



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2018 – 02:07 PM EST

PDB ID : 6B4J  
Title : Crystal structure of human Gle1 CTD-Nup42 GBM-DDX19B(AMPPNP) complex  
Authors : Lin, D.H.; Correia, A.R.; Cai, S.W.; Huber, F.M.; Jette, C.A.; Hoelz, A.  
Deposited on : 2017-09-26  
Resolution : 3.40 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

<https://www.wwpdb.org/validation/2017/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:

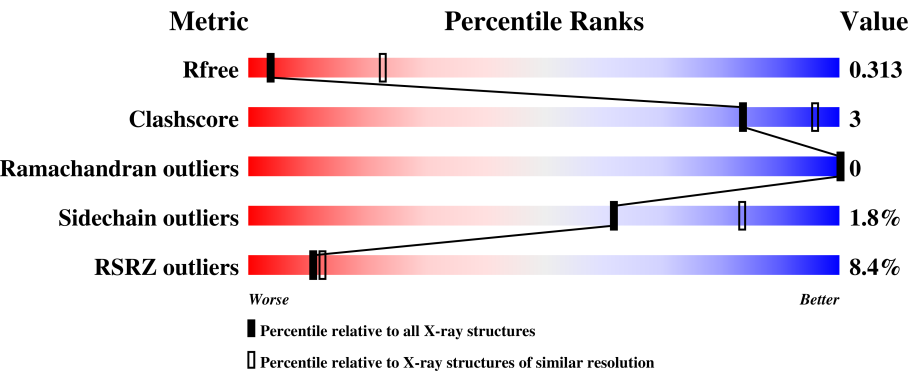
MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031633  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

# 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 3.40 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 <sub>free</sub>	111664	1928 (3.50-3.30)
Clashscore	122126	2051 (3.50-3.30)
Ramachandran outliers	120053	2006 (3.50-3.30)
Sidechain outliers	120020	2006 (3.50-3.30)
RSRZ outliers	108989	1827 (3.50-3.30)

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	317	<div><div>8%</div><div>94%</div><div>5%</div><div></div></div>
1	B	317	<div><div>%</div><div>91%</div><div>9%</div><div></div></div>
2	C	49	<div><div>6%</div><div>80%</div><div>8%</div><div>10%</div></div>
2	D	49	<div><div>4%</div><div>71%</div><div>6%</div><div>22%</div></div>
3	E	430	<div><div>11%</div><div>90%</div><div>8%</div><div></div></div>

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Mol	Chain	Length	Quality of chain
3	F	430	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a red segment at the beginning labeled '11%', a large green segment in the middle labeled '90%', and a small yellow segment at the end labeled '9%'. A small grey dot is visible at the far right end of the bar.

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 25350 atoms, of which 12752 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 Nucleoporin GLE1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	315	Total	C	H	N	O	S	0	0	0
			5099	1640	2558	432	454	15			
1	A	315	Total	C	H	N	O	S	0	0	0
			5099	1640	2558	432	454	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	382	MET	-	initiating methionine	UNP Q53GS7
A	382	MET	-	initiating methionine	UNP Q53GS7

- Molecule 2 is a protein called Nucleoporin like 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	44	Total	C	H	N	O	0	0	0
			735	234	379	56	66			
2	D	38	Total	C	H	N	O	0	0	0
			641	206	333	48	54			

- Molecule 3 is a protein called ATP-dependent RNA helicase DDX19B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	426	Total	C	H	N	O	S	0	1	0
			6824	2132	3445	592	635	20			
3	F	426	Total	C	H	N	O	S	0	1	0
			6825	2132	3446	592	635	20			

There are 8 discrepancies between the modelled and reference sequences:

