Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 06:57 PM GMT

PDB ID	:	1DAP
Title	:	C. GLUTAMICUM DAP DEHYDROGENASE IN COMPLEX WITH NADP+
Authors	:	Scapin, G.; Reddy, S.G.; Blanchard, J.S.
Deposited on	:	1996-07-08
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 ⓘ symbol.

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

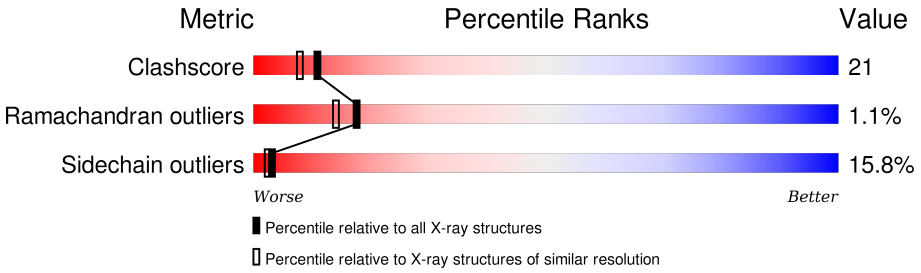
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.20 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	320	63% 30% 8%
1	B	320	52% 36% 11%

2 Entry composition

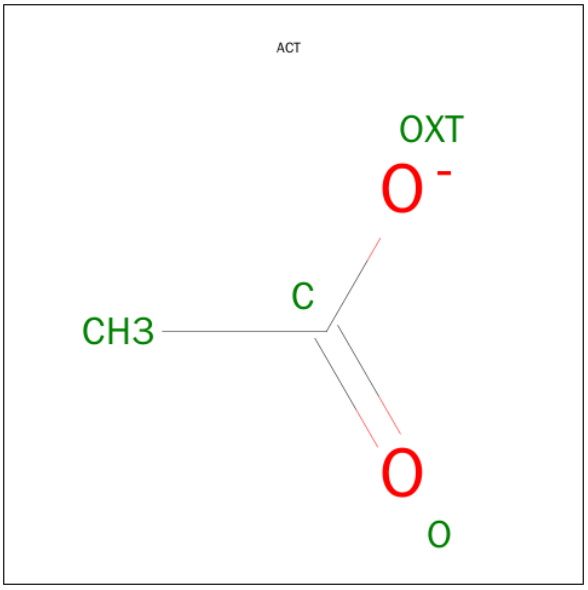
There are 4 unique types of molecules in this entry. The entry contains 5214 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DIAMINOPIMELIC ACID DEHYDROGENASE.

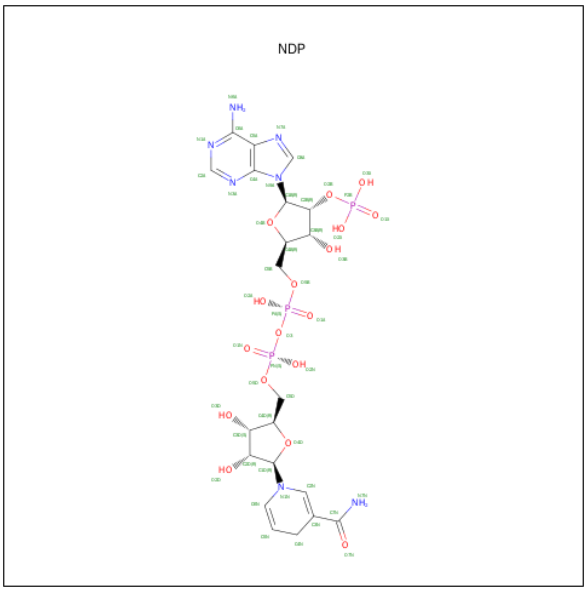
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2467	1538	441	478	10			
1	B	320	Total	C	N	O	S	0	0	0
			2460	1535	441	474	10			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 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
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	92	Total	O	0	0
			92	92		
4	B	91	Total	O	0	0
			91	91		

