



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:33 PM GMT

PDB ID : 1KVS
Title : UDP-GALACTOSE 4-EPIMERASE COMPLEXED WITH UDP-PHENOL
Authors : Thoden, J.B.; Gulick, A.M.; Holden, H.M.
Deposited on : 1997-03-07
Resolution : 2.15 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

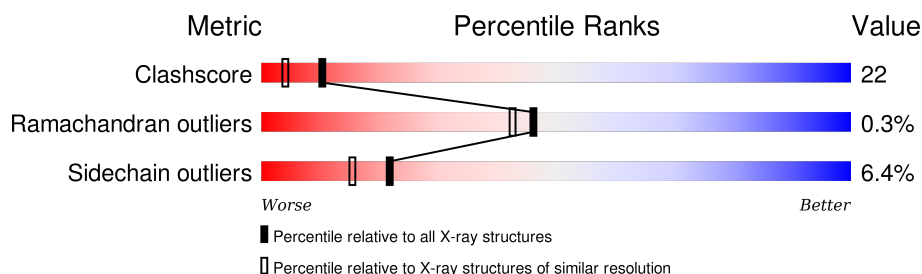
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	338	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PEG	A	410	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3132 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 UDP-GALACTOSE 4-EPIMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2626	1656	463	495	12			

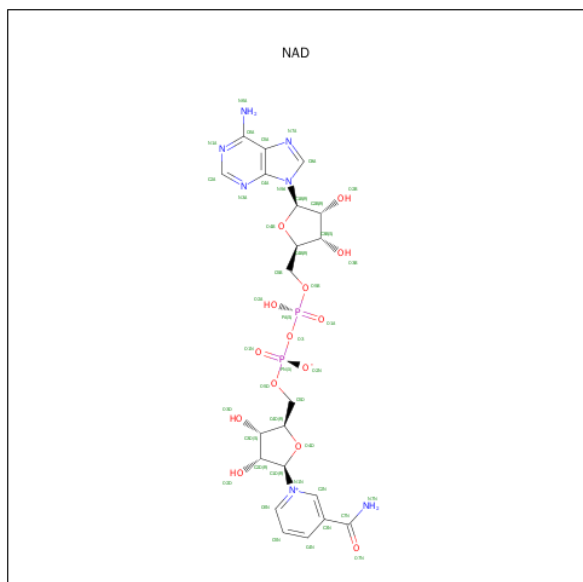
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	124	THR	SER	ENGINEERED	UNP P09147
A	131	ASN	GLN	CONFLICT	UNP P09147

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

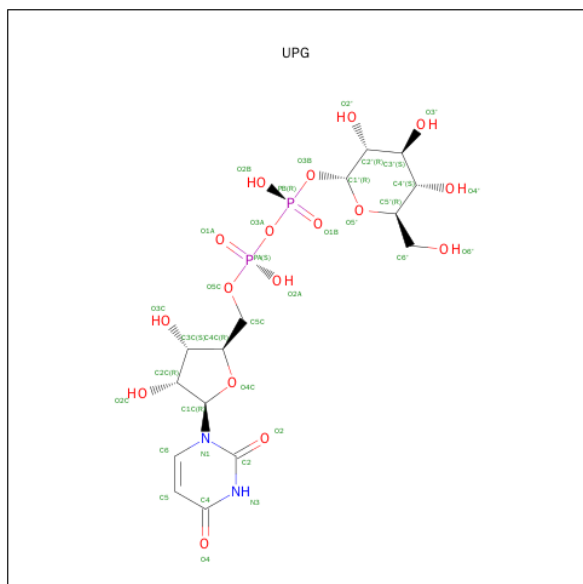
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Na	0	0
			2	2		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



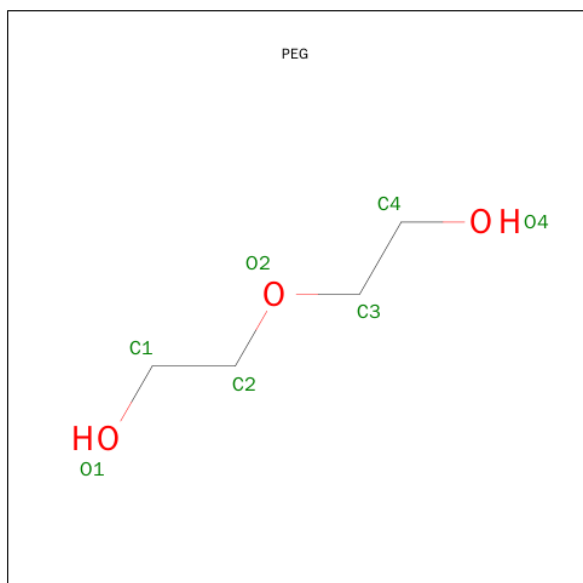
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: UPG) (formula: $C_{15}H_{24}N_2O_{17}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is water.

