE:HA	2.17	0.43
1:C:171:VAL:HG13	1:C:310:VAL:HG23	2.01	0.43
3:D:702:GTP:PA	3:D:702:GTP:H3'	2.58	0.43
1:B:598:TRP:O	1:B:599:ASN:HB2	2.19	0.43
1:B:351:ALA:O	1:B:520:PHE:HA	2.18	0.43
1:C:215:HIS:NE2	2:C:701:DTP:H8	2.34	0.43
1:A:171:VAL:HG13	1:A:310:VAL:HG23	2.01	0.43
1:D:598:TRP:O	1:D:599:ASN:HB2	2.19	0.43
1:C:598:TRP:O	1:C:599:ASN:HB2	2.18	0.42
1:A:598:TRP:O	1:A:599:ASN:HB2	2.18	0.42
1:C:586:VAL:HG11	1:A:525:ALA:HB3	2.01	0.42
1:C:381:ILE:HD12	1:C:381:ILE:HA	1.91	0.42
1:A:320:CYS:HB3	1:A:325:ILE:O	2.18	0.42
1:D:428:LEU:HD12	1:A:425:ASN:HB2	2.01	0.42
1:D:428:LEU:CD1	1:A:425:ASN:HB2	2.50	0.42
1:B:215:HIS:HE1	2:B:704:DTP:O2B	2.03	0.42
1:B:251:LYS:N	1:B:252:PRO:HD2	2.35	0.41
1:D:175:ALA:HB1	1:D:199:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ALA:HB1	1:A:199:VAL:HG12	2.02	0.41
1:D:425:ASN:HB2	1:A:428:LEU:CD1	2.51	0.41
1:C:321:HIS:CE1	1:B:321:HIS:CE1	3.09	0.41
1:B:354:LYS:NZ	2:B:701:DTP:O1A	2.54	0.41
1:B:320:CYS:HB3	1:B:325:ILE:O	2.20	0.41
1:C:175:ALA:HB1	1:C:199:VAL:HG12	2.03	0.41
1:C:150:LEU:CD2	2:C:701:DTP:H2'1	2.51	0.41
1:C:232:THR:HB	1:C:234:GLU:OE1	2.21	0.41
1:B:287:TYR:HB3	1:B:298:TYR:OH	2.21	0.40
1:B:171:VAL:HG13	1:B:310:VAL:HG23	2.02	0.40
1:C:126:ILE:HD13	1:C:126:ILE:HG21	1.89	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	479/514 (93%)	474 (99%)	5 (1%)	0	100	100
1	B	479/514 (93%)	475 (99%)	4 (1%)	0	100	100
1	C	479/514 (93%)	474 (99%)	5 (1%)	0	100	100
1	D	479/514 (93%)	473 (99%)	6 (1%)	0	100	100
All	All	1916/2056 (93%)	1896 (99%)	20 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	429/459 (94%)	412 (96%)	17 (4%)	38	71
1	B	429/459 (94%)	412 (96%)	17 (4%)	38	71
1	C	429/459 (94%)	412 (96%)	17 (4%)	38	71
1	D	429/459 (94%)	412 (96%)	17 (4%)	38	71
All	All	1716/1836 (94%)	1648 (96%)	68 (4%)	38	71

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	115	MET
1	D	180	HIS
1	D	190	GLN
1	D	193	GLU
1	D	277	GLU
1	D	284	LEU
1	D	315	TYR
1	D	342	GLU
1	D	359	LEU
1	D	368	SER
1	D	467	LYS
1	D	478	LYS
1	D	486	LYS
1	D	492	LYS
1	D	496	GLU
1	D	534	LYS
1	D	535	ASN
1	C	115	MET
1	C	180	HIS
1	C	190	GLN
1	C	193	GLU
1	C	277	GLU
1	C	284	LEU
1	C	315	TYR
1	C	342	GLU
1	C	359	LEU
1	C	368	SER
1	C	467	LYS
1	C	478	LYS
1	C	486	LYS

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Mol	Chain	Res	Type
1	C	492	LYS
1	C	496	GLU
1	C	534	LYS
1	C	535	ASN
1	B	115	MET