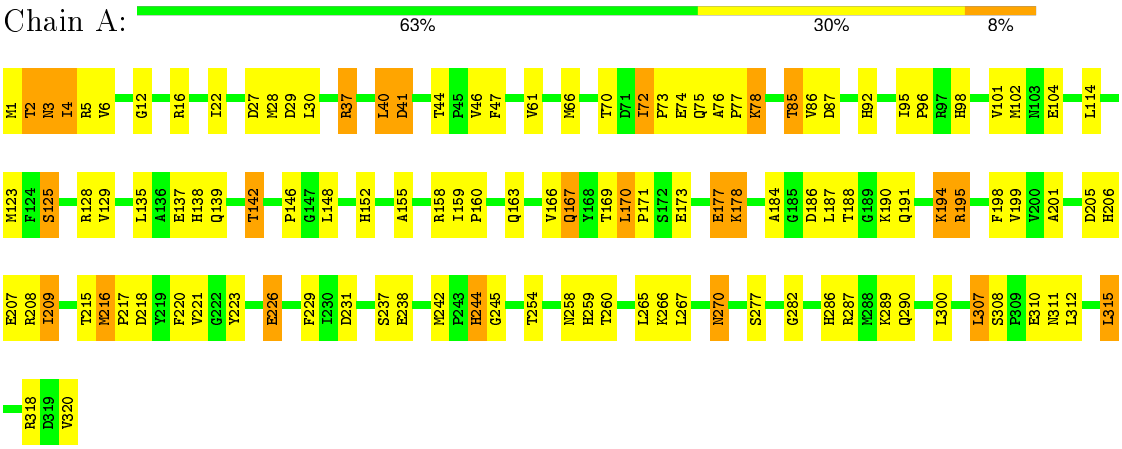
3 Residue-property plots (i)

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.

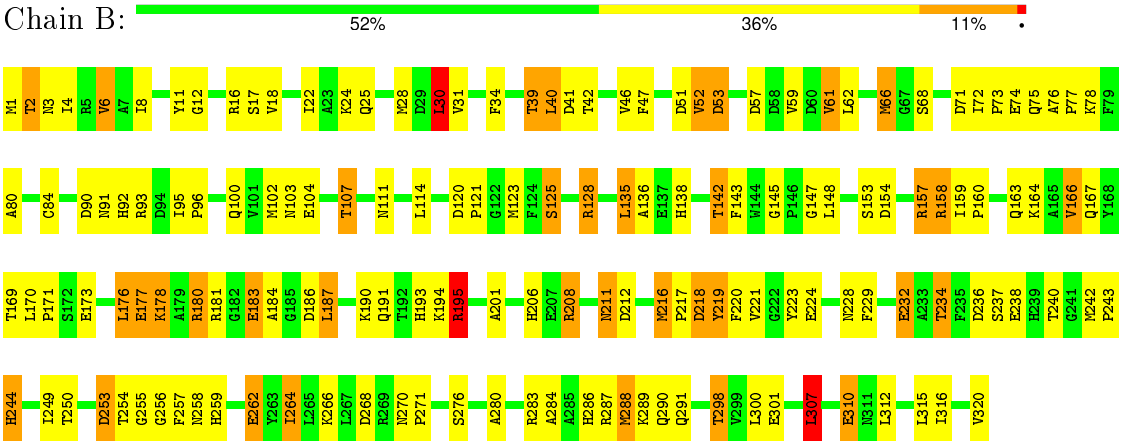
- Molecule 1: DIAMINOPIMELIC ACID DEHYDROGENASE

Chain A:



- Molecule 1: DIAMINOPIMELIC ACID DEHYDROGENASE

Chain B:



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	75.90Å 65.80Å 84.50Å 90.00° 106.60° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	86.0 (20.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.170 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5214	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, ACT

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	0.93	1/2520 (0.0%)	1.02	5/3422 (0.1%)
1	B	0.95	0/2513	1.10	13/3415 (0.4%)
All	All	0.94	1/5033 (0.0%)	1.06	18/6837 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	207	GLU	CG-CD	5.43	1.60	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	128	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	B	145	GLY	C-N-CD	-8.35	102.23	120.60
1	A	5	ARG	NE-CZ-NH2	7.47	124.04	120.30
1	B	157	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	B	195	ARG	NE-CZ-NH2	6.43	123.51	120.30
1	B	30	LEU	CB-CG-CD2	6.37	121.82	111.00
1	A	216	MET	CG-SD-CE	6.34	110.34	100.20
1	B	28	MET	CG-SD-CE	5.99	109.78	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	93	ARG	NE-CZ-NH1	-5.94	117.33	120.30
1	B	102	MET	CG-SD-CE	5.92	109.67	100.20
1	A	28	MET	CG-SD-CE	5.89	109.62	100.20
1	A	123	MET	CG-SD-CE	5.88	109.61	100.20
1	B	123	MET	CG-SD-CE	5.86	109.57	100.20
1	A	102	MET	CG-SD-CE	5.73	109.37	100.20
1	B	288	MET	CG-SD-CE	5.53	109.05	100.20
1	B	216	MET	CG-SD-CE	5.42	108.88	100.20
1	B	307	LEU	CB-CA-C	-5.31	100.11	110.20
1	B	66	MET	CG-SD-CE	5.13	108.40	100.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	277	SER	Mainchain
1	B	52	VAL	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	2467	0	2364	92	5
1	B	2460	0	2354	120	7
2	B	8	0	6	1	0
3	A	48	0	26	2	0
3	B	48	0	26	0	0
4	A	92	0	0	7	0
4	B	91	0	0	6	1
All	All	5214	0	4776	206	7

