



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:27 AM GMT

PDB ID : 3P19
Title : Improved NADPH-dependent Blue Fluorescent Protein
Authors : Kao, T.H.; Chen, Y.; Pai, C.H.; Wang, A.H.J.
Deposited on : 2010-09-30
Resolution : 2.05 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

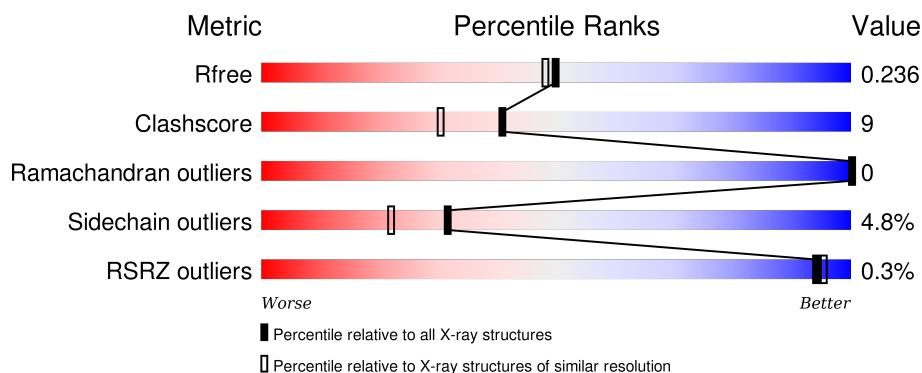
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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 ≥ 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	266	<div> <div>74%</div> <div>14%</div> <div>•</div> <div>10%</div> </div>
1	B	266	<div> <div>65%</div> <div>16%</div> <div>•</div> <div>18%</div> </div>
1	C	266	<div> <div>%</div> <div>64%</div> <div>17%</div> <div>•</div> <div>18%</div> </div>
1	D	266	<div> <div>72%</div> <div>15%</div> <div>•</div> <div>11%</div> </div>

2 Entry composition [i](#)

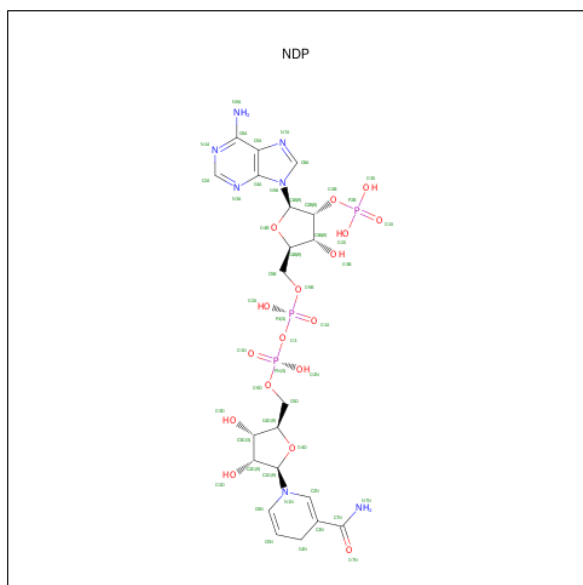
There are 3 unique types of molecules in this entry. The entry contains 7647 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Putative blue fluorescent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	0
			1817	1140	324	341	12			
1	B	218	Total	C	N	O	S	0	0	0
			1643	1033	293	307	10			
1	C	218	Total	C	N	O	S	0	0	0
			1643	1033	293	307	10			
1	D	238	Total	C	N	O	S	0	0	0
			1809	1135	323	340	11			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