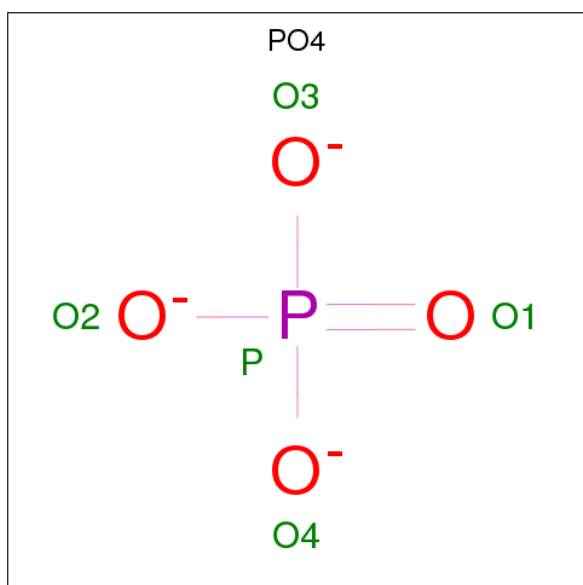
Chain	Residue	Modelled	Actual	Comment	Reference
E	50	GLY	-	expression tag	UNP Q9UMR2
E	51	PRO	-	expression tag	UNP Q9UMR2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	52	HIS	-	expression tag	UNP Q9UMR2
E	53	MET	-	expression tag	UNP Q9UMR2
F	50	GLY	-	expression tag	UNP Q9UMR2
F	51	PRO	-	expression tag	UNP Q9UMR2
F	52	HIS	-	expression tag	UNP Q9UMR2
F	53	MET	-	expression tag	UNP Q9UMR2

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

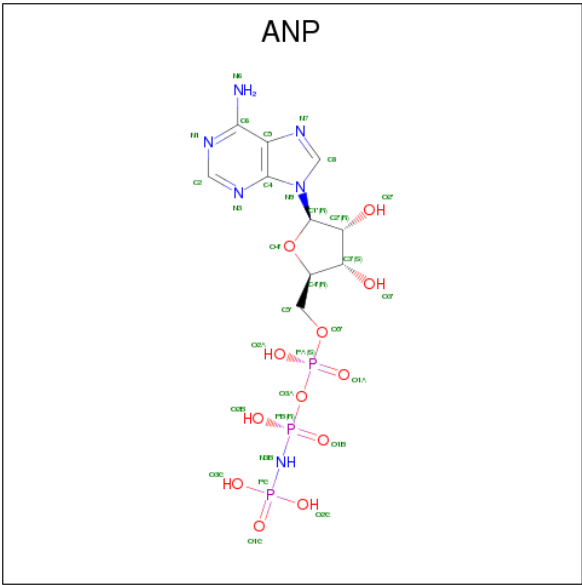


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	E	1	Total O P 5 4 1	0	0
4	E	1	Total O P 5 4 1	0	0
4	F	1	Total O P 5 4 1	0	0
4	F	1	Total O P 5 4 1	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	1	Total	Mg	0	0
			1	1		
5	E	1	Total	Mg	0	0
			1	1		

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).

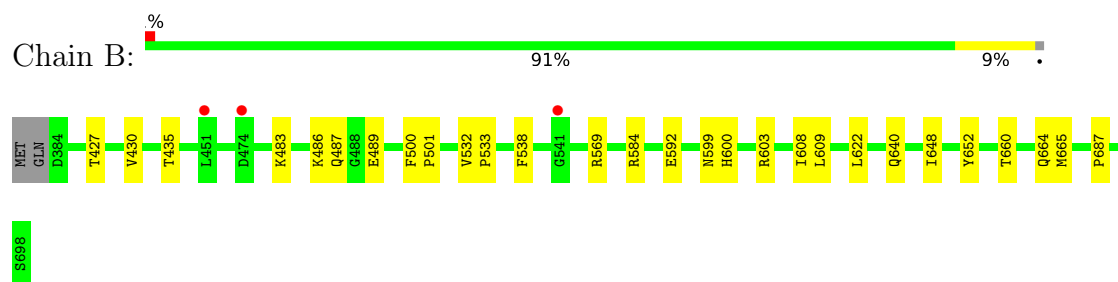


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	E	1	Total 48	C 10	H 17	N 6	O 12	P 3	0	0
6	F	1	Total 47	C 10	H 16	N 6	O 12	P 3	0	0

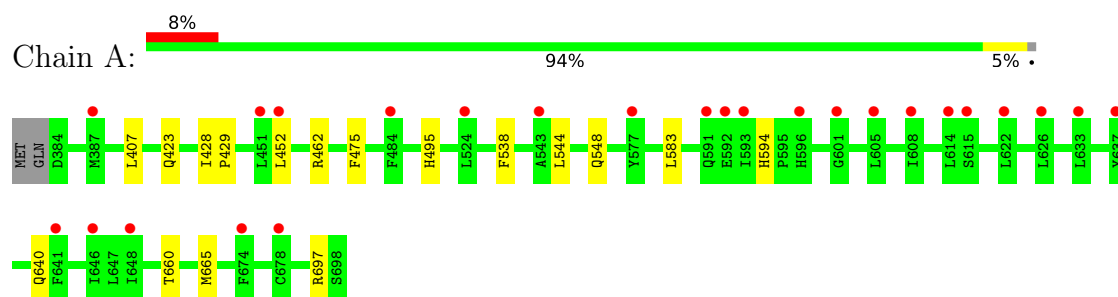
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