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 21.

All (206) 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:167:GLN:HE21	1:B:195:ARG:HG3	1.08	1.09
1:B:194:LYS:HE3	1:B:224:GLU:HG2	1.37	1.05
1:A:3:ASN:ND2	1:A:29:ASP:OD1	1.92	1.03
1:B:167:GLN:NE2	1:B:195:ARG:HG3	1.80	0.96
1:A:152:HIS:HB3	1:A:167:GLN:HG2	1.51	0.93
1:A:1:MET:O	1:A:3:ASN:N	2.09	0.85
1:A:265:LEU:O	1:A:266:LYS:HD3	1.76	0.85
1:A:6:VAL:HG21	1:A:22:ILE:HD13	1.60	0.82
1:A:12:GLY:O	1:A:16:ARG:HG3	1.81	0.80
1:A:128:ARG:HE	1:A:142:THR:HG21	1.47	0.79
1:B:53:ASP:HB2	4:B:472:HOH:O	1.83	0.77
1:B:148:LEU:HD21	1:B:166:VAL:HG22	1.64	0.76
1:B:148:LEU:HD21	1:B:166:VAL:CG2	2.15	0.76
1:B:104:GLU:HG3	4:B:482:HOH:O	1.83	0.76
1:B:12:GLY:O	1:B:16:ARG:HG3	1.86	0.75
1:A:186:ASP:O	1:A:187:LEU:HD23	1.86	0.75
1:A:205:ASP:O	1:A:209:ILE:HG13	1.87	0.75
1:A:85:THR:HG23	4:A:405:HOH:O	1.87	0.74
1:B:194:LYS:HE3	1:B:224:GLU:CG	2.16	0.73
1:A:201:ALA:O	1:A:206:HIS:HE1	1.71	0.73
1:B:170:LEU:N	1:B:170:LEU:HD12	2.03	0.73
1:B:169:THR:C	1:B:170:LEU:HD12	2.10	0.72
1:A:78:LYS:HB2	1:A:78:LYS:NZ	2.04	0.72
1:A:290:GLN:HA	1:A:290:GLN:OE1	1.89	0.72
1:A:216:MET:O	1:A:221:VAL:HG23	1.90	0.72
1:B:181:ARG:O	1:B:183:GLU:HG2	1.90	0.71
1:A:41:ASP:HB2	4:A:461:HOH:O	1.89	0.71
1:A:265:LEU:C	1:A:266:LYS:HD3	2.13	0.69
1:A:72:ILE:HG22	1:A:73:PRO:HD3	1.72	0.69
1:B:178:LYS:HB2	1:B:184:ALA:HB2	1.74	0.69
1:A:6:VAL:HG21	1:A:22:ILE:CD1	2.22	0.69
1:B:68:SER:CB	1:B:90:ASP:OD1	2.41	0.68
1:B:254:THR:O	1:B:256:GLY:N	2.26	0.68
1:A:155:ALA:O	1:A:158:ARG:HG2	1.92	0.68
1:A:178:LYS:HG2	1:A:184:ALA:HB2	1.75	0.67
1:A:173:GLU:HG2	1:A:177:GLU:OE2	1.95	0.67
1:A:160:PRO:O	1:A:208:ARG:NH1	2.27	0.67
1:B:298:THR:HG23	1:B:300:LEU:H	1.61	0.65
1:A:167:GLN:OE1	1:A:195:ARG:HB3	1.96	0.65
1:A:307:LEU:HD23	1:A:307:LEU:N	2.11	0.65
1:B:298:THR:HB	1:B:301:GLU:OE2	1.97	0.65
1:B:310:GLU:HB2	1:B:315:LEU:HD13	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:GLU:N	1:B:74:GLU:OE1	2.28	0.64
1:B:76:ALA:HB3	1:B:77:PRO:HD3	1.79	0.64
1:A:37:ARG:HD3	3:A:400:NDP:O1X	1.97	0.64
1:A:3:ASN:HD22	1:A:29:ASP:CG	2.02	0.63
1:A:85:THR:CG2	4:A:405:HOH:O	2.44	0.63
1:A:159:ILE:HG23	1:A:160:PRO:HD2	1.80	0.63
1:A:216:MET:C	1:A:221:VAL:HG23	2.20	0.62
1:B:310:GLU:HB2	1:B:315:LEU:CD1	2.29	0.61
1:B:6:VAL:HG11	1:B:22:ILE:HD13	1.81	0.61
1:B:75:GLN:O	1:B:78:LYS:HG2	2.01	0.61
