Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 09:20 PM GMT

PDB ID	:	1OHJ
Title	:	HUMAN DIHYDROFOLATE REDUCTASE, MONOCLINIC (P21) CRYSTAL FORM
Authors	:	Cody, V.; Galitsky, N.; Luft, J.R.; Pangborn, W.
Deposited on	:	1997-09-17
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
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:

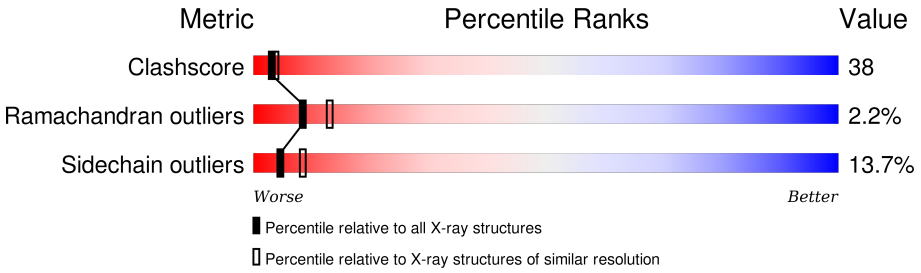
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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 >=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 <=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	186	33% 41% 23% ·

2 Entry composition

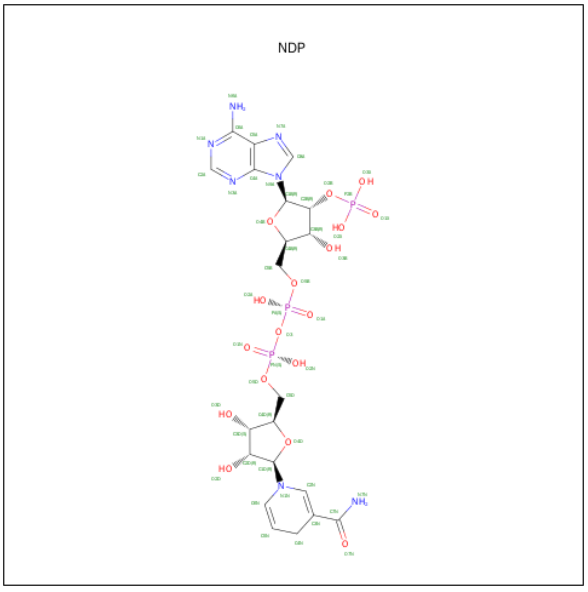
There are 4 unique types of molecules in this entry. The entry contains 1616 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DIHYDROFOLATE REDUCTASE.

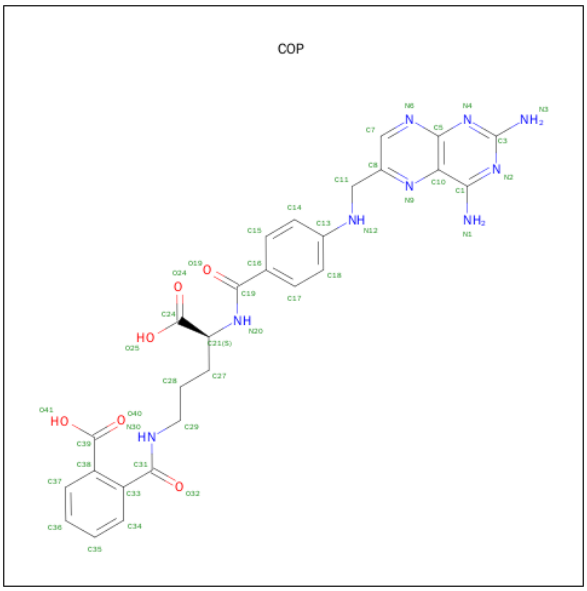
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1502	963	253	279	7			

- 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		

- Molecule 3 is N-(4-CARBOXY-4-{4-[(2,4-DIAMINO-PTERIDIN-6-YLMETHYL)-AMINO]-BENZOYLAMINO}-BUTYL)-PHTHALAMIC ACID (three-letter code: COP) (formula: $C_{27}H_{27}N_9O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			56	37	10	9		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		

