



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 12:57 PM GMT

PDB ID : 3VQT  
Title : Crystal structure analysis of the translation factor RF3  
Authors : Kihira, K.; Shomura, Y.; Shibata, N.; Kitamura, M.; Higuchi, Y.  
Deposited on : 2012-03-30  
Resolution : 1.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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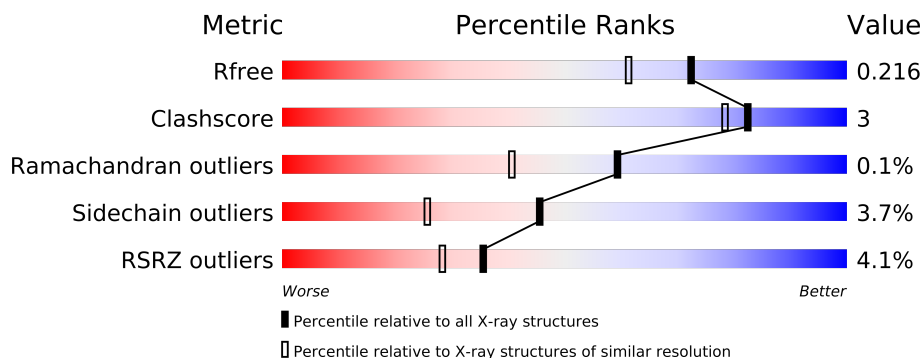
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.80 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))
$R_{free}$	66092	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	548	
1	B	548	
1	C	548	
1	D	548	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16607 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Peptide chain release factor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	0	0
			3899	2471	683	724	21			
1	B	490	Total	C	N	O	S	0	0	0
			3860	2451	674	715	20			
1	C	491	Total	C	N	O	S	0	0	0
			3869	2456	675	718	20			
1	D	494	Total	C	N	O	S	0	0	0
			3900	2471	686	723	20			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	EXPRESSION TAG	UNP B8DIL5
A	-17	SER	-	EXPRESSION TAG	UNP B8DIL5
A	-16	SER	-	EXPRESSION TAG	UNP B8DIL5
A	-15	HIS	-	EXPRESSION TAG	UNP B8DIL5
A	-14	HIS	-	EXPRESSION TAG	UNP B8DIL5
A	-13	HIS	-	EXPRESSION TAG	UNP B8DIL5
A	-12	HIS	-	EXPRESSION TAG	UNP B8DIL5
A	-11	HIS	-	EXPRESSION TAG	UNP B8DIL5
A	-10	HIS	-	EXPRESSION TAG	UNP B8DIL5
A	-9	SER	-	EXPRESSION TAG	UNP B8DIL5
A	-8	SER	-	EXPRESSION TAG	UNP B8DIL5
A	-7	GLY	-	EXPRESSION TAG	UNP B8DIL5
A	-6	LEU	-	EXPRESSION TAG	UNP B8DIL5
A	-5	VAL	-	EXPRESSION TAG	UNP B8DIL5
A	-4	PRO	-	EXPRESSION TAG	UNP B8DIL5
A	-3	ARG	-	EXPRESSION TAG	UNP B8DIL5
A	-2	GLY	-	EXPRESSION TAG	UNP B8DIL5
A	-1	SER	-	EXPRESSION TAG	UNP B8DIL5
A	0	HIS	-	EXPRESSION TAG	UNP B8DIL5
B	-18	GLY	-	EXPRESSION TAG	UNP B8DIL5
B	-17	SER	-	EXPRESSION TAG	UNP B8DIL5