1:B:164:LYS:NZ	1:B:232:GLU:OE2	2.25	0.61
1:B:181:ARG:NH1	1:B:183:GLU:OE2	2.30	0.60
1:B:163:GLN:NE2	1:B:201:ALA:HA	2.15	0.60
1:A:254:THR:OG1	1:A:259:HIS:HE1	1.85	0.60
1:A:37:ARG:HG3	1:A:40:LEU:HD11	1.83	0.59
1:B:208:ARG:HG2	4:B:459:HOH:O	2.03	0.59
1:B:211:ASN:OD1	1:B:212:ASP:N	2.35	0.59
1:A:152:HIS:CB	1:A:167:GLN:HG2	2.29	0.58
1:B:25:GLN:HE21	1:B:283:ARG:HH22	1.50	0.58
1:B:6:VAL:HG11	1:B:22:ILE:CD1	2.33	0.58
1:A:27:ASP:N	1:A:27:ASP:OD1	2.36	0.58
1:A:72:ILE:CD1	4:A:458:HOH:O	2.52	0.57
1:B:217:PRO:O	1:B:219:TYR:N	2.37	0.57
1:A:187:LEU:HD22	1:A:191:GLN:OE1	2.04	0.57
1:A:320:VAL:HA	1:B:125:SER:HB3	1.86	0.57
1:B:286:HIS:O	1:B:290:GLN:HG2	2.05	0.57
1:A:92:HIS:HE1	4:A:466:HOH:O	1.88	0.57
1:B:114:LEU:HD21	1:B:288:MET:CE	2.35	0.57
1:B:136:ALA:HA	4:B:486:HOH:O	2.05	0.56
1:A:75:GLN:O	1:A:78:LYS:HG3	2.05	0.56
1:A:78:LYS:HB2	1:A:78:LYS:HZ3	1.68	0.56
1:A:310:GLU:HA	1:A:310:GLU:OE1	2.06	0.56
1:B:253:ASP:HB2	1:B:258:ASN:ND2	2.21	0.56
1:B:61:VAL:HB	1:B:84:CYS:HB2	1.87	0.55
1:B:280:ALA:HB1	1:B:307:LEU:HB3	1.87	0.55
1:A:188:THR:OG1	1:A:191:GLN:NE2	2.39	0.55
1:B:148:LEU:CD2	1:B:166:VAL:HG22	2.34	0.55
1:B:307:LEU:N	1:B:307:LEU:HD23	2.22	0.55
1:A:216:MET:HB3	1:A:220:PHE:HB2	1.89	0.55
1:A:166:VAL:HG12	1:A:198:PHE:HB2	1.89	0.55
1:B:143:PHE:HA	1:B:193:HIS:CE1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:GLN:NE2	1:B:283:ARG:HH22	2.05	0.54
1:B:142:THR:HG23	4:B:488:HOH:O	2.08	0.54
1:A:4:ILE:HG12	1:A:286:HIS:CD2	2.43	0.54
1:A:190:LYS:HA	1:A:223:TYR:CE1	2.43	0.54
1:A:215:THR:O	1:A:217:PRO:HD3	2.07	0.54
1:A:217:PRO:O	1:A:218:ASP:HB2	2.08	0.54
1:B:211:ASN:OD1	1:B:212:ASP:OD1	2.26	0.54
1:B:164:LYS:HE2	1:B:236:ASP:OD1	2.08	0.53
1:A:125:SER:HB3	1:B:320:VAL:HA	1.90	0.53
1:B:194:LYS:HD2	1:B:224:GLU:HB3	1.90	0.53
1:B:92:HIS:HA	1:B:95:ILE:HD12	1.91	0.53
1:B:194:LYS:CE	1:B:224:GLU:HG2	2.24	0.52
1:B:135:LEU:HD13	1:B:138:HIS:HB3	1.90	0.52
1:A:92:HIS:HD2	1:B:320:VAL:O	1.91	0.52
1:A:287:ARG:NH2	1:A:308:SER:O	2.41	0.52
1:B:216:MET:HG2	1:B:217:PRO:HD2	1.91	0.52
1:A:270:ASN:C	1:A:270:ASN:HD22	2.13	0.52
1:A:104:GLU:HG3	4:A:454:HOH:O	2.10	0.52
1:B:167:GLN:HE21	1:B:195:ARG:CG	2.00	0.51
1:A:72:ILE:N	1:A:73:PRO:HD2	2.25	0.51
1:B:254:THR:OG1	1:B:259:HIS:HE1	1.93	0.51
1:B:1:MET:N	1:B:2:THR:CB	2.73	0.51
1:B:180:ARG:HH11	1:B:180:ARG:HG3	1.75	0.51
