Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:58 PM GMT

PDB ID	:	1DIH
Title	:	THREE-DIMENSIONAL STRUCTURE OF E. COLI DIHYDRODIPICOLINATE REDUCTASE
Authors	:	Scapin, G.; Blanchard, J.S.; Sacchettini, J.C.
Deposited on	:	1994-09-14
Resolution	:	2.20 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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

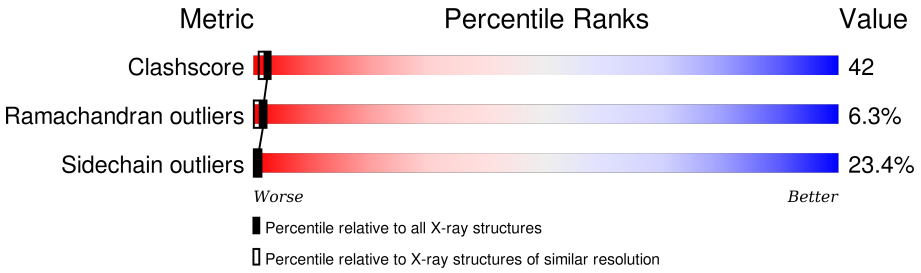
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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	273	44% 34% 17% 5%

2 Entry composition

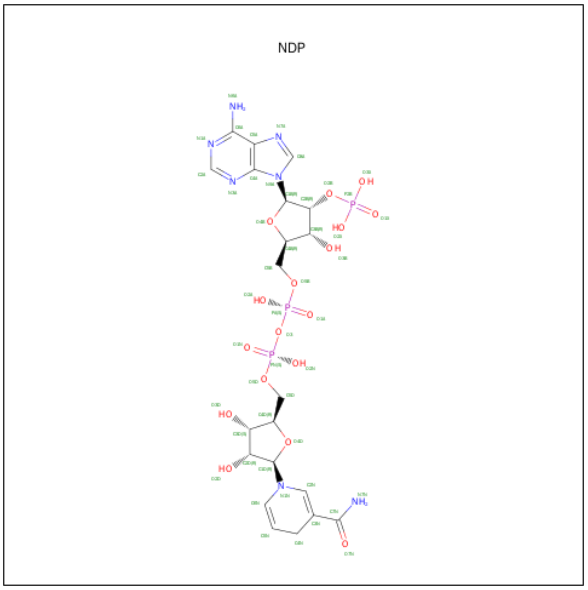
There are 3 unique types of molecules in this entry. The entry contains 2086 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DIHYDRODIPICOLINATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			1979	1232	353	384	10			

- 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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	59	Total	O	0	0
			59	59		

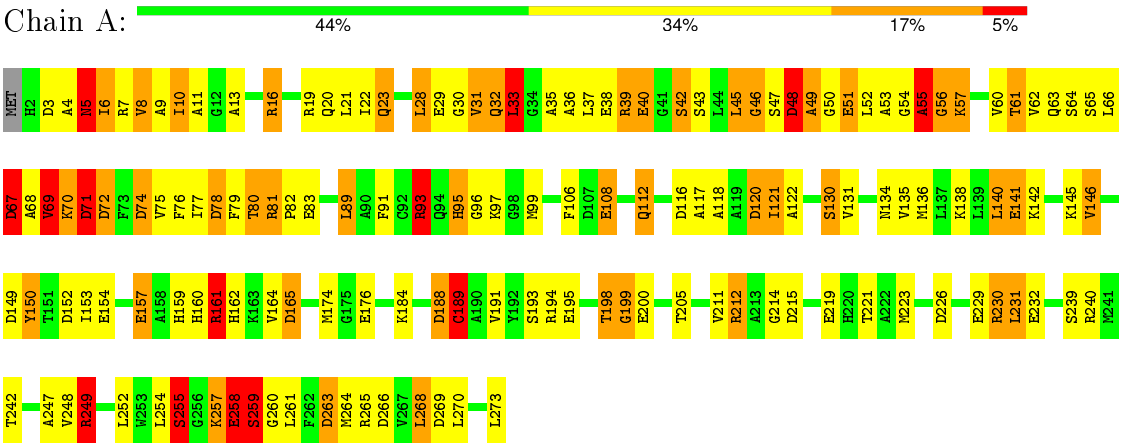
3 Residue-property plots (i)