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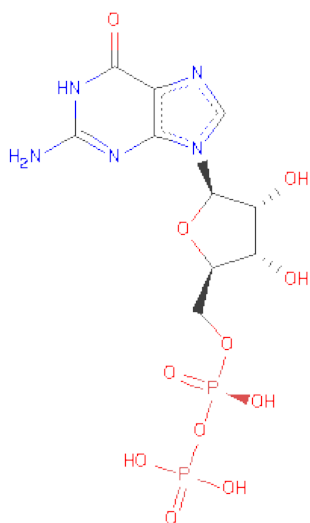
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	EXPRESSION TAG	UNP B8DIL5
B	-15	HIS	-	EXPRESSION TAG	UNP B8DIL5
B	-14	HIS	-	EXPRESSION TAG	UNP B8DIL5
B	-13	HIS	-	EXPRESSION TAG	UNP B8DIL5
B	-12	HIS	-	EXPRESSION TAG	UNP B8DIL5
B	-11	HIS	-	EXPRESSION TAG	UNP B8DIL5
B	-10	HIS	-	EXPRESSION TAG	UNP B8DIL5
B	-9	SER	-	EXPRESSION TAG	UNP B8DIL5
B	-8	SER	-	EXPRESSION TAG	UNP B8DIL5
B	-7	GLY	-	EXPRESSION TAG	UNP B8DIL5
B	-6	LEU	-	EXPRESSION TAG	UNP B8DIL5
B	-5	VAL	-	EXPRESSION TAG	UNP B8DIL5
B	-4	PRO	-	EXPRESSION TAG	UNP B8DIL5
B	-3	ARG	-	EXPRESSION TAG	UNP B8DIL5
B	-2	GLY	-	EXPRESSION TAG	UNP B8DIL5
B	-1	SER	-	EXPRESSION TAG	UNP B8DIL5
B	0	HIS	-	EXPRESSION TAG	UNP B8DIL5
C	-18	GLY	-	EXPRESSION TAG	UNP B8DIL5
C	-17	SER	-	EXPRESSION TAG	UNP B8DIL5
C	-16	SER	-	EXPRESSION TAG	UNP B8DIL5
C	-15	HIS	-	EXPRESSION TAG	UNP B8DIL5
C	-14	HIS	-	EXPRESSION TAG	UNP B8DIL5
C	-13	HIS	-	EXPRESSION TAG	UNP B8DIL5
C	-12	HIS	-	EXPRESSION TAG	UNP B8DIL5
C	-11	HIS	-	EXPRESSION TAG	UNP B8DIL5
C	-10	HIS	-	EXPRESSION TAG	UNP B8DIL5
C	-9	SER	-	EXPRESSION TAG	UNP B8DIL5
C	-8	SER	-	EXPRESSION TAG	UNP B8DIL5
C	-7	GLY	-	EXPRESSION TAG	UNP B8DIL5
C	-6	LEU	-	EXPRESSION TAG	UNP B8DIL5
C	-5	VAL	-	EXPRESSION TAG	UNP B8DIL5
C	-4	PRO	-	EXPRESSION TAG	UNP B8DIL5
C	-3	ARG	-	EXPRESSION TAG	UNP B8DIL5
C	-2	GLY	-	EXPRESSION TAG	UNP B8DIL5
C	-1	SER	-	EXPRESSION TAG	UNP B8DIL5
C	0	HIS	-	EXPRESSION TAG	UNP B8DIL5
D	-18	GLY	-	EXPRESSION TAG	UNP B8DIL5
D	-17	SER	-	EXPRESSION TAG	UNP B8DIL5
D	-16	SER	-	EXPRESSION TAG	UNP B8DIL5
D	-15	HIS	-	EXPRESSION TAG	UNP B8DIL5
D	-14	HIS	-	EXPRESSION TAG	UNP B8DIL5
D	-13	HIS	-	EXPRESSION TAG	UNP B8DIL5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	EXPRESSION TAG	UNP B8DIL5
D	-11	HIS	-	EXPRESSION TAG	UNP B8DIL5
D	-10	HIS	-	EXPRESSION TAG	UNP B8DIL5
D	-9	SER	-	EXPRESSION TAG	UNP B8DIL5
D	-8	SER	-	EXPRESSION TAG	UNP B8DIL5
D	-7	GLY	-	EXPRESSION TAG	UNP B8DIL5
D	-6	LEU	-	EXPRESSION TAG	UNP B8DIL5
D	-5	VAL	-	EXPRESSION TAG	UNP B8DIL5
D	-4	PRO	-	EXPRESSION TAG	UNP B8DIL5
D	-3	ARG	-	EXPRESSION TAG	UNP B8DIL5
D	-2	GLY	-	EXPRESSION TAG	UNP B8DIL5
D	-1	SER	-	EXPRESSION TAG	UNP B8DIL5
D	0	HIS	-	EXPRESSION TAG	UNP B8DIL5

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 3 is water.

