



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:17 PM GMT

PDB ID : 1JNY  
Title : Crystal structure of Sulfolobus solfataricus elongation factor 1 alpha in complex with GDP  
Authors : Vitagliano, L.; Masullo, M.; Sica, F.; Zagari, A.; Bocchini, V.  
Deposited on : 2001-07-26  
Resolution : 1.80 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

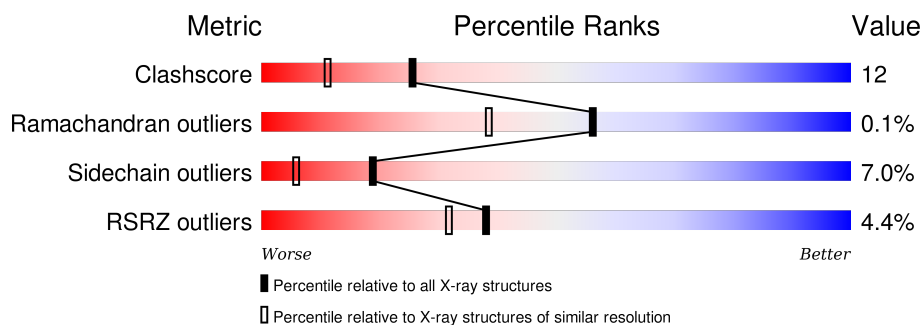
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	435	<div> <div></div> <div>75% 18% • 5%</div> </div>
1	B	435	<div> <div>7%</div> <div>63% 28% • 5%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7001 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.

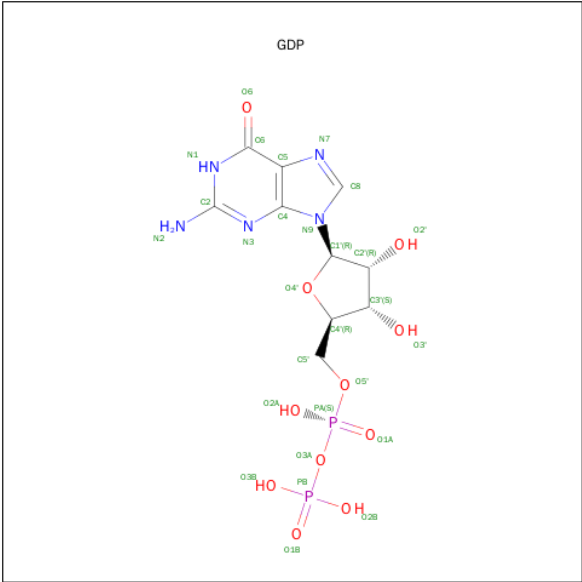
- Molecule 1 is a protein called Elongation factor 1-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	415	Total	C	N	O	S	0	0	0
			3248	2073	563	598	14			
1	B	412	Total	C	N	O	S	0	0	0
			3218	2054	559	591	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	VAL	ILE	CONFLICT	UNP P35021
A	196	SER	ALA	CONFLICT	UNP P35021
A	203	LYS	ARG	CONFLICT	UNP P35021
A	347	LEU	ILE	CONFLICT	UNP P35021
B	15	VAL	ILE	CONFLICT	UNP P35021
B	196	SER	ALA	CONFLICT	UNP P35021
B	203	LYS	ARG	CONFLICT	UNP P35021
B	347	LEU	ILE	CONFLICT	UNP P35021

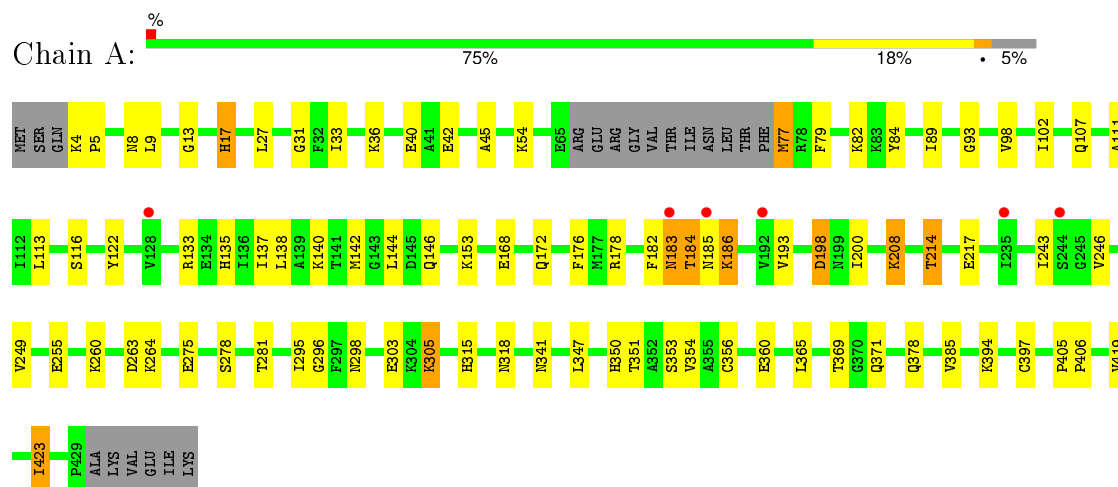
- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



