



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:10 am GMT

PDB ID : 1A2K  
Title : GDPRAN-NTF2 COMPLEX  
Authors : Stewart, M.; Kent, H.M.; Mccoy, A.J.  
Deposited on : 1998-01-06  
Resolution : 2.50 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

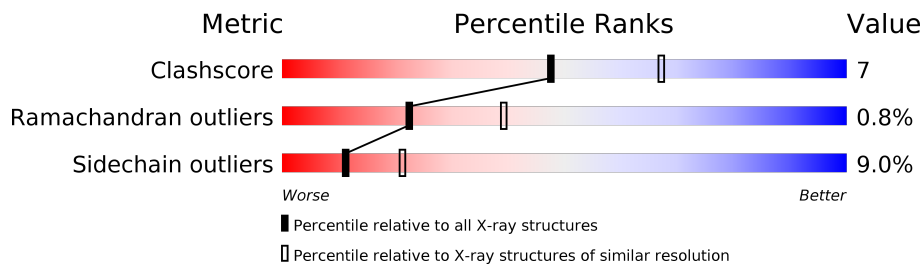
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	127	
1	B	127	
2	C	216	
2	D	216	
2	E	216	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7029 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 NUCLEAR TRANSPORT FACTOR 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	124	Total	C	N	O	S	0	0	0
			993	637	166	183	7			
1	B	124	Total	C	N	O	S	0	0	0
			997	639	167	184	7			

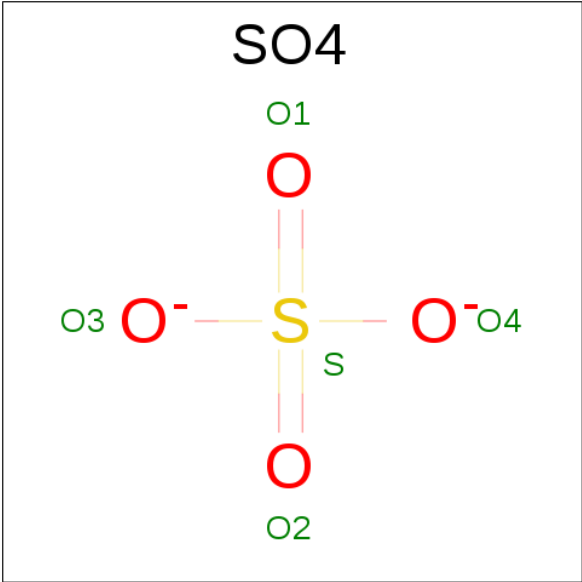
- Molecule 2 is a protein called RAN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	196	Total	C	N	O	S	0	0	0
			1570	1019	271	274	6			
2	D	199	Total	C	N	O	S	0	0	0
			1597	1034	277	280	6			
2	E	205	Total	C	N	O	S	0	0	0
			1632	1056	279	291	6			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

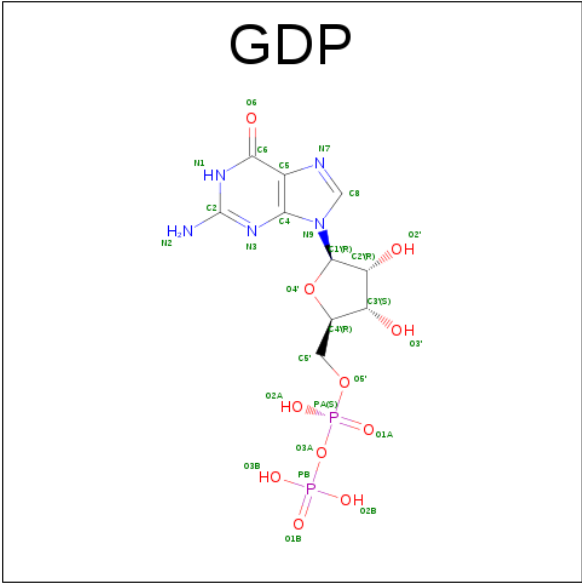
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	O	S		0	0
			5	4	1			

- Molecule 5 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>).



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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	28	Total	O	0	0
			28	28		
6	B	23	Total	O	0	0
			23	23		
6	C	35	Total	O	0	0
			35	35		
6	D	29	Total	O	0	0
			29	29		
6	E	33	Total	O	0	0
			33	33		

### 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.


Note EDS was not executed.