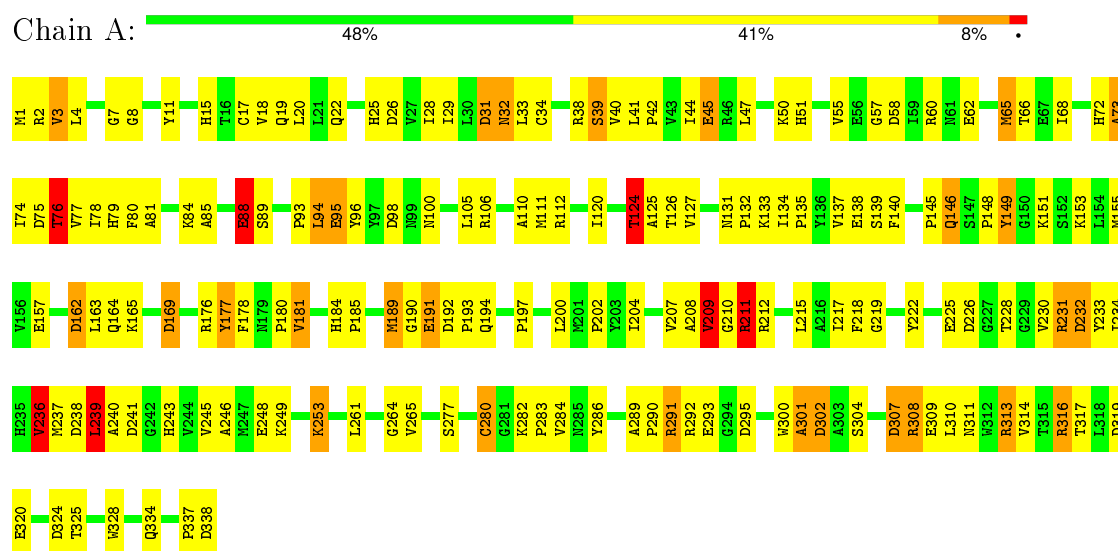
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	417	Total	O	0	0
			417	417		

3 Residue-property plots

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: UDP-GALACTOSE 4-EPIMERASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	83.50Å 83.50Å 108.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.15	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.15)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.188 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3132	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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: UPG, PEG, NAD, NA

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	1.05	12/2692 (0.4%)	1.69	73/3664 (2.0%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	GLU	CD-OE1	9.10	1.35	1.25
1	A	309	GLU	CD-OE1	8.41	1.34	1.25
1	A	62	GLU	CD-OE1	7.57	1.33	1.25
1	A	253	LYS	CE-NZ	-7.49	1.30	1.49
1	A	45	GLU	CD-OE1	6.98	1.33	1.25
1	A	225	GLU	CD-OE2	6.67	1.32	1.25
1	A	88	GLU	CD-OE1	6.34	1.32	1.25
1	A	248	GLU	CD-OE2	6.13	1.32	1.25
1	A	157	GLU	CD-OE1	6.04	1.32	1.25
1	A	95	GLU	CD-OE2	5.56	1.31	1.25
1	A	138	GLU	CD-OE1	5.19	1.31	1.25
1	A	320	GLU	CD-OE2	5.17	1.31	1.25