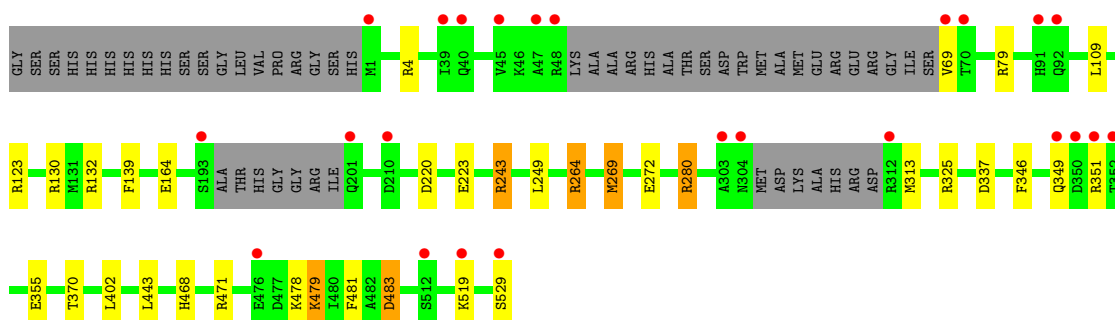
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	266	Total 266	O 266	0	0
3	B	227	Total 227	O 227	0	0
3	C	224	Total 224	O 224	0	0
3	D	250	Total 250	O 250	0	0

### 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.

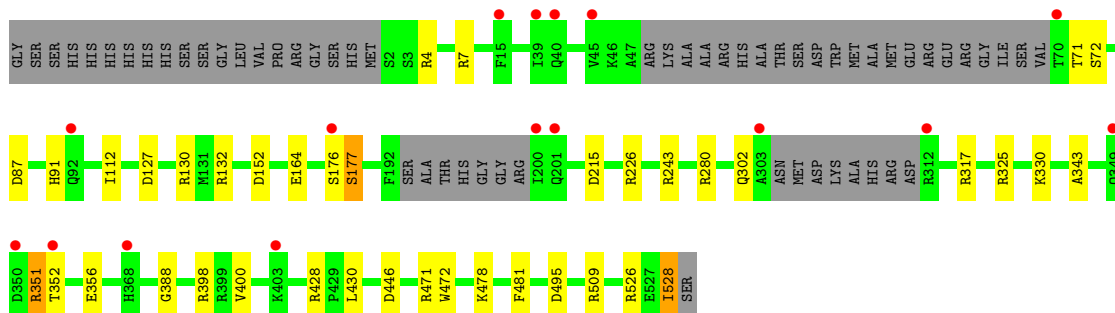
- Molecule 1: Peptide chain release factor 3

Chain A:



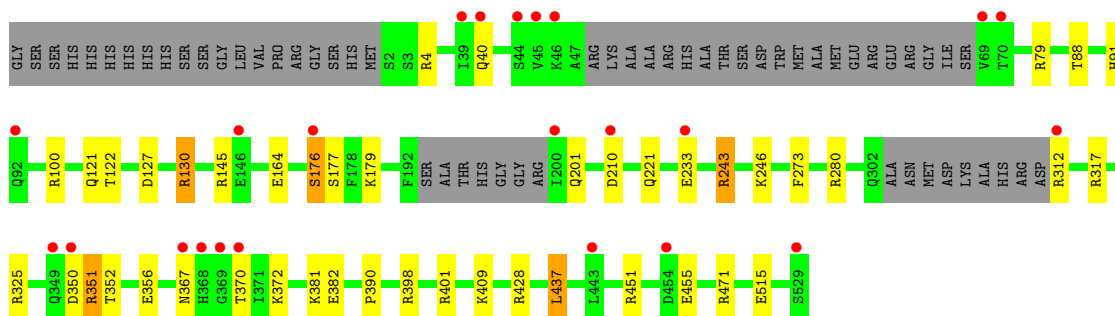
- Molecule 1: Peptide chain release factor 3

Chain B:



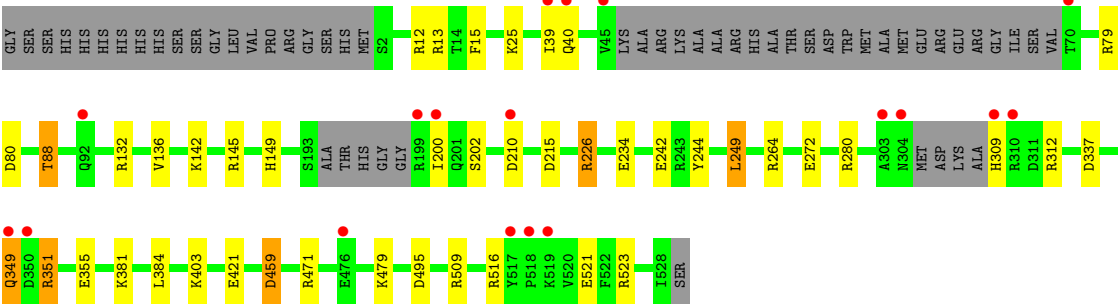
- Molecule 1: Peptide chain release factor 3

