



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2016 – 05:13 AM EDT

PDB ID : 2GVJ  
Title : Crystal Structure of Human NMPRTase in complex with FK866  
Authors : Khan, J.A.; Tao, X.; Tong, L.  
Deposited on : 2006-05-02  
Resolution : 2.10 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028320  
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) : rb-20028320

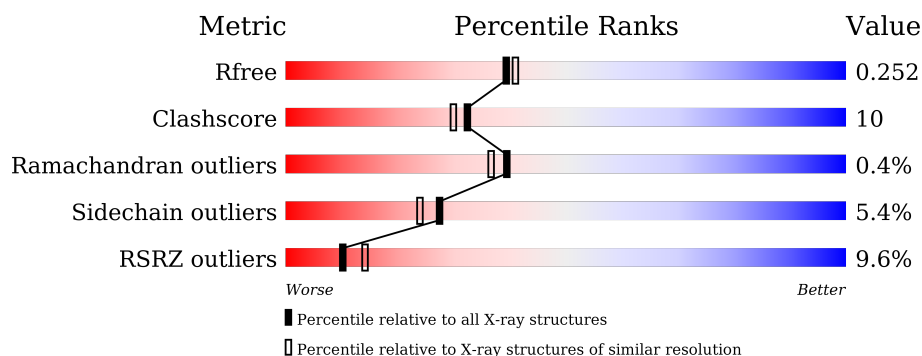
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	491	<div> <div>9%</div> <div>72%</div> <div>20%</div> <div>• 5%</div> </div>
1	B	491	<div> <div>10%</div> <div>75%</div> <div>18%</div> <div>• 5%</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8264 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.

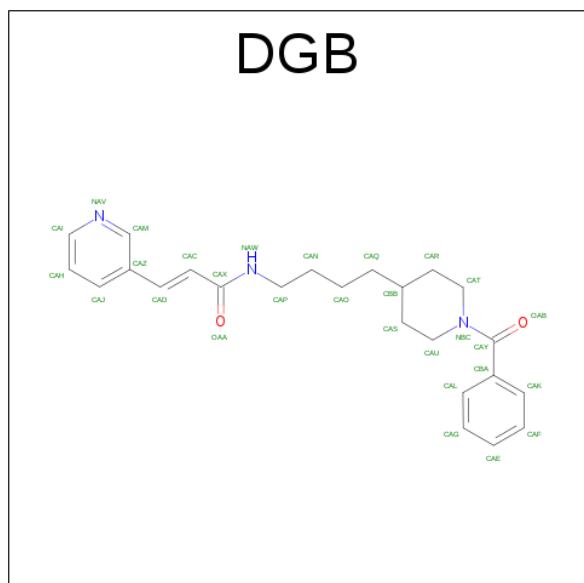
- Molecule 1 is a protein called Nicotinamide phosphoribosyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	Se	0	0	0
			3720	2393	614	706	5	2			
1	B	464	Total	C	N	O	S	Se	0	0	0
			3711	2388	613	703	5	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P43490
A	368	MSE	MET	MODIFIED RESIDUE	UNP P43490
A	372	MSE	MET	MODIFIED RESIDUE	UNP P43490
B	1	MSE	MET	MODIFIED RESIDUE	UNP P43490
B	368	MSE	MET	MODIFIED RESIDUE	UNP P43490
B	372	MSE	MET	MODIFIED RESIDUE	UNP P43490

- Molecule 2 is (2E)-N-{4-[1-(BENZENECARBONYL)PIPERIDIN-4-YL]BUTYL}-3-(PYRIDIN-3-YL)PROP-2-ENAMIDE (three-letter code: DGB) (formula: C<sub>24</sub>H<sub>29</sub>N<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			29	24	3	2		
2	A	1	Total	C	N	O	0	0
			29	24	3	2		

