Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:33 PM GMT

PDB ID	:	4TNQ
Title	:	Structural basis of cellular dNTP regulation, SAMHD1-GTP-dTTP-dTTP complex
Authors	:	Ji, X.; Tang, C.; Zhao, Q.; Wang, W.; Xiong, Y.
Deposited on	:	2014-06-04
Resolution	:	2.55 Å(reported)

The following versions of software and data (see references (i)) 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 2.55 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.
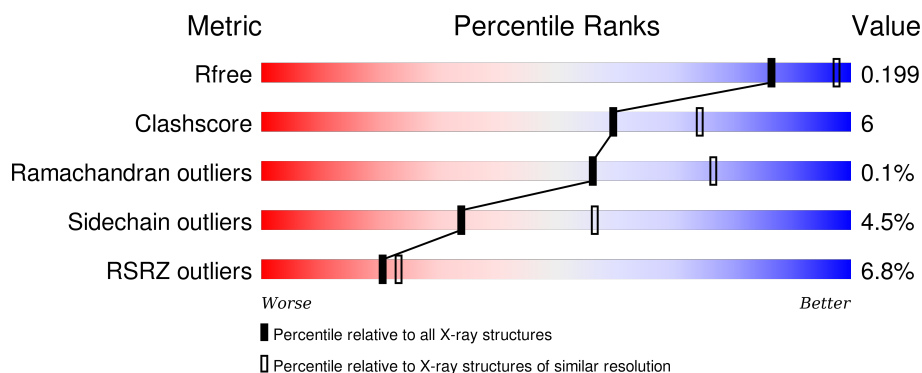
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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 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	6% / 81% / 9% / • / 7%
1	B	514	11% / 82% / 10% / • / 7%
1	C	514	5% / 82% / 11% / 7%
1	D	514	3% / 81% / 11% / • / 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16302 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	480	Total 3923	C 2512	N 683	O 708	S 20	0	0	0
1	C	479	Total 3922	C 2511	N 684	O 706	S 21	0	1	0
1	D	480	Total 3930	C 2515	N 685	O 709	S 21	0	1	0
1	B	480	Total 3925	C 2513	N 684	O 708	S 20	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).
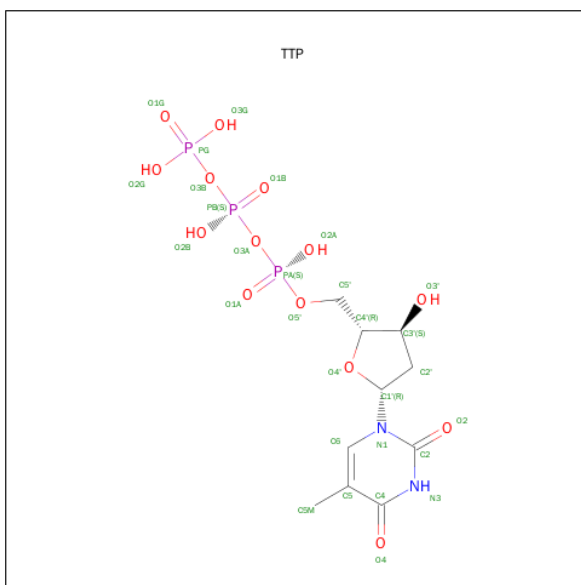
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	C	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	C	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	D	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	D	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	B	1	Total	C	N	O	P	0	0
			29	10	2	14	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	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	D	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	B	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	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	69	Total	O	0	0
			69	69		
5	C	44	Total	O	0	0
			44	44		
5	D	81	Total	O	0	0
			81	81		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	44	Total 44	O 44	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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
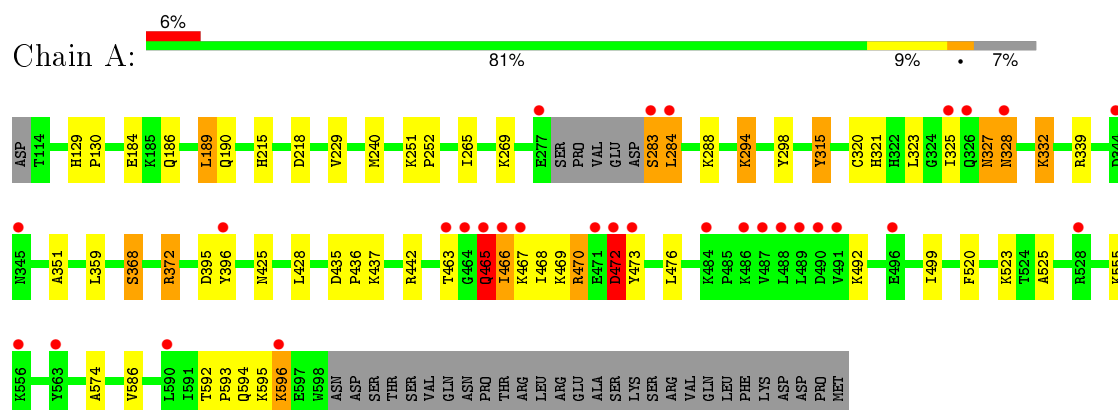
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain B:
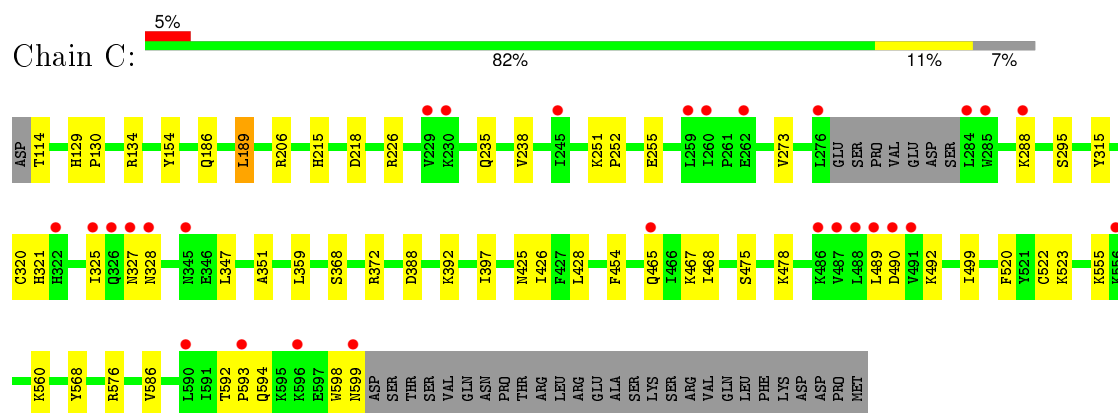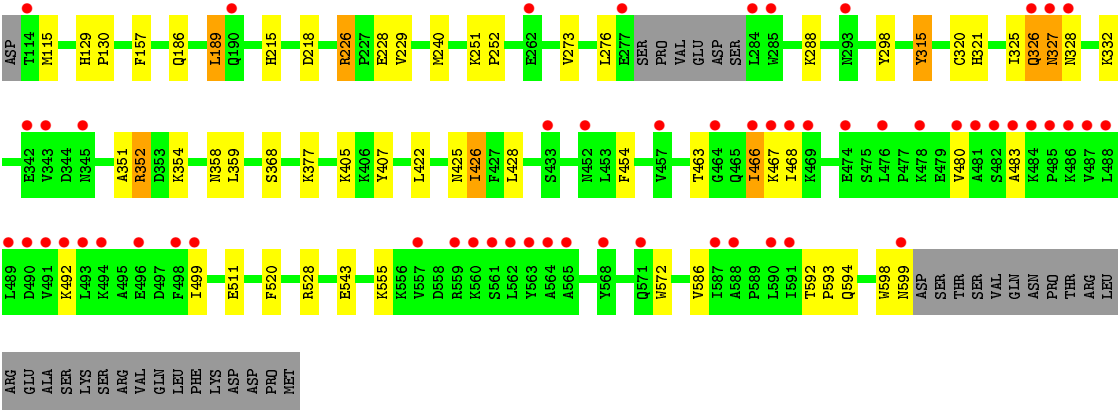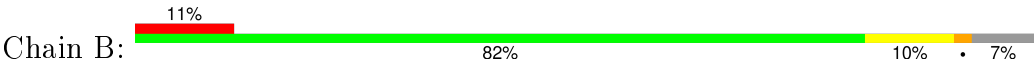
4   Data and refinement statistics (i)