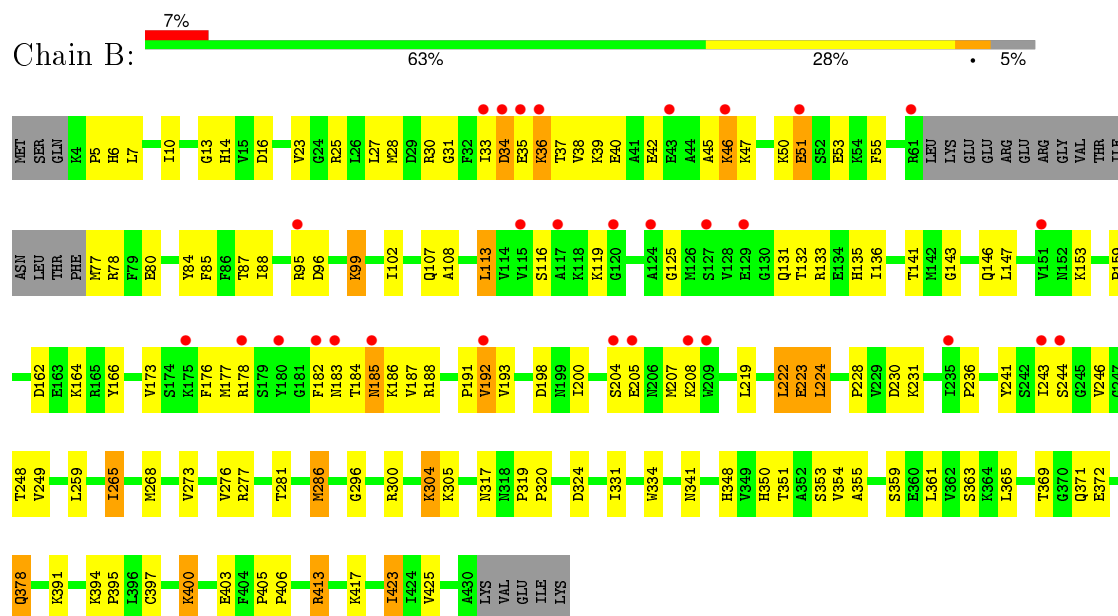
### 3 Residue-property plots

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: Elongation factor 1-alpha



#### • Molecule 1: Elongation factor 1-alpha



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.11Å 113.72Å 80.32Å 90.00° 90.20° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 19.79 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.80) 97.7 (19.79-1.80)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.04 (at 1.80Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.220 , 0.269 0.230 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	24.7	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 60.7	EDS
Estimated twinning fraction	0.021 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 101657 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7001	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.45	0/3316	0.70	1/4479 (0.0%)
1	B	0.43	0/3286	0.72	3/4440 (0.1%)
All	All	0.44	0/6602	0.71	4/8919 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	296	GLY	N-CA-C	-6.11	97.82	113.10
1	A	296	GLY	N-CA-C	-5.47	99.44	113.10
1	B	413	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	B	85	PHE	N-CA-C	-5.00	97.50	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3248	0	3317	65	0
1	B	3218	0	3286	99	0
2	A	28	0	12	1	0
2	B	28	0	12	1	0
3	A	314	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	165	0	0	3	0
All	All	7001	0	6627	164	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 12.