1	B	180	HIS
1	B	190	GLN
1	B	193	GLU
1	B	277	GLU
1	B	284	LEU
1	B	315	TYR
1	B	342	GLU
1	B	359	LEU
1	B	368	SER
1	B	467	LYS
1	B	478	LYS
1	B	486	LYS
1	B	492	LYS
1	B	496	GLU
1	B	534	LYS
1	B	535	ASN
1	A	115	MET
1	A	180	HIS
1	A	190	GLN
1	A	193	GLU
1	A	277	GLU
1	A	284	LEU
1	A	315	TYR
1	A	342	GLU
1	A	359	LEU
1	A	368	SER
1	A	467	LYS
1	A	478	LYS
1	A	486	LYS
1	A	492	LYS
1	A	496	GLU
1	A	534	LYS
1	A	535	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	235	GLN
1	D	364	HIS
1	D	375	GLN
1	D	380	ASN
1	C	235	GLN
1	C	243	HIS
1	C	364	HIS
1	B	235	GLN
1	B	364	HIS
1	B	375	GLN
1	B	380	ASN
1	A	235	GLN
1	A	364	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
2	DTP	A	702	4	24,32,32	1.32	3 (12%)	32,50,50	2.24	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GTP	A	703	4	25,34,34	1.25	3 (12%)	34,54,54	1.92	7 (20%)
2	DTP	B	701	4	24,32,32	1.25	4 (16%)	32,50,50	1.81	6 (18%)
3	GTP	B	703	4	25,34,34	1.06	2 (8%)	34,54,54	1.98	9 (26%)
2	DTP	B	704	-	24,32,32	1.17	2 (8%)	32,50,50	1.91	6 (18%)
2	DTP	C	701	-	24,32,32	1.17	2 (8%)	32,50,50	2.06	6 (18%)
3	GTP	C	703	4	25,34,34	1.09	2 (8%)	34,54,54	1.93	10 (29%)
2	DTP	C	704	4	24,32,32	1.08	2 (8%)	32,50,50	1.71	6 (18%)
2	DTP	D	701	-	24,32,32	1.23	2 (8%)	32,50,50	1.91	5 (15%)
3	GTP	D	702	4	25,34,34	1.32	2 (8%)	34,54,54	2.10	8 (23%)
2	DTP	D	703	4	24,32,32	1.13	2 (8%)	32,50,50	2.53	8 (25%)

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
2	DTP	A	702	4	-	0/18/34/34	0/3/3/3
3	GTP	A	703	4	-	0/18/38/38	0/3/3/3
2	DTP	B	701	4	-	0/18/34/34	0/3/3/3
3	GTP	B	703	4	-	0/18/38/38	0/3/3/3
2	DTP	B	704	-	-	0/18/34/34	0/3/3/3
2	DTP	C	701	-	-	0/18/34/34	0/3/3/3
3	GTP	C	703	4	-	0/18/38/38	0/3/3/3
2	DTP	C	704	4	-	0/18/34/34	0/3/3/3
2	DTP	D	701	-	-	0/18/34/34	0/3/3/3
3	GTP	D	702	4	-	0/18/38/38	0/3/3/3
2	DTP	D	703	4	-	0/18/34/34	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	703	DTP	O4'-C4'	-2.52	1.39	1.45
2	A	702	DTP	PG-O2G	-2.16	1.47	1.54
2	B	701	DTP	PB-O2B	-2.10	1.46	1.54
2	C	704	DTP	PG-O2G	-2.01	1.47	1.54
2	B	704	DTP	C2-N3	2.15	1.36	1.32
2	B	701	DTP	O4'-C1'	2.17	1.47	1.42
2	B	701	DTP	C2-N3	2.24	1.36	1.32
3	A	703	GTP	C6-N1	2.30	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	DTP	C2-N3	2.34	1.36	1.32
3	B	703	GTP	C6-C5	2.34	1.45	1.41
2	A	702	DTP	C2-N3	2.35	1.36	1.32
2	C	701	DTP	C2-N3	2.44	1.36	1.32
3	C	703	GTP	C5-C4	2.44	1.46	1.40