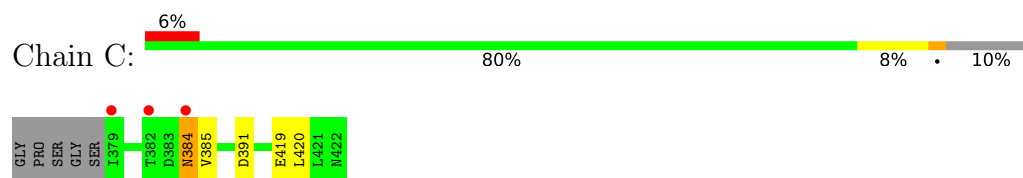
- Molecule 1: Nucleoporin GLE1



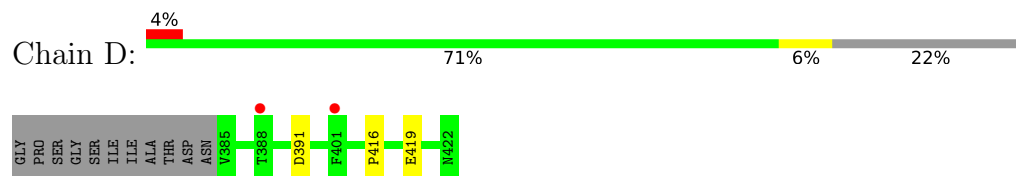
- Molecule 1: Nucleoporin GLE1



- Molecule 2: Nucleoporin like 2

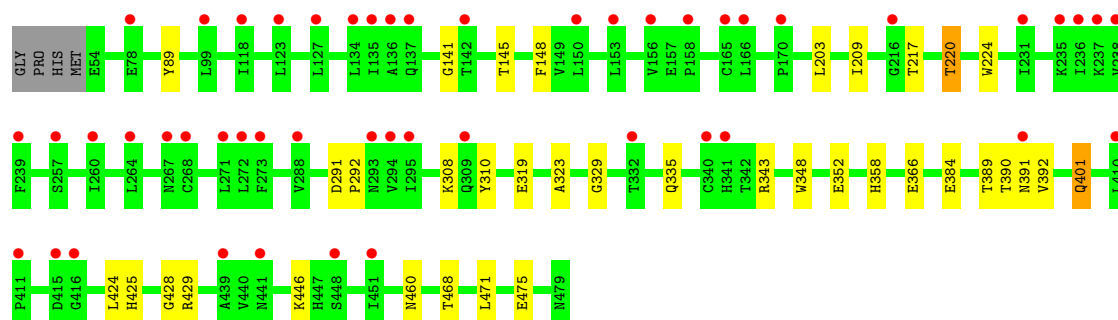


- Molecule 2: Nucleoporin like 2



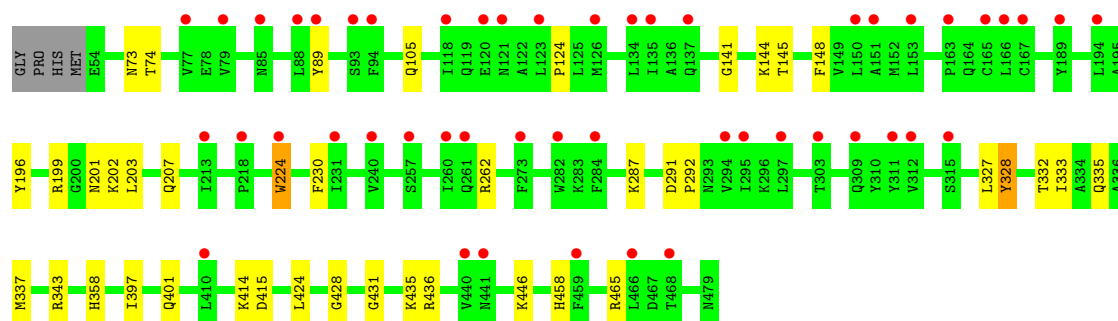
- Molecule 3: ATP-dependent RNA helicase DDX19B