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: DIHYDRODIPICOLINATE 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	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	75.70Å 81.20Å 94.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	89.0 (20.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT, X-PLOR	Depositor
R, R_{free}	0.187 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2086	wwPDB-VP
Average B, all atoms (Å^2)	29.0	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: 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	1.31	17/2005 (0.8%)	1.65	41/2705 (1.5%)

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

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	141	GLU	CD-OE2	8.40	1.34	1.25
1	A	51	GLU	CD-OE2	8.21	1.34	1.25
1	A	108	GLU	CD-OE2	7.95	1.34	1.25
1	A	200	GLU	CD-OE2	7.65	1.34	1.25
1	A	195	GLU	CD-OE2	7.17	1.33	1.25
1	A	29	GLU	CD-OE2	6.90	1.33	1.25
1	A	258	GLU	CD-OE1	6.71	1.33	1.25
1	A	219	GLU	CD-OE2	-6.66	1.18	1.25
1	A	83	GLU	CD-OE2	6.51	1.32	1.25
1	A	229	GLU	CD-OE2	-6.43	1.18	1.25
1	A	40	GLU	CD-OE2	5.90	1.32	1.25
1	A	232	GLU	CD-OE1	-5.55	1.19	1.25
1	A	229	GLU	CD-OE1	5.50	1.31	1.25
1	A	130	SER	CA-CB	-5.36	1.45	1.52
1	A	226	ASP	CG-OD2	5.27	1.37	1.25
1	A	154	GLU	CD-OE2	-5.13	1.20	1.25
1	A	38	GLU	CD-OE1	5.12	1.31	1.25

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	161	ARG	NE-CZ-NH1	11.90	126.25	120.30
1	A	80	THR	CA-CB-CG2	8.78	124.69	112.40
1	A	240	ARG	NE-CZ-NH1	8.75	124.68	120.30
1	A	188	ASP	CB-CG-OD1	-8.20	110.92	118.30
1	A	165	ASP	CB-CG-OD2	-8.15	110.97	118.30
1	A	93	ARG	NE-CZ-NH1	8.05	124.33	120.30
1	A	74	ASP	CB-CG-OD1	-7.83	111.25	118.30
1	A	120	ASP	CB-CG-OD2	-7.76	111.32	118.30
1	A	74	ASP	CB-CG-OD2	7.34	124.91	118.30
1	A	212	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	A	215	ASP	CB-CG-OD2	7.14	124.73	118.30
1	A	226	ASP	CB-CG-OD2	-7.05	111.96	118.30
1	A	16	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	A	263	ASP	CB-CG-OD1	6.71	124.33	118.30
1	A	67	ASP	CB-CG-OD1	-6.58	112.38	118.30
1	A	230	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	71	ASP	CB-CG-OD2	-6.35	112.59	118.30
1	A	72	ASP	CB-CG-OD1	-6.31	112.62	118.30
1	A	149	ASP	CA-CB-CG	-6.17	99.82	113.40
1	A	266	ASP	CB-CG-OD1	6.17	123.86	118.30
1	A	48	ASP	CB-CG-OD2	6.14	123.83	118.30
1	A	249	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	A	150	TYR	CA-CB-CG	-5.97	102.06	113.40
1	A	240	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	A	198	THR	CA-CB-OG1	-5.93	96.55	109.00
1	A	188	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	191	VAL	CA-CB-CG2	5.74	119.52	110.90
1	A	152	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	120	ASP	CB-CG-OD1	5.48	123.24	118.30
1	A	48	ASP	CA-C-N	-5.47	105.16	117.20
1	A	150	TYR	CB-CG-CD1	-5.45	117.73	121.00
1	A	112	GLN	N-CA-CB	5.37	120.26	110.60
1	A	16	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	55	ALA	N-CA-CB	5.35	117.59	110.10
1	A	149	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	A	231	LEU	CB-CG-CD2	5.28	119.97	111.00
1	A	71	ASP	CB-CG-OD1	5.22	122.99	118.30
1	A	152	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	A	189	CYS	N-CA-CB	5.11	119.80	110.60
1	A	78	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	226	ASP	CB-CG-OD1	5.02	122.82	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	247	ALA	Mainchain

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	1979	0	1938	169	0
2	A	48	0	26	2	0
3	A	59	0	0	4	0
All	All	2086	0	1964	169	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 42.