All (164) 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:B:205:GLU:HA	1:B:208:LYS:HE3	1.46	0.96
1:B:224:LEU:H	1:B:224:LEU:HD22	1.44	0.82
1:A:13:GLY:H	1:A:135:HIS:HD2	1.31	0.77
1:A:255:GLU:HB3	3:A:795:HOH:O	1.83	0.77
1:B:359:SER:HB3	1:B:391:LYS:HG3	1.68	0.76
1:A:146:GLN:HG2	1:A:186:LYS:HG2	1.68	0.76
1:B:33:ILE:HD12	1:B:33:ILE:H	1.53	0.73
1:B:14:HIS:HD2	1:B:131:GLN:H	1.35	0.72
1:A:27:LEU:HD11	1:A:77:MET:HE3	1.73	0.70
1:B:243:ILE:HB	1:B:246:VAL:HB	1.74	0.70
1:A:178:ARG:HH11	1:A:184:THR:HG21	1.57	0.70
1:B:259:LEU:HD11	1:B:276:VAL:HG21	1.72	0.70
1:A:214:THR:HG21	3:A:698:HOH:O	1.92	0.69
1:A:406:PRO:HG2	3:A:795:HOH:O	1.93	0.69
1:B:35:GLU:O	1:B:36:LYS:HG3	1.92	0.69
1:A:405:PRO:HB2	1:A:406:PRO:HD3	1.76	0.68
1:B:42:GLU:O	1:B:46:LYS:HG2	1.95	0.67
1:B:277:ARG:HG3	1:B:300:ARG:HG3	1.76	0.67
1:B:241:TYR:HB2	1:B:249:VAL:HG13	1.77	0.66
1:A:33:ILE:H	1:A:33:ILE:HD12	1.62	0.65
1:B:77:MET:HG2	1:B:78:ARG:H	1.63	0.64
1:B:132:THR:O	1:B:136:ILE:HG13	2.00	0.62
1:A:369:THR:OG1	1:A:371:GLN:HG2	2.00	0.62
1:A:350:HIS:CD2	1:A:351:THR:H	2.19	0.61
1:A:260:LYS:HE2	3:A:556:HOH:O	2.01	0.61
1:A:243:ILE:HB	1:A:246:VAL:HB	1.82	0.61
1:B:133:ARG:HB2	1:B:176:PHE:CZ	2.36	0.60
1:A:318:ASN:HB3	3:A:794:HOH:O	1.99	0.60
1:A:45:ALA:HB2	1:A:54:LYS:HG3	1.83	0.60
1:A:17:HIS:CD2	1:A:116:SER:H	2.20	0.59
1:A:183:ASN:HB3	3:A:797:HOH:O	2.01	0.59
1:A:303:GLU:HB3	1:A:305:LYS:HE3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:GLY:H	1:B:135:HIS:HD2	1.50	0.59
1:B:146:GLN:NE2	1:B:223:GLU:HG3	2.17	0.59
1:B:99:LYS:HG3	1:B:331:ILE:HG12	1.84	0.59
1:B:204:SER:O	1:B:205:GLU:HB2	2.03	0.58
1:A:350:HIS:HE1	1:A:397:CYS:O	1.85	0.58
1:B:5:PRO:HG2	1:B:84:TYR:CD1	2.39	0.58
1:B:146:GLN:HE22	1:B:223:GLU:H	1.49	0.57
1:B:23:VAL:HG13	1:B:88:ILE:HD13	1.86	0.57
1:B:28:MET:SD	1:B:55:PHE:HD1	2.27	0.57
1:A:36:LYS:HE2	1:A:40:GLU:OE2	2.05	0.57
1:B:14:HIS:CD2	1:B:131:GLN:H	2.22	0.57
1:B:350:HIS:HE1	1:B:397:CYS:O	1.88	0.57
1:B:38:VAL:O	1:B:42:GLU:HG3	2.06	0.56
1:B:159:PRO:O	1:B:162:ASP:HB2	2.06	0.56
1:A:98:VAL:HG11	1:A:385:VAL:HG11	1.88	0.55
1:B:378:GLN:H	1:B:378:GLN:NE2	2.03	0.55
1:B:153:LYS:HG2	2:B:600:GDP:C6	2.41	0.55
1:B:277:ARG:CG	1:B:300:ARG:HG3	2.37	0.55
1:B:378:GLN:HE21	1:B:378:GLN:H	1.54	0.55
1:B:95:ARG:O	1:B:96:ASP:HB2	2.07	0.54
1:B:277:ARG:HA	1:B:277:ARG:CZ	2.37	0.54
1:A:354:VAL:HG22	1:A:394:LYS:HE2	1.88	0.54
1:B:116:SER:OG	1:B:153:LYS:HD2	2.07	0.54
1:A:17:HIS:HE1	3:A:508:HOH:O	1.91	0.53