2	D	703	DTP	C5-C4	2.64	1.46	1.40
3	B	703	GTP	C5-C4	2.68	1.46	1.40
2	B	701	DTP	C5-C4	2.70	1.46	1.40
2	C	704	DTP	C5-C4	2.77	1.46	1.40
3	A	703	GTP	C6-C5	2.82	1.46	1.41
3	C	703	GTP	C6-C5	3.01	1.47	1.41
2	A	702	DTP	C5-C4	3.26	1.47	1.40
3	D	702	GTP	C5-C4	3.28	1.47	1.40
3	A	703	GTP	C5-C4	3.36	1.48	1.40
2	C	701	DTP	C5-C4	3.47	1.48	1.40
2	B	704	DTP	C5-C4	3.91	1.49	1.40
3	D	702	GTP	C6-C5	3.91	1.49	1.41
2	D	701	DTP	C5-C4	4.01	1.49	1.40

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	703	DTP	N3-C2-N1	-9.89	121.32	128.89
2	C	701	DTP	N3-C2-N1	-8.22	122.60	128.89
2	B	704	DTP	N3-C2-N1	-7.68	123.01	128.89
2	D	701	DTP	N3-C2-N1	-6.96	123.57	128.89
2	A	702	DTP	N3-C2-N1	-6.81	123.68	128.89
3	D	702	GTP	PA-O3A-PB	-6.44	114.63	132.73
2	A	702	DTP	PA-O3A-PB	-5.73	116.64	132.73
2	A	702	DTP	C4-C5-N7	-5.06	104.82	109.48
2	C	704	DTP	N3-C2-N1	-5.03	125.05	128.89
2	B	701	DTP	N3-C2-N1	-5.00	125.06	128.89
3	B	703	GTP	C5-C6-N1	-4.68	117.19	123.59
3	C	703	GTP	PA-O3A-PB	-4.43	120.30	132.73
2	B	701	DTP	PA-O3A-PB	-4.27	120.73	132.73
3	D	702	GTP	C5-C6-N1	-4.25	117.77	123.59
3	A	703	GTP	C5-C6-N1	-4.23	117.80	123.59
2	C	704	DTP	C4-C5-N7	-4.19	105.63	109.48
3	A	703	GTP	N3-C2-N1	-4.07	121.25	127.44
2	D	703	DTP	C1'-N9-C4	-3.95	120.47	127.16
3	A	703	GTP	PA-O3A-PB	-3.88	121.83	132.73
3	B	703	GTP	N3-C2-N1	-3.87	121.55	127.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	703	GTP	C6-C5-C4	-3.80	116.35	120.90
3	C	703	GTP	C6-C5-C4	-3.65	116.53	120.90
3	D	702	GTP	C6-C5-C4	-3.55	116.65	120.90
2	D	701	DTP	PA-O3A-PB	-3.52	122.85	132.73
2	D	701	DTP	C4-C5-N7	-3.48	106.27	109.48
3	A	703	GTP	C6-C5-C4	-3.47	116.75	120.90
3	C	703	GTP	C5-C6-N1	-3.40	118.94	123.59
2	B	704	DTP	C4-C5-N7	-3.37	106.38	109.48
2	B	704	DTP	PA-O3A-PB	-3.30	123.45	132.73
3	C	703	GTP	N3-C2-N1	-3.29	122.44	127.44
2	B	701	DTP	C4-C5-N7	-3.19	106.54	109.48
2	D	701	DTP	PB-O3B-PG	-3.15	122.12	132.67
2	C	701	DTP	PA-O3A-PB	-3.12	123.98	132.73
2	C	701	DTP	C4-C5-N7	-3.08	106.65	109.48
2	C	704	DTP	PB-O3B-PG	-3.00	122.60	132.67
2	D	703	DTP	PB-O3B-PG	-2.99	122.63	132.67
3	B	703	GTP	PB-O3B-PG	-2.99	122.64	132.67
2	C	701	DTP	PB-O3B-PG	-2.98	122.67	132.67
2	A	702	DTP	PB-O3B-PG	-2.98	122.68	132.67
3	C	703	GTP	C4-C5-N7	-2.90	106.81	109.48
2	C	704	DTP	PA-O3A-PB	-2.89	124.62	132.73
2	B	704	DTP	PB-O3B-PG	-2.88	123.01	132.67