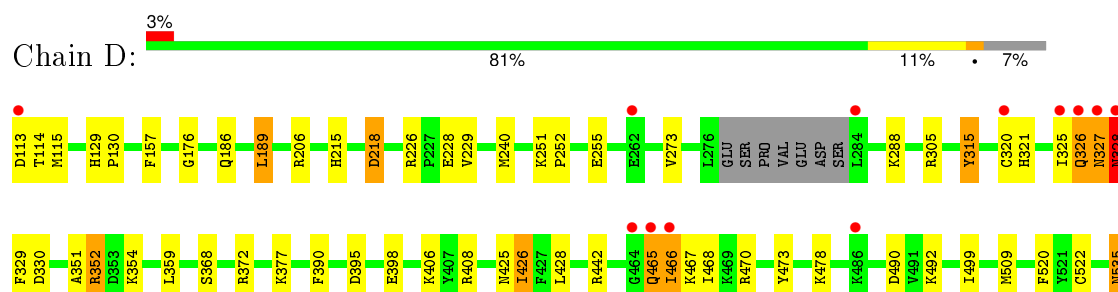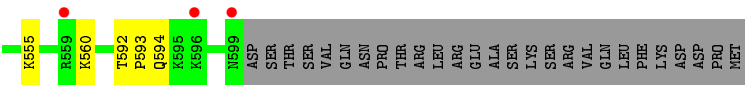| Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.16Å 140.29Å 97.27Å 90.00° 114.56° 90.00°	Depositor
Resolution (Å)	50.00 – 2.55 47.75 – 2.55	Depositor EDS
% Data completeness (in resolution range)	95.1 (50.00-2.55) 95.1 (47.75-2.55)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.80 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.161 , 0.198 0.166 , 0.199	Depositor DCC
R_{free} test set	2966 reflections (5.10%)	DCC
Wilson B-factor (Å^2)	50.4	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 53.9	EDS
Estimated twinning fraction	0.032 for h,-k,-h-l	Xtriage
L-test for twinning [2]	$<|L|> = 0.47, <L^2> = 0.30$	Xtriage
Outliers	0 of 61141 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16302	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG, TTP

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	0.68	0/4015	0.81	9/5419 (0.2%)
1	B	0.61	0/4017	0.77	5/5422 (0.1%)
1	C	0.62	0/4014	0.78	5/5418 (0.1%)
1	D	0.69	1/4022 (0.0%)	0.81	8/5429 (0.1%)
All	All	0.65	1/16068 (0.0%)	0.79	27/21688 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	218	ASP	CB-CG	-6.79	1.37	1.51

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	218	ASP	CB-CG-OD1	-8.63	110.53	118.30
1	C	576	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	A	372	ARG	NE-CZ-NH1	-8.04	116.28	120.30
1	D	218	ASP	CB-CG-OD2	7.55	125.10	118.30
1	B	352	ARG	CG-CD-NE	-7.26	96.55	111.80
1	C	576	ARG	NE-CZ-NH1	7.08	123.84	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	218	ASP	N-CA-CB	-6.67	98.59	110.60
1	A	294	LYS	CD-CE-NZ	6.54	126.74	111.70
1	D	352	ARG	CG-CD-NE	-6.47	98.20	111.80
1	C	218	ASP	CB-CG-OD1	-6.27	112.66	118.30
1	B	405	LYS	CD-CE-NZ	-6.00	97.89	111.70
1	B	218	ASP	CB-CG-OD1	-5.99	112.91	118.30
1	A	218	ASP	CB-CG-OD1	-5.89	113.00	118.30
1	D	470	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	483	ALA	N-CA-C	5.55	126.00	111.00
1	C	226	ARG	NE-CZ-NH2	5.55	123.08	120.30
1	C	218	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	442	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	B	405	LYS	N-CA-CB	-5.37	100.94	110.60
1	A	472	ASP	CB-CG-OD1	-5.36	113.48	118.30
1	D	240	MET	CG-SD-CE	-5.34	91.65	100.20
1	A	218	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	372	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	D	442	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	D	226	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	A	240	MET	CG-SD-CE	-5.12	92.01	100.20
1	A	465	GLN	CB-CA-C	-5.10	100.19	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	465	GLN	Peptide
1	B	276	LEU	Peptide

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	3923	0	3916	58	2
1	B	3925	0	3917	50	2
1	C	3922	0	3915	32	1
1	D	3930	0	3919	45	1

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	58	0	26	5	0
2	B	58	0	26	5	0
2	C	58	0	26	4	0
2	D	58	0	26	6	0
3	A	32	0	12	0	0
3	B	64	0	24	1	0
3	D	32	0	12	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
5	A	69	0	0	4	0
5	B	44	0	0	2	0
5	C	44	0	0	3	0
5	D	81	0	0	5	0
All	All	16302	0	15819	182	3

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 6.