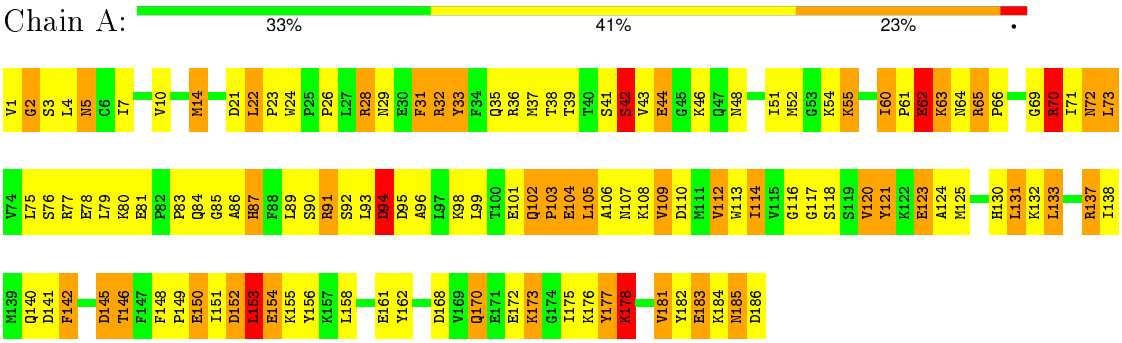
3 Residue-property plots (i)

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.

Note EDS was not executed.

- Molecule 1: DIHYDROFOLATE REDUCTASE

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.82Å 40.35Å 75.15Å 90.00° 109.74° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	93.4 (8.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.208 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1616	wwPDB-VP
Average B, all atoms (Å^2)	17.0	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: COP, 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	0.89	0/1537	2.37	81/2073 (3.9%)