3	D	702	GTP	N3-C2-N1	-2.86	123.08	127.44
2	D	703	DTP	C4-C5-N7	-2.86	106.85	109.48
2	D	703	DTP	PA-O3A-PB	-2.82	124.82	132.73
3	B	703	GTP	PA-O3A-PB	-2.75	125.01	132.73
3	C	703	GTP	O5'-PA-O1A	-2.56	99.68	109.62
3	D	702	GTP	PB-O3B-PG	-2.22	125.22	132.67
3	C	703	GTP	PB-O3B-PG	-2.20	125.30	132.67
2	A	702	DTP	O5'-PA-O1A	-2.12	101.40	109.62
2	B	701	DTP	PB-O3B-PG	-2.06	125.75	132.67
3	B	703	GTP	O2A-PA-O3A	2.05	114.39	105.09
3	A	703	GTP	O2G-PG-O1G	2.08	117.26	110.58
2	B	704	DTP	C2-N1-C6	2.09	122.50	118.77
3	B	703	GTP	O2G-PG-O1G	2.12	117.40	110.58
2	C	701	DTP	O4'-C1'-N9	2.16	111.46	107.72
2	A	702	DTP	O4'-C1'-N9	2.27	111.65	107.72
2	C	701	DTP	C2'-C3'-C4'	2.29	107.51	102.77
2	B	701	DTP	O3G-PG-O1G	2.30	117.98	110.58
3	B	703	GTP	N2-C2-N1	2.32	121.03	117.20
2	D	701	DTP	O3G-PG-O1G	2.32	118.04	110.58
2	C	704	DTP	O3G-PG-O1G	2.36	118.19	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	704	DTP	O3G-PG-O2G	2.37	116.42	107.38
3	C	703	GTP	O4'-C1'-N9	2.41	113.14	108.10
2	A	702	DTP	C2-N1-C6	2.46	123.17	118.77
2	C	704	DTP	C2'-C3'-C4'	2.51	107.98	102.77
3	C	703	GTP	O2G-PG-O1G	2.58	118.88	110.58
3	A	703	GTP	N2-C2-N1	2.76	121.77	117.20
3	D	702	GTP	C4'-O4'-C1'	2.81	112.80	109.72
2	D	703	DTP	C2'-C3'-C4'	3.20	109.41	102.77
2	A	702	DTP	C2'-C3'-C4'	3.27	109.54	102.77
2	D	703	DTP	C2-N1-C6	3.51	125.04	118.77
3	D	702	GTP	O2G-PG-O1G	3.53	121.95	110.58
2	B	701	DTP	O2G-PG-O1G	3.53	121.96	110.58
2	D	703	DTP	O2G-PG-O1G	4.24	124.23	110.58
3	C	703	GTP	C6-N1-C2	4.30	121.91	115.94
3	D	702	GTP	C6-N1-C2	4.61	122.34	115.94
3	A	703	GTP	C6-N1-C2	4.90	122.75	115.94
3	B	703	GTP	C6-N1-C2	5.53	123.61	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	702	DTP	1	0
2	B	701	DTP	2	0
2	B	704	DTP	3	0
2	C	701	DTP	3	0
3	C	703	GTP	1	0
2	C	704	DTP	1	0
2	D	701	DTP	1	0
3	D	702	GTP	2	0
2	D	703	DTP	1	0

5.7 Other polymers (i)

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^{th} 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	481/514 (93%)	1.52	136 (28%) 1 0	43, 114, 190, 223	0
1	B	481/514 (93%)	1.05	97 (20%) 1 1	42, 91, 150, 190	0
1	C	481/514 (93%)	1.09	90 (18%) 2 1	37, 87, 161, 200	0
1	D	481/514 (93%)	0.60	30 (6%) 24 18	37, 74, 115, 162	0
All	All	1924/2056 (93%)	1.07	353 (18%) 2 1	37, 89, 164, 223	0

All (353) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	489	LEU	10.6
1	C	493	LEU	9.5
1	A	573	CYS	8.6