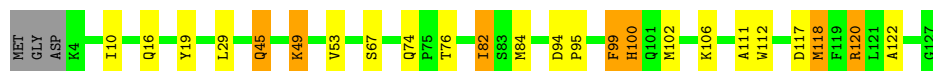
#### • Molecule 1: NUCLEAR TRANSPORT FACTOR 2

Chain A: 



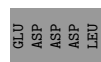
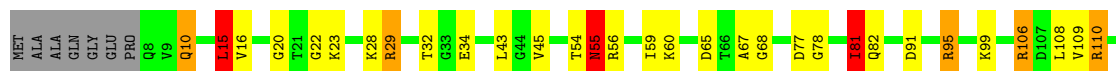
#### • Molecule 1: NUCLEAR TRANSPORT FACTOR 2

Chain B: 



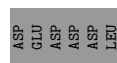
#### • Molecule 2: RAN

Chain C: 



#### • Molecule 2: RAN

Chain D: 



● Molecule 2: RAN

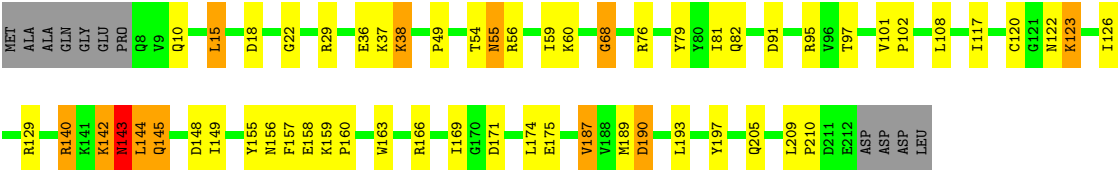
Chain E: 

68%

21%

5%

5%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.15Å 120.54Å 108.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.50	Depositor
% Data completeness (in resolution range)	99.9 (7.00-2.50)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.215 , 0.273	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7029	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, SO4

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	0.59	0/1019	1.36	9/1381 (0.7%)
1	B	0.60	0/1023	1.32	7/1386 (0.5%)
2	C	0.65	0/1610	1.68	24/2182 (1.1%)
2	D	0.63	0/1635	1.52	16/2213 (0.7%)
2	E	0.61	0/1673	1.49	19/2271 (0.8%)
All	All	0.62	0/6960	1.50	75/9433 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
2	C	0	7
2	D	0	7
2	E	0	6
All	All	0	24

There are no bond length outliers.