1:B:184:ALA:O	1:B:187:LEU:HB2	2.11	0.51
1:B:17:SER:OG	1:B:271:PRO:HB2	2.11	0.51
1:B:186:ASP:O	1:B:187:LEU:HD12	2.10	0.51
1:B:6:VAL:HG12	1:B:30:LEU:HA	1.92	0.51
1:A:137:GLU:CD	1:B:24:LYS:HE2	2.31	0.51
1:B:128:ARG:HE	1:B:142:THR:HG21	1.76	0.51
1:B:201:ALA:O	1:B:206:HIS:HE1	1.94	0.50
1:B:4:ILE:HG12	1:B:286:HIS:CD2	2.46	0.50
1:B:287:ARG:O	1:B:291:GLN:HB2	2.10	0.50
1:B:237:SER:OG	1:B:238:GLU:N	2.45	0.50
1:B:167:GLN:HE22	1:B:195:ARG:HE	1.60	0.50
1:A:152:HIS:HB3	1:A:167:GLN:CG	2.34	0.50
1:A:159:ILE:HD11	1:A:216:MET:CE	2.42	0.49
1:B:253:ASP:HA	1:B:257:PHE:O	2.13	0.49
1:B:8:ILE:CD1	1:B:18:VAL:HG22	2.42	0.49
1:A:188:THR:HG23	1:A:191:GLN:HE22	1.78	0.49
1:B:72:ILE:HB	1:B:73:PRO:HD3	1.94	0.49
1:B:170:LEU:N	1:B:170:LEU:CD1	2.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:ASP:CG	1:B:128:ARG:HH22	2.15	0.49
1:B:71:ASP:OD2	1:B:158:ARG:NH2	2.46	0.49
1:B:218:ASP:N	1:B:221:VAL:HG22	2.27	0.49
1:A:169:THR:C	1:A:170:LEU:HD23	2.33	0.49
1:B:153:SER:HB3	1:B:157:ARG:NH2	2.28	0.49
1:B:178:LYS:HB3	1:B:183:GLU:O	2.11	0.48
1:B:31:VAL:HG21	1:B:59:VAL:HG12	1.95	0.48
1:B:148:LEU:HD21	1:B:166:VAL:HG21	1.94	0.48
1:B:298:THR:CG2	1:B:300:LEU:H	2.25	0.48
1:B:217:PRO:C	1:B:219:TYR:H	2.17	0.48
1:A:199:VAL:O	1:A:229:PHE:HA	2.14	0.48
1:B:114:LEU:HD21	1:B:288:MET:HE1	1.96	0.47
1:B:170:LEU:HA	1:B:171:PRO:HD3	1.68	0.47
1:A:311:ASN:OD1	1:A:312:LEU:N	2.47	0.47
1:A:72:ILE:HG22	1:A:73:PRO:CD	2.43	0.47
1:B:180:ARG:NH1	1:B:180:ARG:HG3	2.28	0.47
1:B:270:ASN:N	1:B:271:PRO:HD2	2.29	0.47
1:B:135:LEU:O	1:B:138:HIS:HD2	1.97	0.47
1:B:84:CYS:SG	1:B:289:LYS:HD2	2.54	0.47
1:B:147:GLY:HA3	1:B:244:HIS:HA	1.96	0.47
1:B:135:LEU:O	1:B:138:HIS:CD2	2.69	0.46
1:A:78:LYS:HB2	1:A:78:LYS:HZ2	1.78	0.46
1:B:173:GLU:O	1:B:177:GLU:HG2	2.16	0.46
1:A:46:VAL:HG12	1:A:47:PHE:N	2.30	0.46
1:A:1:MET:O	1:A:2:THR:C	2.52	0.46
1:A:78:LYS:CB	1:A:78:LYS:NZ	2.73	0.46
1:B:1:MET:CA	1:B:2:THR:CB	2.94	0.46
1:B:103:ASN:O	1:B:107:THR:OG1	2.28	0.46
1:B:68:SER:OG	1:B:90:ASP:OD1	2.33	0.45
1:A:95:ILE:HB	1:A:96:PRO:HD3	1.99	0.45
1:A:86:VAL:HG21	1:A:282:GLY:HA2	1.98	0.45
1:B:253:ASP:HB2	1:B:258:ASN:HD21	1.81	0.45
1:A:148:LEU:HD11	1:A:166:VAL:CG2	2.46	0.45
1:A:98:HIS:O	1:A:101:VAL:HG12	2.16	0.45
1:B:154:ASP:O	1:B:158:ARG:HG2	2.17	0.45
1:A:129:VAL:HG21	1:A:300:LEU:CD2	2.46	0.45
1:A:308:SER:CB	1:A:315:LEU:HD21	2.47	0.45