1	B	490	ASP	7.8
1	C	488	LEU	7.8
1	C	598	TRP	7.7
1	C	590	LEU	7.7
1	A	485	PRO	7.5
1	A	569	PHE	7.2
1	C	584	GLY	7.1
1	C	490	ASP	7.1
1	A	275	PRO	7.1
1	A	478	LYS	7.0
1	A	473	TYR	7.0
1	A	341	CYS	7.0
1	A	345	ASN	7.0
1	A	493	LEU	6.9
1	C	498	PHE	6.8
1	C	543	GLU	6.6
1	A	578	PHE	6.5
1	C	572	TRP	6.3

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Mol	Chain	Res	Type	RSRZ
1	B	488	LEU	6.3
1	B	493	LEU	6.3
1	C	485	PRO	6.2
1	B	498	PHE	6.2
1	A	476	LEU	6.2
1	A	480	VAL	6.2
1	A	489	LEU	6.2
1	A	599	ASN	6.2
1	A	230	LYS	6.1
1	A	498	PHE	6.1
1	C	587	ILE	6.0
1	A	572	TRP	6.0
1	B	464	GLY	6.0
1	B	471	GLU	5.9
1	A	457	VAL	5.9
1	A	481	ALA	5.9
1	A	488	LEU	5.8
1	C	484	LYS	5.8
1	D	408	ARG	5.7
1	B	487	VAL	5.7
1	C	487	VAL	5.6
1	C	489	LEU	5.6
1	C	492	LYS	5.6
1	C	557	VAL	5.5
1	B	473	TYR	5.5
1	A	554	CYS	5.5
1	C	589	PRO	5.3
1	B	486	LYS	5.2
1	A	468	ILE	5.2
1	B	113	ASP	5.1
1	B	575	ASP	5.1
1	A	350	CYS	5.1
1	A	563	TYR	5.0
1	B	484	LYS	4.9
1	C	491	VAL	4.8
1	B	263	GLU	4.7
1	B	590	LEU	4.7
1	C	483	ALA	4.7
1	B	255	GLU	4.7
1	A	511[A]	GLU	4.7
1	B	554	CYS	4.7
1	B	599	ASN	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	578	PHE	4.6
1	B	568	TYR	4.6
1	A	530	ILE	4.6
1	A	472	ASP	4.5
1	A	577	ASN	4.4
1	A	586	VAL	4.4
1	C	582	GLN	4.4
1	C	229	VAL	4.4
1	A	340	VAL	4.4
1	B	573	CYS	4.4
1	D	245	ILE	4.4
1	A	484	LYS	4.4
1	C	573	CYS	4.4
1	A	500	VAL	4.3
1	D	255	GLU	4.3
1	C	494	LYS	4.2
1	B	571	GLN	4.2
1	A	592	THR	4.1
1	C	563	TYR	4.1
1	B	468	ILE	4.1
1	A	277	GLU	4.1
1	A	343	VAL	4.1
1	B	572	TRP	4.0
1	B	594	GLN	4.0
1	B	592	THR	4.0
1	C	480	VAL	4.0
1	D	242	GLU	4.0
1	A	347	LEU	3.9
1	C	554	CYS	3.9
1	D	263	GLU	3.9
1	C	478	LYS	3.9
1	A	568	TYR	3.9
1	B	586	VAL	3.9
1	A	467	LYS	3.9
1	A	529	ALA	3.9
1	A	544	LYS	3.8
1	B	500	VAL	3.8
1	A	562	LEU	3.8
1	C	461	GLN	3.8
1	A	349	ILE	3.8
1	A	287	TYR	3.8
1	A	390	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	471	GLU	3.8
1	B	492	LYS	3.7
1	B	276	LEU	3.7
1	C	583	ASP	3.7
1	C	571	GLN	3.7
1	C	465	GLN	3.7
1	A	491	VAL	3.7
1	A	262	GLU	3.7
1	A	492	LYS	3.7
1	A	585	ASP	3.7
1	A	229	VAL	3.6
1	C	471	GLU	3.6
1	D	288	LYS	3.6
1	A	520	PHE	3.6
1	A	531	ARG	3.6
1	B	250	ILE	3.5
1	A	286	PRO	3.5
1	B	565	ALA	3.5
1	B	562	LEU	3.5
1	A	470	ARG	3.5
1	B	491	VAL	3.5
1	B	253	VAL	3.5
1	A	434	THR	3.5
1	B	403	GLY	3.5
1	A	494	LYS	3.5
1	A	487	VAL	3.5
1	B	591	ILE	3.5
1	A	504	ASN	3.5
1	B	483	ALA	3.5
1	C	228	GLU	3.5