All (182) 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:574:ALA:O	1:A:595:LYS:NZ	1.61	1.33
1:B:422:LEU:HD12	1:B:426:ILE:CD1	1.65	1.26
1:A:463:THR:O	1:A:466:ILE:HD13	1.42	1.15
1:A:283:SER:HB2	1:A:284:LEU:HA	1.17	1.15
1:B:226:ARG:HG2	1:B:226:ARG:HH21	1.11	1.14
1:D:390:PHE:CZ	1:D:426:ILE:HD11	1.82	1.13
1:B:422:LEU:HD12	1:B:426:ILE:HD11	1.14	1.12
2:A:701:TTP:O1A	5:A:824:HOH:O	1.70	1.08
2:D:701:TTP:O1G	5:D:836:HOH:O	1.72	1.06
1:A:283:SER:HB2	1:A:284:LEU:CA	1.87	1.03
1:D:390:PHE:CE2	1:D:426:ILE:HD11	1.96	0.99
1:A:283:SER:CB	1:A:284:LEU:HA	1.94	0.98
1:B:422:LEU:CD1	1:B:426:ILE:CD1	2.43	0.96
1:B:228:GLU:CD	1:B:229:VAL:HG23	1.85	0.96
1:B:422:LEU:CD1	1:B:426:ILE:HD11	1.97	0.95
1:D:328:ASN:HD22	1:D:328:ASN:C	1.69	0.94
1:A:463:THR:O	1:A:466:ILE:CD1	2.18	0.91
1:B:298:TYR:O	5:B:814:HOH:O	1.89	0.88
1:B:228:GLU:OE2	1:B:229:VAL:HG23	1.71	0.88
1:B:327:ASN:HD22	1:B:328:ASN:H	1.23	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:390:PHE:CZ	1:D:426:ILE:CD1	2.63	0.82
1:B:466:ILE:N	1:B:466:ILE:HD13	1.96	0.81
1:B:228:GLU:OE2	1:B:229:VAL:CG2	2.30	0.79
1:A:470:ARG:CZ	1:A:470:ARG:HB2	2.12	0.78
1:D:398:GLU:OE2	1:D:406:LYS:HD3	1.83	0.78
1:B:422:LEU:CD1	1:B:426:ILE:HD13	2.13	0.77
1:B:226:ARG:NH2	1:B:226:ARG:HG2	1.90	0.77
1:A:472:ASP:O	1:A:476:LEU:HD12	1.85	0.77
1:A:466:ILE:H	1:A:466:ILE:HD12	1.51	0.76
1:A:466:ILE:N	1:A:466:ILE:HD12	2.02	0.75
1:A:473:TYR:HA	1:A:476:LEU:HD13	1.67	0.74
1:A:298:TYR:O	5:A:851:HOH:O	2.06	0.74
1:D:327:ASN:O	1:D:328:ASN:HB3	1.88	0.73
1:D:466:ILE:N	1:D:466:ILE:HD13	2.03	0.73
1:D:328:ASN:ND2	1:D:328:ASN:C	2.43	0.71
1:A:328:ASN:C	1:A:328:ASN:HD22	1.94	0.70
1:C:328:ASN:O	5:C:832:HOH:O	2.10	0.69
1:A:473:TYR:HA	1:A:476:LEU:CD1	2.21	0.69
1:D:327:ASN:O	1:D:328:ASN:CB	2.42	0.68
1:B:422:LEU:HD12	1:B:426:ILE:HD13	1.69	0.67
1:A:320:CYS:SG	1:A:327:ASN:O	2.53	0.66
1:B:327:ASN:HD22	1:B:328:ASN:N	1.93	0.66
1:A:470:ARG:HA	1:A:473:TYR:CE2	2.31	0.66
1:B:463:THR:O	1:B:466:ILE:HG12	1.96	0.65
1:A:596:LYS:H	1:A:596:LYS:HD3	1.61	0.65
1:A:466:ILE:CD1	1:A:466:ILE:H	2.10	0.65
1:B:326:GLN:HG3	1:B:326:GLN:O	1.96	0.65
2:D:703:TTP:O1B	1:B:377:LYS:NZ	2.30	0.65
1:A:472:ASP:O	1:A:476:LEU:CD1	2.46	0.64
1:A:574:ALA:C	1:A:595:LYS:NZ	2.50	0.63