1:B:39:LYS:N	1:B:39:LYS:HD2	2.24	0.53
1:B:224:LEU:H	1:B:224:LEU:CD2	2.17	0.53
1:B:248:THR:HG22	1:B:304:LYS:HB2	1.91	0.53
1:A:263:ASP:OD2	1:A:315:HIS:HE1	1.92	0.53
1:B:33:ILE:O	1:B:35:GLU:N	2.42	0.53
1:A:133:ARG:HG3	1:A:176:PHE:CZ	2.43	0.52
1:B:10:ILE:HG23	1:B:108:ALA:HB2	1.91	0.52
1:B:231:LYS:HE3	1:B:403:GLU:O	2.09	0.52
1:B:28:MET:SD	1:B:55:PHE:CD1	3.02	0.52
1:A:137:ILE:O	1:A:140:LYS:HB3	2.08	0.52
1:A:111:ALA:HB2	1:A:144:LEU:HD13	1.91	0.52
1:A:27:LEU:HD11	1:A:77:MET:CE	2.39	0.52
1:B:228:PRO:HB3	1:B:231:LYS:HD3	1.91	0.52
1:B:228:PRO:CB	1:B:231:LYS:HD3	2.39	0.52
1:B:173:VAL:O	1:B:177:MET:HG3	2.10	0.52
1:B:369:THR:OG1	1:B:371:GLN:HG2	2.10	0.52
1:B:400:LYS:HE3	3:B:616:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ILE:HG12	1:A:249:VAL:CG1	2.39	0.52
1:A:93:GLY:HA2	3:A:779:HOH:O	2.09	0.52
1:A:31:GLY:HA2	1:A:79:PHE:HA	1.92	0.52
1:A:183:ASN:O	1:A:184:THR:HB	2.11	0.51
1:A:341:ASN:HD21	1:A:360:GLU:HA	1.75	0.51
1:A:378:GLN:H	1:A:378:GLN:CD	2.13	0.51
1:A:214:THR:HG22	1:A:217:GLU:H	1.75	0.51
1:B:277:ARG:HG3	1:B:300:ARG:CG	2.40	0.51
1:A:243:ILE:HG12	1:A:249:VAL:HG11	1.92	0.51
1:A:200:ILE:O	1:A:214:THR:HG23	2.11	0.51
1:B:350:HIS:CD2	1:B:351:THR:H	2.28	0.51
1:A:305:LYS:H	1:A:305:LYS:HE3	1.76	0.51
1:B:185:ASN:HD22	1:B:185:ASN:N	2.09	0.51
1:B:35:GLU:C	1:B:37:THR:H	2.14	0.50
1:A:135:HIS:HE1	3:A:539:HOH:O	1.94	0.50
1:B:192:VAL:HG13	1:B:200:ILE:HD11	1.93	0.50
1:A:193:VAL:HB	1:A:198:ASP:HB2	1.93	0.50
1:B:30:ARG:HB3	1:B:80:GLU:O	2.12	0.50
1:A:208:LYS:H	1:A:208:LYS:HE2	1.77	0.50
1:A:178:ARG:NH1	1:A:184:THR:HG21	2.26	0.49
1:A:350:HIS:HD2	1:A:351:THR:H	1.59	0.49
1:B:113:LEU:HB2	1:B:147:LEU:HD11	1.93	0.49
1:A:341:ASN:HD21	1:A:360:GLU:CA	2.25	0.48
1:B:6:HIS:CE1	1:B:87:THR:OG1	2.67	0.48
1:B:363:SER:HB2	1:B:372:GLU:HG3	1.96	0.48
1:B:277:ARG:NE	1:B:277:ARG:HA	2.28	0.48
1:A:42:GLU:HA	1:A:54:LYS:HG2	1.95	0.48
1:B:236:PRO:HB3	1:B:350:HIS:CD2	2.49	0.48
1:A:138:LEU:HG	1:A:142:MET:CE	2.43	0.48
1:A:27:LEU:O	1:A:33:ILE:HD11	2.14	0.48
1:B:166:TYR:CZ	1:B:191:PRO:HD3	2.48	0.47
1:B:143:GLY:HA2	3:B:700:HOH:O	2.14	0.47
1:B:405:PRO:HB2	1:B:406:PRO:HD3	1.96	0.47
1:B:102:ILE:O	1:B:423:ILE:HD13	2.14	0.47
1:B:265:ILE:O	1:B:273:VAL:HA	2.13	0.47
1:B:359:SER:CB	1:B:391:LYS:HG3	2.42	0.47
1:B:355:ALA:H	1:B:394:LYS:HZ3	1.63	0.47
1:A:102:ILE:O	1:A:423:ILE:HD13	2.15	0.47
1:B:304:LYS:HB3	1:B:305:LYS:HE2	1.97	0.47
1:B:413:ARG:NH2	1:B:417:LYS:HA	2.31	0.46
