Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:15 AM GMT

PDB ID	:	3DZH
Title	:	Crystal structure of human CD38 extracellular domain, GTP complex
Authors	:	Liu, Q.; Kriksunov, I.A.; Jiang, H.; Graeff, R.; Lin, H.; Lee, H.C.; Hao, Q.
Deposited on	:	2008-07-29
Resolution	:	1.60 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 (i) symbol.

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

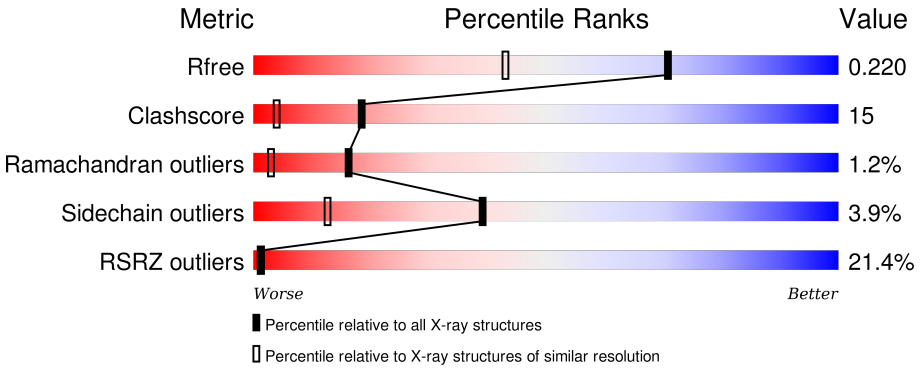
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.60 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	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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 <=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	262	19% 68% 25%
1	B	262	22% 70% 21% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GTP	A	301	-	-	-	X
2	GTP	B	301	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4542 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.

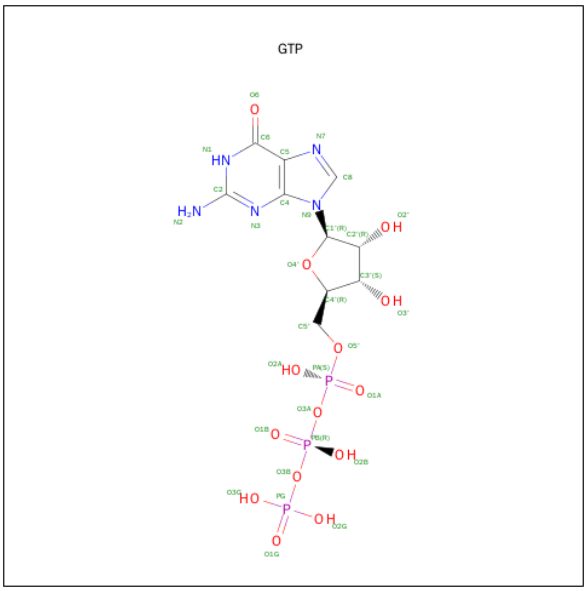
- Molecule 1 is a protein called ADP-ribosyl cyclase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			2050	1290	358	386	16			
1	B	252	Total	C	N	O	S	0	0	0
			2050	1290	358	386	16			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	LYS	-	EXPRESSION TAG	UNP P28907
A	40	ARG	-	EXPRESSION TAG	UNP P28907
A	41	GLU	-	EXPRESSION TAG	UNP P28907
A	42	ALA	-	EXPRESSION TAG	UNP P28907
A	43	GLU	-	EXPRESSION TAG	UNP P28907
A	44	ALA	-	EXPRESSION TAG	UNP P28907
A	49	THR	GLN	ENGINEERED	UNP P28907
A	100	ASP	ASN	ENGINEERED	UNP P28907
A	164	ASP	ASN	ENGINEERED	UNP P28907
A	209	ASP	ASN	ENGINEERED	UNP P28907
A	219	ASP	ASN	ENGINEERED	UNP P28907
B	39	LYS	-	EXPRESSION TAG	UNP P28907
B	40	ARG	-	EXPRESSION TAG	UNP P28907
B	41	GLU	-	EXPRESSION TAG	UNP P28907
B	42	ALA	-	EXPRESSION TAG	UNP P28907
B	43	GLU	-	EXPRESSION TAG	UNP P28907
B	44	ALA	-	EXPRESSION TAG	UNP P28907
B	49	THR	GLN	ENGINEERED	UNP P28907
B	100	ASP	ASN	ENGINEERED	UNP P28907
B	164	ASP	ASN	ENGINEERED	UNP P28907
B	209	ASP	ASN	ENGINEERED	UNP P28907
B	219	ASP	ASN	ENGINEERED	UNP P28907