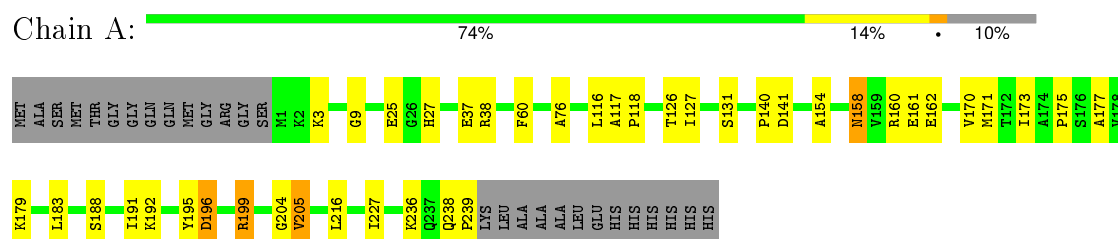
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	132	Total	O	0	0
			132	132		
3	B	128	Total	O	0	0
			128	128		
3	C	137	Total	O	0	0
			137	137		
3	D	146	Total	O	0	0
			146	146		

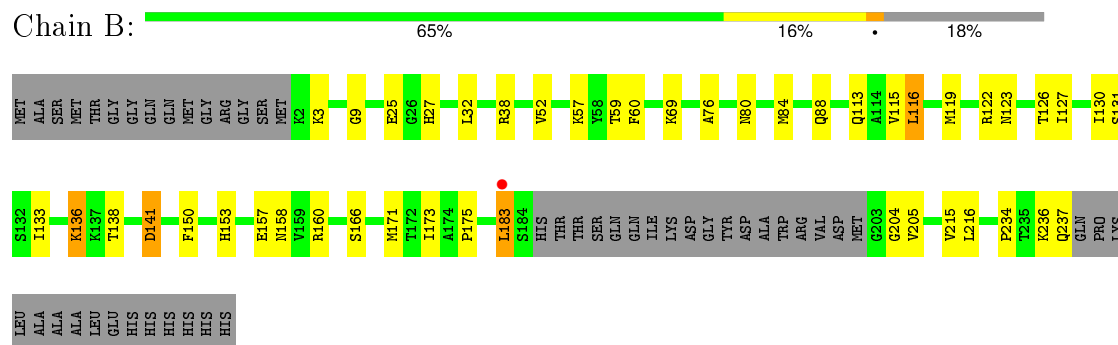
3 Residue-property plots [i](#)

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.

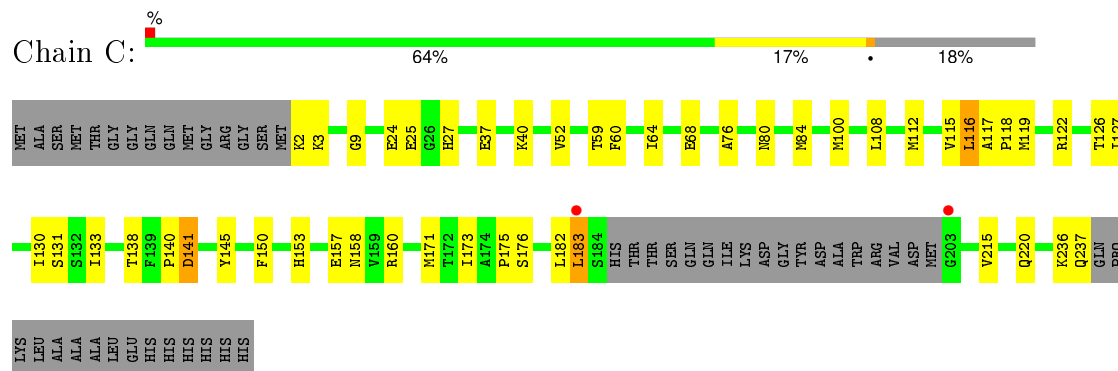
- Molecule 1: Putative blue fluorescent protein