Chain C:



● Molecule 1: Peptide chain release factor 3

Chain D: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.39Å 82.80Å 148.29Å 104.21° 89.78° 89.63°	Depositor
Resolution (Å)	33.87 – 1.80 33.86 – 1.80	Depositor EDS
% Data completeness (in resolution range)	93.5 (33.87-1.80) 93.5 (33.86-1.80)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.52 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.177 , 0.218 0.178 , 0.216	Depositor DCC
$R_{free}$ test set	9597 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.2	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 48.8	EDS
Estimated twinning fraction	0.026 for h,-k,-l 0.037 for -h,k,-k-l 0.003 for -h,-k,k+l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 189405 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16607	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP

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	1.05	3/3978 (0.1%)	0.98	10/5376 (0.2%)
1	B	1.04	4/3939 (0.1%)	0.99	10/5326 (0.2%)
1	C	1.06	4/3948 (0.1%)	1.09	17/5337 (0.3%)
1	D	1.07	3/3980 (0.1%)	1.00	14/5381 (0.3%)
All	All	1.06	14/15845 (0.1%)	1.02	51/21420 (0.2%)

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	C	0	1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	479	LYS	CE-NZ	10.05	1.74	1.49
1	B	176	SER	CB-OG	8.60	1.53	1.42
1	C	176	SER	CB-OG	-7.89	1.31	1.42
1	C	177	SER	N-CA	7.18	1.60	1.46
1	C	176	SER	CA-CB	7.03	1.63	1.52
1	A	519	LYS	N-CA	6.00	1.58	1.46
1	C	273	PHE	CE2-CZ	5.96	1.48	1.37
1	B	472	TRP	CE3-CZ3	5.62	1.48	1.38
1	B	400	VAL	CB-CG2	-5.35	1.41	1.52
1	D	136	VAL	CB-CG1	5.35	1.64	1.52
1	A	139	PHE	CD1-CE1	5.25	1.49	1.39
1	D	242	GLU	CB-CG	5.13	1.61	1.52
1	B	177	SER	N-CA	5.12	1.56	1.46
1	D	244	TYR	CE1-CZ	5.06	1.45	1.38

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	100	ARG	NE-CZ-NH1	20.65	130.62	120.30
1	C	100	ARG	NE-CZ-NH2	-16.62	111.99	120.30
1	C	130	ARG	NE-CZ-NH2	-12.58	114.01	120.30
1	C	130	ARG	NE-CZ-NH1	10.58	125.59	120.30
1	D	249	LEU	CA-CB-CG	10.57	139.62	115.30
1	B	471	ARG	NE-CZ-NH1	9.81	125.20	120.30
1	C	210	ASP	CB-CG-OD1	9.77	127.09	118.30
1	B	471	ARG	NE-CZ-NH2	-9.19	115.70	120.30
1	B	398	ARG	NE-CZ-NH1	8.97	124.78	120.30
1	B	317	ARG	NE-CZ-NH2	-8.79	115.91	120.30
1	D	471	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	C	317	ARG	NE-CZ-NH2	-8.37	116.12	120.30
1	D	264	ARG	NE-CZ-NH1	8.31	124.46	120.30
1	D	132	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	C	437	LEU	CB-CG-CD1	7.14	123.14	111.00
1	A	313	MET	CG-SD-CE	-6.98	89.04	100.20
1	C	100	ARG	CD-NE-CZ	6.88	133.23	123.60
1	D	280	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	C	210	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	C	79	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	D	280	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	4	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	A	351	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	D	145	ARG	CG-CD-NE	-6.04	99.11	111.80
1	A	123	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	C	471	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	C	372	LYS	CD-CE-NZ	5.76	124.96	111.70
1	B	428	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	A	280	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	C	317	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	C	398	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	D	495	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	B	495	ASP	CB-CG-OD2	5.54	123.29	118.30
1	D	471	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	D	226	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	C	243	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	D	15	PHE	CB-CG-CD2	5.38	124.56	120.80
1	C	176	SER	N-CA-CB	-5.37	102.44	110.50
1	A	109	LEU	CB-CG-CD2	-5.30	101.99	111.00
1	D	13	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	D	384	LEU	CB-CG-CD1	-5.24	102.10	111.00
1	B	87	ASP	CB-CG-OD2	-5.23	113.59	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	12	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	A	471	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	130	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	351	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	243	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	C	471	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	249	LEU	CB-CG-CD1	-5.05	102.41	111.00
1	B	509	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	B	398	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	351	ARG	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3899	0	0	13	0
1	B	3860	0	0	13	1
1	C	3869	0	0	12	0
1	D	3900	0	0	13	0
2	A	28	0	12	0	0
2	B	28	0	12	1	0
2	C	28	0	12	1	0
2	D	28	0	12	0	0
3	A	266	0	0	5	0
3	B	227	0	0	3	0
3	C	224	0	0	4	0
3	D	250	0	0	4	0
All	All	16607	0	48	49	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 3.