1:A:372:ARG:HD2	2:C:701:TTP:O4	1.99	0.63
1:B:466:ILE:CD1	1:B:466:ILE:N	2.61	0.63
1:B:327:ASN:ND2	1:B:328:ASN:H	1.96	0.63
1:A:596:LYS:N	1:A:596:LYS:HD3	2.15	0.61
1:C:397:ILE:HG21	1:C:426:ILE:HD11	1.82	0.61
1:A:470:ARG:NH1	1:A:470:ARG:HB2	2.15	0.61
1:D:115:MET:SD	1:D:115:MET:C	2.79	0.60
2:C:703:TTP:PA	2:C:703:TTP:O1G	2.60	0.59
1:C:215:HIS:CD2	2:C:703:TTP:C6	2.91	0.59
1:B:422:LEU:HD11	1:B:426:ILE:HD13	1.85	0.58
1:B:466:ILE:H	1:B:466:ILE:HD13	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:GLN:O	1:A:294:LYS:NZ	2.37	0.58
1:B:226:ARG:NH2	1:B:229:VAL:HG21	2.19	0.57
1:C:490:ASP:OD2	1:C:560:LYS:HE2	2.04	0.57
1:D:535:ASN:OD1	1:D:535:ASN:N	2.27	0.56
1:A:596:LYS:N	1:A:596:LYS:CD	2.69	0.56
1:D:473:TYR:OH	5:D:865:HOH:O	2.16	0.56
1:C:206:ARG:NH1	2:C:703:TTP:O2B	2.38	0.56
1:A:321:HIS:CE1	1:D:321:HIS:CE1	2.93	0.56
1:B:354:LYS:NZ	5:B:842:HOH:O	2.39	0.56
1:A:396:TYR:CE2	1:A:437:LYS:HB3	2.41	0.55
1:D:465:GLN:OE1	1:D:465:GLN:HA	2.06	0.55
1:D:390:PHE:CE1	1:D:426:ILE:CD1	2.91	0.54
1:D:395:ASP:OD1	1:D:408:ARG:NH1	2.38	0.53
1:C:235:GLN:O	1:C:238:VAL:HG22	2.09	0.53
1:D:466:ILE:N	1:D:466:ILE:CD1	2.71	0.53
1:D:113:ASP:HB3	1:D:130:PRO:HB3	1.91	0.53
1:C:154:TYR:O	5:C:839:HOH:O	2.18	0.53
1:C:388:ASP:OD2	1:C:392:LYS:HE3	2.10	0.51
1:D:522[A]:CYS:SG	1:B:586:VAL:HG11	2.50	0.51
2:D:703:TTP:H2'1	1:B:157:PHE:CE1	2.45	0.51
1:D:390:PHE:CE1	1:D:426:ILE:HD11	2.40	0.51
1:D:592:THR:OG1	1:D:593:PRO:HD3	2.11	0.51
1:C:327:ASN:O	1:C:328:ASN:HB2	2.11	0.51
1:A:425:ASN:HB2	1:D:428:LEU:HD13	1.93	0.50
1:B:467:LYS:HG3	1:B:468:ILE:N	2.27	0.50
1:C:592:THR:OG1	1:C:593:PRO:HD3	2.12	0.50
1:A:574:ALA:C	1:A:595:LYS:HZ2	2.13	0.50
1:D:466:ILE:HD13	1:D:466:ILE:H	1.77	0.50
1:B:215:HIS:CD2	2:B:705:TTP:C6	2.99	0.50
1:A:396:TYR:CZ	1:A:437:LYS:HB3	2.47	0.50
1:C:295:SER:HB2	5:C:831:HOH:O	2.12	0.50
1:D:467:LYS:HG3	1:D:468:ILE:N	2.26	0.50
2:A:701:TTP:O5'	2:A:701:TTP:O1B	2.29	0.49
1:A:470:ARG:CZ	1:A:470:ARG:CB	2.87	0.49
1:D:499:ILE:HD11	1:D:555:LYS:HE2	1.94	0.49
1:A:315:TYR:CE2	2:A:701:TTP:H5'1	2.47	0.49
1:D:305:ARG:HG2	1:D:305:ARG:NH2	2.27	0.49
1:B:592:THR:OG1	1:B:593:PRO:HD3	2.12	0.49
1:D:351:ALA:O	1:D:520:PHE:HA	2.13	0.49
1:C:186:GLN:HB2	1:C:189:LEU:HD22	1.95	0.49
1:D:186:GLN:HB2	1:D:189:LEU:HD22	1.94	0.49