- Molecule 1: Putative blue fluorescent protein



- Molecule 1: Putative blue fluorescent protein



- Molecule 1: Putative blue fluorescent protein



MET	ALA	SER	MET	THR	GLY	GLY	GLN	GLN	MET	GLY	ARG	GLY	SER	MET	K2	K3	G9	E16	E25	G26	H27	P28	R38	I43	I46	I47	F60	K69	N79	G111	A117	P118	M123	M129	I130	S131	S132	I133	T138	H153	A154	M158	V159
R160	E161	S166	N167	V170	M171	S176	A177	V178	K179	T180	E181	L182	L183	S188	I191	Y195	D196	R199	G204	V205	L216	I227	Q238	P239	LYS	LEU	ALA	ALA	ALA	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	64.40 Å 64.40 Å 262.59 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.32 – 2.05 24.32 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.5 (24.32-2.05) 99.5 (24.32-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.04 Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.186 , 0.239 0.185 , 0.236	Depositor DCC
R_{free} test set	3352 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	33.9	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.5	EDS
Estimated twinning fraction	0.489 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 66194 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7647	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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

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	0.52	0/1844	0.58	0/2500
1	B	0.54	0/1664	0.60	0/2254
1	C	0.53	0/1664	0.57	0/2254
1	D	0.55	0/1836	0.60	0/2490
All	All	0.54	0/7008	0.59	0/9498

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	C	0	1
1	D	0	2
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	204	GLY	Peptide
1	C	182	LEU	Peptide
1	D	204	GLY	Peptide
1	D	46	ASN	Peptide

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	1817	0	1853	30	0
1	B	1643	0	1689	32	0
1	C	1643	0	1689	39	0
1	D	1809	0	1841	28	0
2	A	48	0	26	2	0
2	B	48	0	26	3	0
2	C	48	0	26	3	0
2	D	48	0	26	2	0
3	A	132	0	0	1	0
3	B	128	0	0	4	0
3	C	137	0	0	7	0
3	D	146	0	0	1	0
All	All	7647	0	7176	123	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 9.