1:B:35:GLU:O	1:B:37:THR:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:VAL:HG13	1:B:394:LYS:HE2	1.97	0.45
1:B:178:ARG:HH11	1:B:184:THR:HG21	1.82	0.45
1:A:116:SER:O	1:A:122:TYR:HB2	2.16	0.45
1:A:315:HIS:HD2	3:A:548:HOH:O	1.99	0.45
1:A:168:GLU:O	1:A:172:GLN:HG3	2.17	0.45
1:B:13:GLY:H	1:B:135:HIS:CD2	2.32	0.44
1:B:219:LEU:O	1:B:222:LEU:HB2	2.18	0.44
1:A:45:ALA:CB	1:A:54:LYS:HG3	2.47	0.44
1:B:191:PRO:HB2	1:B:207:MET:SD	2.57	0.44
1:B:178:ARG:NH1	1:B:184:THR:HG21	2.32	0.44
1:B:281:THR:HB	1:B:286:MET:CE	2.47	0.44
1:B:25:ARG:HD2	1:B:25:ARG:HA	1.75	0.44
1:B:177:MET:HB3	1:B:182:PHE:HB3	1.99	0.44
1:B:45:ALA:HB1	1:B:51:GLU:HA	1.99	0.44
1:B:141:THR:HG23	1:B:425:VAL:HG12	2.00	0.43
1:B:193:VAL:HB	1:B:198:ASP:HB2	1.99	0.43
1:A:405:PRO:CB	1:A:406:PRO:HD3	2.48	0.43
1:A:5:PRO:HB2	1:A:84:TYR:HD1	1.83	0.43
1:A:183:ASN:HD22	1:A:183:ASN:C	2.21	0.43
1:A:281:THR:OG1	1:A:295:ILE:HG22	2.19	0.43
1:B:14:HIS:CD2	1:B:125:GLY:HA2	2.54	0.43
1:B:146:GLN:HE22	1:B:223:GLU:HG3	1.84	0.43
1:A:153:LYS:HG2	2:A:500:GDP:C6	2.53	0.42
1:B:268:MET:HG2	1:B:320:PRO:HD2	2.02	0.42
1:B:224:LEU:N	1:B:224:LEU:HD22	2.25	0.42
1:B:146:GLN:HE22	1:B:223:GLU:N	2.17	0.42
1:B:36:LYS:O	1:B:40:GLU:HG3	2.19	0.42
1:B:185:ASN:ND2	1:B:186:LYS:H	2.17	0.42
1:A:365:LEU:HB2	1:A:385:VAL:HG12	2.02	0.42
1:A:8:ASN:HB3	1:A:89:ILE:HD13	2.01	0.42
1:B:395:PRO:HA	3:B:714:HOH:O	2.19	0.42
1:A:341:ASN:HD21	1:A:360:GLU:N	2.17	0.42
1:A:138:LEU:HG	1:A:142:MET:HE2	2.02	0.42
1:B:348:HIS:CD2	1:B:413:ARG:HG3	2.55	0.41
1:B:34:ASP:HB3	1:B:37:THR:OG1	2.19	0.41
1:B:185:ASN:ND2	1:B:186:LYS:N	2.68	0.41
1:A:4:LYS:HA	1:A:5:PRO:HD3	1.90	0.41
1:A:278:SER:OG	1:A:298:ASN:HB3	2.20	0.41
1:B:7:LEU:HD21	1:B:224:LEU:HD13	2.02	0.41
1:B:281:THR:HB	1:B:286:MET:HE2	2.02	0.41
1:B:23:VAL:HG13	1:B:88:ILE:CD1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:PRO:HA	1:B:320:PRO:HD3	1.98	0.41
1:B:147:LEU:HB3	1:B:187:VAL:HG22	2.02	0.41
1:A:264:LYS:NZ	1:A:275:GLU:HB2	2.35	0.41
1:B:27:LEU:O	1:B:31:GLY:HA3	2.21	0.41
1:B:355:ALA:H	1:B:394:LYS:NZ	2.19	0.40
1:B:45:ALA:HA	1:B:53:GLU:HB3	2.03	0.40
1:B:391:LYS:HB3	1:B:391:LYS:HE2	1.97	0.40
1:B:334:TRP:CD2	1:B:417:LYS:HE2	2.57	0.40
1:A:347:LEU:HD13	1:A:356:CYS:HB2	2.04	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	411/435 (94%)	395 (96%)	16 (4%)	0	100	100
1	B	408/435 (94%)	387 (95%)	20 (5%)	1 (0%)	52	35
All	All	819/870 (94%)	782 (96%)	36 (4%)	1 (0%)	56	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	34	ASP