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	ARG	NE-CZ-NH2	11.47	126.04	120.30
1	A	302	ASP	CB-CG-OD1	-11.07	108.34	118.30
1	A	162	ASP	CB-CG-OD2	10.67	127.90	118.30
1	A	31	ASP	CB-CG-OD2	10.58	127.82	118.30
1	A	231	ARG	NE-CZ-NH2	9.37	124.98	120.30
1	A	26	ASP	CB-CG-OD1	-9.33	109.90	118.30
1	A	176	ARG	NE-CZ-NH1	-9.30	115.65	120.30
1	A	302	ASP	CB-CG-OD2	9.25	126.63	118.30
1	A	226	ASP	CB-CG-OD2	-8.46	110.69	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	A	232	ASP	CB-CG-OD1	-8.28	110.85	118.30
1	A	313	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	A	231	ARG	CD-NE-CZ	-7.87	112.58	123.60
1	A	60	ARG	NE-CZ-NH1	7.85	124.23	120.30
1	A	307	ASP	CB-CG-OD2	7.63	125.17	118.30
1	A	162	ASP	CB-CG-OD1	-7.58	111.48	118.30
1	A	75	ASP	CB-CG-OD1	-7.42	111.62	118.30
1	A	291	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	A	31	ASP	CB-CG-OD1	-7.38	111.66	118.30
1	A	338	ASP	CB-CG-OD2	7.32	124.89	118.30
1	A	319	ASP	CB-CG-OD1	7.12	124.71	118.30
1	A	88	GLU	N-CA-CB	6.88	122.99	110.60
1	A	26	ASP	CB-CG-OD2	6.87	124.48	118.30
1	A	169	ASP	CB-CG-OD1	-6.83	112.15	118.30
1	A	324	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	A	325	THR	CA-CB-CG2	-6.68	103.05	112.40
1	A	177	TYR	CB-CG-CD1	6.60	124.96	121.00
1	A	236	VAL	CG1-CB-CG2	-6.58	100.38	110.90
1	A	295	ASP	CB-CG-OD1	6.47	124.12	118.30
1	A	233	TYR	CB-CG-CD1	-6.34	117.20	121.00
1	A	209	VAL	CA-CB-CG1	-6.31	101.44	110.90
1	A	319	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	A	79	HIS	N-CA-CB	-6.20	99.45	110.60
1	A	58	ASP	CB-CG-OD1	6.15	123.84	118.30
1	A	58	ASP	CB-CG-OD2	-6.11	112.81	118.30
1	A	239	LEU	N-CA-CB	-6.05	98.31	110.40
1	A	149	TYR	CB-CG-CD1	-6.04	117.37	121.00
1	A	226	ASP	CB-CG-OD1	6.03	123.72	118.30
1	A	316	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	140	PHE	CB-CA-C	-5.96	98.49	110.40
1	A	192	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	A	283	PRO	N-CA-CB	5.93	110.42	103.30
1	A	181	VAL	CG1-CB-CG2	-5.88	101.48	110.90
1	A	291	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	A	301	ALA	CB-CA-C	-5.63	101.66	110.10
1	A	211	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	A	217	ILE	CA-CB-CG2	-5.60	99.70	110.90
1	A	60	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	A	145	PRO	CB-CA-C	5.49	125.73	112.00
1	A	124	THR	CB-CA-C	-5.49	96.79	111.60
1	A	44	ILE	CG1-CB-CG2	-5.48	99.35	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	THR	CA-CB-CG2	-5.48	104.73	112.40
1	A	232	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	324	ASP	CB-CG-OD1	5.47	123.22	118.30
1	A	280	CYS	N-CA-CB	5.41	120.34	110.60
1	A	80	PHE	CB-CG-CD2	5.40	124.58	120.80
1	A	228	THR	CA-CB-CG2	-5.40	104.84	112.40
1	A	81	ALA	CB-CA-C	-5.39	102.01	110.10
1	A	212	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	A	192	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	98	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	316	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	73	ALA	N-CA-CB	-5.23	102.78	110.10
1	A	169	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	286	TYR	CB-CG-CD2	-5.19	117.89	121.00
1	A	162	ASP	CB-CA-C	-5.15	100.10	110.40
1	A	189	MET	CA-CB-CG	5.14	122.05	113.30
1	A	65	MET	CG-SD-CE	-5.13	91.98	100.20
1	A	178	PHE	CB-CA-C	5.12	120.64	110.40
1	A	338	ASP	CB-CG-OD1	-5.11	113.70	118.30
1	A	286	TYR	CB-CG-CD1	5.11	124.07	121.00
1	A	181	VAL	CA-CB-CG1	-5.07	103.29	110.90
1	A	76	THR	CA-CB-CG2	-5.06	105.31	112.40

There are no chirality outliers.

There are no planarity outliers.

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	2626	0	2557	112	21
2	A	2	0	0	0	0
3	A	44	0	26	2	0
4	A	36	0	22	3	0
5	A	7	0	10	3	1
6	A	417	0	0	16	17
All	All	3132	0	2615	115	27

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 22.