All (123) 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:A:238:GLN:HB2	1:A:239:PRO:HD2	1.12	1.05
1:A:238:GLN:HB2	1:A:239:PRO:CD	1.94	0.96
1:C:100:MET:HE3	1:C:145:TYR:HD1	1.31	0.95
1:C:100:MET:HE1	1:C:145:TYR:HA	1.44	0.95
1:D:38:ARG:NH2	1:D:181:GLU:OE2	2.06	0.88
1:A:177:ALA:HB1	1:A:205:VAL:HG22	1.55	0.86
1:C:37:GLU:HB3	3:C:328:HOH:O	1.75	0.84
1:A:179:LYS:HG3	1:A:205:VAL:HG12	1.61	0.81
1:B:236:LYS:O	1:B:237:GLN:HB2	1.82	0.80
1:B:115:VAL:O	1:B:119:MET:HG3	1.82	0.79
1:C:116:LEU:HD13	1:C:127:ILE:HD11	1.66	0.78
1:D:238:GLN:HB3	1:D:239:PRO:HD2	1.67	0.76
1:C:100:MET:CE	1:C:145:TYR:HD1	2.00	0.74
1:A:177:ALA:HB1	1:A:205:VAL:CG2	2.17	0.73
1:A:188:SER:HB3	1:A:191:ILE:HD12	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:ARG:NH2	3:C:303:HOH:O	2.15	0.70
1:D:177:ALA:HB1	1:D:205:VAL:CG2	2.21	0.70
1:A:158:ASN:OD1	1:B:138:THR:HB	1.92	0.69
1:A:117:ALA:HB3	1:A:118:PRO:HD3	1.73	0.69
1:B:116:LEU:HD13	1:B:127:ILE:HD11	1.73	0.69
1:C:84:MET:CE	1:C:183:LEU:HD13	2.24	0.68
1:D:177:ALA:HB1	1:D:205:VAL:HG22	1.74	0.68
1:C:9:GLY:HA2	2:C:2001:NDP:H1B	1.76	0.68
1:D:196:ASP:HA	1:D:199:ARG:HD3	1.75	0.67
1:B:171:MET:HE1	3:B:253:HOH:O	1.93	0.67
1:D:117:ALA:HB3	1:D:118:PRO:HD3	1.75	0.67
1:D:79:ASN:HD21	1:D:111:GLY:HA3	1.62	0.65
1:C:3:LYS:O	1:C:27:HIS:HD2	1.81	0.64
1:D:79:ASN:HB2	1:D:129:ASN:HD22	1.63	0.64
1:A:196:ASP:HA	1:A:199:ARG:HD3	1.79	0.63
1:C:100:MET:HE1	1:C:145:TYR:CA	2.25	0.63
1:C:158:ASN:OD1	1:D:138:THR:HB	1.98	0.63
1:A:238:GLN:CB	1:A:239:PRO:HD2	2.05	0.62
1:B:3:LYS:O	1:B:27:HIS:HD2	1.84	0.61
1:C:157:GLU:OE2	1:C:160:ARG:NH1	2.34	0.61
1:A:183:LEU:HD22	1:A:195:TYR:CD2	2.36	0.60
1:B:84:MET:CE	1:B:183:LEU:HD13	2.32	0.59
1:D:47:THR:HG22	1:D:47:THR:O	2.02	0.59
1:B:131:SER:O	2:B:2001:NDP:H6N	2.02	0.59
1:A:9:GLY:HA2	2:A:2001:NDP:H1B	1.84	0.58
1:B:9:GLY:HA2	2:B:2001:NDP:H1B	1.86	0.58
1:A:27:HIS:HE1	3:A:273:HOH:O	1.87	0.58
1:D:188:SER:HB3	1:D:191:ILE:HD12	1.86	0.58
1:A:158:ASN:O	1:A:162:GLU:HG3	2.04	0.57
1:C:131:SER:O	2:C:2001:NDP:H6N	2.05	0.56
1:D:131:SER:O	2:D:2001:NDP:H6N	2.06	0.56
1:C:160:ARG:HD2	3:C:418:HOH:O	2.06	0.56
1:A:160:ARG:NH2	1:A:161:GLU:HG3	2.21	0.56
1:C:100:MET:HE3	1:C:145:TYR:CD1	2.24	0.55
1:C:100:MET:CE	1:C:145:TYR:CD1	2.86	0.55
1:B:25:GLU:HG3	1:B:216:LEU:HD21	1.87	0.55
1:C:138:THR:HB	1:D:158:ASN:OD1	2.07	0.55
1:A:131:SER:O	2:A:2001:NDP:H6N	2.07	0.55
1:B:32:LEU:HD22	1:B:52:VAL:HG21	1.88	0.54
1:C:115:VAL:O	1:C:119:MET:HG3	2.06	0.54
1:D:171:MET:HG2	1:D:227:ILE:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:PRO:HA	1:D:46:ASN:O	2.08	0.53
1:A:177:ALA:O	1:A:205:VAL:HG13	2.09	0.52
1:C:157:GLU:CD	1:C:160:ARG:NH1	2.63	0.52
1:D:183:LEU:HD22	1:D:195:TYR:CD2	2.45	0.52
1:A:140:PRO:O	1:A:141:ASP:HB2	2.09	0.52
1:C:76:ALA:HA	1:C:126:THR:O	2.10	0.52
1:A:37:GLU:HG2	1:A:38:ARG:N	2.23	0.52
1:D:3:LYS:O	1:D:27:HIS:HD2	1.92	0.51
1:B:204:GLY:HA2	1:B:234:PRO:HB3	1.93	0.51
1:B:236:LYS:O	1:B:237:GLN:CB	2.54	0.51
1:A:177:ALA:CB	1:A:205:VAL:HG22	2.36	0.51