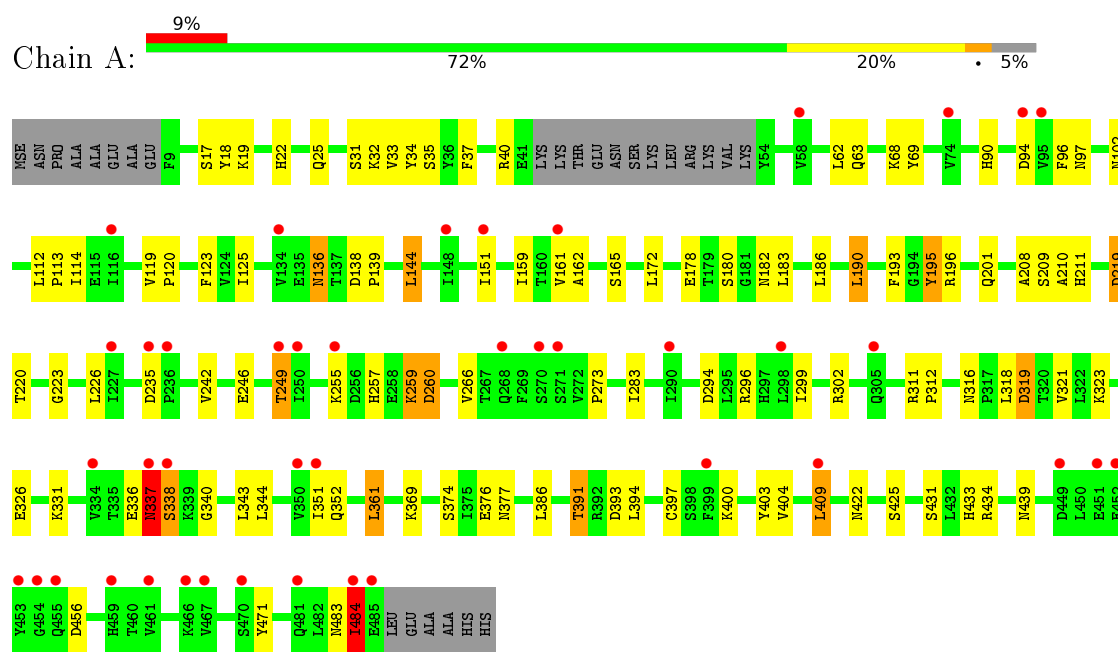
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	388	Total	O	0	0
			388	388		
3	B	387	Total	O	0	0
			387	387		

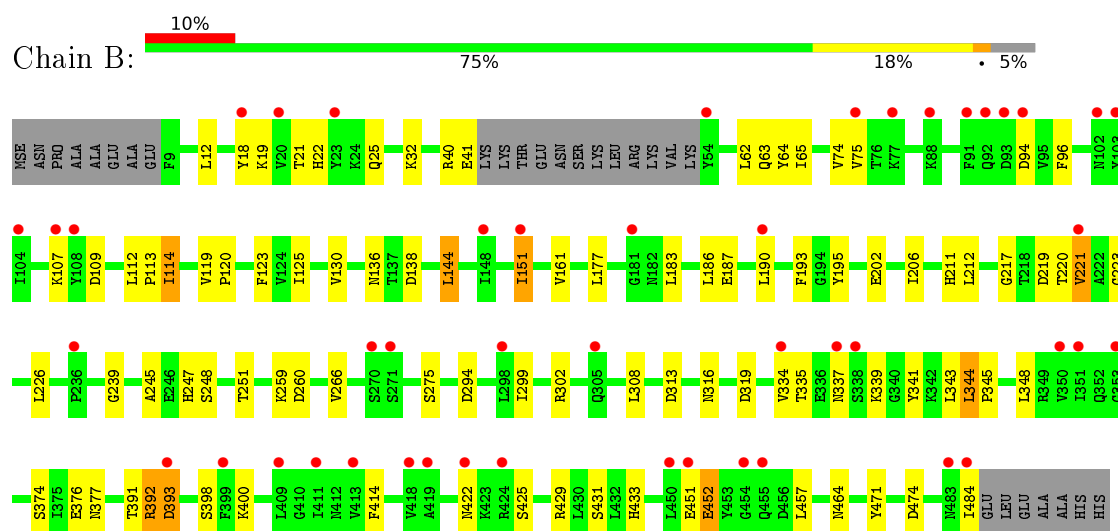
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Nicotinamide phosphoribosyltransferase