1:A:2:THR:HG22	4:A:447:HOH:O	2.16	0.44
1:A:2:THR:OG1	1:A:3:ASN:N	2.51	0.44
1:A:128:ARG:NE	1:A:142:THR:HG21	2.23	0.44
1:A:170:LEU:N	1:A:170:LEU:HD23	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:ARG:NH2	2:B:402:ACT:OXT	2.50	0.44
1:A:160:PRO:HB2	1:A:208:ARG:NH1	2.32	0.44
1:A:201:ALA:O	1:A:206:HIS:CE1	2.60	0.44
1:B:135:LEU:HD11	1:B:250:THR:CG2	2.47	0.44
1:A:135:LEU:O	1:A:138:HIS:HD2	2.00	0.44
1:A:146:PRO:HD2	1:A:266:LYS:NZ	2.33	0.44
1:B:135:LEU:CD1	1:B:138:HIS:HB3	2.48	0.44
1:B:284:ALA:O	1:B:288:MET:HG3	2.17	0.44
1:B:216:MET:HB3	1:B:220:PHE:HB2	2.00	0.43
1:B:176:LEU:HD21	1:B:249:ILE:HD11	2.01	0.43
1:B:195:ARG:NH1	1:B:223:TYR:CZ	2.86	0.43
1:B:163:GLN:HE21	1:B:201:ALA:HA	1.81	0.43
1:B:135:LEU:HD11	1:B:250:THR:HG21	1.99	0.43
1:A:92:HIS:CD2	1:B:320:VAL:O	2.72	0.43
1:B:181:ARG:HH12	1:B:183:GLU:CD	2.18	0.43
1:A:307:LEU:CD2	1:A:307:LEU:N	2.82	0.43
1:B:262:GLU:HG3	4:B:451:HOH:O	2.18	0.43
1:B:262:GLU:OE1	1:B:264:ILE:HG12	2.19	0.42
1:A:270:ASN:HD21	3:A:400:NDP:H5N	1.83	0.42
1:B:312:LEU:HG	1:B:316:ILE:HD12	2.01	0.42
1:A:258:ASN:O	1:B:268:ASP:HB2	2.19	0.42
1:A:265:LEU:HD23	1:A:265:LEU:HA	1.79	0.42
1:A:135:LEU:O	1:A:138:HIS:CD2	2.73	0.42
1:B:76:ALA:N	1:B:77:PRO:CD	2.82	0.42
1:A:152:HIS:CB	1:A:167:GLN:CG	2.94	0.41
1:B:181:ARG:NH1	1:B:183:GLU:CD	2.74	0.41
1:A:244:HIS:CD2	1:A:245:GLY:H	2.38	0.41
1:A:266:LYS:C	1:A:267:LEU:HD23	2.41	0.41
1:B:1:MET:CB	1:B:2:THR:CA	2.98	0.41
1:B:11:TYR:CD2	1:B:40:LEU:HG	2.54	0.41
1:A:135:LEU:HA	1:A:135:LEU:HD23	1.87	0.41
1:B:242:MET:N	1:B:243:PRO:CD	2.83	0.41
1:B:34:PHE:CD1	1:B:47:PHE:HB2	2.56	0.41
1:B:114:LEU:HD21	1:B:288:MET:HE3	2.01	0.41
1:A:76:ALA:HB3	1:A:77:PRO:HD3	2.01	0.41
1:B:159:ILE:HA	1:B:160:PRO:HD2	1.82	0.41
1:A:159:ILE:HG23	1:A:160:PRO:CD	2.47	0.41
1:A:194:LYS:HB2	1:A:194:LYS:HE2	1.91	0.40
1:B:92:HIS:CE1	1:B:121:PRO:HD3	2.57	0.40
1:B:95:ILE:N	1:B:96:PRO:CD	2.85	0.40
1:B:80:ALA:O	1:B:111:ASN:ND2	2.46	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:ASP:OD2	1:B:190:LYS:NZ[2_646]	1.97	0.23
1:A:226:GLU:OE2	1:B:234:THR:OG1[2_556]	2.04	0.16
1:B:39:THR:N	4:B:416:HOH:O[2_646]	2.11	0.09
1:A:229:PHE:N	1:B:229:PHE:O[2_556]	2.11	0.09
1:A:206:HIS:CD2	1:B:206:HIS:CD2[2_556]	2.12	0.08
1:A:231:ASP:N	1:B:228:ASN:OD1[2_556]	2.14	0.06
1:A:229:PHE:O	1:B:229:PHE:N[2_556]	2.17	0.03