- Molecule 3: ATP-dependent RNA helicase DDX19B

Chain F: 11% 90% 9%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.94Å 73.56Å 145.86Å 90.00° 95.07° 90.00°	Depositor
Resolution (Å)	48.43 – 3.40 48.43 – 3.40	Depositor EDS
% Data completeness (in resolution range)	82.3 (48.43-3.40) 99.6 (48.43-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.30	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 3.40Å)	Xtriage
Refinement program	PHENIX (dev_2006: ???)	Depositor
R, $R_{free}$	0.261 , 0.313 0.268 , 0.313	Depositor DCC
$R_{free}$ test set	2362 reflections (9.16%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	115.5	Xtriage
Anisotropy	0.550	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 47.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	25350	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: PO4, ANP, MG

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	0.23	0/2604	0.36	0/3514
1	B	0.24	0/2604	0.37	0/3514
2	C	0.23	0/363	0.41	0/491
2	D	0.23	0/315	0.39	0/426
3	E	0.23	0/3442	0.39	0/4645
3	F	0.23	0/3442	0.40	0/4645
All	All	0.23	0/12770	0.38	0/17235

There are no bond length outliers.

There are no bond angle outliers.

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	2541	2558	2558	9	0
1	B	2541	2558	2558	17	0
2	C	356	379	379	4	0
2	D	308	333	331	2	0
3	E	3379	3445	3438	21	0
3	F	3379	3446	3438	22	0
4	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	10	0	0	1	0
4	F	10	0	0	1	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	E	31	17	13	1	0
6	F	31	16	13	2	0
All	All	12598	12752	12728	67	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (67) 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:489:GLU:OE2	1:B:569:ARG:NH1	2.18	0.77
3:F:199:ARG:NH2	4:F:502:PO4:O1	2.20	0.74
1:B:584:ARG:NH2	1:B:592:GLU:O	2.22	0.72
1:A:423:GLN:NE2	3:E:329:GLY:O	2.25	0.69
1:A:697:ARG:O	3:F:105:GLN:NE2	2.32	0.62
3:E:335:GLN:OE1	3:E:401:GLN:NE2	2.34	0.60
1:B:640:GLN:NE2	2:C:420:LEU:O	2.35	0.57
3:E:429:ARG:NH1	4:E:501:PO4:O2	2.37	0.56
1:A:495:HIS:HB2	3:E:401:GLN:HG2	1.87	0.56
1:A:660:THR:OG1	1:A:665:MET:SD	2.58	0.55
1:A:583:LEU:O	1:A:594:HIS:NE2	2.37	0.54
3:F:196:TYR:O	3:F:201:ASN:ND2	2.34	0.54
3:E:424:LEU:O	3:E:428:GLY:N	2.36	0.53
3:E:471:LEU:H	3:E:471:LEU:HD12	1.73	0.53