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:HIS:CE1	2:A:701:TTP:O2A	2.66	0.49
1:A:283:SER:HB2	1:A:284:LEU:C	2.33	0.48
1:D:305:ARG:HH21	1:D:305:ARG:HG2	1.79	0.48
1:A:186:GLN:HB2	1:A:189:LEU:HD22	1.96	0.48
1:C:499:ILE:HD11	1:C:555:LYS:HE2	1.96	0.48
1:A:592:THR:OG1	1:A:593:PRO:HD3	2.13	0.48
1:B:186:GLN:HB2	1:B:189:LEU:HD22	1.95	0.48
1:A:323:LEU:HB3	1:A:325:ILE:HD12	1.96	0.47
1:A:351:ALA:O	1:A:520:PHE:HA	2.14	0.47
1:C:467:LYS:HG3	1:C:468:ILE:N	2.29	0.47
1:A:499:ILE:HD11	1:A:555:LYS:HE2	1.96	0.47
1:A:368:SER:O	1:A:372:ARG:HG3	2.15	0.47
1:D:490:ASP:OD2	1:D:560:LYS:HD3	2.15	0.47
1:D:327:ASN:ND2	1:D:328:ASN:H	2.12	0.47
1:A:332:LYS:HG2	5:A:847:HOH:O	2.14	0.47
1:A:586:VAL:HG11	1:C:522[A]:CYS:SG	2.55	0.47
1:B:351:ALA:O	1:B:520:PHE:HA	2.15	0.47
1:D:215:HIS:CD2	2:D:701:TTP:C6	3.03	0.47
1:C:351:ALA:O	1:C:520:PHE:HA	2.14	0.47
1:D:251:LYS:HB2	1:D:252:PRO:HD3	1.97	0.47
1:D:315:TYR:CE2	2:D:701:TTP:H5'1	2.51	0.46
2:B:705:TTP:O2G	2:B:705:TTP:O2B	2.33	0.46
1:B:327:ASN:ND2	1:B:328:ASN:N	2.61	0.46
1:D:329:PHE:HA	5:D:870:HOH:O	2.14	0.46
1:A:320:CYS:HB3	1:A:325:ILE:O	2.15	0.46
5:A:858:HOH:O	1:C:372:ARG:HD2	2.14	0.46
1:A:428:LEU:HD13	1:D:425:ASN:HB2	1.97	0.46
1:A:467:LYS:HG3	1:A:468:ILE:N	2.30	0.46
1:A:473:TYR:CA	1:A:476:LEU:CD1	2.92	0.45
1:C:251:LYS:HB2	1:C:252:PRO:HD3	1.98	0.45
1:D:352:ARG:HG3	1:D:354:LYS:HG2	1.98	0.45
1:B:499:ILE:HD11	1:B:555:LYS:HE2	1.98	0.45
1:D:320:CYS:HB3	1:D:325:ILE:O	2.16	0.45
1:A:251:LYS:HB2	1:A:252:PRO:HD3	1.99	0.45
1:C:592:THR:N	1:C:593:PRO:CD	2.80	0.45
1:A:328:ASN:ND2	1:A:328:ASN:C	2.65	0.44
1:B:352:ARG:HG3	1:B:354:LYS:HG2	1.99	0.44
1:D:330:ASP:N	5:D:870:HOH:O	1.99	0.44
1:C:489:LEU:CD1	1:C:568:TYR:HE2	2.30	0.44
3:B:706:GTP:O1B	3:B:706:GTP:O3G	2.35	0.44
1:D:129:HIS:CG	1:D:130:PRO:HD2	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:ARG:HA	1:A:473:TYR:CD2	2.52	0.44
1:B:592:THR:N	1:B:593:PRO:CD	2.81	0.44
1:A:265:ILE:O	1:A:269:LYS:HG3	2.18	0.44
1:B:251:LYS:HB2	1:B:252:PRO:HD3	1.99	0.44
2:B:705:TTP:O1B	2:B:705:TTP:O2A	2.36	0.43
1:D:176:GLY:HA3	5:D:849:HOH:O	2.18	0.43
1:D:372:ARG:HD3	1:B:358:ASN:OD1	2.18	0.43
1:D:157:PHE:CE1	2:B:703:TTP:H2'1	2.53	0.43
1:C:129:HIS:CG	1:C:130:PRO:HD2	2.54	0.43
1:C:295:SER:OG	1:C:347:LEU:O	2.36	0.43
1:A:129:HIS:CG	1:A:130:PRO:HD2	2.53	0.43
1:B:226:ARG:NH2	1:B:228:GLU:OE2	2.51	0.43
2:A:703:TTP:O4	1:C:372:ARG:HG2	2.19	0.43
1:C:598:TRP:O	1:C:599:ASN:CB	2.66	0.43
1:C:321:HIS:CE1	1:B:321:HIS:CE1	3.07	0.43
1:B:228:GLU:CD	1:B:229:VAL:CG2	2.70	0.43
1:A:466:ILE:N	1:A:466:ILE:CD1	2.68	0.42
1:A:396:TYR:CE2	1:A:437:LYS:O	2.72	0.42
1:B:598:TRP:O	1:B:599:ASN:CB	2.68	0.42
1:B:129:HIS:CG	1:B:130:PRO:HD2	2.55	0.42
1:B:454:PHE:CD2	1:B:499:ILE:CD1	3.03	0.42
1:B:320:CYS:HB3	1:B:325:ILE:O	2.19	0.42
1:C:598:TRP:O	1:C:599:ASN:HB2	2.20	0.42
1:B:315:TYR:OH	2:B:705:TTP:O3G	2.19	0.41
1:A:469:LYS:HD3	1:A:469:LYS:HA	1.86	0.41
1:D:326:GLN:O	1:D:327:ASN:HB2	2.19	0.41
1:C:454:PHE:CD2	1:C:499:ILE:CD1	3.02	0.41
1:C:475:SER:O	1:C:478:LYS:HB3	2.21	0.41
1:B:226:ARG:NH2	1:B:229:VAL:CG2	2.83	0.41
1:A:525:ALA:HB3	1:C:586:VAL:HG11	2.02	0.41
1:D:390:PHE:CE1	1:D:426:ILE:HD12	2.56	0.41
1:B:480:VAL:HG22	1:B:572:TRP:CD2	2.56	0.41
1:A:435:ASP:HA	1:A:436:PRO:HD3	1.95	0.41
1:C:320:CYS:HB3	1:C:325:ILE:O	2.21	0.41
2:D:703:TTP:H2'1	1:B:157:PHE:CZ	2.56	0.40
1:A:592:THR:N	1:A:593:PRO:CD	2.84	0.40
1:C:428:LEU:HD13	1:B:425:ASN:HB2	2.02	0.40
1:C:425:ASN:HB2	1:B:428:LEU:HD13	2.03	0.40
1:A:476:LEU:HD12	1:A:476:LEU:H	1.86	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:478:LYS:CE	1:D:395:ASP:O[1_454]	2.01	0.19
1:A:395:ASP:OD2	1:B:407:TYR:OH[1_556]	2.13	0.07
1:A:465:GLN:OE1	1:B:543:GLU:OE2[1_455]	2.18	0.02