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 3 is water.

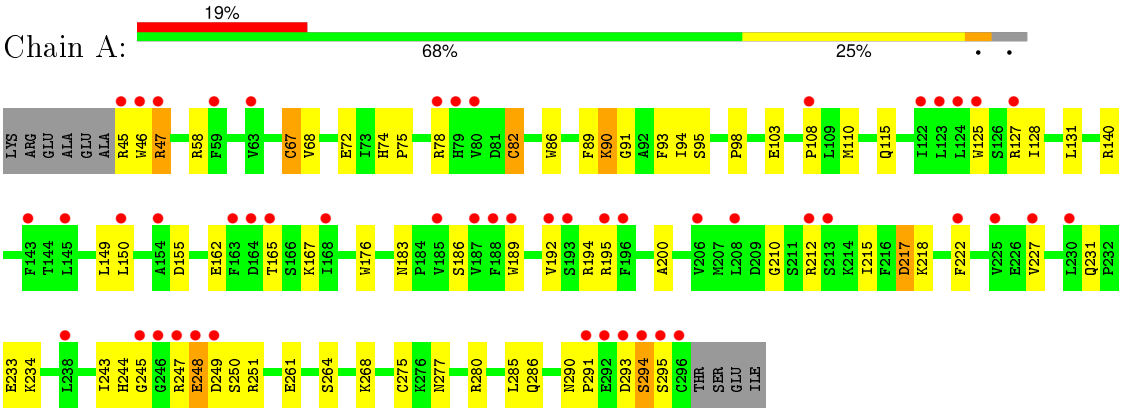
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	199	Total	O	0	0
			199	199		
3	B	179	Total	O	0	0
			179	179		

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.

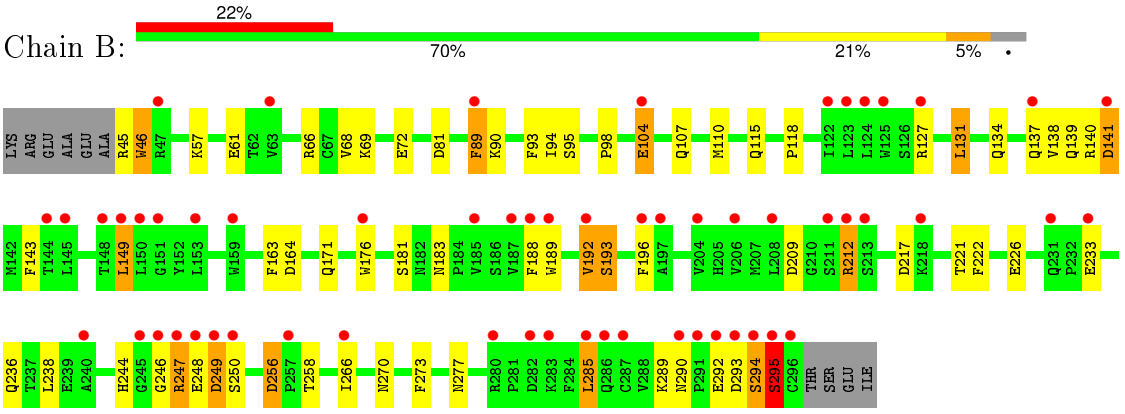
- Molecule 1: ADP-ribosyl cyclase 1

Chain A:



- Molecule 1: ADP-ribosyl cyclase 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	41.68Å 52.65Å 65.23Å 106.14° 91.83° 95.02°	Depositor
Resolution (Å)	20.00 – 1.60 28.06 – 1.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.60) 86.5 (28.06-1.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.64 (at 1.61Å)	Xtriage
Refinement program	REFMAC 5.4.0067	Depositor
R, R_{free}	0.176 , 0.218 0.179 , 0.220	Depositor DCC
R_{free} test set	3345 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	18.4	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 52.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 65992 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4542	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.40% 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

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	1.35	9/2101 (0.4%)	1.26	7/2846 (0.2%)
1	B	1.32	12/2101 (0.6%)	1.22	8/2846 (0.3%)
All	All	1.33	21/4202 (0.5%)	1.24	15/5692 (0.3%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	171	GLN	CG-CD	8.01	1.69	1.51
1	B	57	LYS	CB-CG	-7.47	1.32	1.52
1	A	233	GLU	CG-CD	6.49	1.61	1.51
1	A	82	CYS	CB-SG	6.48	1.93	1.82
1	B	181	SER	CB-OG	-6.38	1.33	1.42
1	B	61	GLU	CG-CD	6.21	1.61	1.51
1	A	67	CYS	CB-SG	-6.12	1.71	1.82
1	B	66	ARG	CZ-NH2	6.09	1.41	1.33
1	B	104	GLU	CG-CD	5.94	1.60	1.51
1	B	196	PHE	CE1-CZ	5.85	1.48	1.37
1	A	275	CYS	CB-SG	-5.64	1.72	1.81
1	A	93	PHE	CG-CD2	5.60	1.47	1.38
1	B	89	PHE	CD2-CE2	5.55	1.50	1.39
1	B	192	VAL	CB-CG1	-5.54	1.41	1.52
1	B	46	TRP	CE3-CZ3	5.45	1.47	1.38
1	A	125	TRP	CE3-CZ3	5.38	1.47	1.38
1	A	222	PHE	CE2-CZ	5.36	1.47	1.37
1	B	193	SER	CA-CB	5.25	1.60	1.52
1	A	189	TRP	CE3-CZ3	5.19	1.47	1.38
1	A	264	SER	CB-OG	5.15	1.49	1.42
1	B	93	PHE	CE2-CZ	5.04	1.47	1.37

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	227	VAL	CA-CB-CG2	-8.18	98.63	110.90
1	B	188	PHE	CB-CG-CD1	-7.69	115.42	120.80
1	B	141	ASP	CB-CG-OD1	-6.68	112.29	118.30
1	B	66	ARG	NE-CZ-NH1	-6.63	116.99	120.30
1	A	140	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	B	81	ASP	CB-CG-OD2	6.22	123.90	118.30
1	B	193	SER	CA-CB-OG	-6.01	94.97	111.20
1	B	57	LYS	CG-CD-CE	5.99	129.85	111.90
1	A	131	LEU	CB-CG-CD1	5.92	121.06	111.00
1	B	188	PHE	CZ-CE2-CD2	-5.57	113.42	120.10
1	A	155	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	217	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	245	GLY	N-CA-C	-5.17	100.18	113.10
1	B	149	LEU	CB-CG-CD2	-5.11	102.32	111.00
1	A	285	LEU	CB-CG-CD1	-5.06	102.40	111.00

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	2050	0	1976	78	0
1	B	2050	0	1978	51	0
2	A	32	0	12	1	0
2	B	32	0	12	0	0
3	A	199	0	0	15	0
3	B	179	0	0	6	0
All	All	4542	0	3978	125	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 15.