2:D:419:GLU:OE1	2:D:419:GLU:N	2.43	0.52
1:B:532:VAL:O	1:B:603:ARG:NH1	2.37	0.51
3:F:424:LEU:O	3:F:428:GLY:N	2.40	0.51
3:E:471:LEU:O	3:E:475:GLU:N	2.34	0.50
3:F:141:GLY:H	6:F:504:ANP:PB	2.35	0.50
1:B:435:THR:HG22	1:B:501:PRO:HG3	1.95	0.49
3:E:323:ALA:HB1	3:E:468:THR:HG21	1.96	0.47
3:E:319:GLU:O	3:E:323:ALA:N	2.41	0.47
1:A:544:LEU:O	1:A:548:GLN:N	2.40	0.47
3:E:343:ARG:NH1	3:F:207:GLN:OE1	2.47	0.47
3:E:335:GLN:NE2	3:E:384:GLU:O	2.47	0.47
3:F:337:MET:SD	3:F:397:ILE:HG22	2.54	0.47
3:E:217:THR:OG1	3:E:220:THR:OG1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:328:TYR:CD1	3:F:333:ILE:HG21	2.51	0.45
2:C:419:GLU:OE1	2:C:419:GLU:N	2.49	0.45
1:B:599:ASN:OD1	1:B:600:HIS:ND1	2.50	0.45
3:F:335:GLN:OE1	3:F:401:GLN:NE2	2.46	0.45
3:F:262:ARG:NH2	3:F:287:LYS:O	2.49	0.44
1:B:486:LYS:HB3	3:F:332:THR:HG22	1.99	0.44
3:E:389:THR:OG1	3:E:392:VAL:O	2.36	0.44
1:B:609:LEU:HD22	1:B:648:ILE:HG22	2.00	0.43
3:F:144:LYS:NZ	6:F:504:ANP:O3G	2.43	0.43
3:E:366:GLU:HA	3:F:203:LEU:HD13	2.00	0.43
3:F:73:ASN:OD1	3:F:74:THR:N	2.51	0.43
1:B:500:PHE:CZ	1:B:687:PRO:HB2	2.54	0.43
1:A:407:LEU:HD23	1:A:475:PHE:CG	2.54	0.43
2:C:384:ASN:OD1	2:C:384:ASN:N	2.52	0.43
3:E:348:TRP:NE1	3:E:352:GLU:OE1	2.52	0.43
3:E:390:THR:O	3:E:391:ASN:HB2	2.19	0.43
1:B:430:VAL:HG12	1:B:487:GLN:HG3	2.01	0.43
2:C:385:VAL:HG12	2:C:385:VAL:O	2.19	0.42
3:F:327:LEU:HD23	3:F:327:LEU:O	2.20	0.42
3:E:291:ASP:N	3:E:292:PRO:HD3	2.34	0.42
1:B:500:PHE:N	1:B:501:PRO:HD2	2.35	0.42
3:E:141:GLY:H	6:E:504:ANP:PB	2.43	0.42
1:B:648:ILE:HA	1:B:652:TYR:CB	2.50	0.42
3:F:431:GLY:HA2	3:F:435:LYS:HB2	2.02	0.42
3:F:89:TYR:HB3	3:F:124:PRO:HB2	2.02	0.42
1:B:660:THR:OG1	1:B:665:MET:SD	2.64	0.41
3:E:308:LYS:HB3	3:E:310:TYR:CE2	2.56	0.41
3:E:145:THR:HA	3:E:148:PHE:CE2	2.55	0.41
3:F:224:TRP:O	3:F:230:PHE:N	2.53	0.41
1:A:640:GLN:HG3	2:D:416:PRO:CB	2.51	0.41
1:A:428:ILE:N	1:A:429:PRO:CD	2.84	0.41
3:F:291:ASP:N	3:F:292:PRO:HD3	2.36	0.41
1:B:608:ILE:CD1	1:B:622:LEU:HD13	2.51	0.41
3:F:145:THR:HA	3:F:148:PHE:CE2	2.55	0.41
3:F:203:LEU:HD11	3:F:207:GLN:OE1	2.21	0.41
1:B:608:ILE:HD11	1:B:622:LEU:HD13	2.02	0.40
1:B:532:VAL:N	1:B:533:PRO:HA	2.36	0.40
3:E:203:LEU:HD21	3:E:209:ILE:HD11	2.04	0.40
3:F:414:LYS:O	3:F:415:ASP:HB2	2.22	0.40
1:B:427:THR:HB	1:B:483:LYS:HG3	2.02	0.40