All (169) 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:42:SER:CB	1:A:45:LEU:HD22	1.55	1.32
1:A:42:SER:CB	1:A:45:LEU:CD2	2.24	1.16
1:A:70:LYS:HB2	1:A:91:PHE:HZ	1.21	1.03
1:A:61:THR:HG23	1:A:63:GLN:HE21	1.19	1.02
1:A:80:THR:HG22	1:A:81:ARG:H	1.24	1.00
1:A:69:VAL:HG22	1:A:72:ASP:HB2	1.50	0.91
1:A:80:THR:CG2	1:A:81:ARG:H	1.83	0.91
1:A:6:ILE:HD11	1:A:75:VAL:HG23	1.52	0.91
1:A:70:LYS:HB2	1:A:91:PHE:CZ	2.07	0.89
1:A:89:LEU:HD23	1:A:99:MET:CE	2.05	0.87
1:A:112:GLN:NE2	1:A:116:ASP:HB2	1.90	0.85
1:A:112:GLN:HE21	1:A:116:ASP:HB2	1.41	0.85
1:A:70:LYS:NZ	1:A:71:ASP:HB3	1.93	0.84
1:A:28:LEU:HD12	1:A:248:VAL:HG12	1.61	0.83
1:A:160:HIS:HD2	1:A:162:HIS:H	1.27	0.83
1:A:37:LEU:HD21	1:A:66:LEU:HD23	1.59	0.82
1:A:65:SER:HB3	1:A:68:ALA:HB2	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:SER:HB3	1:A:68:ALA:CB	2.12	0.80
1:A:89:LEU:HD23	1:A:99:MET:HE1	1.63	0.78
1:A:97:LYS:N	1:A:121:ILE:HD11	1.98	0.77
1:A:9:ALA:C	1:A:10:ILE:HD13	2.05	0.77
1:A:273:LEU:HA	3:A:456:HOH:O	1.86	0.76
1:A:160:HIS:CD2	1:A:162:HIS:H	2.04	0.74
1:A:3:ASP:CA	1:A:32:GLN:HB2	2.18	0.74
1:A:56:GLY:C	1:A:57:LYS:HE3	2.09	0.73
1:A:51:GLU:HB3	1:A:56:GLY:O	1.87	0.73
1:A:23:GLN:HG2	1:A:53:ALA:CB	2.18	0.73
1:A:3:ASP:HA	1:A:32:GLN:CG	2.18	0.73
1:A:131:VAL:HG13	1:A:268:LEU:HD21	1.71	0.73
1:A:259:SER:HA	3:A:452:HOH:O	1.88	0.72
1:A:28:LEU:HD13	1:A:31:VAL:HG13	1.71	0.72
1:A:61:THR:CG2	1:A:63:GLN:HE21	1.98	0.72
1:A:4:ALA:HB1	1:A:30:GLY:HA2	1.72	0.70
1:A:45:LEU:HD12	1:A:46:GLY:H	1.57	0.69
1:A:4:ALA:O	1:A:6:ILE:N	2.26	0.69
1:A:3:ASP:HA	1:A:32:GLN:HG3	1.76	0.68
1:A:61:THR:HG23	1:A:63:GLN:NE2	2.03	0.68
1:A:22:ILE:HG22	1:A:53:ALA:CB	2.24	0.68
1:A:6:ILE:HG13	1:A:7:ARG:N	2.08	0.67
1:A:93:ARG:NH2	1:A:116:ASP:OD2	2.28	0.66
1:A:122:ALA:HB2	1:A:258:GLU:HA	1.76	0.66
1:A:70:LYS:HZ3	1:A:71:ASP:HB3	1.59	0.66
1:A:3:ASP:HA	1:A:32:GLN:HB2	1.78	0.65
1:A:122:ALA:N	1:A:258:GLU:OE1	2.29	0.65
1:A:264:MET:O	1:A:268:LEU:HB2	1.96	0.65
1:A:93:ARG:NH1	1:A:120:ASP:OD2	2.30	0.65
1:A:10:ILE:HD13	1:A:10:ILE:N	2.10	0.65
1:A:6:ILE:HD11	1:A:75:VAL:CG2	2.24	0.64
1:A:80:THR:CG2	1:A:81:ARG:N	2.59	0.64
1:A:37:LEU:HD21	1:A:66:LEU:CD2	2.27	0.63
1:A:122:ALA:HA	1:A:259:SER:O	1.99	0.63
1:A:45:LEU:HD11	1:A:63:GLN:O	1.99	0.63
1:A:268:LEU:HB3	1:A:270:LEU:HG	1.81	0.62
1:A:89:LEU:HD23	1:A:99:MET:HE2	1.82	0.62
1:A:4:ALA:H	1:A:32:GLN:HE21	1.48	0.61
1:A:70:LYS:HG3	1:A:95:HIS:CD2	2.36	0.61