All (125) 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:231:GLN:HG3	3:A:367:HOH:O	1.57	1.05
1:B:45:ARG:HD3	3:B:478:HOH:O	1.59	1.00
1:B:176:TRP:HB3	3:B:393:HOH:O	1.66	0.95
1:A:165:THR:HG23	1:A:167:LYS:H	1.33	0.93
1:B:137:GLN:HG2	3:B:388:HOH:O	1.70	0.89
1:A:115:GLN:HE22	1:A:149:LEU:H	1.23	0.87
1:B:127:ARG:HH11	1:B:212:ARG:HD2	1.41	0.85
1:A:128:ILE:HD13	1:A:243:ILE:HG13	1.58	0.85
1:A:261:GLU:HG3	1:B:163:PHE:HZ	1.45	0.82
1:B:290:ASN:HB3	1:B:293:ASP:HB2	1.61	0.81
1:B:238:LEU:HB3	1:B:266:ILE:HD13	1.63	0.81
1:B:115:GLN:HE22	1:B:149:LEU:H	1.24	0.81
1:A:127:ARG:HD2	3:A:429:HOH:O	1.81	0.80
1:A:128:ILE:CD1	1:A:243:ILE:HG13	2.12	0.78
1:A:176:TRP:HH2	3:A:481:HOH:O	1.65	0.78
1:A:110:MET:HE1	1:A:150:LEU:HD13	1.66	0.77
1:A:212:ARG:HD3	3:A:344:HOH:O	1.82	0.77
1:A:127:ARG:CB	1:A:212:ARG:HE	2.04	0.71
1:A:261:GLU:HG3	1:B:163:PHE:CZ	2.26	0.70
1:A:212:ARG:HG2	1:A:212:ARG:HH11	1.57	0.70
1:A:127:ARG:HG2	1:A:212:ARG:HE	1.58	0.69
1:A:127:ARG:CG	1:A:212:ARG:HE	2.04	0.69
1:A:110:MET:HE1	1:A:192:VAL:HG12	1.74	0.69
1:A:290:ASN:O	1:A:293:ASP:HB2	1.93	0.68
1:A:162:GLU:HB2	1:A:165:THR:HG22	1.75	0.66
1:A:244:HIS:HE1	1:A:277:ASN:OD1	1.79	0.66
1:A:195:ARG:HD3	3:A:426:HOH:O	1.95	0.66
1:A:127:ARG:CD	3:A:429:HOH:O	2.42	0.65
1:A:128:ILE:HD11	1:A:243:ILE:HG21	1.79	0.63
1:B:115:GLN:NE2	1:B:149:LEU:H	1.95	0.63
1:A:127:ARG:HG2	1:A:212:ARG:NE	2.13	0.63
1:A:183:ASN:HD21	1:A:186:SER:H	1.47	0.62
1:B:127:ARG:HD3	1:B:212:ARG:NH1	2.14	0.62
1:B:246:GLY:O	1:B:247:ARG:C	2.38	0.60
1:A:162:GLU:OE2	1:A:165:THR:HG21	2.02	0.60
1:A:127:ARG:NE	3:A:429:HOH:O	2.35	0.60
1:B:256:ASP:OD1	1:B:258:THR:N	2.34	0.60
1:A:127:ARG:NH1	1:A:217:ASP:OD2	2.34	0.60
1:A:45:ARG:HA	3:A:392:HOH:O	2.02	0.59
1:A:183:ASN:ND2	1:A:186:SER:H	2.00	0.59
1:A:127:ARG:NH2	1:A:217:ASP:OD2	2.36	0.58
1:A:127:ARG:HB3	1:A:212:ARG:HE	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:MET:CE	1:A:192:VAL:HG12	2.33	0.58