#### • Molecule 1: Nicotinamide phosphoribosyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.78 Å 105.90 Å 83.43 Å 90.00° 96.45° 90.00°	Depositor
Resolution (Å)	82.76 – 2.10 29.84 – 2.09	Depositor EDS
% Data completeness (in resolution range)	98.2 (82.76-2.10) 91.8 (29.84-2.09)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.12 (at 2.10 Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, $R_{free}$	0.247 , 0.298 0.247 , 0.252	Depositor DCC
$R_{free}$ test set	4346 reflections (8.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	12.7	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	8264	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.57% 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

### 5.1 Standard geometry

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

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	0.46	0/3806	0.73	8/5155 (0.2%)
1	B	0.46	0/3797	0.73	7/5143 (0.1%)
All	All	0.46	0/7603	0.73	15/10298 (0.1%)

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

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	456	ASP	CB-CG-OD2	7.22	124.80	118.30
1	A	138	ASP	CB-CG-OD2	6.45	124.10	118.30
1	B	474	ASP	CB-CG-OD2	6.08	123.77	118.30
1	B	138	ASP	CB-CG-OD2	6.03	123.73	118.30
1	A	409	LEU	CA-CB-CG	5.79	128.60	115.30
1	B	109	ASP	CB-CG-OD2	5.75	123.47	118.30
1	A	219	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	313	ASP	CB-CG-OD2	5.48	123.23	118.30
1	B	260	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	235	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	260	ASP	CB-CG-OD2	5.16	122.95	118.30
1	A	94	ASP	CB-CG-OD2	5.11	122.89	118.30
1	B	94	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	319	ASP	CB-CG-OD2	5.08	122.87	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	393	ASP	CB-CG-OD2	5.06	122.85	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	337	ASN	Peptide

## 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	3720	0	3692	87	0
1	B	3711	0	3686	74	0
2	A	29	0	31	1	0
2	B	29	0	31	2	0
3	A	388	0	0	26	0
3	B	387	0	0	19	0
All	All	8264	0	7440	156	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 10.