1:A:78:ASP:OD1	1:A:80:THR:HB	2.00	0.61
1:A:82:PRO:HB3	1:A:106:PHE:CD2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ARG:HD3	1:A:249:ARG:N	2.15	0.61
1:A:121:ILE:HA	1:A:258:GLU:OE1	2.01	0.61
1:A:42:SER:O	1:A:45:LEU:HB2	2.02	0.60
1:A:10:ILE:HD12	1:A:77:ILE:HB	1.83	0.60
1:A:23:GLN:HG2	1:A:53:ALA:HB1	1.82	0.60
1:A:49:ALA:HB1	1:A:60:VAL:O	2.02	0.59
1:A:70:LYS:HG3	1:A:95:HIS:HD2	1.67	0.59
1:A:263:ASP:OD1	1:A:265:ARG:HB2	2.02	0.58
1:A:130:SER:O	1:A:134:ASN:ND2	2.36	0.58
1:A:198:THR:O	1:A:199:GLY:O	2.22	0.58
1:A:3:ASP:HA	1:A:32:GLN:CB	2.33	0.58
1:A:19:ARG:CB	1:A:52:LEU:HD22	2.34	0.58
1:A:28:LEU:HD13	1:A:31:VAL:CG1	2.34	0.57
1:A:22:ILE:HG22	1:A:53:ALA:HB2	1.85	0.57
1:A:67:ASP:HA	1:A:70:LYS:HB3	1.86	0.56
1:A:19:ARG:CB	1:A:52:LEU:HD13	2.35	0.56
1:A:11:ALA:HB2	1:A:76:PHE:CZ	2.40	0.56
1:A:70:LYS:O	1:A:70:LYS:HG2	2.05	0.56
1:A:95:HIS:ND1	1:A:95:HIS:N	2.54	0.56
1:A:42:SER:CB	1:A:45:LEU:HD23	2.29	0.56
1:A:21:LEU:HD22	1:A:77:ILE:HG21	1.88	0.56
1:A:4:ALA:N	1:A:32:GLN:HB2	2.20	0.56
1:A:70:LYS:HZ2	1:A:71:ASP:HB3	1.69	0.55
1:A:70:LYS:CB	1:A:91:PHE:HZ	2.08	0.55
1:A:46:GLY:N	1:A:62:VAL:O	2.41	0.54
1:A:45:LEU:O	1:A:47:SER:N	2.28	0.54
1:A:23:GLN:HG2	1:A:53:ALA:HB2	1.88	0.54
1:A:96:GLY:C	1:A:121:ILE:HD11	2.27	0.54
1:A:66:LEU:HB3	1:A:91:PHE:CZ	2.43	0.53
1:A:164:VAL:O	1:A:164:VAL:HG22	2.07	0.53
1:A:65:SER:HB3	1:A:68:ALA:HB3	1.88	0.53
1:A:39:ARG:HH11	1:A:39:ARG:HG2	1.74	0.53
1:A:269:ASP:HA	3:A:457:HOH:O	2.09	0.52
1:A:52:LEU:O	1:A:52:LEU:HD23	2.09	0.52
1:A:39:ARG:O	1:A:42:SER:N	2.31	0.52
1:A:117:ALA:O	1:A:121:ILE:HG22	2.10	0.51
1:A:36:ALA:O	1:A:62:VAL:HA	2.11	0.51
1:A:80:THR:HG22	1:A:81:ARG:N	2.07	0.51
1:A:33:LEU:O	1:A:60:VAL:HG21	2.11	0.51
1:A:3:ASP:O	1:A:4:ALA:HB2	2.12	0.50
1:A:255:SER:OG	1:A:255:SER:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LEU:HA	1:A:99:MET:CE	2.42	0.50
1:A:69:VAL:HG22	1:A:69:VAL:O	2.11	0.50
1:A:66:LEU:O	1:A:70:LYS:N	2.45	0.49
1:A:160:HIS:HD2	1:A:162:HIS:N	2.03	0.49
1:A:7:ARG:O	1:A:74:ASP:HB2	2.12	0.49
1:A:6:ILE:CG2	1:A:252:LEU:HD12	2.42	0.49
1:A:23:GLN:CG	1:A:53:ALA:HB1	2.43	0.49
1:A:89:LEU:CD2	1:A:99:MET:HE1	2.40	0.48
1:A:47:SER:O	1:A:48:ASP:HB2	2.14	0.48
1:A:69:VAL:HG13	1:A:69:VAL:O	2.13	0.48
1:A:122:ALA:HB2	1:A:258:GLU:CA	2.44	0.48
1:A:69:VAL:CG2	1:A:72:ASP:HB2	2.33	0.47
1:A:82:PRO:HB3	1:A:106:PHE:CE2	2.49	0.47
1:A:16:ARG:HG3	2:A:301:NDP:O1A	2.15	0.47
1:A:45:LEU:HA	1:A:45:LEU:HD13	1.51	0.47