1:A:128:ILE:CD1	1:A:243:ILE:CG1	2.81	0.58
1:B:90:LYS:HG2	1:B:94:ILE:HG13	1.84	0.58
1:A:261:GLU:CG	1:B:163:PHE:HZ	2.15	0.57
1:B:244:HIS:HE1	1:B:277:ASN:OD1	1.87	0.57
1:B:104:GLU:HA	1:B:107:GLN:HG2	1.86	0.57
1:A:86:TRP:CZ2	1:A:90:LYS:HG3	2.39	0.57
1:B:45:ARG:HG3	1:B:46:TRP:H	1.70	0.56
1:A:115:GLN:NE2	1:A:149:LEU:H	1.99	0.56
1:A:294:SER:O	1:A:295:SER:OG	2.08	0.56
1:B:45:ARG:HG3	1:B:46:TRP:N	2.20	0.56
1:B:90:LYS:CG	1:B:94:ILE:HG13	2.35	0.56
1:B:266:ILE:HD11	1:B:273:PHE:HB2	1.89	0.55
1:B:98:PRO:O	1:B:183:ASN:HA	2.06	0.55
1:A:286:GLN:NE2	1:A:290:ASN:HD22	2.04	0.54
1:A:110:MET:HE1	1:A:192:VAL:CG1	2.38	0.53
1:A:45:ARG:HG2	1:A:46:TRP:N	2.24	0.52
1:A:294:SER:C	1:A:295:SER:HG	2.08	0.52
1:A:47:ARG:O	1:A:47:ARG:HG2	2.10	0.52
1:A:68:VAL:O	1:A:72:GLU:HG3	2.10	0.51
1:B:110:MET:CE	1:B:192:VAL:HG12	2.40	0.51
1:A:291:PRO:C	1:A:293:ASP:H	2.13	0.51
1:A:45:ARG:HG2	1:A:46:TRP:H	1.75	0.51
1:A:194:ARG:HD2	3:A:414:HOH:O	2.10	0.51
1:B:189:TRP:O	1:B:193:SER:HB2	2.12	0.50
1:A:290:ASN:HB3	1:A:293:ASP:OD2	2.11	0.50
1:A:212:ARG:HG2	1:A:212:ARG:NH1	2.25	0.50
1:B:293:ASP:O	1:B:294:SER:C	2.51	0.49
1:A:268:LYS:NZ	1:B:95:SER:O	2.25	0.49
1:A:200:ALA:O	1:A:234:LYS:HE3	2.12	0.49
1:A:127:ARG:C	3:A:360:HOH:O	2.50	0.49
1:B:110:MET:SD	1:B:192:VAL:HG12	2.53	0.49
1:A:176:TRP:CH2	3:A:481:HOH:O	2.50	0.48
1:A:103:GLU:OE1	1:A:194:ARG:NH1	2.36	0.48
1:B:209:ASP:OD2	1:B:212:ARG:NE	2.39	0.48
1:B:233:GLU:CD	1:B:233:GLU:H	2.17	0.48
1:B:193:SER:OG	1:B:221:THR:HG21	2.13	0.48
1:B:68:VAL:O	1:B:72:GLU:HG3	2.13	0.48
1:A:45:ARG:HD3	1:A:47:ARG:O	2.13	0.48
1:A:248:GLU:HG2	1:A:280:ARG:NH2	2.29	0.47
1:B:45:ARG:HB2	3:B:478:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:SER:O	1:B:295:SER:C	2.52	0.47
1:A:91:GLY:HA3	3:A:356:HOH:O	2.14	0.47
1:B:139:GLN:C	1:B:141:ASP:H	2.18	0.47