All (156) 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:114:ILE:HD13	1:B:144:LEU:HD13	1.40	1.04
1:A:283:ILE:HG12	3:A:1358:HOH:O	1.57	1.03
1:A:119:VAL:HG21	1:A:125:ILE:HD11	1.42	0.99
1:B:40:ARG:HD3	1:B:422:ASN:O	1.67	0.93
1:A:338:SER:HB3	3:A:1182:HOH:O	1.70	0.90
1:A:165:SER:HA	3:A:1359:HOH:O	1.71	0.89
1:A:249:THR:HG21	1:B:25:GLN:OE1	1.73	0.88
1:B:344:LEU:H	1:B:377:ASN:HD21	1.22	0.85
1:A:223:GLY:HA2	3:A:813:HOH:O	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:LEU:HD13	1:A:376:GLU:HG3	1.59	0.82
1:B:32:LYS:HD3	3:B:844:HOH:O	1.81	0.81
1:B:343:LEU:HD13	1:B:376:GLU:HG3	1.64	0.79
1:A:344:LEU:H	1:A:377:ASN:HD21	1.28	0.79
1:B:316:ASN:HD22	1:B:319:ASP:H	1.33	0.77
1:A:336:GLU:HG2	1:A:337:ASN:CB	2.15	0.77
1:B:64:TYR:CE2	1:B:206:ILE:HD11	2.19	0.77
1:B:343:LEU:CD1	1:B:376:GLU:HG3	2.15	0.76
1:A:63:GLN:HE22	1:A:471:TYR:H	1.33	0.75
1:A:209:SER:HB3	3:A:813:HOH:O	1.89	0.72
1:A:40:ARG:HD3	1:A:422:ASN:O	1.90	0.72
1:B:221:VAL:C	3:B:1298:HOH:O	2.28	0.72
3:A:815:HOH:O	1:B:251:THR:HG21	1.89	0.72
1:A:196:ARG:HG2	3:A:1301:HOH:O	1.90	0.71
1:A:312:PRO:HB3	3:A:1358:HOH:O	1.90	0.71
1:A:226:LEU:HB3	3:A:813:HOH:O	1.90	0.71
1:A:220:THR:HG22	3:A:708:HOH:O	1.89	0.70
1:A:374:SER:OG	1:A:376:GLU:HG2	1.91	0.70
1:B:130:VAL:HG22	3:B:1332:HOH:O	1.91	0.70
1:A:25:GLN:HE22	1:B:245:ALA:HA	1.57	0.70
1:A:17:SER:OG	1:A:90:HIS:HE1	1.75	0.70
1:B:211:HIS:HA	3:B:1304:HOH:O	1.92	0.69
1:A:259:LYS:HB2	1:A:259:LYS:HZ2	1.56	0.69
1:A:336:GLU:HG2	1:A:337:ASN:N	2.06	0.69
1:A:259:LYS:HB2	1:A:259:LYS:NZ	2.08	0.68
1:B:63:GLN:HE22	1:B:471:TYR:H	1.40	0.67
1:A:40:ARG:CD	1:A:422:ASN:O	2.43	0.67
1:B:400:LYS:HD2	1:B:425:SER:HB3	1.77	0.67
1:A:338:SER:HB2	3:A:1005:HOH:O	1.94	0.66
1:B:344:LEU:H	1:B:377:ASN:ND2	1.92	0.66
1:B:348:LEU:HB3	3:B:1343:HOH:O	1.96	0.66
1:A:136:ASN:HD22	1:A:136:ASN:H	1.44	0.65
1:B:64:TYR:CZ	1:B:206:ILE:HD11	2.31	0.65
1:B:161:VAL:HG12	3:B:1304:HOH:O	1.97	0.65
1:A:302:ARG:NH1	3:A:1448:HOH:O	2.17	0.64
1:A:316:ASN:HD22	1:A:319:ASP:H	1.45	0.64
1:A:400:LYS:HD2	1:A:425:SER:HB3	1.79	0.63
1:A:195:TYR:OH	1:A:201:GLN:NE2	2.31	0.62
1:B:193:PHE:CZ	2:B:501:DGB:HAD1	2.34	0.62
1:B:220:THR:HG22	3:B:769:HOH:O	1.98	0.62
1:A:249:THR:HG23	1:B:25:GLN:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ASN:HA	1:A:340:GLY:H	1.66	0.61
1:A:296:ARG:NH1	1:A:331:LYS:O	2.34	0.61
1:B:348:LEU:CB	3:B:1343:HOH:O	2.49	0.60