1:B:69:LYS:HB3	3:B:304:HOH:O	2.10	0.51
1:D:183:LEU:HD22	1:D:195:TYR:HD2	1.76	0.51
1:B:133:ILE:HA	1:B:136:LYS:HD3	1.93	0.50
1:D:16:GLU:OE1	3:D:490:HOH:O	2.18	0.50
1:B:171:MET:CE	3:B:253:HOH:O	2.54	0.50
1:B:27:HIS:HE1	3:B:339:HOH:O	1.94	0.50
1:C:173:ILE:HG13	1:C:215:VAL:HG22	1.95	0.49
1:D:160:ARG:HB2	1:D:170:VAL:HB	1.94	0.49
1:C:2:LYS:HB3	3:C:317:HOH:O	2.12	0.49
1:A:3:LYS:O	1:A:27:HIS:HD2	1.95	0.49
1:C:25:GLU:HG2	1:C:220:GLN:NE2	2.27	0.49
1:B:84:MET:HE1	1:B:183:LEU:HD13	1.94	0.49
1:C:108:LEU:O	1:C:112:MET:HG3	2.13	0.48
1:A:25:GLU:CG	1:A:216:LEU:HD21	2.44	0.48
1:C:116:LEU:HD13	1:C:127:ILE:CD1	2.40	0.48
1:B:116:LEU:HD13	1:B:127:ILE:CD1	2.41	0.48
1:B:236:LYS:HE2	1:D:167:ASN:HB2	1.96	0.48
1:C:80:ASN:HD22	1:C:130:ILE:HG13	1.79	0.48
1:C:175:PRO:O	2:C:2001:NDP:H5N	2.13	0.48
1:B:57:LYS:NZ	1:B:113:GLN:HE21	2.12	0.47
1:D:25:GLU:HG3	1:D:216:LEU:HD21	1.96	0.47
1:D:9:GLY:HA2	2:D:2001:NDP:H1B	1.94	0.47
1:C:157:GLU:CD	1:C:160:ARG:HH12	2.17	0.47
1:D:133:ILE:HD12	1:D:176:SER:HB2	1.97	0.47
1:C:64:ILE:O	1:C:68:GLU:HG3	2.15	0.47
1:B:175:PRO:O	2:B:2001:NDP:H5N	2.14	0.46
1:C:133:ILE:HD12	1:C:176:SER:HB2	1.97	0.46
1:C:84:MET:HE1	1:C:183:LEU:HD13	1.95	0.46
1:B:32:LEU:HD22	1:B:52:VAL:CG2	2.46	0.46
1:B:157:GLU:OE1	1:B:160:ARG:NH1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:LYS:HE2	3:C:280:HOH:O	2.17	0.45
1:B:80:ASN:HD22	1:B:130:ILE:HG13	1.81	0.45
1:A:171:MET:HG2	1:A:227:ILE:O	2.15	0.45
1:D:177:ALA:O	1:D:205:VAL:HG22	2.17	0.45
1:B:204:GLY:HA2	1:B:234:PRO:CB	2.45	0.45
1:B:76:ALA:HA	1:B:126:THR:O	2.17	0.44
1:C:117:ALA:HB3	1:C:118:PRO:CD	2.48	0.44
1:C:150:PHE:CG	1:D:154:ALA:HB2	2.52	0.44
1:C:140:PRO:O	1:C:141:ASP:HB2	2.18	0.44
1:A:154:ALA:HB2	1:B:150:PHE:CG	2.53	0.44
1:A:116:LEU:HD13	1:A:127:ILE:HD11	1.99	0.43
1:C:171:MET:CE	3:C:259:HOH:O	2.65	0.43
1:C:27:HIS:HE1	3:C:275:HOH:O	2.01	0.43
1:D:123:ASN:HA	1:D:166:SER:O	2.19	0.43
1:C:236:LYS:O	1:C:237:GLN:HB3	2.18	0.43
1:A:160:ARG:HB2	1:A:170:VAL:HB	2.00	0.42
1:A:76:ALA:HA	1:A:126:THR:O	2.20	0.42
1:B:88:GLN:NE2	1:B:141:ASP:OD1	2.48	0.42
1:A:183:LEU:HD22	1:A:195:TYR:HD2	1.81	0.42
1:B:52:VAL:HG22	1:B:59:THR:HG22	2.02	0.42
1:C:52:VAL:HG22	1:C:59:THR:HG22	2.03	0.41
1:D:160:ARG:HH11	1:D:160:ARG:HG2	1.86	0.41
1:C:140:PRO:O	1:C:141:ASP:CB	2.69	0.41
1:B:123:ASN:HA	1:B:166:SER:O	2.20	0.40
1:B:173:ILE:HG13	1:B:215:VAL:HG22	2.04	0.40
1:A:173:ILE:O	1:A:175:PRO:HD3	2.21	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	237/266 (89%)	230 (97%)	7 (3%)	0	100	100
1	B	214/266 (80%)	210 (98%)	4 (2%)	0	100	100
1	C	214/266 (80%)	209 (98%)	5 (2%)	0	100	100
1	D	236/266 (89%)	228 (97%)	8 (3%)	0	100	100
All	All	901/1064 (85%)	877 (97%)	24 (3%)	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	192/211 (91%)	186 (97%)	6 (3%)	47	39
1	B	173/211 (82%)	163 (94%)	10 (6%)	25	14
1	C	173/211 (82%)	166 (96%)	7 (4%)	38	29
1	D	191/211 (90%)	179 (94%)	12 (6%)	22	12
All	All	729/844 (86%)	694 (95%)	35 (5%)	31	22