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	129	ARG	NE-CZ-NH1	23.04	131.82	120.30
2	C	56	ARG	CD-NE-CZ	19.59	151.03	123.60
2	C	29	ARG	NE-CZ-NH1	14.75	127.67	120.30
2	C	129	ARG	CD-NE-CZ	12.98	141.77	123.60
2	C	129	ARG	NE-CZ-NH2	-12.34	114.13	120.30
2	D	29	ARG	NE-CZ-NH1	10.78	125.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	56	ARG	NE-CZ-NH2	10.76	125.68	120.30
2	C	29	ARG	CD-NE-CZ	10.38	138.13	123.60
2	C	29	ARG	CG-CD-NE	10.30	133.44	111.80
2	E	56	ARG	CD-NE-CZ	9.76	137.26	123.60
2	D	29	ARG	NE-CZ-NH2	-9.39	115.60	120.30
1	A	120	ARG	NE-CZ-NH2	-9.08	115.76	120.30
2	D	29	ARG	CD-NE-CZ	8.87	136.02	123.60
2	D	95	ARG	CD-NE-CZ	8.72	135.81	123.60
2	C	56	ARG	NE-CZ-NH1	-8.65	115.97	120.30
2	E	76	ARG	NE-CZ-NH1	8.19	124.39	120.30
2	D	95	ARG	NE-CZ-NH1	8.12	124.36	120.30
2	C	110	ARG	CD-NE-CZ	7.86	134.61	123.60
1	B	100	HIS	CA-CB-CG	7.84	126.92	113.60
1	A	100	HIS	CA-CB-CG	7.64	126.58	113.60
2	D	146	TYR	CB-CG-CD1	-7.52	116.49	121.00
2	D	29	ARG	CG-CD-NE	7.35	127.24	111.80
2	C	55	ASN	C-N-CA	6.84	138.81	121.70
2	E	140	ARG	CD-NE-CZ	6.71	133.00	123.60
2	E	91	ASP	CB-CG-OD1	6.70	124.33	118.30
2	E	157	PHE	C-N-CA	6.59	138.18	121.70
2	E	95	ARG	NE-CZ-NH1	6.56	123.58	120.30
2	E	190	ASP	CB-CG-OD1	6.51	124.16	118.30
1	A	120	ARG	CA-CB-CG	6.33	127.32	113.40
2	E	129	ARG	CD-NE-CZ	6.28	132.38	123.60
1	A	26	ARG	C-N-CA	6.26	137.36	121.70
2	C	146	TYR	CB-CG-CD1	-6.23	117.27	121.00
2	C	81	ILE	N-CA-CB	6.22	125.11	110.80
2	C	65	ASP	CB-CG-OD1	6.16	123.85	118.30
1	A	109	ASN	CA-CB-CG	6.10	126.82	113.40
2	D	157	PHE	C-N-CA	5.92	136.51	121.70
1	A	117	ASP	CB-CG-OD1	5.90	123.61	118.30
2	C	77	ASP	C-N-CA	5.87	134.63	122.30
2	E	68	GLY	O-C-N	-5.79	113.43	122.70
2	C	29	ARG	NE-CZ-NH2	-5.71	117.44	120.30
2	D	110	ARG	NE-CZ-NH1	5.70	123.15	120.30
2	D	136	ILE	C-N-CA	5.69	135.93	121.70
2	D	53	HIS	CA-CB-CG	-5.69	103.93	113.60
2	D	129	ARG	CD-NE-CZ	5.67	131.53	123.60
2	D	137	VAL	C-N-CA	5.66	135.84	121.70
2	D	147	TYR	N-CA-CB	5.58	120.64	110.60
2	E	140	ARG	C-N-CA	5.57	135.63	121.70
1	B	118	MET	CA-CB-CG	5.55	122.73	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	120	ARG	CD-NE-CZ	5.54	131.36	123.60
2	E	143	ASN	CA-C-O	5.52	131.70	120.10
2	E	171	ASP	CB-CG-OD2	-5.51	113.34	118.30
2	C	91	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	33	TYR	CB-CG-CD1	5.37	124.22	121.00
1	B	120	ARG	CA-CB-CG	5.37	125.21	113.40
2	E	29	ARG	NE-CZ-NH1	5.34	122.97	120.30
2	E	142	LYS	C-N-CA	5.33	135.03	121.70
2	C	95	ARG	CD-NE-CZ	5.32	131.05	123.60
1	A	33	TYR	CB-CG-CD2	-5.30	117.82	121.00
2	D	171	ASP	CB-CG-OD1	5.26	123.04	118.30
2	E	79	TYR	CB-CG-CD1	-5.26	117.85	121.00
2	C	139	HIS	CA-CB-CG	5.22	122.48	113.60
2	E	171	ASP	CB-CG-OD1	5.22	123.00	118.30
2	D	24	THR	CA-CB-CG2	5.18	119.65	112.40
1	B	117	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	102	MET	CA-CB-CG	5.11	121.98	113.30
1	B	122	ALA	C-N-CA	5.10	134.45	121.70
2	E	143	ASN	C-N-CA	5.08	134.39	121.70
2	C	147	TYR	N-CA-CB	5.07	119.72	110.60
1	B	99	PHE	CB-CG-CD1	5.06	124.34	120.80
2	C	151	ALA	O-C-N	-5.06	114.60	122.70
2	C	175	GLU	CA-CB-CG	5.06	124.54	113.40
2	E	166	ARG	NE-CZ-NH2	-5.04	117.78	120.30
2	C	200	ASP	O-C-N	-5.03	114.66	122.70
2	E	187	VAL	CA-CB-CG1	5.03	118.44	110.90
2	C	147	TYR	CB-CG-CD2	-5.02	117.99	121.00