1:A:336:GLU:HG2	1:A:337:ASN:HB2	1.83	0.60
1:A:338:SER:CB	3:A:1005:HOH:O	2.49	0.60
1:A:35:SER:HB3	3:A:1324:HOH:O	2.02	0.59
1:B:206:ILE:HD13	1:B:226:LEU:HD11	1.86	0.58
1:B:113:PRO:HA	1:B:464:ASN:HD22	1.69	0.58
1:B:398:SER:HA	3:B:1322:HOH:O	2.03	0.58
1:B:221:VAL:O	1:B:221:VAL:HG12	2.03	0.58
3:A:611:HOH:O	1:B:391:THR:HG23	2.05	0.57
1:A:161:VAL:HG12	3:A:722:HOH:O	2.05	0.56
1:A:266:VAL:HB	1:A:302:ARG:HH21	1.69	0.55
1:B:64:TYR:CE2	1:B:206:ILE:CD1	2.88	0.55
1:A:178:GLU:HG3	3:A:888:HOH:O	2.05	0.55
1:A:32:LYS:HA	1:A:136:ASN:HD21	1.71	0.55
1:A:182:ASN:ND2	3:A:952:HOH:O	2.40	0.54
1:A:400:LYS:HD2	1:A:425:SER:CB	2.37	0.54
1:A:34:TYR:HB3	1:A:403:TYR:HB3	1.90	0.54
1:A:343:LEU:CD1	1:A:376:GLU:HG3	2.33	0.53
1:B:248:SER:HA	1:B:251:THR:HG22	1.89	0.53
1:B:343:LEU:HD13	1:B:376:GLU:CG	2.36	0.53
1:A:336:GLU:CG	1:A:337:ASN:N	2.72	0.53
1:A:19:LYS:HA	1:A:22:HIS:CD2	2.44	0.53
1:B:433:HIS:HA	1:B:457:LEU:HD13	1.90	0.53
1:A:321:VAL:HG23	1:A:352:GLN:HE21	1.74	0.52
1:B:247:HIS:O	1:B:251:THR:HG22	2.09	0.52
1:A:193:PHE:CZ	2:A:502:DGB:HAD1	2.45	0.52
1:A:190:LEU:CD1	3:A:1359:HOH:O	2.57	0.52
1:A:255:LYS:HG2	3:A:1314:HOH:O	2.09	0.51
1:B:21:THR:HA	3:B:1341:HOH:O	2.11	0.51
1:B:337:ASN:HB3	1:B:339:LYS:H	1.76	0.51
1:B:316:ASN:ND2	1:B:319:ASP:H	2.06	0.50
1:A:32:LYS:O	1:A:404:VAL:HG23	2.12	0.50
1:B:19:LYS:HA	1:B:22:HIS:CD2	2.46	0.50
1:A:33:VAL:H	1:A:136:ASN:HD21	1.59	0.50
1:A:299:ILE:HA	1:A:302:ARG:HD2	1.94	0.50
1:B:374:SER:OG	1:B:376:GLU:HG2	2.12	0.49
1:A:172:LEU:HD21	1:A:361:LEU:HD21	1.94	0.49
1:B:40:ARG:O	1:B:41:GLU:HB3	2.13	0.49
1:A:344:LEU:H	1:A:377:ASN:ND2	2.04	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:LEU:HD23	1:B:96:PHE:HZ	1.76	0.49
1:A:33:VAL:H	1:A:136:ASN:ND2	2.11	0.48
1:B:275:SER:CB	2:B:501:DGB:HAP1	2.43	0.48
1:A:136:ASN:H	1:A:136:ASN:ND2	2.10	0.48
1:A:17:SER:OG	1:A:90:HIS:CE1	2.62	0.48
1:A:63:GLN:HE22	1:A:471:TYR:N	2.06	0.48
1:A:159:ILE:HD11	3:A:773:HOH:O	2.14	0.48
1:A:316:ASN:HB3	1:A:319:ASP:HB2	1.96	0.48
1:B:120:PRO:O	1:B:123:PHE:HB2	2.13	0.48
1:A:90:HIS:HD2	1:B:239:GLY:O	1.97	0.48
1:B:266:VAL:HB	1:B:302:ARG:HH21	1.79	0.48
1:B:40:ARG:CD	1:B:422:ASN:O	2.50	0.47
1:A:40:ARG:HD2	1:A:422:ASN:O	2.14	0.47
1:B:414:PHE:CB	3:B:1317:HOH:O	2.62	0.47
1:B:113:PRO:HD2	1:B:144:LEU:CD1	2.45	0.47
1:B:259:LYS:HD2	1:B:294:ASP:HB3	1.96	0.47
1:A:391:THR:CG2	1:A:393:ASP:H	2.28	0.46
1:B:74:VAL:HG23	1:B:75:VAL:HG23	1.97	0.46