All (49) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:479:LYS:NZ	1:A:479:LYS:CE	1.74	1.47
1:A:264:ARG:NH1	1:A:264:ARG:CG	2.31	0.91
1:C:145:ARG:NH1	3:C:762:HOH:O	2.10	0.82
1:C:164:GLU:OE1	1:C:243:ARG:NH2	2.11	0.82
1:A:269:MET:CE	3:A:760:HOH:O	2.32	0.77
1:D:351:ARG:NH2	3:D:1017:HOH:O	2.18	0.75
1:B:215:ASP:OD1	1:B:226:ARG:NH2	2.20	0.74
1:A:164:GLU:OE1	1:A:243:ARG:NH2	2.25	0.70
1:A:478:LYS:CE	3:A:852:HOH:O	2.38	0.70
1:B:91:HIS:NE2	2:B:601:GDP:O1B	2.27	0.68
1:A:264:ARG:NH1	3:A:807:HOH:O	2.29	0.65
1:D:40:GLN:OE1	1:D:349:GLN:NE2	2.30	0.65
1:B:164:GLU:OE2	1:B:243:ARG:NH2	2.33	0.62
1:B:325:ARG:NH2	1:B:343:ALA:O	2.36	0.58
1:C:127:ASP:OD1	1:C:130:ARG:NH2	2.37	0.57
1:A:479:LYS:NZ	1:A:479:LYS:CD	2.65	0.55
1:B:4:ARG:NH2	1:B:356:GLU:OE2	2.39	0.55
1:C:325:ARG:NH2	3:C:835:HOH:O	2.40	0.54
1:A:402:LEU:O	3:A:962:HOH:O	2.19	0.53
1:C:312:ARG:CB	1:C:367:ASN:OD1	2.57	0.53
1:A:325:ARG:NE	1:A:355:GLU:OE2	2.42	0.52
1:D:215:ASP:OD1	1:D:226:ARG:NH2	2.43	0.52
1:D:149:HIS:NE2	3:D:1234:HOH:O	2.34	0.51
1:B:351:ARG:NH2	3:B:741:HOH:O	2.44	0.51
1:A:346:PHE:O	3:A:914:HOH:O	2.19	0.50
1:C:179:LYS:NZ	1:C:221:GLN:OE1	2.45	0.50
1:B:132:ARG:NH1	1:B:388:GLY:O	2.44	0.50
1:C:451:ARG:NE	1:C:455:GLU:OE2	2.46	0.49
1:D:403:LYS:NZ	1:D:459:ASP:OD2	2.45	0.49
1:B:7:ARG:NH1	3:B:725:HOH:O	2.47	0.48
1:C:428:ARG:NH2	3:C:903:HOH:O	2.46	0.47
1:D:521:GLU:OE1	1:D:523:ARG:NH2	2.48	0.47
1:B:71:THR:CG2	1:B:71:THR:O	2.62	0.46
1:C:164:GLU:OE1	1:C:243:ARG:CZ	2.63	0.46
1:A:468:HIS:NE2	1:B:152:ASP:OD1	2.49	0.45
1:D:142:LYS:NZ	3:D:1049:HOH:O	2.48	0.45
1:D:25:LYS:NZ	1:D:88:THR:O	2.50	0.44
1:D:312:ARG:NH1	1:D:421:GLU:CD	2.71	0.44
1:B:280:ARG:NH1	3:B:859:HOH:O	2.50	0.43
1:A:483:ASP:OD1	1:A:483:ASP:C	2.57	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:312:ARG:NH1	1:D:421:GLU:OE1	2.52	0.42
1:D:79:ARG:NH1	1:D:272:GLU:OE2	2.53	0.42
1:D:381:LYS:NZ	3:D:1057:HOH:O	2.51	0.42
1:C:130:ARG:CD	3:C:872:HOH:O	2.67	0.42
1:A:79:ARG:NH1	1:A:272:GLU:OE2	2.53	0.41
1:B:127:ASP:OD1	1:B:130:ARG:NH1	2.54	0.41
1:B:526:ARG:NH1	1:B:528:ILE:CG2	2.84	0.40
1:C:91:HIS:NE2	2:C:601:GDP:O1B	2.54	0.40
1:C:164:GLU:OE2	1:D:509:ARG:NH1	2.55	0.40