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 (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	36	ARG	NE-CZ-NH1	18.21	129.41	120.30
1	A	137	ARG	NE-CZ-NH1	15.16	127.88	120.30
1	A	141	ASP	CB-CG-OD1	14.68	131.51	118.30
1	A	77	ARG	NE-CZ-NH1	-13.81	113.39	120.30
1	A	77	ARG	NE-CZ-NH2	13.57	127.08	120.30
1	A	145	ASP	CB-CG-OD1	13.31	130.28	118.30
1	A	32	ARG	NE-CZ-NH2	-12.77	113.92	120.30
1	A	28	ARG	NE-CZ-NH1	11.86	126.23	120.30
1	A	36	ARG	NE-CZ-NH2	-11.08	114.76	120.30
1	A	62	GLU	C-N-CA	8.73	143.52	121.70
1	A	70	ARG	CD-NE-CZ	-8.70	111.42	123.60
1	A	145	ASP	CB-CG-OD2	-8.63	110.53	118.30
1	A	141	ASP	CB-CG-OD2	-8.53	110.62	118.30
1	A	183	GLU	OE1-CD-OE2	8.50	133.50	123.30
1	A	32	ARG	NH1-CZ-NH2	8.23	128.45	119.40
1	A	77	ARG	CD-NE-CZ	-8.10	112.26	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	140	GLN	CA-CB-CG	7.92	130.83	113.40
1	A	28	ARG	CD-NE-CZ	7.91	134.67	123.60
1	A	65	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	A	137	ARG	NH1-CZ-NH2	-7.62	111.02	119.40
1	A	84	GLN	CA-CB-CG	7.30	129.45	113.40
1	A	78	GLU	OE1-CD-OE2	7.29	132.04	123.30
1	A	31	PHE	CA-CB-CG	7.21	131.20	113.90
1	A	3	SER	N-CA-CB	-7.15	99.78	110.50
1	A	172	GLU	CA-CB-CG	7.11	129.04	113.40
1	A	133	LEU	CA-CB-CG	7.03	131.47	115.30
1	A	94	ASP	CB-CG-OD2	-6.97	112.03	118.30
1	A	77	ARG	C-N-CA	6.90	138.95	121.70
1	A	123	GLU	OE1-CD-OE2	6.87	131.55	123.30
1	A	109	VAL	CB-CA-C	-6.79	98.49	111.40
1	A	78	GLU	CB-CA-C	-6.74	96.92	110.40
1	A	150	GLU	CB-CG-CD	6.72	132.34	114.20
1	A	132	LYS	N-CA-CB	6.63	122.54	110.60
1	A	81	GLU	CA-CB-CG	6.58	127.88	113.40
1	A	78	GLU	N-CA-C	6.54	128.67	111.00
1	A	154	GLU	CA-CB-CG	6.53	127.77	113.40
1	A	123	GLU	CG-CD-OE1	-6.53	105.25	118.30
1	A	36	ARG	CD-NE-CZ	6.52	132.72	123.60
1	A	22	LEU	CB-CA-C	6.37	122.30	110.20
1	A	95	ASP	CB-CG-OD1	6.36	124.02	118.30
1	A	65	ARG	NH1-CZ-NH2	6.23	126.25	119.40
1	A	28	ARG	NH1-CZ-NH2	-6.18	112.60	119.40
1	A	177	TYR	CB-CG-CD2	-6.17	117.30	121.00
1	A	140	GLN	N-CA-CB	6.05	121.49	110.60
1	A	44	GLU	CB-CG-CD	6.05	130.52	114.20
1	A	168	ASP	CA-C-O	6.04	132.78	120.10
1	A	33	TYR	CB-CG-CD1	-6.02	117.39	121.00
1	A	91	ARG	CD-NE-CZ	-6.01	115.19	123.60
1	A	62	GLU	O-C-N	-5.98	113.14	122.70
1	A	32	ARG	NE-CZ-NH1	-5.97	117.31	120.30
1	A	2	GLY	C-N-CA	5.93	136.53	121.70
1	A	87	HIS	CA-CB-CG	5.92	123.67	113.60
1	A	60	ILE	N-CA-CB	5.88	124.32	110.80
1	A	65	ARG	NE-CZ-NH1	-5.87	117.36	120.30
1	A	168	ASP	CB-CG-OD2	5.85	123.56	118.30
1	A	162	TYR	N-CA-CB	-5.78	100.19	110.60
1	A	121	TYR	CB-CG-CD1	-5.75	117.55	121.00
1	A	141	ASP	CA-CB-CG	5.75	126.04	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	91	ARG	CA-CB-CG	-5.64	100.99	113.40
1	A	73	LEU	CB-CG-CD1	5.62	120.56	111.00
1	A	181	VAL	CA-CB-CG2	5.60	119.30	110.90
1	A	89	LEU	O-C-N	5.60	131.66	122.70
1	A	131	LEU	CA-C-O	-5.55	108.44	120.10
1	A	91	ARG	NE-CZ-NH2	5.55	123.07	120.30
1	A	177	TYR	CB-CG-CD1	5.50	124.30	121.00
1	A	14	MET	N-CA-CB	-5.50	100.70	110.60
1	A	78	GLU	CA-CB-CG	5.41	125.30	113.40
1	A	91	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	A	29	ASN	CA-CB-CG	-5.33	101.67	113.40
1	A	140	GLN	CA-C-N	-5.32	105.49	117.20
1	A	178	LYS	CA-CB-CG	5.25	124.95	113.40
1	A	152	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	A	142	PHE	O-C-N	5.19	131.00	122.70
1	A	117	GLY	CA-C-O	5.18	129.92	120.60
1	A	137	ARG	CA-CB-CG	5.17	124.78	113.40
1	A	7	ILE	CB-CA-C	5.16	121.92	111.60
1	A	101	GLU	CB-CA-C	-5.16	100.08	110.40
1	A	109	VAL	O-C-N	5.09	130.84	122.70
1	A	62	GLU	CG-CD-OE1	5.04	128.38	118.30
1	A	62	GLU	OE1-CD-OE2	-5.04	117.25	123.30
1	A	33	TYR	CB-CG-CD2	5.02	124.01	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	70	ARG	Sidechain

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	1502	0	1510	116	0
2	A	48	0	26	7	0
3	A	56	0	20	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	10	0	0	1	0
All	All	1616	0	1556	121	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 38.