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	ASN	Mainchain
1	B	19	TYR	Mainchain
1	B	45	GLN	Mainchain
1	B	76	THR	Mainchain
2	C	109	VAL	Mainchain
2	C	15	LEU	Mainchain
2	C	156	ASN	Mainchain
2	C	16	VAL	Mainchain
2	C	34	GLU	Mainchain
2	C	54	THR	Mainchain

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Mol	Chain	Res	Type	Group
2	C	68	GLY	Mainchain
2	D	123	LYS	Mainchain
2	D	15	LEU	Mainchain
2	D	171	ASP	Mainchain
2	D	54	THR	Mainchain
2	D	65	ASP	Mainchain
2	D	66	THR	Mainchain
2	D	91	ASP	Mainchain
2	E	123	LYS	Mainchain
2	E	15	LEU	Mainchain
2	E	155	TYR	Mainchain
2	E	156	ASN	Mainchain
2	E	54	THR	Mainchain
2	E	68	GLY	Mainchain

## 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	993	0	955	15	0
1	B	997	0	961	10	0
2	C	1570	0	1574	29	0
2	D	1597	0	1613	24	0
2	E	1632	0	1628	25	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	E	5	0	0	0	0
5	C	28	0	12	1	0
5	D	28	0	12	1	0
5	E	28	0	12	0	0
6	A	28	0	0	0	0
6	B	23	0	0	0	0
6	C	35	0	0	0	0
6	D	29	0	0	0	0
6	E	33	0	0	1	0
All	All	7029	0	6767	96	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 7.