1	C	599	ASN	3.4
1	C	569	PHE	3.4
1	A	590	LEU	3.4
1	B	497	ASP	3.4
1	D	466	ILE	3.4
1	A	490	ASP	3.4
1	B	262	GLU	3.4
1	B	556	LYS	3.4
1	A	403	GLY	3.3
1	A	469	LYS	3.3
1	C	113	ASP	3.3
1	D	287	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	556	LYS	3.3
1	B	557	VAL	3.2
1	A	502	VAL	3.2
1	A	465	GLN	3.2
1	B	257	TYR	3.2
1	B	553	TYR	3.2
1	A	483	ALA	3.2
1	A	496	GLU	3.2
1	B	560	LYS	3.2
1	B	485	PRO	3.2
1	B	478	LYS	3.2
1	C	594	GLN	3.2
1	A	284	LEU	3.2
1	D	113	ASP	3.2
1	A	291	PRO	3.2
1	D	252	PRO	3.2
1	C	497	ASP	3.2
1	B	593	PRO	3.2
1	A	497	ASP	3.2
1	B	480	VAL	3.2
1	D	465	GLN	3.2
1	A	499	ILE	3.1
1	C	586	VAL	3.1
1	A	557	VAL	3.1
1	A	574	ALA	3.1
1	C	562	LEU	3.1
1	A	528	ARG	3.1
1	C	482	SER	3.1
1	B	285	TRP	3.1
1	C	288	LYS	3.1
1	D	201	ILE	3.0
1	C	595	LYS	3.0
1	A	587	ILE	3.0
1	D	114	THR	3.0
1	C	597	GLU	3.0
1	C	568	TYR	3.0
1	C	462	PRO	3.0
1	A	595	LYS	3.0
1	B	259	LEU	3.0
1	A	548	GLN	3.0
1	A	507	TYR	3.0
1	D	262	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	486	LYS	2.9
1	C	555	LYS	2.9
1	A	395	ASP	2.9
1	B	286	PRO	2.9
1	C	544	LYS	2.9
1	D	347	LEU	2.9
1	B	129	HIS	2.9
1	A	189	LEU	2.9
1	A	288	LYS	2.9
1	C	397	ILE	2.9
1	B	345	ASN	2.9
1	A	388	ASP	2.8
1	D	464	GLY	2.8
1	A	508	GLY	2.8
1	C	328	ASN	2.8
1	A	440	ASP	2.8
1	B	287	TYR	2.8
1	A	266	CYS	2.8
1	A	299	GLU	2.8
1	B	563	TYR	2.8
1	A	399	ILE	2.8
1	C	481	ALA	2.8
1	A	524	THR	2.8
1	A	413	ILE	2.8
1	A	342	GLU	2.8
1	B	584	GLY	2.8
1	C	553	TYR	2.7
1	A	591	ILE	2.7
1	B	569	PHE	2.7
1	A	224	LEU	2.7
1	C	574	ALA	2.7
1	B	481	ALA	2.7
1	C	567	GLN	2.7
1	C	593	PRO	2.7
1	A	273	VAL	2.7
1	D	298	TYR	2.7
1	C	396	TYR	2.7
1	A	545	PHE	2.7
1	D	326	GLN	2.7
1	A	191	ILE	2.7
1	D	205	CYS	2.6
1	C	263	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	555	LYS	2.6
1	B	564	ALA	2.6
1	C	470	ARG	2.6
1	C	400	THR	2.6
1	A	348	ARG	2.6
1	A	326	GLN	2.6
1	B	245	ILE	2.6
1	A	462	PRO	2.6
1	C	524	THR	2.6
1	A	576	ARG	2.6
1	A	244	LEU	2.5
1	A	276	LEU	2.5
1	A	475	SER	2.5
1	C	526	PRO	2.5
1	A	466	ILE	2.5
1	A	526	PRO	2.5
1	A	510	GLN	2.5
1	C	570	VAL	2.5
1	D	490	ASP	2.5
1	B	190	GLN	2.5
1	C	564	ALA	2.5
1	B	228	GLU	2.5
1	B	252	PRO	2.5
1	B	293	ASN	2.5
1	B	241	PHE	2.5
1	D	259	LEU	2.5
1	A	519	SER	2.5
1	A	598	TRP	2.5
1	A	565	ALA	2.5
1	A	267	PHE	2.5
1	D	286	PRO	2.4
1	B	495	ALA	2.4
1	B	496	GLU	2.4
1	C	275	PRO	2.4
1	C	581	PRO	2.4
1	B	284	LEU	2.4
1	A	584	GLY	2.4
1	A	298	TYR	2.4
1	C	585	ASP	2.4