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	PHE
1	A	158	ASN
1	A	192	LYS
1	A	196	ASP
1	A	199	ARG
1	A	205	VAL
1	B	38	ARG
1	B	60	PHE
1	B	116	LEU
1	B	122	ARG
1	B	136	LYS
1	B	141	ASP
1	B	153	HIS

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Mol	Chain	Res	Type
1	B	158	ASN
1	B	183	LEU
1	B	205	VAL
1	C	24	GLU
1	C	40	LYS
1	C	60	PHE
1	C	116	LEU
1	C	141	ASP
1	C	153	HIS
1	C	183	LEU
1	D	38	ARG
1	D	43	ASN
1	D	47	THR
1	D	60	PHE
1	D	69	LYS
1	D	153	HIS
1	D	158	ASN
1	D	161	GLU
1	D	179	LYS
1	D	196	ASP
1	D	199	ARG
1	D	205	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	80	ASN
1	A	88	GLN
1	A	189	GLN
1	B	27	HIS
1	B	80	ASN
1	B	113	GLN
1	C	27	HIS
1	C	80	ASN
1	C	98	GLN
1	C	220	GLN
1	C	237	GLN
1	D	27	HIS
1	D	46	ASN
1	D	79	ASN
1	D	80	ASN

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Mol	Chain	Res	Type
1	D	129	ASN
1	D	189	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NDP	A	2001	-	42,52,52	1.30	4 (9%)	55,80,80	1.87	5 (9%)
2	NDP	B	2001	-	42,52,52	1.37	3 (7%)	55,80,80	1.79	7 (12%)
2	NDP	C	2001	-	42,52,52	1.41	4 (9%)	55,80,80	1.66	6 (10%)
2	NDP	D	2001	-	42,52,52	1.34	4 (9%)	55,80,80	1.87	5 (9%)

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	NDP	A	2001	-	-	0/30/77/77	0/5/5/5
2	NDP	B	2001	-	-	0/30/77/77	0/5/5/5
2	NDP	C	2001	-	-	0/30/77/77	0/5/5/5
2	NDP	D	2001	-	-	0/30/77/77	0/5/5/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	NDP	C4N-C5N	-4.15	1.40	1.49
2	C	2001	NDP	C4N-C5N	-4.09	1.40	1.49
2	D	2001	NDP	C4N-C5N	-3.84	1.40	1.49
2	A	2001	NDP	C4N-C5N	-3.81	1.40	1.49
2	C	2001	NDP	O4D-C1D	2.04	1.47	1.42
2	A	2001	NDP	C2N-C3N	2.31	1.40	1.34
2	D	2001	NDP	O4B-C1B	2.33	1.44	1.41
2	A	2001	NDP	C6N-C5N	3.28	1.39	1.33
2	D	2001	NDP	C6N-C5N	3.48	1.40	1.33
2	C	2001	NDP	C6N-C5N	3.56	1.40	1.33
2	B	2001	NDP	C6N-C5N	3.60	1.40	1.33
2	D	2001	NDP	O7N-C7N	3.74	1.33	1.24
2	A	2001	NDP	O7N-C7N	3.96	1.34	1.24
2	B	2001	NDP	O7N-C7N	4.55	1.35	1.24
2	C	2001	NDP	O7N-C7N	4.58	1.36	1.24