All (96) 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)
2:D:141:LYS:CA	2:D:142:LYS:N	2.45	0.80
2:E:59:ILE:HD12	2:E:169:ILE:HD11	1.68	0.76
2:D:141:LYS:CA	2:D:141:LYS:O	2.38	0.71
2:D:141:LYS:O	2:D:142:LYS:N	2.24	0.69
2:D:59:ILE:HD12	2:D:169:ILE:HD11	1.75	0.67
1:A:102:MET:HG3	1:A:118:MET:HB2	1.77	0.66
2:E:140:ARG:HA	2:E:142:LYS:HE2	1.77	0.66
2:E:55:ASN:ND2	2:E:175:GLU:H	1.98	0.62
2:C:106:ARG:HE	2:C:110:ARG:NH2	1.98	0.62
2:E:120:CYS:HB3	2:E:149:ILE:HG12	1.83	0.61
2:D:118:VAL:HG11	2:D:160:PRO:HB3	1.83	0.59
2:C:159:LYS:HB2	2:C:160:PRO:HD3	1.88	0.55
2:C:106:ARG:HE	2:C:110:ARG:HH22	1.55	0.55
2:C:55:ASN:HD21	2:C:174:LEU:HA	1.70	0.55
2:C:20:GLY:HA2	5:C:220:GDP:H5'	1.89	0.54
2:C:10:GLN:HE21	2:C:60:LYS:HD2	1.72	0.54
2:C:190:ASP:HB3	2:C:193:LEU:HB2	1.90	0.54
2:E:55:ASN:H	2:E:55:ASN:HD22	1.55	0.54
1:B:111:ALA:HB2	2:E:140:ARG:HH22	1.73	0.53
2:C:117:ILE:HB	2:C:144:LEU:HD22	1.91	0.53
2:C:29:ARG:HD2	2:C:151:ALA:O	2.08	0.53
2:E:159:LYS:HB2	2:E:160:PRO:HD3	1.90	0.52
2:C:55:ASN:ND2	2:C:175:GLU:H	2.07	0.52
2:C:15:LEU:HD13	2:C:23:LYS:HB3	1.91	0.52
1:A:108:ILE:O	1:A:109:ASN:HB2	2.10	0.52
2:D:190:ASP:HB3	2:D:193:LEU:HB2	1.92	0.52
2:E:22:GLY:HA3	2:E:122:ASN:ND2	2.25	0.51
2:C:153:SER:O	2:C:154:ASN:HB2	2.09	0.51
2:D:55:ASN:HD21	2:D:174:LEU:HA	1.76	0.51
2:C:29:ARG:HD3	2:C:154:ASN:OD1	2.10	0.51
2:C:43:LEU:HB2	2:C:45:VAL:HG12	1.94	0.50
1:A:42:GLU:HA	1:A:120:ARG:HD2	1.93	0.50
2:C:22:GLY:HA3	2:C:122:ASN:HD22	1.76	0.50
1:B:94:ASP:HB3	1:B:95:PRO:HD2	1.93	0.50
2:E:55:ASN:HD21	2:E:174:LEU:HA	1.77	0.50
2:D:127:LYS:HD3	2:D:193:LEU:HD11	1.93	0.49
2:D:29:ARG:HD2	2:D:151:ALA:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:142:LYS:O	2:E:143:ASN:HB3	2.13	0.49
2:C:145:GLN:HG3	2:C:163:TRP:NE1	2.28	0.48
2:D:145:GLN:HG3	2:D:163:TRP:NE1	2.28	0.48
2:C:10:GLN:HB3	2:C:60:LYS:HB3	1.95	0.47
2:E:145:GLN:HG3	2:E:163:TRP:NE1	2.28	0.47
2:C:150:SER:HB3	2:C:155:TYR:HB3	1.97	0.47
2:C:22:GLY:HA3	2:C:122:ASN:ND2	2.30	0.47
2:E:123:LYS:HB3	2:E:126:ILE:HD12	1.98	0.46
2:C:108:LEU:HD11	2:C:115:ILE:HD11	1.97	0.46
2:E:145:GLN:HG3	2:E:163:TRP:CD1	2.50	0.46
2:D:78:GLY:HA2	2:D:81:ILE:HG23	1.96	0.46
1:A:76:THR:HB	1:A:77:PRO:HD2	1.98	0.46
2:C:140:ARG:HH21	2:C:146:TYR:HB3	1.80	0.46
1:A:82:ILE:HD12	1:A:104:LEU:HD13	1.98	0.46
1:B:74:GLN:HB2	1:B:82:ILE:HG22	1.97	0.45
2:D:124:VAL:HG23	2:D:189:MET:HE1	1.99	0.45
2:E:18:ASP:OD2	2:E:97:THR:HA	2.16	0.45
2:C:137:VAL:HG12	2:C:140:ARG:HE	1.82	0.45
2:E:140:ARG:HD2	2:E:205:GLN:NE2	2.32	0.45
2:C:127:LYS:HD3	2:C:193:LEU:HD11	1.99	0.44
1:B:95:PRO:HG2	2:C:67:ALA:HB1	1.98	0.44
2:C:156:ASN:O	2:C:157:PHE:C	2.55	0.44
1:A:39:LEU:HD22	1:A:52:ILE:HG23	2.00	0.44
2:D:85:CYS:HB2	2:D:164:LEU:HD22	1.99	0.44
1:A:60:PRO:HG2	2:D:71:LYS:HB3	2.00	0.44
2:D:10:GLN:HE21	2:D:60:LYS:HD3	1.83	0.43
2:E:55:ASN:HD21	2:E:174:LEU:HD12	1.83	0.43
2:E:38:LYS:NZ	2:E:49:PRO:HD3	2.33	0.43
1:A:100:HIS:HD2	1:B:100:HIS:HB3	1.83	0.43
1:A:102:MET:HB3	1:B:84:MET:SD	2.58	0.43
2:D:29:ARG:HD3	2:D:154:ASN:OD1	2.19	0.43
2:D:43:LEU:HB2	2:D:45:VAL:HG12	2.01	0.43
1:A:21:LEU:HB3	1:A:29:LEU:HD13	2.01	0.42
2:D:10:GLN:HG2	2:D:60:LYS:HD2	2.01	0.42
2:C:81:ILE:O	2:C:82:GLN:HB2	2.19	0.42
2:D:34:GLU:O	2:D:37:LYS:HD3	2.19	0.42
1:A:118:MET:HB3	1:B:84:MET:HE2	2.01	0.42
1:A:4:LYS:HA	1:A:5:PRO:HD3	1.85	0.42
2:E:101:VAL:HB	2:E:102:PRO:HD3	2.01	0.42
2:E:117:ILE:HB	2:E:144:LEU:HD22	2.01	0.42
1:A:82:ILE:O	1:B:118:MET:HE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:ILE:HD13	1:B:112:TRP:NE1	2.34	0.41
2:E:189:MET:O	2:E:190:ASP:C	2.59	0.41
2:C:55:ASN:HD22	2:C:55:ASN:H	1.67	0.41
2:C:137:VAL:HG12	2:C:140:ARG:NE	2.35	0.41
2:C:78:GLY:HA2	2:C:81:ILE:HG23	2.01	0.41
2:D:117:ILE:HB	2:D:144:LEU:HD22	2.03	0.41
2:D:123:LYS:HG2	5:D:220:GDP:C5	2.55	0.41
2:D:137:VAL:HB	2:D:138:PHE:HD1	1.85	0.41
2:E:148:ASP:HB2	6:E:456:HOH:O	2.21	0.41
1:B:49:LYS:O	1:B:53:VAL:HG23	2.21	0.40
2:E:10:GLN:HE21	2:E:60:LYS:HD3	1.86	0.40
1:A:52:ILE:O	1:A:56:LEU:HG	2.21	0.40
2:D:93:THR:HG22	2:D:128:ASP:O	2.21	0.40
2:D:24:THR:HG23	2:D:28:LYS:HE3	2.03	0.40
2:E:193:LEU:HD22	2:E:197:TYR:CZ	2.57	0.40
2:E:81:ILE:O	2:E:82:GLN:HB2	2.21	0.40
1:A:37:SER:HA	1:A:115:THR:O	2.21	0.40
2:E:209:LEU:HB3	2:E:210:PRO:HD2	2.03	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	122/127 (96%)	116 (95%)	5 (4%)	1 (1%)	22	39
1	B	122/127 (96%)	114 (93%)	8 (7%)	0	100	100
2	C	194/216 (90%)	184 (95%)	9 (5%)	1 (0%)	32	53
2	D	195/216 (90%)	182 (93%)	9 (5%)	4 (2%)	8	13
2	E	203/216 (94%)	187 (92%)	15 (7%)	1 (0%)	32	53
All	All	836/902 (93%)	783 (94%)	46 (6%)	7 (1%)	22	39