All (121) 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:79:LEU:O	1:A:91:ARG:NH2	1.81	1.12
2:A:187:NDP:H8A	2:A:187:NDP:H52A	1.50	0.94
1:A:1:VAL:HG13	1:A:2:GLY:H	1.30	0.93
1:A:4:LEU:HD12	1:A:112:VAL:CG2	1.99	0.92
1:A:62:GLU:OE2	1:A:65:ARG:NH2	2.03	0.92
1:A:54:LYS:HD3	2:A:187:NDP:O2X	1.73	0.88
1:A:35:GLN:O	1:A:39:THR:OG1	1.94	0.85
1:A:72:ASN:H	1:A:87:HIS:HD2	1.29	0.81
1:A:72:ASN:H	1:A:87:HIS:CD2	2.03	0.74
1:A:114:ILE:HD13	1:A:124:ALA:HB1	1.71	0.71
1:A:161:GLU:HG2	1:A:161:GLU:O	1.88	0.71
1:A:91:ARG:HG2	1:A:91:ARG:NH1	2.07	0.69
1:A:145:ASP:OD1	1:A:146:THR:HG22	1.92	0.69
1:A:96:ALA:O	1:A:99:LEU:HB3	1.93	0.68
1:A:151:ILE:HA	4:A:193:HOH:O	1.92	0.68
1:A:28:ARG:O	1:A:32:ARG:HG3	1.94	0.68
1:A:42:SER:OG	1:A:110:ASP:OD2	2.13	0.66
1:A:114:ILE:HD13	1:A:124:ALA:CB	2.26	0.65
1:A:76:SER:O	1:A:91:ARG:NH1	2.30	0.65
1:A:72:ASN:N	1:A:72:ASN:HD22	1.94	0.64
1:A:52:MET:HA	1:A:116:GLY:O	1.97	0.64
1:A:130:HIS:HB2	1:A:185:ASN:CG	2.19	0.64
1:A:109:VAL:O	1:A:109:VAL:HG13	1.99	0.63
1:A:60:ILE:HG21	1:A:64:ASN:HB3	1.81	0.63
1:A:54:LYS:NZ	2:A:187:NDP:O2X	2.30	0.62
1:A:130:HIS:HB2	1:A:185:ASN:ND2	2.14	0.62
1:A:93:LEU:HD22	1:A:123:GLU:HG3	1.82	0.62
1:A:66:PRO:HG3	1:A:85:GLY:O	1.99	0.62
1:A:21:ASP:OD1	1:A:22:LEU:N	2.28	0.62
1:A:46:LYS:HE2	1:A:107:ASN:O	2.01	0.60
1:A:4:LEU:HD12	1:A:112:VAL:HG21	1.83	0.60
1:A:91:ARG:HG2	1:A:91:ARG:HH11	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:VAL:O	1:A:124:ALA:HB2	2.04	0.58
1:A:60:ILE:HG22	1:A:61:PRO:HD2	1.86	0.57
1:A:161:GLU:O	1:A:161:GLU:CG	2.51	0.57
3:A:188[A]:COP:O32	3:A:188[A]:COP:O40	2.22	0.57
1:A:109:VAL:O	1:A:109:VAL:CG1	2.53	0.56
1:A:61:PRO:O	1:A:63:LYS:N	2.38	0.56
1:A:44:GLU:O	1:A:44:GLU:HG3	2.05	0.56
1:A:99:LEU:HG	1:A:105:LEU:HD23	1.86	0.56
1:A:60:ILE:HG22	1:A:64:ASN:HB2	1.87	0.56
1:A:118:SER:HB3	2:A:187:NDP:O1N	2.06	0.55
1:A:133:LEU:O	1:A:181:VAL:HA	2.06	0.55
1:A:10:VAL:CG2	1:A:14:MET:HA	2.36	0.55
1:A:4:LEU:CD1	1:A:112:VAL:CG2	2.81	0.55
1:A:170:GLN:O	1:A:176:LYS:HA	2.08	0.54
1:A:121:TYR:O	1:A:124:ALA:HB3	2.08	0.53
1:A:60:ILE:CG2	1:A:64:ASN:HB3	2.39	0.53
1:A:131:LEU:HD23	1:A:184:LYS:HE2	1.91	0.53
1:A:69:GLY:C	1:A:70:ARG:HG3	2.29	0.52
1:A:4:LEU:CD1	1:A:112:VAL:HG21	2.40	0.52
1:A:94:ASP:O	1:A:98:LYS:HE3	2.08	0.52
1:A:1:VAL:CG1	1:A:2:GLY:H	2.09	0.52
1:A:152:ASP:HB3	1:A:155:LYS:HB3	1.91	0.52
1:A:93:LEU:HD13	1:A:120:VAL:HG12	1.91	0.52
1:A:51:ILE:HG12	1:A:73:LEU:HD22	1.91	0.51
1:A:93:LEU:O	1:A:96:ALA:HB3	2.11	0.51
2:A:187:NDP:H6N	2:A:187:NDP:H52N	1.93	0.51
1:A:105:LEU:O	1:A:109:VAL:HG12	2.11	0.50