### 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	357/375 (95%)	339 (95%)	18 (5%)	30	13
1	B	353/375 (94%)	321 (91%)	32 (9%)	12	3
All	All	710/750 (95%)	660 (93%)	50 (7%)	19	6

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	17	HIS
1	A	77	MET
1	A	82	LYS
1	A	107	GLN
1	A	113	LEU
1	A	182	PHE
1	A	183	ASN
1	A	184	THR
1	A	185	ASN
1	A	186	LYS
1	A	198	ASP
1	A	208	LYS
1	A	214	THR
1	A	305	LYS
1	A	353	SER
1	A	419	VAL
1	A	423	ILE
1	B	16	ASP
1	B	36	LYS
1	B	46	LYS
1	B	47	LYS
1	B	50	LYS
1	B	51	GLU
1	B	99	LYS
1	B	107	GLN
1	B	113	LEU
1	B	119	LYS
1	B	164	LYS
1	B	183	ASN
1	B	185	ASN
1	B	188	ARG
1	B	192	VAL
1	B	222	LEU

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Mol	Chain	Res	Type
1	B	223	GLU
1	B	224	LEU
1	B	230	ASP
1	B	244	SER
1	B	265	ILE
1	B	286	MET
1	B	304	LYS
1	B	317	ASN
1	B	324	ASP
1	B	341	ASN
1	B	353	SER
1	B	361	LEU
1	B	365	LEU
1	B	378	GLN
1	B	400	LYS
1	B	423	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	100	ASN
1	A	135	HIS
1	A	183	ASN
1	A	185	ASN
1	A	202	HIS
1	A	282	HIS
1	A	294	ASN
1	A	315	HIS
1	A	317	ASN
1	A	341	ASN
1	A	350	HIS
1	B	6	HIS
1	B	14	HIS
1	B	135	HIS
1	B	146	GLN
1	B	183	ASN
1	B	185	ASN
1	B	202	HIS
1	B	221	GLN
1	B	315	HIS
1	B	350	HIS

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Mol	Chain	Res	Type
1	B	378	GLN

### 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	GDP	A	500	-	23,30,30	2.79	8 (34%)	30,47,47	3.36	12 (40%)
2	GDP	B	600	-	23,30,30	2.91	10 (43%)	30,47,47	3.32	13 (43%)

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	500	-	-	0/12/32/32	0/3/3/3
2	GDP	B	600	-	-	0/12/32/32	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	GDP	PB-O2B	-3.81	1.41	1.54
2	A	500	GDP	PB-O2B	-3.72	1.41	1.54
2	B	600	GDP	C5-C4	2.02	1.45	1.40
2	B	600	GDP	O3'-C3'	2.19	1.48	1.43
2	A	500	GDP	C3'-C4'	2.25	1.59	1.53
2	A	500	GDP	O4'-C4'	2.31	1.50	1.45
2	B	600	GDP	O4'-C4'	2.37	1.50	1.45
2	B	600	GDP	C3'-C4'	2.60	1.60	1.53
2	A	500	GDP	PB-O3B	2.67	1.64	1.54
2	B	600	GDP	PB-O3B	2.92	1.65	1.54
2	A	500	GDP	C8-N7	3.44	1.41	1.34
2	B	600	GDP	C8-N7	3.73	1.41	1.34
2	A	500	GDP	O6-C6	3.88	1.34	1.24
2	B	600	GDP	O6-C6	3.97	1.34	1.24
2	A	500	GDP	O4'-C1'	6.30	1.49	1.41
2	B	600	GDP	O4'-C1'	6.85	1.49	1.41
2	B	600	GDP	C2-N1	7.73	1.49	1.35
2	A	500	GDP	C2-N1	8.05	1.49	1.35