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	138	PHE
2	E	143	ASN
2	D	113	GLU
2	D	204	ALA
1	A	109	ASN
2	C	128	ASP
2	D	143	ASN

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	108/111 (97%)	104 (96%)	4 (4%)	39	66
1	B	109/111 (98%)	99 (91%)	10 (9%)	11	20
2	C	167/185 (90%)	145 (87%)	22 (13%)	5	8
2	D	172/185 (93%)	153 (89%)	19 (11%)	7	13
2	E	174/185 (94%)	163 (94%)	11 (6%)	21	38
All	All	730/777 (94%)	664 (91%)	66 (9%)	11	21

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	62	GLN
1	A	100	HIS
1	A	120	ARG
1	B	16	GLN
1	B	29	LEU
1	B	45	GLN
1	B	49	LYS
1	B	67	SER
1	B	82	ILE
1	B	99	PHE

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Mol	Chain	Res	Type
1	B	102	MET
1	B	106	LYS
1	B	120	ARG
2	C	10	GLN
2	C	15	LEU
2	C	28	LYS
2	C	32	THR
2	C	55	ASN
2	C	59	ILE
2	C	81	ILE
2	C	95	ARG
2	C	99	LYS
2	C	106	ARG
2	C	129	ARG
2	C	134	LYS
2	C	135	SER
2	C	138	PHE
2	C	139	HIS
2	C	140	ARG
2	C	144	LEU
2	C	145	GLN
2	C	158	GLU
2	C	167	LYS
2	C	196	GLN
2	C	201	LEU
2	D	8	GLN
2	D	9	VAL
2	D	15	LEU
2	D	37	LYS
2	D	38	LYS
2	D	42	THR
2	D	55	ASN
2	D	81	ILE
2	D	99	LYS
2	D	108	LEU
2	D	114	ASN
2	D	134	LYS
2	D	140	ARG
2	D	144	LEU
2	D	145	GLN
2	D	158	GLU
2	D	187	VAL