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	318/320 (99%)	295 (93%)	20 (6%)	3 (1%)	21	19
1	B	318/320 (99%)	301 (95%)	13 (4%)	4 (1%)	15	11
All	All	636/640 (99%)	596 (94%)	33 (5%)	7 (1%)	17	14

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	B	53	ASP
1	B	218	ASP
1	B	255	GLY
1	A	4	ILE
1	B	2	THR
1	A	41	ASP

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	258/261 (99%)	221 (86%)	37 (14%)	4 3
1	B	256/261 (98%)	212 (83%)	44 (17%)	2 2
All	All	514/522 (98%)	433 (84%)	81 (16%)	3 2

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	30	LEU
1	A	37	ARG
1	A	40	LEU
1	A	44	THR
1	A	61	VAL
1	A	66	MET
1	A	70	THR
1	A	72	ILE
1	A	74	GLU
1	A	78	LYS
1	A	85	THR
1	A	87	ASP
1	A	114	LEU
1	A	125	SER
1	A	139	GLN
1	A	142	THR
1	A	163	GLN
1	A	167	GLN
1	A	170	LEU
1	A	171	PRO
1	A	177	GLU
1	A	178	LYS
1	A	194	LYS
1	A	195	ARG
1	A	209	ILE
1	A	226	GLU

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Mol	Chain	Res	Type
1	A	237	SER
1	A	238	GLU
1	A	242	MET
1	A	244	HIS
1	A	260	THR
1	A	270	ASN
1	A	289	LYS
1	A	307	LEU
1	A	315	LEU
1	A	318	ARG
1	B	3	ASN
1	B	6	VAL
1	B	30	LEU
1	B	39	THR
1	B	40	LEU
1	B	41	ASP
1	B	42	THR
1	B	46	VAL
1	B	52	VAL
1	B	57	ASP
1	B	61	VAL
1	B	62	LEU
1	B	66	MET
1	B	91	ASN
1	B	100	GLN
1	B	107	THR
1	B	125	SER
1	B	135	LEU
1	B	142	THR
1	B	158	ARG
1	B	166	VAL
1	B	176	LEU
1	B	177	GLU
1	B	178	LYS
1	B	180	ARG
1	B	183	GLU
1	B	187	LEU
1	B	191	GLN
1	B	195	ARG
1	B	208	ARG
1	B	211	ASN
1	B	219	TYR

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Mol	Chain	Res	Type
1	B	232	GLU
1	B	234	THR
1	B	240	THR
1	B	244	HIS
1	B	253	ASP
1	B	262	GLU
1	B	264	ILE
1	B	266	LYS
1	B	276	SER
1	B	298	THR
1	B	307	LEU
1	B	310	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	92	HIS
1	A	100	GLN
1	A	138	HIS
1	A	191	GLN
1	A	206	HIS
1	A	244	HIS
1	A	258	ASN
1	A	259	HIS
1	A	270	ASN
1	A	286	HIS
1	B	25	GLN
1	B	91	ASN
1	B	138	HIS
1	B	152	HIS
1	B	163	GLN
1	B	167	GLN
1	B	206	HIS
1	B	258	ASN
1	B	259	HIS
1	B	286	HIS
1	B	291	GLN
1	B	293	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
3	NDP	A	400	-	42,52,52	1.78	4 (9%)	55,80,80	2.05	17 (30%)
3	NDP	B	400	-	42,52,52	1.83	6 (14%)	55,80,80	2.17	13 (23%)
2	ACT	B	401	-	1,3,3	4.32	1 (100%)	0,3,3	0.00	-
2	ACT	B	402	-	1,3,3	4.94	1 (100%)	0,3,3	0.00	-