1:A:251:ARG:HD3	1:A:251:ARG:H	1.80	0.47
1:B:266:ILE:HD11	1:B:273:PHE:CB	2.45	0.46
1:A:195:ARG:HG3	3:A:382:HOH:O	2.15	0.46
1:A:46:TRP:HE1	1:A:47:ARG:NH1	2.13	0.46
1:A:128:ILE:HD13	1:A:243:ILE:CG1	2.35	0.46
1:B:266:ILE:HD11	1:B:273:PHE:CA	2.46	0.46
1:A:261:GLU:CG	1:B:163:PHE:CZ	2.93	0.46
1:A:210:GLY:HA2	1:A:215:ILE:HG12	1.98	0.46
1:A:94:ILE:O	1:A:95:SER:HB2	2.16	0.45
1:A:110:MET:CE	1:A:150:LEU:HD13	2.42	0.45
1:A:128:ILE:CD1	1:A:243:ILE:CB	2.94	0.45
1:B:94:ILE:HD12	1:B:94:ILE:HG23	1.53	0.45
1:B:118:PRO:HD2	1:B:143:PHE:CE2	2.52	0.45
1:A:45:ARG:NH1	1:A:47:ARG:O	2.48	0.45
1:A:248:GLU:HG2	1:A:280:ARG:HH21	1.81	0.45
1:A:98:PRO:O	1:A:183:ASN:HA	2.17	0.45
1:B:69:LYS:NZ	3:B:473:HOH:O	2.49	0.45
1:A:75:PRO:HA	1:A:78:ARG:HG3	2.00	0.44
1:B:137:GLN:NE2	3:B:471:HOH:O	2.50	0.44
1:B:217:ASP:C	1:B:217:ASP:OD1	2.54	0.44
1:B:138:VAL:HG21	1:B:289:LYS:HG2	1.99	0.44
1:A:244:HIS:HD2	1:A:250:SER:CB	2.30	0.44
1:A:110:MET:CE	1:A:192:VAL:CG1	2.95	0.43
2:A:301:GTP:PG	3:A:471:HOH:O	2.75	0.43
1:B:248:GLU:HG3	1:B:249:ASP:H	1.83	0.43
1:A:67:CYS:C	1:A:82:CYS:SG	2.98	0.43
1:B:164:ASP:OD1	1:B:164:ASP:N	2.45	0.42
1:A:128:ILE:HD12	1:A:243:ILE:HB	2.00	0.42
1:A:74:HIS:HA	1:A:75:PRO:HD2	1.96	0.42
1:B:134:GLN:HE21	1:B:285:LEU:HD11	1.84	0.41
1:B:212:ARG:HD3	1:B:212:ARG:HA	1.89	0.41
1:A:244:HIS:HD2	1:A:250:SER:HB2	1.85	0.41
1:B:222:PHE:HA	1:B:226:GLU:HB2	2.02	0.41
1:B:266:ILE:HD11	1:B:273:PHE:HA	2.03	0.41
1:B:110:MET:CE	1:B:192:VAL:CG1	2.98	0.41
1:A:212:ARG:CD	3:A:344:HOH:O	2.54	0.40
1:A:127:ARG:CG	1:A:212:ARG:NE	2.76	0.40
1:B:131:LEU:O	1:B:131:LEU:HD22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ARG:HD3	1:A:58:ARG:HH11	1.74	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	250/262 (95%)	237 (95%)	11 (4%)	2 (1%)	24 6
1	B	250/262 (95%)	238 (95%)	8 (3%)	4 (2%)	12 2
All	All	500/524 (95%)	475 (95%)	19 (4%)	6 (1%)	16 3