1:A:103:PRO:HA	1:A:106:ALA:HB3	1.93	0.50
1:A:152:ASP:O	1:A:154:GLU:N	2.46	0.49
1:A:83:PRO:HG2	1:A:86:ALA:HB2	1.95	0.49
1:A:33:TYR:O	1:A:37:MET:HG2	2.13	0.48
1:A:1:VAL:HG13	1:A:2:GLY:N	2.12	0.48
1:A:4:LEU:HA	1:A:112:VAL:HG22	1.94	0.48
1:A:10:VAL:HG22	1:A:14:MET:HA	1.96	0.48
1:A:75:LEU:HA	1:A:90:SER:O	2.14	0.47
1:A:72:ASN:N	1:A:87:HIS:HD2	2.06	0.47
1:A:148:PHE:CD1	1:A:149:PRO:HD2	2.49	0.47
1:A:170:GLN:HA	1:A:170:GLN:HE21	1.80	0.47
1:A:155:LYS:HE3	1:A:184:LYS:HD2	1.97	0.47
1:A:38:THR:O	1:A:48:ASN:ND2	2.33	0.46
1:A:153:LEU:H	1:A:153:LEU:HD23	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ILE:HG23	1:A:175:ILE:CG2	2.45	0.46
1:A:60:ILE:HG22	1:A:64:ASN:CB	2.45	0.46
1:A:24:TRP:HB3	1:A:142:PHE:CZ	2.51	0.46
1:A:114:ILE:HG22	1:A:114:ILE:O	2.16	0.46
1:A:108:LYS:HB2	1:A:108:LYS:NZ	2.31	0.46
1:A:5:ASN:N	1:A:5:ASN:ND2	2.63	0.45
1:A:102:GLN:O	1:A:104:GLU:N	2.50	0.45
1:A:177:TYR:O	1:A:177:TYR:CD1	2.69	0.45
1:A:4:LEU:HD12	1:A:112:VAL:HG22	1.91	0.45
1:A:71:ILE:C	1:A:72:ASN:HD22	2.20	0.45
1:A:60:ILE:CG2	1:A:64:ASN:CB	2.94	0.45
1:A:51:ILE:HG21	1:A:51:ILE:HD13	1.57	0.44
2:A:187:NDP:C5B	2:A:187:NDP:H8A	2.33	0.44
1:A:26:PRO:O	1:A:173:LYS:CE	2.65	0.44
1:A:60:ILE:HG22	1:A:61:PRO:CD	2.48	0.44
1:A:103:PRO:HA	1:A:106:ALA:CB	2.48	0.44
1:A:104:GLU:HG2	1:A:104:GLU:H	1.29	0.44
1:A:158:LEU:HB2	1:A:182:TYR:CE2	2.53	0.43
1:A:23:PRO:HB2	1:A:142:PHE:HB3	2.00	0.43
1:A:94:ASP:O	1:A:98:LYS:HB2	2.18	0.43
1:A:55:LYS:HB2	1:A:55:LYS:NZ	2.33	0.43
1:A:170:GLN:CA	1:A:170:GLN:HE21	2.31	0.43
1:A:131:LEU:CD2	1:A:156:TYR:OH	2.67	0.42
1:A:151:ILE:HD13	1:A:151:ILE:HG21	1.77	0.42
1:A:138:ILE:CG2	1:A:142:PHE:HE1	2.32	0.42
1:A:175:ILE:HD13	1:A:175:ILE:HG21	1.67	0.42
1:A:124:ALA:O	1:A:131:LEU:HD22	2.19	0.42
1:A:98:LYS:HB2	1:A:98:LYS:HE3	1.65	0.42
1:A:5:ASN:O	1:A:113:TRP:HA	2.19	0.42
1:A:152:ASP:C	1:A:154:GLU:H	2.23	0.42
1:A:177:TYR:CD1	1:A:177:TYR:C	2.92	0.42
1:A:42:SER:HG	1:A:110:ASP:CG	2.19	0.41
1:A:137:ARG:HG3	1:A:178:LYS:NZ	2.35	0.41
1:A:60:ILE:O	1:A:65:ARG:NH2	2.44	0.41
1:A:54:LYS:CD	2:A:187:NDP:O2X	2.58	0.41
1:A:43:VAL:HG11	1:A:46:LYS:HD2	2.03	0.41
1:A:125:MET:HA	1:A:131:LEU:HD21	2.02	0.41
1:A:102:GLN:H	1:A:102:GLN:HG2	1.62	0.41
1:A:62:GLU:CD	1:A:62:GLU:H	2.25	0.41
1:A:152:ASP:C	1:A:154:GLU:N	2.74	0.41
1:A:186:ASP:OD1	1:A:186:ASP:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:VAL:O	1:A:124:ALA:CB	2.67	0.40
1:A:183:GLU:CG	1:A:184:LYS:N	2.84	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	184/186 (99%)	168 (91%)	12 (6%)	4 (2%)	8 13