All (1) 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	Distance(Å)	Clash(Å)
1:B:446:ASP:OD2	1:B:478:LYS:NZ[1_655]	2.14	0.06

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	487/548 (89%)	475 (98%)	12 (2%)	0	100	100
1	B	482/548 (88%)	475 (98%)	7 (2%)	0	100	100
1	C	483/548 (88%)	475 (98%)	7 (1%)	1 (0%)	56	38
1	D	486/548 (89%)	478 (98%)	8 (2%)	0	100	100
All	All	1938/2192 (88%)	1903 (98%)	34 (2%)	1 (0%)	59	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	390	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	412/453 (91%)	398 (97%)	14 (3%)	49	29
1	B	407/453 (90%)	398 (98%)	9 (2%)	64	48
1	C	409/453 (90%)	388 (95%)	21 (5%)	33	14
1	D	412/453 (91%)	396 (96%)	16 (4%)	43	23
All	All	1640/1812 (90%)	1580 (96%)	60 (4%)	45	26

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	VAL
1	A	132	ARG
1	A	220	ASP
1	A	223	GLU
1	A	264	ARG
1	A	269	MET
1	A	280	ARG
1	A	337	ASP
1	A	349	GLN
1	A	370	THR
1	A	443	LEU
1	A	481	PHE
1	A	483	ASP
1	A	529	SER
1	B	72	SER
1	B	112	ILE
1	B	177	SER
1	B	302	GLN
1	B	330	LYS
1	B	352	THR
1	B	430	LEU
1	B	481	PHE
1	B	528	ILE
1	C	4	ARG
1	C	40	GLN
1	C	88	THR

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Mol	Chain	Res	Type
1	C	121	GLN
1	C	122	THR
1	C	176	SER
1	C	201	GLN
1	C	233	GLU
1	C	246	LYS
1	C	280	ARG
1	C	350	ASP
1	C	351	ARG
1	C	352	THR
1	C	356	GLU
1	C	370	THR
1	C	381	LYS
1	C	382	GLU
1	C	401	ARG
1	C	409	LYS
1	C	437	LEU
1	C	515	GLU
1	D	39	ILE
1	D	80	ASP
1	D	88	THR
1	D	200	ILE
1	D	202	SER
1	D	210	ASP
1	D	234	GLU
1	D	249	LEU
1	D	309	HIS
1	D	337	ASP
1	D	349	GLN
1	D	351	ARG
1	D	355	GLU
1	D	459	ASP
1	D	479	LYS
1	D	516	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