1	A	570	VAL	2.4
1	C	344	ASP	2.4
1	C	559	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	469	LYS	2.3
1	A	512	LYS	2.3
1	A	596	LYS	2.3
1	D	241	PHE	2.3
1	C	460	THR	2.3
1	C	548	GLN	2.3
1	A	594	GLN	2.3
1	B	390	PHE	2.3
1	B	326	GLN	2.3
1	A	495	ALA	2.3
1	B	466	ILE	2.3
1	A	438	LEU	2.3
1	A	223	PRO	2.3
1	B	288	LYS	2.3
1	C	409	ILE	2.3
1	C	579	THR	2.3
1	B	494	LYS	2.3
1	C	588	ALA	2.2
1	A	274	GLY	2.2
1	B	465	GLN	2.2
1	C	438	LEU	2.2
1	A	221	PHE	2.2
1	C	577	ASN	2.2
1	B	179	VAL	2.2
1	B	340	VAL	2.2
1	B	260	ILE	2.2
1	C	545	PHE	2.2
1	A	327	ASN	2.2
1	B	574	ALA	2.2
1	C	253	VAL	2.2
1	D	285	TRP	2.2
1	B	566	ARG	2.2
1	A	559	ARG	2.2
1	C	327	ASN	2.2
1	C	560	LYS	2.2
1	D	253	VAL	2.2
1	A	460	THR	2.2
1	D	594	GLN	2.2
1	C	547	GLU	2.2
1	D	327	ASN	2.2
1	B	114	THR	2.2
1	A	285	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	419	TYR	2.2
1	A	456	TYR	2.2
1	C	463	THR	2.2
1	A	486	LYS	2.1
1	A	231	TRP	2.1
1	A	553	TYR	2.1
1	A	402	ALA	2.1
1	C	540	LEU	2.1
1	C	591	ILE	2.1
1	B	325	ILE	2.1
1	A	503	ILE	2.1
1	C	441	ALA	2.1
1	C	531	ARG	2.1
1	B	402	ALA	2.1
1	B	476	LEU	2.1
1	D	260	ILE	2.1
1	D	560	LYS	2.1
1	C	399	ILE	2.1
1	B	598	TRP	2.1
1	A	396	TYR	2.1
1	A	417	GLU	2.1
1	B	587	ILE	2.1
1	B	189	LEU	2.0
1	B	579	THR	2.0
1	A	386	ILE	2.0
1	B	347	LEU	2.0
1	B	461	GLN	2.0
1	C	466	ILE	2.0
1	B	277	GLU	2.0
1	B	550	ILE	2.0
1	B	558	ASP	2.0
1	B	585	ASP	2.0
1	A	328	ASN	2.0
1	A	549	LEU	2.0
1	C	520	PHE	2.0
1	B	291	PRO	2.0
1	B	578	PHE	2.0
1	B	441	ALA	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^{th} 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
2	DTP	C	701	30/30	0.70	0.31	3.01	84,115,131,132	0
2	DTP	B	704	30/30	0.78	0.28	2.63	81,126,144,148	0
2	DTP	D	701	30/30	0.80	0.23	2.36	56,84,110,114	0
2	DTP	A	702	30/30	0.97	0.20	-0.37	60,67,89,90	0
3	GTP	A	703	32/32	0.95	0.17	-0.82	63,72,89,93	0
2	DTP	B	701	30/30	0.98	0.17	-1.05	41,42,45,46	0
3	GTP	B	703	32/32	0.95	0.16	-1.16	63,73,91,94	0
2	DTP	C	704	30/30	0.97	0.16	-1.41	52,60,75,79	0
2	DTP	D	703	30/30	0.99	0.16	-1.51	42,48,61,63	0
3	GTP	D	702	32/32	0.98	0.14	-1.69	37,41,45,46	0
3	GTP	C	703	32/32	0.97	0.13	-2.02	39,43,54,57	0
4	MG	D	704	1/1	0.90	0.08	-	72,72,72,72	0
4	MG	C	702	1/1	0.94	0.07	-	46,46,46,46	0
4	MG	A	701	1/1	0.93	0.09	-	46,46,46,46	0
4	MG	B	702	1/1	0.94	0.12	-	88,88,88,88	0

6.5 Other polymers (i)

There are no such residues in this entry.