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	GLU
1	A	153	LEU
1	A	42	SER
1	A	103	PRO

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	168/168 (100%)	145 (86%)	23 (14%)	4 8

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	41	SER
1	A	42	SER
1	A	55	LYS
1	A	62	GLU
1	A	63	LYS
1	A	72	ASN
1	A	80	LYS
1	A	92	SER
1	A	94	ASP
1	A	102	GLN
1	A	104	GLU
1	A	105	LEU
1	A	112	VAL
1	A	114	ILE
1	A	120	VAL
1	A	146	THR
1	A	150	GLU
1	A	153	LEU
1	A	170	GLN
1	A	173	LYS
1	A	178	LYS
1	A	185	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	87	HIS
1	A	102	GLN
1	A	170	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

3 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	187	-	42,52,52	2.38	13 (30%)	55,80,80	2.68	17 (30%)
3	COP	A	188[A]	-	37,45,45	1.32	4 (10%)	43,62,62	3.47	10 (23%)
3	COP	A	188[B]	-	37,45,45	1.34	4 (10%)	43,62,62	3.20	14 (32%)

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	187	-	-	0/30/77/77	0/5/5/5
3	COP	A	188[A]	-	-	0/24/32/32	0/4/4/4
3	COP	A	188[B]	-	-	0/24/32/32	0/4/4/4

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	187	NDP	O4B-C4B	-9.10	1.24	1.45
2	A	187	NDP	C5A-C4A	-4.43	1.30	1.40
3	A	188[A]	COP	C5-N6	-3.96	1.30	1.37
3	A	188[B]	COP	C5-N6	-3.96	1.30	1.37
2	A	187	NDP	PN-O1N	-3.19	1.39	1.51
2	A	187	NDP	C6A-N1A	-3.02	1.22	1.37
2	A	187	NDP	O2B-C2B	-2.48	1.36	1.44
2	A	187	NDP	P2B-O2X	-2.46	1.45	1.54
3	A	188[A]	COP	C3-N2	-2.34	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	188[B]	COP	C3-N2	-2.34	1.31	1.35
2	A	187	NDP	PA-O2A	-2.24	1.45	1.54
2	A	187	NDP	C4N-C5N	2.05	1.53	1.49
2	A	187	NDP	PA-O5B	2.23	1.69	1.59
3	A	188[B]	COP	C29-N30	2.57	1.52	1.46
3	A	188[A]	COP	C29-N30	2.59	1.52	1.46
2	A	187	NDP	C1D-N1N	2.99	1.55	1.46
3	A	188[A]	COP	C31-N30	3.08	1.40	1.33
3	A	188[B]	COP	C31-N30	3.33	1.41	1.33
2	A	187	NDP	P2B-O2B	3.71	1.71	1.60
2	A	187	NDP	O3B-C3B	3.81	1.52	1.43
2	A	187	NDP	C3B-C4B	3.87	1.63	1.53