1:B:391:THR:HG22	1:B:392:ARG:N	2.29	0.46
1:A:483:ASN:O	1:A:484:ILE:C	2.53	0.46
1:A:162:ALA:HA	3:A:722:HOH:O	2.16	0.45
1:B:119:VAL:HG22	1:B:120:PRO:HD2	1.98	0.45
1:A:431:SER:OG	1:A:433:HIS:HE1	2.00	0.45
1:B:187:GLU:HG2	3:B:933:HOH:O	2.17	0.45
1:B:223:GLY:N	3:B:769:HOH:O	2.50	0.45
1:A:211:HIS:HA	3:A:722:HOH:O	2.17	0.44
1:B:119:VAL:HG21	1:B:125:ILE:HD11	1.99	0.44
1:B:202:GLU:O	1:B:206:ILE:HG12	2.18	0.44
1:B:113:PRO:HD2	1:B:144:LEU:HD12	2.00	0.43
1:A:178:GLU:OE1	1:A:369:LYS:HE3	2.18	0.43
1:B:429:ARG:NH1	3:B:786:HOH:O	2.51	0.43
1:A:311:ARG:HG3	1:A:351:ILE:HG23	2.00	0.43
1:B:114:ILE:HD12	1:B:136:ASN:HA	2.01	0.43
1:B:345:PRO:HG2	3:B:1343:HOH:O	2.19	0.43
1:A:63:GLN:NE2	1:A:471:TYR:H	2.09	0.42
1:A:336:GLU:HG2	1:A:337:ASN:CA	2.49	0.42
1:A:112:LEU:HA	1:A:113:PRO:HD3	1.86	0.42
1:B:211:HIS:CA	3:B:1304:HOH:O	2.60	0.42
1:A:323:LYS:HA	1:A:326:GLU:HG2	2.01	0.42
1:A:31:SER:O	1:A:139:PRO:HA	2.20	0.42
1:A:208:ALA:HB3	3:A:708:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:VAL:HG11	1:A:273:PRO:HB2	2.01	0.41
1:A:37:PHE:CZ	1:A:397:CYS:HB3	2.55	0.41
1:B:431:SER:OG	1:B:433:HIS:CE1	2.73	0.41
1:B:65:ILE:HG23	1:B:151:ILE:HD13	2.02	0.41
1:A:120:PRO:HB2	1:A:123:PHE:CD1	2.56	0.41
1:A:484:ILE:HG13	1:A:484:ILE:H	1.57	0.41
1:B:299:ILE:CD1	1:B:308:LEU:HD22	2.51	0.41
1:A:400:LYS:CD	1:A:425:SER:HB3	2.48	0.41
1:A:210:ALA:C	3:A:722:HOH:O	2.58	0.41
1:B:65:ILE:HG23	1:B:151:ILE:CD1	2.49	0.41
1:A:246:GLU:OE2	1:B:19:LYS:NZ	2.35	0.41
1:B:337:ASN:HB2	1:B:341:TYR:H	1.86	0.41
1:A:114:ILE:HG12	1:A:144:LEU:HD13	2.03	0.41
1:B:112:LEU:HA	1:B:113:PRO:HD3	1.87	0.41
1:B:266:VAL:O	1:B:302:ARG:NH2	2.55	0.40
1:B:452:GLU:HB2	3:B:1204:HOH:O	2.21	0.40
1:B:484:ILE:H	1:B:484:ILE:HD12	1.86	0.40
1:B:217:GLY:HA3	3:B:631:HOH:O	2.22	0.40
1:B:392:ARG:NH1	3:B:803:HOH:O	2.42	0.40
1:A:257:HIS:HD2	1:A:260:ASP:OD2	2.04	0.40
1:A:68:LYS:HD3	1:A:69:TYR:CZ	2.56	0.40
1:B:316:ASN:HB3	1:B:319:ASP:HB2	2.03	0.40
1:A:259:LYS:HZ1	1:A:294:ASP:HB3	1.85	0.40
1:A:439:ASN:HB3	3:A:1450:HOH:O	2.22	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	461/491 (94%)	440 (95%)	18 (4%)	3 (1%)	26 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	460/491 (94%)	443 (96%)	16 (4%)	1 (0%)	52	53
All	All	921/982 (94%)	883 (96%)	34 (4%)	4 (0%)	39	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	484	ILE
1	A	96	PHE
1	A	337	ASN
1	B	221	VAL