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
3	NDP	A	400	-	-	0/30/77/77	0/5/5/5
3	NDP	B	400	-	-	0/30/77/77	0/5/5/5
2	ACT	B	401	-	-	0/0/0/0	0/0/0/0
2	ACT	B	402	-	-	0/0/0/0	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	400	NDP	C4N-C5N	-4.70	1.38	1.49
3	A	400	NDP	C4N-C5N	-4.59	1.39	1.49
3	B	400	NDP	O3B-C3B	-2.26	1.37	1.43
3	B	400	NDP	P2B-O3X	-2.10	1.47	1.54
3	B	400	NDP	C6N-C5N	4.27	1.41	1.33
2	B	401	ACT	CH3-C	4.32	1.54	1.48
3	B	400	NDP	O7N-C7N	4.35	1.35	1.24
3	A	400	NDP	C6N-C5N	4.67	1.42	1.33
3	A	400	NDP	C2A-N3A	4.87	1.40	1.32
2	B	402	ACT	CH3-C	4.94	1.55	1.48
3	B	400	NDP	C2A-N3A	6.02	1.42	1.32
3	A	400	NDP	O7N-C7N	6.66	1.41	1.24

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	400	NDP	N3A-C2A-N1A	-10.19	121.09	128.89
3	A	400	NDP	N3A-C2A-N1A	-8.06	122.72	128.89
3	B	400	NDP	O2D-C2D-C1D	-3.82	96.59	109.94
3	B	400	NDP	C2D-C1D-N1N	-3.56	103.73	113.34
3	B	400	NDP	O5D-PN-O1N	-3.51	95.99	109.62
3	B	400	NDP	C1D-N1N-C2N	-3.39	115.00	120.91
3	B	400	NDP	C1B-N9A-C4A	-2.89	122.59	126.94
3	B	400	NDP	O4B-C1B-N9A	-2.76	102.33	108.10
3	A	400	NDP	O4D-C1D-C2D	-2.74	100.22	106.58
3	A	400	NDP	C4N-C5N-C6N	-2.74	118.06	122.58
3	A	400	NDP	C2D-C3D-C4D	-2.65	97.17	102.61
3	A	400	NDP	C4D-O4D-C1D	-2.16	104.77	109.52
3	A	400	NDP	O5D-PN-O1N	-2.09	101.50	109.62
3	B	400	NDP	O5B-PA-O1A	-2.07	101.59	109.62
3	A	400	NDP	O2A-PA-O3	2.01	114.21	105.09
3	A	400	NDP	N6A-C6A-N1A	2.05	123.59	119.20
3	B	400	NDP	O2N-PN-O3	2.13	114.77	105.09
3	B	400	NDP	C5D-C4D-C3D	2.36	124.56	115.21
3	A	400	NDP	O4D-C4D-C3D	2.62	110.43	105.15
3	A	400	NDP	C2A-N1A-C6A	2.81	123.78	118.77
3	A	400	NDP	O3D-C3D-C4D	2.87	119.65	111.05
3	A	400	NDP	O3-PA-O5B	2.96	110.79	102.94
3	A	400	NDP	O3X-P2B-O1X	3.08	120.48	110.58
3	A	400	NDP	C4A-C5A-N7A	3.11	112.34	109.48
3	B	400	NDP	C5N-C4N-C3N	3.16	121.24	112.52
3	A	400	NDP	C1B-N9A-C4A	3.18	131.74	126.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	400	NDP	O3X-P2B-O1X	3.22	120.96	110.58
3	B	400	NDP	C2A-N1A-C6A	3.40	124.85	118.77
3	A	400	NDP	C5N-C4N-C3N	3.67	122.63	112.52
3	A	400	NDP	C3D-C2D-C1D	4.58	110.61	101.40

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
3	A	400	NDP	2	0
2	B	402	ACT	1	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.