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	476/514 (93%)	471 (99%)	5 (1%)	0	100	100
1	B	476/514 (93%)	468 (98%)	8 (2%)	0	100	100
1	C	476/514 (93%)	468 (98%)	8 (2%)	0	100	100
1	D	477/514 (93%)	469 (98%)	7 (2%)	1 (0%)	52	73
All	All	1905/2056 (93%)	1876 (98%)	28 (2%)	1 (0%)	56	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	328	ASN

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	426/459 (93%)	405 (95%)	21 (5%)	31	52
1	B	426/459 (93%)	408 (96%)	18 (4%)	36	60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	426/459 (93%)	413 (97%)	13 (3%)	47	73
1	D	427/459 (93%)	403 (94%)	24 (6%)	26	45
All	All	1705/1836 (93%)	1629 (96%)	76 (4%)	34	56

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	184	GLU
1	A	189	LEU
1	A	229	VAL
1	A	283	SER
1	A	284	LEU
1	A	288	LYS
1	A	315	TYR
1	A	327	ASN
1	A	328	ASN
1	A	332	LYS
1	A	339	ARG
1	A	359	LEU
1	A	368	SER
1	A	465	GLN
1	A	466	ILE
1	A	470	ARG
1	A	472	ASP
1	A	492	LYS
1	A	523	LYS
1	A	594	GLN
1	A	596	LYS
1	C	114	THR
1	C	134	ARG
1	C	189	LEU
1	C	255	GLU
1	C	273	VAL
1	C	288	LYS
1	C	315	TYR
1	C	359	LEU
1	C	368	SER
1	C	465	GLN
1	C	492	LYS
1	C	523	LYS
1	C	594	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	114	THR
1	D	189	LEU
1	D	206	ARG
1	D	218	ASP
1	D	228	GLU
1	D	229	VAL
1	D	255	GLU
1	D	273	VAL
1	D	288	LYS
1	D	315	TYR
1	D	326	GLN
1	D	327	ASN
1	D	328	ASN
1	D	359	LEU
1	D	368	SER
1	D	377	LYS
1	D	426	ILE
1	D	465	GLN
1	D	466	ILE
1	D	478	LYS
1	D	492	LYS
1	D	509	MET
1	D	535	ASN
1	D	594	GLN
1	B	115	MET
1	B	189	LEU
1	B	226	ARG
1	B	240	MET
1	B	273	VAL
1	B	288	LYS
1	B	315	TYR
1	B	326	GLN
1	B	327	ASN
1	B	332	LYS
1	B	359	LEU
1	B	368	SER
1	B	426	ILE
1	B	466	ILE
1	B	492	LYS
1	B	511	GLU
1	B	528	ARG
1	B	594	GLN

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

Mol	Chain	Res	Type
1	A	215	HIS
1	A	327	ASN
1	A	328	ASN
1	A	425	ASN
1	C	215	HIS
1	C	326	GLN
1	C	425	ASN
1	D	190	GLN
1	D	327	ASN
1	D	328	ASN
1	D	425	ASN
1	B	233	HIS
1	B	327	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 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	TTP	A	701	-	21,30,30	0.68	0	31,47,47	2.08	5 (16%)
3	GTP	A	702	4	25,34,34	1.11	2 (8%)	34,54,54	1.96	10 (29%)
2	TTP	A	703	4	21,30,30	1.05	2 (9%)	31,47,47	2.18	6 (19%)
3	GTP	B	702	4	25,34,34	1.58	3 (12%)	34,54,54	2.02	10 (29%)
2	TTP	B	703	4	21,30,30	1.07	2 (9%)	31,47,47	1.81	5 (16%)
2	TTP	B	705	-	21,30,30	0.78	1 (4%)	31,47,47	2.13	7 (22%)
3	GTP	B	706	4	25,34,34	1.32	2 (8%)	34,54,54	2.16	9 (26%)
2	TTP	C	701	4	21,30,30	1.24	2 (9%)	31,47,47	2.02	6 (19%)
2	TTP	C	703	-	21,30,30	0.85	1 (4%)	31,47,47	2.22	5 (16%)
2	TTP	D	701	-	21,30,30	0.89	0	31,47,47	2.04	7 (22%)
3	GTP	D	702	4	25,34,34	1.39	4 (16%)	34,54,54	2.01	9 (26%)
2	TTP	D	703	4	21,30,30	0.78	0	31,47,47	2.15	5 (16%)

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	TTP	A	701	-	-	0/18/34/34	0/2/2/2
3	GTP	A	702	4	-	0/18/38/38	0/3/3/3
2	TTP	A	703	4	-	0/18/34/34	0/2/2/2
3	GTP	B	702	4	-	0/18/38/38	0/3/3/3
2	TTP	B	703	4	-	0/18/34/34	0/2/2/2
2	TTP	B	705	-	-	0/18/34/34	0/2/2/2
3	GTP	B	706	4	-	0/18/38/38	0/3/3/3
2	TTP	C	701	4	-	0/18/34/34	0/2/2/2
2	TTP	C	703	-	-	0/18/34/34	0/2/2/2
2	TTP	D	701	-	-	0/18/34/34	0/2/2/2
3	GTP	D	702	4	-	0/18/38/38	0/3/3/3
2	TTP	D	703	4	-	0/18/34/34	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	703	TTP	C6-N1	-2.47	1.31	1.35
2	C	701	TTP	C6-N1	-2.33	1.31	1.35
2	A	703	TTP	C6-N1	-2.31	1.31	1.35
2	A	703	TTP	PG-O2G	-2.20	1.46	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	703	TTP	O4'-C4'	-2.15	1.40	1.45
2	B	703	TTP	O4'-C4'	-2.12	1.40	1.45
2	B	705	TTP	O4'-C4'	-2.09	1.40	1.45
3	D	702	GTP	C2-N2	2.21	1.38	1.34
2	C	701	TTP	O4'-C1'	2.27	1.47	1.42
3	A	702	GTP	C5-C4	2.61	1.46	1.40
3	D	702	GTP	C6-C5	2.64	1.46	1.41
3	B	706	GTP	C6-C5	2.97	1.47	1.41
3	A	702	GTP	C6-C5	3.00	1.47	1.41
3	D	702	GTP	O4'-C1'	3.27	1.45	1.41
3	B	706	GTP	C5-C4	3.46	1.48	1.40
3	B	702	GTP	C5-C4	3.53	1.48	1.40
3	D	702	GTP	C5-C4	3.69	1.48	1.40
3	B	702	GTP	C6-C5	4.09	1.49	1.41
3	B	702	GTP	O4'-C1'	4.72	1.47	1.41