### 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	409/427 (96%)	385 (94%)	24 (6%)	24	20
1	B	408/427 (96%)	388 (95%)	20 (5%)	31	28
All	All	817/854 (96%)	773 (95%)	44 (5%)	27	24

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	TYR
1	A	62	LEU
1	A	97	ASN
1	A	102	ASN
1	A	136	ASN
1	A	144	LEU
1	A	151	ILE
1	A	180	SER
1	A	183	LEU
1	A	186	LEU
1	A	190	LEU
1	A	195	TYR

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Mol	Chain	Res	Type
1	A	219	ASP
1	A	249	THR
1	A	259	LYS
1	A	318	LEU
1	A	338	SER
1	A	361	LEU
1	A	386	LEU
1	A	391	THR
1	A	394	LEU
1	A	409	LEU
1	A	434	ARG
1	A	484	ILE
1	B	18	TYR
1	B	62	LEU
1	B	107	LYS
1	B	114	ILE
1	B	144	LEU
1	B	151	ILE
1	B	177	LEU
1	B	183	LEU
1	B	186	LEU
1	B	190	LEU
1	B	195	TYR
1	B	212	LEU
1	B	219	ASP
1	B	334	VAL
1	B	335	THR
1	B	344	LEU
1	B	392	ARG
1	B	393	ASP
1	B	451	GLU
1	B	452	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	25	GLN
1	A	63	GLN
1	A	90	HIS
1	A	97	ASN
1	A	102	ASN

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Mol	Chain	Res	Type
1	A	129	ASN
1	A	136	ASN
1	A	201	GLN
1	A	257	HIS
1	A	268	GLN
1	A	316	ASN
1	A	362	GLN
1	A	377	ASN
1	A	433	HIS
1	A	464	ASN
1	A	479	ASN
1	B	22	HIS
1	B	63	GLN
1	B	90	HIS
1	B	97	ASN
1	B	129	ASN
1	B	146	ASN
1	B	257	HIS
1	B	316	ASN
1	B	337	ASN
1	B	370	GLN
1	B	377	ASN
1	B	412	ASN
1	B	433	HIS
1	B	464	ASN
1	B	479	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	DGB	A	502	-	31,31,31	1.28	1 (3%)	39,39,39	1.32	6 (15%)
2	DGB	B	501	-	31,31,31	1.29	1 (3%)	39,39,39	1.46	5 (12%)

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	DGB	A	502	-	-	0/21/31/31	0/3/3/3
2	DGB	B	501	-	-	0/21/31/31	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	DGB	CAC-CAX	-6.78	1.34	1.48
2	B	501	DGB	CAC-CAX	-6.61	1.35	1.48