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	SER
1	B	249	ASP
1	B	294	SER
1	B	295	SER
1	A	247	ARG
1	B	247	ARG

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	233/241 (97%)	226 (97%)	7 (3%)	48 19
1	B	233/241 (97%)	222 (95%)	11 (5%)	32 9
All	All	466/482 (97%)	448 (96%)	18 (4%)	39 13

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	89	PHE
1	A	90	LYS
1	A	108	PRO
1	A	218	LYS
1	A	248	GLU
1	A	249	ASP
1	B	89	PHE
1	B	131	LEU
1	B	140	ARG
1	B	212	ARG
1	B	236	GLN
1	B	250	SER
1	B	256	ASP
1	B	270	ASN
1	B	285	LEU
1	B	292	GLU
1	B	295	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	134	GLN
1	A	137	GLN
1	A	183	ASN
1	A	244	HIS
1	A	286	GLN
1	A	290	ASN
1	B	83	GLN
1	B	115	GLN
1	B	134	GLN
1	B	229	ASN
1	B	231	GLN

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Mol	Chain	Res	Type
1	B	244	HIS
1	B	270	ASN

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

2 ligands are modelled in this entry.

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	GTP	A	301	-	25,34,34	1.29	3 (12%)	34,54,54	2.49	15 (44%)
2	GTP	B	301	-	25,34,34	1.41	3 (12%)	34,54,54	2.73	14 (41%)

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	GTP	A	301	-	-	0/18/38/38	0/3/3/3
2	GTP	B	301	-	-	0/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	GTP	C6-C5	-3.96	1.33	1.41
2	B	301	GTP	C4-N3	-3.35	1.30	1.35
2	A	301	GTP	C6-C5	-3.30	1.34	1.41
2	A	301	GTP	C2'-C3'	-2.59	1.46	1.53
2	A	301	GTP	C8-N7	2.72	1.39	1.34
2	B	301	GTP	C2-N1	2.95	1.40	1.35

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	GTP	PA-O3A-PB	-6.23	115.23	132.73
2	A	301	GTP	PA-O3A-PB	-6.22	115.27	132.73
2	B	301	GTP	C1'-N9-C4	-5.99	117.91	126.94
2	A	301	GTP	C1'-N9-C4	-5.83	118.14	126.94
2	B	301	GTP	N3-C2-N1	-5.66	118.82	127.44
2	A	301	GTP	PB-O3B-PG	-4.39	117.93	132.67
2	B	301	GTP	O3'-C3'-C2'	-4.10	98.51	111.83
2	A	301	GTP	N3-C2-N1	-3.96	121.41	127.44
2	B	301	GTP	PB-O3B-PG	-3.81	119.89	132.67
2	A	301	GTP	C2'-C3'-C4'	-3.41	95.60	102.61
2	B	301	GTP	C2'-C1'-N9	-3.34	109.18	114.29
2	A	301	GTP	O3'-C3'-C2'	-3.15	101.57	111.83
2	A	301	GTP	C4'-O4'-C1'	-3.08	106.33	109.72
2	A	301	GTP	C4-C5-N7	-2.81	106.89	109.48
2	B	301	GTP	C5-C6-N1	-2.74	119.84	123.59
2	B	301	GTP	N2-C2-N1	-2.65	112.82	117.20
2	A	301	GTP	C2'-C1'-N9	-2.49	110.49	114.29
2	A	301	GTP	C5-C6-N1	-2.39	120.32	123.59
2	A	301	GTP	C6-C5-C4	-2.05	118.44	120.90
2	B	301	GTP	O2A-PA-O3A	2.16	114.89	105.09
2	A	301	GTP	O2A-PA-O3A	2.56	116.71	105.09
2	B	301	GTP	O3'-C3'-C4'	2.69	119.12	111.05
2	B	301	GTP	O3G-PG-O3B	2.71	117.41	105.09
2	A	301	GTP	O3A-PA-O5'	2.76	110.27	102.94
2	A	301	GTP	N2-C2-N3	2.95	123.46	117.80
2	B	301	GTP	O3A-PA-O5'	3.00	110.89	102.94
2	A	301	GTP	C6-N1-C2	3.36	120.60	115.94
2	B	301	GTP	C6-N1-C2	3.62	120.96	115.94
2	B	301	GTP	N2-C2-N3	5.48	128.32	117.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	GTP	1	0