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	703	TTP	C5-C4-N3	-6.43	117.98	125.14
2	C	701	TTP	C5-C4-N3	-6.15	118.30	125.14
2	B	703	TTP	C5-C4-N3	-6.14	118.31	125.14
2	A	701	TTP	C5-C4-N3	-5.72	118.77	125.14
2	D	701	TTP	PB-O3A-PA	-5.71	116.71	132.73
2	C	703	TTP	C5-C4-N3	-5.69	118.80	125.14
2	D	703	TTP	C5-C4-N3	-5.59	118.91	125.14
2	B	705	TTP	PB-O3A-PA	-5.47	117.36	132.73
3	B	702	GTP	C5-C6-N1	-5.28	116.38	123.59
2	A	701	TTP	PB-O3B-PG	-5.22	115.15	132.67
3	B	706	GTP	C5-C6-N1	-5.08	116.64	123.59
2	B	705	TTP	PB-O3B-PG	-5.04	115.77	132.67
2	D	701	TTP	C5-C4-N3	-4.56	120.06	125.14
2	A	701	TTP	PB-O3A-PA	-4.47	120.17	132.73
3	D	702	GTP	C5-C6-N1	-4.44	117.52	123.59
3	A	702	GTP	C5-C6-N1	-4.42	117.55	123.59
2	B	705	TTP	C5-C4-N3	-4.41	120.23	125.14
3	D	702	GTP	PA-O3A-PB	-4.34	120.55	132.73
3	B	706	GTP	PA-O3A-PB	-4.32	120.60	132.73
3	B	706	GTP	N3-C2-N1	-3.95	121.42	127.44
3	D	702	GTP	C6-C5-C4	-3.82	116.33	120.90
3	B	706	GTP	PB-O3B-PG	-3.81	119.90	132.67
2	D	701	TTP	PB-O3B-PG	-3.79	119.95	132.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	703	TTP	PB-O3A-PA	-3.79	122.09	132.73
3	A	702	GTP	PA-O3A-PB	-3.69	122.38	132.73
3	B	702	GTP	PA-O3A-PB	-3.63	122.55	132.73
3	A	702	GTP	N3-C2-N1	-3.46	122.17	127.44
3	D	702	GTP	N3-C2-N1	-3.41	122.25	127.44
3	B	706	GTP	C6-C5-C4	-3.30	116.95	120.90
2	C	703	TTP	PB-O3B-PG	-3.22	121.88	132.67
3	A	702	GTP	C4-C5-N7	-3.11	106.61	109.48
2	A	703	TTP	PB-O3B-PG	-3.03	122.51	132.67
3	B	702	GTP	N3-C2-N1	-2.98	122.91	127.44
3	A	702	GTP	C6-C5-C4	-2.95	117.37	120.90
3	B	702	GTP	C6-C5-C4	-2.81	117.54	120.90
3	D	702	GTP	PB-O3B-PG	-2.69	123.65	132.67
2	D	703	TTP	PB-O3B-PG	-2.69	123.65	132.67
3	B	702	GTP	O3A-PA-O5'	-2.62	95.97	102.94
2	B	703	TTP	PB-O3B-PG	-2.61	123.92	132.67
3	B	702	GTP	PB-O3B-PG	-2.60	123.95	132.67
3	B	702	GTP	C4-C5-N7	-2.55	107.14	109.48
2	D	703	TTP	PB-O3A-PA	-2.47	125.79	132.73
3	B	706	GTP	C4-C5-N7	-2.23	107.43	109.48
2	C	701	TTP	PB-O3B-PG	-2.14	125.49	132.67
3	A	702	GTP	O5'-PA-O1A	-2.09	101.52	109.62
3	A	702	GTP	O2G-PG-O3B	-2.07	95.69	105.09
3	B	702	GTP	C2'-C1'-N9	-2.04	111.17	114.29
2	C	701	TTP	O3G-PG-O1G	2.02	117.09	110.58
3	B	702	GTP	O2B-PB-O3A	2.03	114.31	105.09
2	A	703	TTP	O2B-PB-O1B	2.05	123.62	112.53
3	D	702	GTP	N2-C2-N3	2.05	121.74	117.80
2	A	701	TTP	O3G-PG-O2G	2.07	115.25	107.38
2	B	703	TTP	C2'-C3'-C4'	2.13	107.18	102.77
2	C	703	TTP	O4'-C1'-N1	2.16	111.46	107.72
2	D	701	TTP	O2B-PB-O3A	2.17	114.93	105.09
2	B	705	TTP	O3G-PG-O2G	2.17	115.64	107.38
2	D	701	TTP	C5M-C5-C6	2.17	122.99	118.62
2	D	701	TTP	O4'-C1'-N1	2.20	111.53	107.72
2	B	705	TTP	C2'-C3'-C4'	2.29	107.52	102.77
2	C	701	TTP	O3G-PG-O2G	2.34	116.28	107.38
3	D	702	GTP	O3G-PG-O1G	2.37	118.20	110.58
3	A	702	GTP	N2-C2-N1	2.39	121.15	117.20
2	C	701	TTP	O2A-PA-O1A	2.50	126.07	112.53
2	D	703	TTP	O2G-PG-O1G	2.56	118.81	110.58
3	D	702	GTP	O2B-PB-O3B	2.64	117.08	105.09

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	703	TTP	O3G-PG-O2G	2.73	117.77	107.38
3	B	706	GTP	O2G-PG-O1G	2.79	119.56	110.58
2	B	705	TTP	O3G-PG-O1G	2.88	119.85	110.58
2	A	703	TTP	O3G-PG-O2G	2.93	118.52	107.38
3	A	702	GTP	O2G-PG-O1G	3.04	120.35	110.58
2	A	703	TTP	C2'-C3'-C4'	3.10	109.20	102.77
3	B	706	GTP	N2-C2-N1	3.40	122.82	117.20
2	B	703	TTP	C4-N3-C2	5.10	119.66	115.25
3	B	702	GTP	C6-N1-C2	5.22	123.18	115.94
3	A	702	GTP	C6-N1-C2	5.24	123.22	115.94
2	B	705	TTP	C4-N3-C2	5.45	119.96	115.25
2	D	701	TTP	C4-N3-C2	5.66	120.14	115.25
3	B	706	GTP	C6-N1-C2	5.79	123.98	115.94
3	D	702	GTP	C6-N1-C2	5.91	124.14	115.94
2	A	701	TTP	C4-N3-C2	6.03	120.46	115.25
2	C	701	TTP	C4-N3-C2	6.60	120.95	115.25
2	A	703	TTP	C4-N3-C2	7.17	121.45	115.25
2	C	703	TTP	C4-N3-C2	8.03	122.19	115.25
2	D	703	TTP	C4-N3-C2	8.53	122.62	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	TTP	4	0
2	A	703	TTP	1	0
2	B	703	TTP	1	0
2	B	705	TTP	4	0
3	B	706	GTP	1	0
2	C	701	TTP	1	0
2	C	703	TTP	3	0
2	D	701	TTP	3	0
2	D	703	TTP	3	0