4 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	GDP	A	601	-	30,30,30	1.37	4 (13%)	44,47,47	3.64	11 (25%)
2	GDP	B	601	-	30,30,30	1.62	5 (16%)	44,47,47	3.96	11 (25%)
2	GDP	C	601	-	30,30,30	1.80	8 (26%)	44,47,47	4.06	14 (31%)
2	GDP	D	601	-	30,30,30	1.55	6 (20%)	44,47,47	2.20	11 (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	GDP	A	601	-	-	0/16/32/32	0/1/3/3
2	GDP	B	601	-	-	0/16/32/32	0/1/3/3
2	GDP	C	601	-	-	0/16/32/32	0/1/3/3
2	GDP	D	601	-	-	0/16/32/32	0/1/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	GDP	C4-N9	-4.94	1.30	1.37
2	C	601	GDP	C6-C5	4.79	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	GDP	C6-C5	4.71	1.48	1.41
2	C	601	GDP	C5-C4	4.23	1.50	1.40
2	B	601	GDP	C4-N9	-4.23	1.31	1.37
2	A	601	GDP	C4-N9	-3.76	1.32	1.37
2	B	601	GDP	C5-C4	3.72	1.48	1.40
2	A	601	GDP	C6-C5	3.71	1.47	1.41
2	C	601	GDP	C2'-C1'	-2.90	1.49	1.53
2	C	601	GDP	C2-N3	2.88	1.37	1.33
2	D	601	GDP	C6-C5	2.84	1.45	1.41
2	D	601	GDP	C2-N2	2.84	1.36	1.32
2	D	601	GDP	C5-C4	2.75	1.46	1.40
2	C	601	GDP	C4-N9	-2.68	1.33	1.37
2	A	601	GDP	C2-N2	2.66	1.36	1.32
2	D	601	GDP	C4-N3	2.66	1.40	1.35
2	C	601	GDP	C2-N2	2.59	1.36	1.32
2	C	601	GDP	PB-O3A	2.50	1.64	1.60
2	B	601	GDP	C2-N3	2.48	1.36	1.33
2	B	601	GDP	C2-N2	2.35	1.36	1.32
2	C	601	GDP	PB-O3B	-2.26	1.46	1.54
2	A	601	GDP	PB-O3A	2.18	1.64	1.60
2	D	601	GDP	PB-O3A	2.08	1.63	1.60