There are no symmetry-related clashes.

## 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	313/317 (99%)	293 (94%)	20 (6%)	0	100	100
1	B	313/317 (99%)	293 (94%)	20 (6%)	0	100	100
2	C	42/49 (86%)	39 (93%)	3 (7%)	0	100	100
2	D	36/49 (74%)	34 (94%)	2 (6%)	0	100	100
3	E	425/430 (99%)	408 (96%)	17 (4%)	0	100	100
3	F	425/430 (99%)	410 (96%)	15 (4%)	0	100	100
All	All	1554/1592 (98%)	1477 (95%)	77 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	277/279 (99%)	274 (99%)	3 (1%)	76	89
1	B	277/279 (99%)	275 (99%)	2 (1%)	85	93
2	C	42/45 (93%)	40 (95%)	2 (5%)	28	64
2	D	36/45 (80%)	35 (97%)	1 (3%)	47	77
3	E	376/378 (100%)	368 (98%)	8 (2%)	56	82
3	F	376/378 (100%)	367 (98%)	9 (2%)	52	80
All	All	1384/1404 (99%)	1359 (98%)	25 (2%)	62	83

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	538	PHE
1	B	664	GLN
2	C	384	ASN
2	C	391	ASP
1	A	452	LEU
1	A	462	ARG
1	A	538	PHE
2	D	391	ASP
3	E	89	TYR
3	E	220	THR
3	E	224	TRP
3	E	358	HIS
3	E	401	GLN
3	E	425	HIS
3	E	446	LYS
3	E	460	ASN
3	F	202	LYS
3	F	224	TRP
3	F	328	TYR
3	F	343	ARG
3	F	358	HIS
3	F	436	ARG
3	F	446	LYS
3	F	458	HIS
3	F	465	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 molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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
4	PO4	B	701	-	4,4,4	0.76	0	6,6,6	0.42	0
4	PO4	B	702	-	4,4,4	0.76	0	6,6,6	0.39	0
4	PO4	E	501	-	4,4,4	0.75	0	6,6,6	0.40	0
4	PO4	E	502	-	4,4,4	0.75	0	6,6,6	0.41	0
6	ANP	E	504	5	29,33,33	0.87	1 (3%)	29,52,52	3.18	4 (13%)
4	PO4	F	501	-	4,4,4	0.75	0	6,6,6	0.35	0
4	PO4	F	502	-	4,4,4	0.76	0	6,6,6	0.34	0
6	ANP	F	504	5	29,33,33	0.78	1 (3%)	29,52,52	3.16	4 (13%)

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
4	PO4	B	701	-	-	0/0/0/0	0/0/0/0
4	PO4	B	702	-	-	0/0/0/0	0/0/0/0
4	PO4	E	501	-	-	0/0/0/0	0/0/0/0
4	PO4	E	502	-	-	0/0/0/0	0/0/0/0
6	ANP	E	504	5	-	1/13/38/38	0/3/3/3
4	PO4	F	501	-	-	0/0/0/0	0/0/0/0
4	PO4	F	502	-	-	0/0/0/0	0/0/0/0
6	ANP	F	504	5	-	0/13/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	504	ANP	PB-O3A	2.79	1.62	1.59
6	E	504	ANP	PB-O3A	3.58	1.63	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	504	ANP	O2B-PB-O1B	-14.95	78.94	109.88
6	F	504	ANP	O2B-PB-O1B	-14.80	79.25	109.88
6	E	504	ANP	O1B-PB-N3B	-4.59	104.92	111.79
6	F	504	ANP	O1B-PB-N3B	-4.57	104.96	111.79
6	E	504	ANP	O3A-PB-N3B	3.82	117.19	106.59
6	F	504	ANP	O3A-PB-N3B	3.97	117.62	106.59
6	F	504	ANP	O2B-PB-O3A	4.82	123.25	104.54
6	E	504	ANP	O2B-PB-O3A	4.89	123.53	104.54