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	480/514 (93%)	0.17	30 (6%)	23	27	27, 51, 102, 144	0
1	B	480/514 (93%)	0.51	57 (11%)	6	6	32, 60, 103, 130	0
1	C	479/514 (93%)	0.24	28 (5%)	26	31	35, 59, 92, 122	0
1	D	480/514 (93%)	0.07	15 (3%)	52	58	27, 48, 82, 116	0
All	All	1919/2056 (93%)	0.25	130 (6%)	20	23	27, 55, 94, 144	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	464	GLY	10.5
1	B	464	GLY	7.5
1	B	488	LEU	6.6
1	B	489	LEU	6.3
1	B	562	LEU	6.2
1	B	483	ALA	6.1
1	B	486	LYS	6.0
1	B	487	VAL	5.5
1	D	284	LEU	4.9
1	C	490	ASP	4.9
1	A	465	GLN	4.8
1	B	485	PRO	4.8
1	C	487	VAL	4.6
1	B	284	LEU	4.6
1	B	563	TYR	4.5
1	C	488	LEU	4.4
1	A	487	VAL	4.3
1	C	284	LEU	4.2
1	D	466	ILE	4.1
1	A	466	ILE	4.1
1	A	326	GLN	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	590	LEU	4.1
1	C	326	GLN	4.0
1	A	590	LEU	4.0
1	C	327	ASN	4.0
1	A	596	LYS	3.9
1	B	490	ASP	3.9
1	C	491	VAL	3.8
1	C	596	LYS	3.8
1	B	590	LEU	3.8
1	A	491	VAL	3.8
1	B	466	ILE	3.8
1	C	230	LYS	3.7
1	A	464	GLY	3.7
1	B	327	ASN	3.7
1	A	473	TYR	3.6
1	B	285	TRP	3.6
1	A	472	ASP	3.6
1	A	489	LEU	3.6
1	B	484	LYS	3.5
1	A	486	LYS	3.5
1	B	469	LYS	3.5
1	A	471	GLU	3.4
1	B	559	ARG	3.3
1	B	492	LYS	3.3
1	A	345	ASN	3.3
1	C	599	ASN	3.3
1	A	488	LEU	3.3
1	A	490	ASP	3.2
1	B	277	GLU	3.2
1	A	328	ASN	3.2
1	A	463	THR	3.2
1	B	457	VAL	3.2
1	B	478	LYS	3.2
1	B	293	ASN	3.1
1	C	325	ILE	3.1
1	D	325	ILE	3.1
1	B	328	ASN	3.1
1	B	591	ILE	3.0
1	B	491	VAL	3.0
1	D	465	GLN	3.0
1	D	262	GLU	3.0
1	B	565	ALA	3.0

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	326	GLN	2.9
1	D	113	ASP	2.9
1	D	559	ARG	2.8
1	C	259	LEU	2.8
1	B	557	VAL	2.8
1	B	496	GLU	2.8
1	B	326	GLN	2.8
1	A	484	LYS	2.8
1	D	599	ASN	2.7
1	C	465	GLN	2.7
1	B	342	GLU	2.7
1	B	190	GLN	2.7
1	A	563	TYR	2.7
1	B	345	ASN	2.7
1	C	593	PRO	2.6
1	B	561	SER	2.6
1	D	327	ASN	2.6
1	B	498	PHE	2.6
1	B	499	ILE	2.6
1	B	262	GLU	2.6
1	C	328	ASN	2.5
1	C	245	ILE	2.5
1	C	288	LYS	2.5
1	B	343	VAL	2.5
1	B	571	GLN	2.5
1	A	283	SER	2.4
1	B	474	GLU	2.4
1	B	588	ALA	2.4
1	C	276	LEU	2.4
1	B	476	LEU	2.4
1	A	344	ASP	2.4
1	B	468	ILE	2.4
1	B	493	LEU	2.3
1	B	482	SER	2.3
1	A	284	LEU	2.3
1	C	262	GLU	2.3
1	B	599	ASN	2.3
1	A	496	GLU	2.3
1	D	328	ASN	2.3
1	B	433	SER	2.3
1	B	560	LYS	2.3
1	A	325	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	285	TRP	2.2
1	B	467	LYS	2.2
1	B	568	TYR	2.2
1	B	587	ILE	2.2
1	C	345	ASN	2.2
1	A	277	GLU	2.2
1	D	320	CYS	2.2
1	C	486	LYS	2.2
1	B	480	VAL	2.1
1	A	396	TYR	2.1
1	A	467	LYS	2.1
1	C	556	LYS	2.1
1	C	322	HIS	2.1
1	B	494	LYS	2.1
1	D	486	LYS	2.1
1	A	528	ARG	2.1
1	A	556	LYS	2.1
1	B	481	ALA	2.1
1	B	452	ASN	2.0
1	B	564	ALA	2.0
1	C	229	VAL	2.0
1	C	260	ILE	2.0
1	C	489	LEU	2.0
1	B	114	THR	2.0
1	D	596	LYS	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
2	TTP	A	701	29/29	0.93	0.16	0.63	41,59,95,101	0
2	TTP	B	705	29/29	0.88	0.17	0.45	49,62,110,118	0
2	TTP	C	703	29/29	0.87	0.16	-0.07	45,68,95,99	0
2	TTP	C	701	29/29	0.98	0.15	-0.30	32,36,44,46	0
2	TTP	D	701	29/29	0.93	0.15	-0.32	38,53,85,109	0
2	TTP	A	703	29/29	0.98	0.13	-0.65	34,38,40,49	0
2	TTP	B	703	29/29	0.99	0.12	-0.85	29,34,40,41	0
3	GTP	A	702	32/32	0.99	0.11	-0.92	31,32,41,42	0
2	TTP	D	703	29/29	0.99	0.14	-0.92	38,45,49,50	0
3	GTP	D	702	32/32	0.98	0.12	-1.26	28,33,42,49	0
3	GTP	B	706	32/32	0.98	0.11	-1.45	36,43,56,57	0
3	GTP	B	702	32/32	0.98	0.09	-2.45	35,39,47,49	0
4	MG	C	704	1/1	0.92	0.11	-	59,59,59,59	0
4	MG	B	701	1/1	0.98	0.06	-	40,40,40,40	0
4	MG	C	702	1/1	0.91	0.06	-	41,41,41,41	0
4	MG	B	704	1/1	0.98	0.06	-	49,49,49,49	0

6.5 Other polymers (i)

There are no such residues in this entry.