1:A:161:ARG:HH11	1:A:214:GLY:HA2	1.79	0.47
1:A:9:ALA:HA	1:A:35:ALA:O	2.15	0.47
1:A:118:ALA:HA	1:A:121:ILE:O	2.15	0.46
1:A:198:THR:O	1:A:198:THR:HG23	2.14	0.46
1:A:145:LYS:NZ	1:A:145:LYS:CB	2.77	0.46
1:A:188:ASP:O	1:A:189:CYS:HB3	2.15	0.46
1:A:8:VAL:HG13	1:A:10:ILE:HD11	1.97	0.46
1:A:249:ARG:HD3	1:A:249:ARG:H	1.80	0.46
1:A:79:PHE:HB3	2:A:301:NDP:H51N	1.99	0.45
1:A:66:LEU:HB2	1:A:91:PHE:CE2	2.50	0.45
1:A:138:LYS:HA	1:A:138:LYS:HD3	1.60	0.45
1:A:239:SER:O	1:A:242:THR:HG22	2.17	0.45
1:A:159:HIS:O	1:A:212:ARG:HA	2.16	0.45
1:A:6:ILE:HG21	1:A:252:LEU:HD12	1.98	0.45
1:A:142:LYS:HE2	1:A:273:LEU:OXT	2.17	0.45
1:A:153:ILE:HA	1:A:223:MET:O	2.17	0.45
1:A:69:VAL:HG22	1:A:72:ASP:CB	2.36	0.45
1:A:80:THR:HG22	1:A:81:ARG:O	2.17	0.45
1:A:22:ILE:CG2	1:A:53:ALA:HB2	2.46	0.45
1:A:257:LYS:HE2	1:A:257:LYS:HB3	1.77	0.45
1:A:39:ARG:CG	1:A:39:ARG:HH11	2.30	0.45
1:A:141:GLU:O	1:A:145:LYS:HD3	2.16	0.44
1:A:254:LEU:O	1:A:257:LYS:N	2.50	0.44
1:A:45:LEU:C	1:A:47:SER:H	2.12	0.44
1:A:157:GLU:OE1	1:A:159:HIS:ND1	2.46	0.44
1:A:150:TYR:CD1	1:A:150:TYR:N	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ALA:H	1:A:32:GLN:HB2	1.83	0.43
1:A:66:LEU:CB	1:A:91:PHE:CE2	3.01	0.43
1:A:189:CYS:HB2	1:A:205:THR:HA	2.00	0.43
1:A:145:LYS:HB2	1:A:145:LYS:HE3	1.78	0.43
1:A:136:MET:HE1	1:A:174:MET:SD	2.58	0.43
1:A:4:ALA:CB	1:A:30:GLY:CA	2.97	0.43
1:A:4:ALA:HB3	1:A:30:GLY:C	2.39	0.43
1:A:19:ARG:CB	1:A:52:LEU:CD2	2.97	0.43
1:A:135:VAL:O	1:A:138:LYS:HB3	2.19	0.43
1:A:188:ASP:O	1:A:189:CYS:CB	2.66	0.42
1:A:54:GLY:O	1:A:55:ALA:HB3	2.20	0.42
1:A:28:LEU:HD12	1:A:248:VAL:CG1	2.43	0.42
1:A:136:MET:HE3	1:A:174:MET:HG2	2.01	0.42
1:A:145:LYS:NZ	1:A:145:LYS:HB3	2.35	0.41
1:A:211:VAL:O	1:A:212:ARG:NH1	2.48	0.41
1:A:37:LEU:CD2	1:A:66:LEU:CD2	2.96	0.41
1:A:49:ALA:HB1	3:A:468:HOH:O	2.20	0.41
1:A:9:ALA:O	1:A:10:ILE:HD13	2.21	0.41
1:A:194:ARG:HD2	1:A:194:ARG:HH11	1.68	0.41
1:A:5:ASN:HA	1:A:5:ASN:HD22	1.48	0.41
1:A:3:ASP:CA	1:A:32:GLN:HG3	2.49	0.41
1:A:10:ILE:HD11	1:A:77:ILE:HD12	2.03	0.41
1:A:45:LEU:HD13	1:A:62:VAL:HG12	2.03	0.41
1:A:140:LEU:HD12	1:A:140:LEU:HA	1.85	0.41
1:A:19:ARG:O	1:A:22:ILE:HB	2.20	0.40
1:A:45:LEU:C	1:A:47:SER:N	2.73	0.40
1:A:69:VAL:O	1:A:71:ASP:N	2.54	0.40
1:A:146:VAL:O	1:A:150:TYR:HE2	2.04	0.40
1:A:69:VAL:C	1:A:71:ASP:N	2.75	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	270/273 (99%)	233 (86%)	20 (7%)	17 (6%)	2 0