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	GDP	C6-C5-C4	-10.33	108.55	120.90
2	B	600	GDP	C6-C5-C4	-9.38	109.68	120.90
2	B	600	GDP	C4-C5-N7	-8.11	102.02	109.48
2	A	500	GDP	N2-C2-N1	-5.68	107.79	117.20
2	B	600	GDP	O3A-PA-O5'	-5.37	88.69	102.94
2	A	500	GDP	N3-C2-N1	-5.36	119.28	127.44
2	B	600	GDP	N2-C2-N1	-5.18	108.63	117.20
2	A	500	GDP	C4-C5-N7	-4.80	105.07	109.48
2	B	600	GDP	N3-C2-N1	-3.76	121.71	127.44
2	A	500	GDP	C1'-N9-C4	-3.26	122.02	126.94
2	B	600	GDP	O4'-C1'-N9	-2.93	101.97	108.10
2	B	600	GDP	O3B-PB-O3A	-2.68	92.93	105.09
2	B	600	GDP	C1'-N9-C4	-2.68	122.90	126.94
2	A	500	GDP	O3'-C3'-C4'	-2.35	104.01	111.05
2	B	600	GDP	O3'-C3'-C2'	-2.07	105.10	111.83
2	A	500	GDP	C5-C6-N1	2.42	126.90	123.59
2	A	500	GDP	O2B-PB-O1B	2.51	118.65	110.58
2	B	600	GDP	O2'-C2'-C3'	2.55	120.12	111.83
2	A	500	GDP	O3B-PB-O2B	2.79	117.99	107.38
2	B	600	GDP	C2'-C3'-C4'	2.85	108.46	102.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	GDP	O5'-PA-O1A	3.39	122.76	109.62
2	A	500	GDP	O2'-C2'-C3'	3.89	124.48	111.83
2	A	500	GDP	C4'-O4'-C1'	4.79	114.98	109.72
2	B	600	GDP	N2-C2-N3	6.18	129.66	117.80
2	A	500	GDP	N2-C2-N3	7.88	132.92	117.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	GDP	1	0
2	B	600	GDP	1	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 ⓘ

### 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	415/435 (95%)	-0.04	6 (1%) 78 74	16, 27, 53, 84	0
1	B	412/435 (94%)	0.35	30 (7%) 18 14	18, 35, 67, 92	0
All	All	827/870 (95%)	0.16	36 (4%) 38 32	16, 31, 61, 92	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	61	ARG	6.4
1	B	36	LYS	5.5
1	A	244	SER	4.8
1	B	129	GLU	4.5
1	B	33	ILE	4.0
1	B	51	GLU	3.9
1	B	178	ARG	3.6
1	B	117	ALA	3.4
1	B	124	ALA	3.4
1	B	95	ARG	3.3
1	B	175	LYS	3.2
1	B	182	PHE	3.0
1	B	35	GLU	3.0
1	B	180	TYR	2.9
1	B	185	ASN	2.8
1	B	120	GLY	2.8
1	A	128	VAL	2.7
1	B	183	ASN	2.6
1	B	127	SER	2.6
1	B	43	GLU	2.6
1	B	34	ASP	2.5
1	B	46	LYS	2.4
1	B	208	LYS	2.4
1	B	205	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	185	ASN	2.3
1	B	243	ILE	2.2
1	B	209	TRP	2.1
1	B	244	SER	2.1
1	B	204	SER	2.0
1	A	192	VAL	2.0
1	B	151	VAL	2.0
1	B	192	VAL	2.0
1	A	235	ILE	2.0
1	B	235	ILE	2.0
1	A	183	ASN	2.0
1	B	115	VAL	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<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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	GDP	B	600	28/28	0.94	0.10	-0.82	37,44,51,53	0
2	GDP	A	500	28/28	0.97	0.06	-0.87	22,24,26,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.