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	504	ANP	O1B-PB-N3B-PG

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	501	PO4	1	0
6	E	504	ANP	1	0
4	F	502	PO4	1	0
6	F	504	ANP	2	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	315/317 (99%)	0.54	25 (7%) 12 14	69, 118, 151, 165	0
1	B	315/317 (99%)	0.36	3 (0%) 82 80	37, 79, 137, 153	0
2	C	44/49 (89%)	0.28	3 (6%) 17 19	55, 83, 104, 114	0
2	D	38/49 (77%)	0.47	2 (5%) 26 26	119, 144, 155, 171	0
3	E	426/430 (99%)	0.72	49 (11%) 5 5	64, 110, 150, 177	0
3	F	426/430 (99%)	0.66	49 (11%) 5 5	53, 112, 140, 156	0
All	All	1564/1592 (98%)	0.58	131 (8%) 11 12	37, 109, 147, 177	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	123	LEU	5.4
3	E	238	VAL	5.4
3	E	295	ILE	5.3
3	E	268	CYS	5.0
3	E	236	ILE	4.9
3	E	216	GLY	4.8
3	F	257	SER	4.6
3	E	123	LEU	4.5
1	A	615	SER	4.3
1	A	593	ILE	4.2
3	E	158	PRO	4.2
1	A	608	ILE	4.2
3	F	459	PHE	4.1
3	E	135	ILE	4.1
3	E	165	CYS	4.0
3	F	153	LEU	4.0
1	A	626	LEU	3.9
3	E	264	LEU	3.9
3	F	121	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	541	GLY	3.8
3	F	189	TYR	3.7
3	F	273	PHE	3.7
3	E	260	ILE	3.6
3	E	294	VAL	3.6
3	E	136	ALA	3.6
3	F	134	LEU	3.5
3	F	166	LEU	3.5
3	F	77	VAL	3.5
3	F	260	ILE	3.5
3	F	89	TYR	3.5
3	F	94	PHE	3.5
3	F	440	VAL	3.4
1	A	577	TYR	3.3
3	E	288	VAL	3.3
2	C	384	ASN	3.2
3	F	150	LEU	3.2
3	E	156	VAL	3.2
3	E	153	LEU	3.1
3	F	88	LEU	3.1
3	F	194	LEU	3.1
3	F	151	ALA	3.1
3	E	273	PHE	3.1
1	A	641	PHE	3.1
3	E	415	ASP	3.1
3	F	224	TRP	3.1
1	A	605	LEU	3.1
3	E	267	ASN	3.0
3	F	231	ILE	3.0
3	E	309	GLN	3.0
1	A	592	GLU	3.0
3	E	127	LEU	2.9
3	F	468	THR	2.9
1	A	596	HIS	2.9
3	F	79	VAL	2.9
1	A	633	LEU	2.9
3	E	411	PRO	2.8
1	A	484	PHE	2.8
1	A	591	GLN	2.8
3	F	303	THR	2.8
1	A	622	LEU	2.8
3	E	340	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
3	E	332	THR	2.8
1	A	543	ALA	2.7
3	E	293	ASN	2.7
3	E	439	ALA	2.6
3	E	271	LEU	2.6
1	A	451	LEU	2.6
3	E	78	GLU	2.6
1	A	452	LEU	2.6
3	F	218	PRO	2.6
1	A	387	MET	2.6
2	C	379	ILE	2.6
3	E	150	LEU	2.5
1	B	451	LEU	2.5
3	F	126	MET	2.5
3	E	99	LEU	2.5
3	F	167	CYS	2.5
2	D	388	THR	2.5
1	A	601	GLY	2.5
3	F	165	CYS	2.5
3	F	410	LEU	2.4
3	F	93	SER	2.4
3	E	410	LEU	2.4
3	F	137	GLN	2.4
3	F	441	ASN	2.4
3	F	309	GLN	2.3
3	E	441	ASN	2.3
1	A	614	LEU	2.3
3	E	257	SER	2.3
3	E	237	LYS	2.3
1	A	637	TYR	2.3
3	F	294	VAL	2.3
2	D	401	PHE	2.3
3	E	239	PHE	2.3
3	F	315	SER	2.3
3	E	166	LEU	2.3
3	E	451	ILE	2.2
3	E	231	ILE	2.2
1	B	474	ASP	2.2
3	E	118	ILE	2.2
3	F	261	GLN	2.2
3	F	295	ILE	2.2
3	E	235	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
3	F	297	LEU	2.2
2	C	382	THR	2.2
3	E	134	LEU	2.2
3	E	448	SER	2.2
3	E	416	GLY	2.2
1	A	524	LEU	2.1
3	F	135	ILE	2.1
3	F	163	PRO	2.1
3	E	272	LEU	2.1
3	E	137	GLN	2.1
3	E	170	PRO	2.1
3	F	118	ILE	2.1
1	A	678	CYS	2.1
3	F	312	VAL	2.1
1	A	674	PHE	2.1
3	F	284	PHE	2.1
1	A	648	ILE	2.1
3	F	466	LEU	2.1
3	E	391	ASN	2.1
3	F	311	TYR	2.1
1	A	646	ILE	2.1
3	F	213	ILE	2.1
3	F	120	GLU	2.0
3	F	85	ASN	2.0
3	E	142	THR	2.0
3	F	282	TRP	2.0
3	F	240	VAL	2.0
3	E	341	HIS	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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
4	PO4	B	702	5/5	0.51	0.28	102,117,124,132	0
4	PO4	F	501	5/5	0.76	0.22	115,118,124,131	0
4	PO4	E	501	5/5	0.77	0.24	120,122,125,136	0
5	MG	E	503	1/1	0.82	0.14	86,86,86,86	0
4	PO4	B	701	5/5	0.83	0.17	75,86,97,114	0
4	PO4	F	502	5/5	0.91	0.18	96,99,108,114	0
6	ANP	E	504	31/31	0.91	0.18	71,92,124,128	0
4	PO4	E	502	5/5	0.92	0.15	104,112,120,127	0
6	ANP	F	504	31/31	0.94	0.17	81,99,119,129	0
5	MG	F	503	1/1	0.98	0.15	76,76,76,76	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.