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	GDP	C6-C5-N7	23.77	137.34	134.14
2	C	601	GDP	C6-C5-N7	23.47	137.30	134.14
2	A	601	GDP	C6-C5-N7	20.65	136.92	134.14
2	D	601	GDP	C8-N9-C4	6.83	112.11	106.90
2	D	601	GDP	C6-C5-N7	6.58	135.03	134.14
2	D	601	GDP	N3-C4-N9	5.42	134.86	126.91
2	C	601	GDP	N3-C4-N9	5.23	134.58	126.91
2	A	601	GDP	N3-C4-N9	5.14	134.44	126.91
2	C	601	GDP	C8-N9-C4	4.92	110.65	106.90
2	A	601	GDP	C2-N3-C4	4.81	121.85	115.09
2	A	601	GDP	C8-N9-C4	4.55	110.37	106.90
2	B	601	GDP	C8-N9-C4	4.52	110.35	106.90
2	B	601	GDP	N3-C4-N9	4.42	133.39	126.91
2	A	601	GDP	C5-C4-N3	-4.28	119.74	125.94
2	C	601	GDP	C5-C4-N3	-3.74	120.52	125.94
2	D	601	GDP	O4'-C1'-N9	3.71	111.89	108.44
2	C	601	GDP	C2-N3-C4	3.56	120.09	115.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	GDP	O3B-PB-O2B	3.44	121.02	107.61
2	B	601	GDP	C5-C4-N3	-3.36	121.07	125.94
2	C	601	GDP	O2B-PB-O1B	-3.29	99.70	110.44
2	B	601	GDP	C2-N3-C4	3.26	119.68	115.09
2	C	601	GDP	PA-O3A-PB	-3.23	122.21	131.68
2	A	601	GDP	C4-C5-N7	-3.14	106.83	109.52
2	C	601	GDP	C4-C5-N7	-3.06	106.90	109.52
2	B	601	GDP	C4-C5-N7	-2.94	107.01	109.52
2	A	601	GDP	O2A-PA-O3A	2.83	118.56	105.14
2	A	601	GDP	O2'-C2'-C3'	2.78	120.87	111.83
2	D	601	GDP	C5-C4-N3	-2.78	121.92	125.94
2	D	601	GDP	C1'-N9-C4	-2.77	121.85	126.64
2	D	601	GDP	C5-C4-N9	-2.74	103.21	107.16
2	B	601	GDP	O2A-PA-O3A	2.63	117.64	105.14
2	C	601	GDP	C1'-N9-C4	-2.52	122.28	126.64
2	B	601	GDP	C1'-N9-C4	-2.51	122.30	126.64
2	C	601	GDP	O2A-PA-O3A	2.48	116.90	105.14
2	C	601	GDP	C6-N1-C2	2.48	123.84	119.51
2	D	601	GDP	C2-N3-C4	2.45	118.53	115.09
2	A	601	GDP	O4'-C1'-N9	2.38	110.65	108.44
2	D	601	GDP	C6-N1-C2	2.28	123.50	119.51
2	D	601	GDP	O3B-PB-O2B	2.24	116.35	107.61
2	B	601	GDP	O3B-PB-O2B	2.24	116.34	107.61
2	D	601	GDP	O3B-PB-O1B	2.15	117.46	110.44
2	A	601	GDP	N7-C8-N9	-2.12	108.35	114.36
2	C	601	GDP	O4'-C1'-N9	-2.08	106.51	108.44
2	B	601	GDP	O2B-PB-O1B	-2.05	103.76	110.44
2	C	601	GDP	O3A-PA-O5'	-2.04	94.27	103.41
2	B	601	GDP	O4'-C1'-N9	2.03	110.33	108.44
2	A	601	GDP	N2-C2-N3	-2.00	117.59	120.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	495/548 (90%)	0.07	24 (4%)	29 23	15, 28, 53, 73	0
1	B	490/548 (89%)	0.05	16 (3%)	44 36	16, 31, 51, 71	0
1	C	491/548 (89%)	0.10	23 (4%)	30 23	16, 30, 53, 70	0
1	D	494/548 (90%)	0.04	18 (3%)	41 33	15, 28, 52, 75	0
All	All	1970/2192 (89%)	0.06	81 (4%)	35 28	15, 29, 53, 75	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	368	HIS	9.0
1	C	200	ILE	7.9
1	B	200	ILE	6.7
1	B	92	GLN	6.3
1	B	350	ASP	5.8
1	C	92	GLN	5.4
1	C	369	GLY	5.1
1	D	350	ASP	5.0
1	A	69	VAL	4.9
1	C	69	VAL	4.9
1	A	1	MET	4.8
1	D	39	ILE	4.8
1	B	39	ILE	4.8
1	D	200	ILE	4.7
1	B	312	ARG	4.7
1	A	304	ASN	4.7
1	A	350	ASP	4.6
1	B	303	ALA	4.5
1	A	529	SER	4.5
1	D	70	THR	4.4
1	A	352	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	370	THR	4.4
1	C	70	THR	4.3
1	A	48	ARG	4.1
1	A	70	THR	3.9
1	A	47	ALA	3.9
1	B	368	HIS	3.8
1	D	309	HIS	3.8
1	A	39	ILE	3.7
1	C	46	LYS	3.5
1	D	349	GLN	3.5
1	D	199	ARG	3.4
1	A	476	GLU	3.3
1	A	312	ARG	3.2
1	D	45	VAL	3.2
1	C	40	GLN	3.2
1	C	44	SER	3.2
1	A	349	GLN	3.2
1	B	40	GLN	3.2
1	D	92	GLN	3.1
1	A	45	VAL	3.1
1	B	45	VAL	3.1
1	D	310	ARG	3.1
1	D	40	GLN	3.1
1	C	454	ASP	3.0
1	A	201	GLN	3.0
1	C	367	ASN	3.0
1	B	176	SER	3.0
1	B	352	THR	2.9
1	A	210	ASP	2.9
1	D	304	ASN	2.8
1	A	92	GLN	2.8
1	C	39	ILE	2.8
1	A	40	GLN	2.8
1	A	519	LYS	2.8
1	D	303	ALA	2.8
1	D	210	ASP	2.7
1	D	518	PRO	2.7
1	C	312	ARG	2.6
1	C	146	GLU	2.6
1	A	512	SER	2.5
1	B	15	PHE	2.5
1	A	303	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	529	SER	2.5
1	C	45	VAL	2.5
1	C	176	SER	2.5
1	C	443	LEU	2.5
1	A	193	SER	2.4
1	B	349	GLN	2.4
1	D	517	TYR	2.4
1	D	519	LYS	2.3
1	C	233	GLU	2.2
1	B	70	THR	2.2
1	C	210	ASP	2.2
1	D	476	GLU	2.2
1	B	403	LYS	2.1
1	B	201	GLN	2.1
1	C	350	ASP	2.1
1	C	349	GLN	2.1
1	A	91	HIS	2.0
1	A	351	ARG	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	GDP	C	601	28/28	0.08	-0.35	24,34,39,44	0
2	GDP	B	601	28/28	0.08	-0.46	26,35,37,41	0
2	GDP	A	601	28/28	0.07	-0.54	22,27,31,33	0
2	GDP	D	601	28/28	0.06	-0.78	21,26,30,32	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.