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, 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	252/262 (96%)	1.15	50 (19%) 1 1	22, 26, 38, 54	0
1	B	252/262 (96%)	1.36	58 (23%) 1 1	22, 27, 42, 58	0
All	All	504/524 (96%)	1.25	108 (21%) 1 1	22, 27, 41, 58	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	247	ARG	12.2
1	B	295	SER	11.0
1	A	249	ASP	10.9
1	B	291	PRO	9.1
1	B	246	GLY	8.4
1	B	293	ASP	7.5
1	A	246	GLY	7.4
1	B	213	SER	6.8
1	A	294	SER	6.6
1	B	248	GLU	6.2
1	A	248	GLU	6.1
1	B	176	TRP	5.9
1	B	294	SER	5.9
1	B	292	GLU	5.7
1	B	249	ASP	5.4
1	B	296	CYS	5.4
1	B	290	ASN	5.2
1	A	124	LEU	4.9
1	A	47	ARG	4.8
1	B	282	ASP	4.5
1	A	247	ARG	4.4
1	A	293	ASP	4.3
1	A	79	HIS	4.3
1	B	189	TRP	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	212	ARG	4.1
1	A	123	LEU	4.1
1	B	245	GLY	4.0
1	A	78	ARG	3.7
1	B	211	SER	3.6
1	A	143	PHE	3.6
1	B	123	LEU	3.6
1	A	80	VAL	3.5
1	A	206	VAL	3.5
1	B	124	LEU	3.5
1	A	145	LEU	3.4
1	B	145	LEU	3.4
1	A	245	GLY	3.4
1	B	153	LEU	3.4
1	A	189	TRP	3.3
1	A	213	SER	3.2
1	B	204	VAL	3.1
1	A	212	ARG	3.1
1	B	150	LEU	3.1
1	B	287	CYS	3.1
1	A	122	ILE	3.1
1	A	291	PRO	3.1
1	A	225	VAL	3.0
1	B	196	PHE	3.0
1	B	285	LEU	3.0
1	B	104	GLU	3.0
1	B	250	SER	2.9
1	A	125	TRP	2.9
1	A	296	CYS	2.9
1	B	208	LEU	2.8
1	A	165	THR	2.8
1	B	127	ARG	2.8
1	A	127	ARG	2.7
1	B	144	THR	2.7
1	A	150	LEU	2.7
1	B	149	LEU	2.7
1	B	257	PRO	2.7
1	B	188	PHE	2.6
1	B	125	TRP	2.6
1	B	192	VAL	2.6
1	A	187	VAL	2.6
1	A	227	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	222	PHE	2.6
1	B	206	VAL	2.5
1	A	185	VAL	2.5
1	B	283	LYS	2.5
1	A	208	LEU	2.5
1	A	196	PHE	2.5
1	A	164	ASP	2.4
1	A	168	ILE	2.4
1	B	159	TRP	2.4
1	B	240	ALA	2.4
1	A	195	ARG	2.4
1	B	141	ASP	2.4
1	B	151	GLY	2.3
1	B	280	ARG	2.3
1	B	89	PHE	2.3
1	B	148	THR	2.3
1	B	187	VAL	2.3
1	A	292	GLU	2.3
1	A	238	LEU	2.3
1	B	218	LYS	2.3
1	A	45	ARG	2.3
1	A	230	LEU	2.2
1	A	193	SER	2.2
1	A	295	SER	2.2
1	B	286	GLN	2.2
1	A	192	VAL	2.2
1	B	47	ARG	2.2
1	A	188	PHE	2.1
1	B	197	ALA	2.1
1	B	266	ILE	2.1
1	A	46	TRP	2.1
1	A	108	PRO	2.1
1	B	63	VAL	2.1
1	B	185	VAL	2.1
1	A	59	PHE	2.1
1	A	154	ALA	2.1
1	B	137	GLN	2.1
1	A	63	VAL	2.1
1	A	163	PHE	2.1
1	B	122	ILE	2.0
1	B	233	GLU	2.0
1	B	231	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	GTP	A	301	32/32	0.77	0.26	2.15	21,36,83,84	0
2	GTP	B	301	32/32	0.82	0.24	2.03	18,34,82,85	0

6.5 Other polymers (i)

There are no such residues in this entry.