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	NDP	N3A-C2A-N1A	-10.55	120.82	128.89
2	D	2001	NDP	N3A-C2A-N1A	-10.53	120.83	128.89
2	B	2001	NDP	N3A-C2A-N1A	-9.64	121.51	128.89
2	C	2001	NDP	N3A-C2A-N1A	-8.81	122.15	128.89
2	B	2001	NDP	C5B-C4B-C3B	-2.81	104.04	115.21
2	A	2001	NDP	O4D-C1D-C2D	-2.80	100.10	106.58
2	A	2001	NDP	C5B-C4B-C3B	-2.63	104.79	115.21
2	C	2001	NDP	O4D-C1D-C2D	-2.62	100.50	106.58
2	C	2001	NDP	C5B-C4B-C3B	-2.48	105.37	115.21
2	B	2001	NDP	O4D-C1D-C2D	-2.40	101.01	106.58
2	D	2001	NDP	PN-O3-PA	-2.21	126.52	132.73
2	B	2001	NDP	C5D-C4D-C3D	-2.14	106.72	115.21
2	C	2001	NDP	C4B-O4B-C1B	-2.07	107.44	109.72
2	D	2001	NDP	C5B-C4B-C3B	-2.02	107.21	115.21
2	B	2001	NDP	O4B-C1B-N9A	2.35	113.02	108.10
2	B	2001	NDP	P2B-O2B-C2B	2.44	127.42	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2001	NDP	P2B-O2B-C2B	2.47	127.48	121.56
2	A	2001	NDP	C5N-C4N-C3N	2.56	119.56	112.52
2	D	2001	NDP	C5N-C4N-C3N	2.56	119.57	112.52
2	B	2001	NDP	C5N-C4N-C3N	2.72	120.03	112.52
2	C	2001	NDP	C5N-C4N-C3N	2.74	120.06	112.52
2	D	2001	NDP	P2B-O2B-C2B	2.74	128.14	121.56
2	A	2001	NDP	P2B-O2B-C2B	3.29	129.45	121.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	NDP	2	0
2	B	2001	NDP	3	0
2	C	2001	NDP	3	0
2	D	2001	NDP	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²)	Q<0.9
1	A	239/266 (89%)	-0.33	0 100 100	22, 34, 55, 67	0
1	B	218/266 (81%)	-0.33	1 (0%) 91 93	20, 32, 46, 60	0
1	C	218/266 (81%)	-0.34	2 (0%) 85 89	21, 31, 48, 63	0
1	D	238/266 (89%)	-0.33	0 100 100	22, 34, 54, 63	0
All	All	913/1064 (85%)	-0.33	3 (0%) 94 95	20, 33, 51, 67	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	183	LEU	3.9
1	C	203	GLY	2.3
1	B	183	LEU	2.2

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, 95th 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(\AA^2)	Q<0.9
2	NDP	D	2001	48/48	0.98	0.09	-0.47	21,31,37,40	0
2	NDP	A	2001	48/48	0.98	0.09	-0.56	19,29,35,40	0
2	NDP	C	2001	48/48	0.98	0.09	-0.69	20,32,41,50	0
2	NDP	B	2001	48/48	0.98	0.09	-0.71	24,32,41,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.