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Mol	Chain	Res	Type
2	D	196	GLN
2	D	206	THR
2	E	15	LEU
2	E	36	GLU
2	E	37	LYS
2	E	38	LYS
2	E	55	ASN
2	E	108	LEU
2	E	143	ASN
2	E	144	LEU
2	E	145	GLN
2	E	158	GLU
2	E	187	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	100	HIS
1	A	116	ASN
1	B	45	GLN
1	B	116	ASN
1	B	124	HIS
2	C	10	GLN
2	C	55	ASN
2	C	82	GLN
2	C	103	ASN
2	D	10	GLN
2	D	55	ASN
2	D	62	ASN
2	D	82	GLN
2	D	103	ASN
2	D	105	HIS
2	E	10	GLN
2	E	55	ASN
2	E	62	ASN
2	E	103	ASN
2	E	143	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 ⓘ

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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$
5	GDP	C	220	3	25,30,30	1.36	5 (20%)	26,47,47	2.81	7 (26%)
5	GDP	D	220	3	25,30,30	1.40	5 (20%)	26,47,47	2.64	9 (34%)
5	GDP	E	220	3	25,30,30	1.59	5 (20%)	26,47,47	2.73	8 (30%)
4	SO4	E	222	-	4,4,4	0.40	0	6,6,6	0.54	0

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
5	GDP	C	220	3	-	0/12/32/32	0/3/3/3
5	GDP	D	220	3	-	0/12/32/32	0/3/3/3
5	GDP	E	220	3	-	0/12/32/32	0/3/3/3
4	SO4	E	222	-	-	0/0/0/0	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	220	GDP	PB-O3B	-3.20	1.41	1.54
5	D	220	GDP	PB-O3B	-2.89	1.42	1.54
5	C	220	GDP	PB-O3B	-2.72	1.43	1.54
5	E	220	GDP	C8-N7	-2.43	1.30	1.34
5	D	220	GDP	C8-N7	-2.38	1.30	1.34
5	C	220	GDP	PB-O3A	2.20	1.63	1.60
5	C	220	GDP	C2'-C1'	2.21	1.57	1.53
5	C	220	GDP	C2-N1	2.27	1.39	1.35
5	D	220	GDP	C2-N1	2.36	1.39	1.35
5	D	220	GDP	C2'-C1'	2.64	1.57	1.53
5	E	220	GDP	C2-N1	2.64	1.40	1.35
5	E	220	GDP	PB-O3A	2.68	1.64	1.60
5	D	220	GDP	C6-N1	3.40	1.39	1.33
5	C	220	GDP	C6-N1	3.42	1.39	1.33
5	E	220	GDP	C6-N1	3.77	1.39	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	220	GDP	C5-C6-N1	-9.58	109.85	123.48
5	D	220	GDP	C5-C6-N1	-9.08	110.55	123.48
5	E	220	GDP	C5-C6-N1	-9.07	110.56	123.48
5	E	220	GDP	C2-N3-C4	-3.46	111.12	115.16
5	C	220	GDP	C2-N3-C4	-3.11	111.53	115.16
5	E	220	GDP	O3A-PB-O1B	-3.04	92.74	111.44
5	E	220	GDP	N2-C2-N1	-3.02	112.41	117.24
5	C	220	GDP	N2-C2-N1	-2.94	112.54	117.24
5	D	220	GDP	N3-C2-N1	-2.86	123.28	127.46
5	C	220	GDP	O3A-PB-O1B	-2.34	97.03	111.44
5	D	220	GDP	C2-N3-C4	-2.18	112.61	115.16
5	D	220	GDP	N2-C2-N1	-2.02	114.01	117.24
5	E	220	GDP	N2-C2-N3	2.06	121.56	117.75
5	D	220	GDP	C1'-N9-C4	2.08	130.23	126.64
5	D	220	GDP	C4-C5-N7	2.35	111.68	109.41
5	D	220	GDP	N2-C2-N3	2.68	122.71	117.75
5	C	220	GDP	N2-C2-N3	2.76	122.84	117.75
5	E	220	GDP	C1'-N9-C4	3.38	132.48	126.64
5	D	220	GDP	O5'-C5'-C4'	3.45	121.24	109.00
5	C	220	GDP	O5'-C5'-C4'	3.98	123.10	109.00
5	E	220	GDP	O5'-C5'-C4'	4.93	126.49	109.00
5	E	220	GDP	C6-N1-C2	5.41	123.84	116.06
5	C	220	GDP	C6-N1-C2	6.34	125.19	116.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	220	GDP	C6-N1-C2	6.51	125.42	116.06

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
5	C	220	GDP	1	0
5	D	220	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.