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	40	GLU
1	A	48	ASP
1	A	55	ALA
1	A	189	CYS
1	A	46	GLY
1	A	199	GLY
1	A	255	SER
1	A	33	LEU
1	A	49	ALA
1	A	56	GLY
1	A	69	VAL
1	A	42	SER
1	A	259	SER
1	A	13	ALA
1	A	260	GLY
1	A	50	GLY

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	192/201 (96%)	147 (77%)	45 (23%)	1 0

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	6	ILE
1	A	8	VAL
1	A	10	ILE

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Mol	Chain	Res	Type
1	A	20	GLN
1	A	23	GLN
1	A	28	LEU
1	A	31	VAL
1	A	32	GLN
1	A	33	LEU
1	A	39	ARG
1	A	43	SER
1	A	45	LEU
1	A	48	ASP
1	A	57	LYS
1	A	61	THR
1	A	64	SER
1	A	67	ASP
1	A	69	VAL
1	A	70	LYS
1	A	71	ASP
1	A	81	ARG
1	A	89	LEU
1	A	93	ARG
1	A	95	HIS
1	A	108	GLU
1	A	121	ILE
1	A	140	LEU
1	A	146	VAL
1	A	157	GLU
1	A	161	ARG
1	A	165	ASP
1	A	176	GLU
1	A	184	LYS
1	A	193	SER
1	A	221	THR
1	A	230	ARG
1	A	231	LEU
1	A	249	ARG
1	A	255	SER
1	A	257	LYS
1	A	258	GLU
1	A	259	SER
1	A	261	LEU
1	A	268	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	32	GLN
1	A	63	GLN
1	A	88	HIS
1	A	112	GLN
1	A	134	ASN
1	A	160	HIS
1	A	197	HIS

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)

1 ligand is 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	301	-	42,52,52	1.83	6 (14%)	55,80,80	2.02	11 (20%)

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	301	-	-	0/30/77/77	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NDP	C4N-C5N	-4.62	1.39	1.49
2	A	301	NDP	C4A-N3A	-2.92	1.31	1.35
2	A	301	NDP	C8A-N7A	-2.41	1.30	1.34
2	A	301	NDP	O3B-C3B	-2.04	1.38	1.43
2	A	301	NDP	C6N-C5N	3.30	1.39	1.33
2	A	301	NDP	O7N-C7N	7.97	1.44	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	NDP	C1D-N1N-C2N	-8.61	105.91	120.91
2	A	301	NDP	C4N-C5N-C6N	-3.23	117.25	122.58
2	A	301	NDP	O3X-P2B-O2X	-2.70	97.09	107.38
2	A	301	NDP	C3B-C2B-C1B	-2.20	98.48	102.73
2	A	301	NDP	O2X-P2B-O1X	2.38	118.25	110.58
2	A	301	NDP	C3N-C2N-N1N	2.58	126.83	123.14
2	A	301	NDP	O3-PA-O5B	2.67	110.03	102.94
2	A	301	NDP	O2N-PN-O3	2.71	117.40	105.09
2	A	301	NDP	O2A-PA-O3	3.28	119.99	105.09
2	A	301	NDP	C5N-C4N-C3N	4.88	125.96	112.52
2	A	301	NDP	C1D-N1N-C6N	6.18	134.63	120.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NDP	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.