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	DGB	CAN-CAP-NAW	-3.40	102.68	112.29
2	A	502	DGB	CAN-CAP-NAW	-3.22	103.17	112.29
2	A	502	DGB	CAR-CAT-NBC	-3.20	106.31	110.99
2	A	502	DGB	CAZ-CAD-CAC	-2.84	120.42	126.98
2	B	501	DGB	CAS-CAU-NBC	-2.47	107.39	110.99
2	B	501	DGB	CAR-CAT-NBC	-2.32	107.61	110.99
2	A	502	DGB	CAS-CAU-NBC	-2.08	107.95	110.99
2	A	502	DGB	CAJ-CAZ-CAM	2.02	119.13	117.00
2	B	501	DGB	CAI-NAV-CAM	2.03	120.56	116.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502	DGB	CAP-NAW-CAX	3.31	127.04	122.39
2	B	501	DGB	CAP-NAW-CAX	5.71	130.41	122.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	DGB	1	0
2	B	501	DGB	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	463/491 (94%)	0.96	42 (9%) 11 16	4, 13, 21, 34	0
1	B	462/491 (94%)	0.88	47 (10%) 9 12	5, 13, 21, 31	0
All	All	925/982 (94%)	0.92	89 (9%) 10 14	4, 13, 21, 34	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	484	ILE	6.4
1	A	337	ASN	5.9
1	A	95	VAL	5.4
1	B	484	ILE	5.2
1	A	451	GLU	4.8
1	B	451	GLU	4.5
1	B	305	GLN	4.1
1	A	485	GLU	3.9
1	A	454	GLY	3.9
1	A	338	SER	3.8
1	A	409	LEU	3.7
1	B	411	ILE	3.6
1	B	221	VAL	3.6
1	A	298	LEU	3.4
1	B	338	SER	3.2
1	A	449	ASP	3.2
1	A	236	PRO	3.1
1	B	455	GLN	3.1
1	A	470	SER	3.0
1	A	94	ASP	2.9
1	A	250	ILE	2.9
1	B	104	ILE	2.9
1	A	453	TYR	2.9
1	B	236	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	409	LEU	2.8
1	B	77	LYS	2.8
1	B	413	VAL	2.8
1	B	148	ILE	2.8
1	B	102	ASN	2.8
1	B	23	TYR	2.7
1	B	271	SER	2.7
1	A	235	ASP	2.6
1	B	424	ARG	2.6
1	B	20	VAL	2.6
1	B	399	PHE	2.6
1	A	305	GLN	2.6
1	A	116	ILE	2.6
1	A	271	SER	2.5
1	B	103	TYR	2.5
1	B	337	ASN	2.5
1	A	290	ILE	2.5
1	A	466	LYS	2.5
1	A	134	VAL	2.5
1	B	450	LEU	2.4
1	B	454	GLY	2.4
1	A	334	VAL	2.4
1	A	467	VAL	2.4
1	B	88	LYS	2.4
1	B	151	ILE	2.4
1	A	452	GLU	2.4
1	A	459	HIS	2.4
1	A	255	LYS	2.3
1	A	461	VAL	2.3
1	B	18	TYR	2.3
1	A	481	GLN	2.3
1	A	350	VAL	2.3
1	B	92	GLN	2.3
1	B	351	ILE	2.3
1	B	91	PHE	2.3
1	A	148	ILE	2.3
1	A	270	SER	2.3
1	B	181	GLY	2.3
1	B	270	SER	2.3
1	B	107	LYS	2.3
1	B	422	ASN	2.2
1	B	393	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	455	GLN	2.2
1	A	58	VAL	2.2
1	A	399	PHE	2.2
1	A	249	THR	2.2
1	B	94	ASP	2.2
1	B	75	VAL	2.1
1	B	419	ALA	2.1
1	B	353	GLY	2.1
1	A	351	ILE	2.1
1	B	298	LEU	2.1
1	B	334	VAL	2.1
1	B	54	TYR	2.1
1	B	93	ASP	2.1
1	B	418	VAL	2.1
1	B	483	ASN	2.1
1	A	74	VAL	2.1
1	A	227	ILE	2.0
1	B	108	TYR	2.0
1	B	190	LEU	2.0
1	B	350	VAL	2.0
1	A	151	ILE	2.0
1	A	161	VAL	2.0
1	A	268	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<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( $\text{\AA}^2$ )	Q<0.9
2	DGB	A	502	29/29	0.82	0.23	1.27	11,12,13,14	0
2	DGB	B	501	29/29	0.87	0.19	0.53	11,12,14,14	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.