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	187	NDP	O3B-C3B-C4B	-5.78	93.70	111.05
3	A	188[A]	COP	O19-C19-C16	-4.81	112.75	120.97
3	A	188[B]	COP	O19-C19-C16	-4.81	112.75	120.97
2	A	187	NDP	O2B-P2B-O1X	-4.65	95.49	107.11
3	A	188[B]	COP	O32-C31-C33	-3.99	113.31	120.95
2	A	187	NDP	O5B-PA-O1A	-3.70	95.26	109.62
2	A	187	NDP	O4B-C1B-C2B	-3.58	100.12	106.60
3	A	188[A]	COP	O32-C31-C33	-3.46	114.31	120.95
2	A	187	NDP	C5B-C4B-C3B	-3.46	101.47	115.21
3	A	188[A]	COP	N4-C3-N2	-3.39	122.28	127.44
3	A	188[B]	COP	N4-C3-N2	-3.39	122.28	127.44
3	A	188[A]	COP	C27-C28-C29	-3.33	101.88	112.13
2	A	187	NDP	O2B-C2B-C1B	-3.18	97.62	110.02
2	A	187	NDP	O5B-C5B-C4B	-2.74	99.01	109.12
3	A	188[B]	COP	C27-C28-C29	-2.69	103.85	112.13
2	A	187	NDP	O4D-C4D-C3D	-2.43	100.24	105.15
3	A	188[A]	COP	C11-N12-C13	-2.42	115.59	122.15
3	A	188[B]	COP	C11-N12-C13	-2.42	115.59	122.15
3	A	188[B]	COP	C37-C38-C39	-2.34	116.64	120.23
2	A	187	NDP	C2B-C3B-C4B	-2.22	96.59	101.85
2	A	187	NDP	O3-PA-O5B	-2.22	97.04	102.94
2	A	187	NDP	C1D-N1N-C2N	-2.20	117.07	120.91
3	A	188[A]	COP	C10-C5-N4	-2.01	118.86	122.11
3	A	188[B]	COP	C10-C5-N4	-2.01	118.86	122.11
3	A	188[B]	COP	C38-C33-C31	2.48	126.21	121.58
2	A	187	NDP	O2A-PA-O1A	2.66	126.92	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	188[A]	COP	N6-C5-N4	2.86	120.23	116.14
3	A	188[B]	COP	N6-C5-N4	2.86	120.23	116.14
3	A	188[B]	COP	C37-C38-C33	3.65	122.20	118.03
2	A	187	NDP	C4A-C5A-N7A	3.74	112.92	109.48
2	A	187	NDP	O3X-P2B-O2X	3.89	122.18	107.38
3	A	188[B]	COP	C33-C31-N30	3.98	125.65	117.52
3	A	188[A]	COP	C16-C19-N20	4.00	124.05	116.93
3	A	188[B]	COP	C16-C19-N20	4.00	124.05	116.93
3	A	188[A]	COP	C28-C29-N30	4.65	125.82	112.19
2	A	187	NDP	N6A-C6A-N1A	5.99	132.06	119.20
3	A	188[B]	COP	C28-C29-N30	6.27	130.55	112.19
2	A	187	NDP	C4B-O4B-C1B	8.30	118.84	109.72
2	A	187	NDP	P2B-O2B-C2B	8.40	141.70	121.56
3	A	188[B]	COP	C29-N30-C31	15.65	157.21	122.15
3	A	188[A]	COP	C29-N30-C31	19.58	165.99	122.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	187	NDP	7	0
3	A	188[A]	COP	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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.