All (115) 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:2:ARG:HD3	6:A:418:HOH:O	1.42	1.19
1:A:28:ILE:HD13	1:A:74:ILE:HD11	1.39	1.02
1:A:146:GLN:NE2	1:A:146:GLN:HA	1.80	0.94
1:A:169:ASP:OD1	6:A:553:HOH:O	1.92	0.85
1:A:181:VAL:HG12	6:A:560:HOH:O	1.76	0.85
5:A:410:PEG:H41	5:A:410:PEG:H12	1.55	0.85
1:A:28:ILE:HD13	1:A:74:ILE:CD1	2.07	0.84
1:A:100:ASN:HB3	6:A:823:HOH:O	1.84	0.77
1:A:100:ASN:HA	6:A:700:HOH:O	1.87	0.75
1:A:124:THR:O	1:A:127:VAL:HG22	1.87	0.74
1:A:151:LYS:O	1:A:155:MET:HG3	1.86	0.73
5:A:410:PEG:C4	5:A:410:PEG:H12	2.18	0.73
1:A:209:VAL:HG13	1:A:209:VAL:O	1.89	0.72
1:A:146:GLN:CA	1:A:146:GLN:NE2	2.54	0.69
1:A:191:GLU:HG2	1:A:193:PRO:HD3	1.77	0.67
1:A:124:THR:HG22	1:A:125:ALA:N	2.09	0.67
1:A:124:THR:HG22	1:A:125:ALA:H	1.60	0.66
1:A:334:GLN:O	6:A:575:HOH:O	2.13	0.66
1:A:31:ASP:OD1	3:A:340:NAD:H1B	1.96	0.66
1:A:124:THR:HB	1:A:126:THR:HG22	1.76	0.65
1:A:133:LYS:C	1:A:134:ILE:HD12	2.18	0.65
1:A:180:PRO:HB3	1:A:239:LEU:HD23	1.81	0.62
1:A:124:THR:HG21	4:A:341:UPG:O4'	1.99	0.62
1:A:314:VAL:O	1:A:314:VAL:HG23	2.00	0.60
1:A:17:CYS:HA	1:A:20:LEU:HD12	1.83	0.60
1:A:135:PRO:HD2	6:A:714:HOH:O	2.02	0.60
1:A:72:HIS:O	1:A:73:ALA:HB3	2.00	0.59
1:A:180:PRO:HB3	1:A:239:LEU:CD2	2.32	0.59
1:A:264:GLY:HA2	1:A:301:ALA:O	2.03	0.58
1:A:8:GLY:HA3	1:A:29:ILE:HG23	1.85	0.58
1:A:28:ILE:CD1	1:A:74:ILE:CD1	2.81	0.58
1:A:2:ARG:CD	6:A:418:HOH:O	2.21	0.58
1:A:32:ASN:C	1:A:32:ASN:HD22	2.07	0.58
5:A:410:PEG:H41	5:A:410:PEG:C1	2.31	0.58
1:A:41:LEU:HB2	1:A:42:PRO:HD3	1.85	0.58
1:A:146:GLN:CA	1:A:146:GLN:HE21	2.17	0.57
1:A:200:LEU:HG	1:A:204:ILE:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ASP:C	1:A:302:ASP:OD1	2.43	0.57
1:A:3:VAL:HB	1:A:76:THR:HG23	1.87	0.56
1:A:208:ALA:O	1:A:282:LYS:NZ	2.37	0.56
1:A:289:ALA:HB1	1:A:290:PRO:CD	2.35	0.56
1:A:15:HIS:CE1	1:A:189:MET:HE2	2.40	0.56
1:A:249:LYS:NZ	6:A:628:HOH:O	2.23	0.56
1:A:197:PRO:HB3	1:A:202:PRO:HB2	1.87	0.56
1:A:184:HIS:CG	1:A:185:PRO:HD2	2.42	0.55
1:A:238:ASP:OD2	1:A:316:ARG:HB2	2.07	0.55
1:A:146:GLN:N	1:A:146:GLN:HE21	2.05	0.54
1:A:38:ARG:O	1:A:40:VAL:N	2.40	0.54
1:A:38:ARG:O	1:A:41:LEU:HG	2.07	0.54
1:A:124:THR:CB	1:A:126:THR:HG22	2.37	0.54
1:A:94:LEU:HB2	6:A:493:HOH:O	2.08	0.53
1:A:2:ARG:CG	6:A:418:HOH:O	2.54	0.52
1:A:4:LEU:HB3	1:A:77:VAL:HG22	1.92	0.52
1:A:177:TYR:HH	1:A:243:HIS:CE1	2.27	0.51
1:A:153:LYS:HD3	6:A:823:HOH:O	2.10	0.51
1:A:253:LYS:HE2	6:A:578:HOH:O	2.11	0.51
1:A:265:VAL:HG23	6:A:620:HOH:O	2.10	0.50
1:A:66:THR:HG22	1:A:66:THR:O	2.10	0.50
1:A:232:ASP:HB2	1:A:300:TRP:HB2	1.93	0.50
1:A:310:LEU:O	1:A:311:ASN:HB3	2.12	0.50
1:A:135:PRO:HB3	1:A:300:TRP:CD1	2.48	0.49
1:A:232:ASP:HB2	1:A:300:TRP:CB	2.43	0.49
1:A:240:ALA:O	1:A:241:ASP:C	2.51	0.49
1:A:218:PHE:CE2	1:A:292:ARG:HD3	2.47	0.48
1:A:78:ILE:HG12	1:A:120:ILE:HD12	1.94	0.48
1:A:32:ASN:ND2	1:A:34:CYS:H	2.12	0.48
1:A:131:ASN:OD1	1:A:133:LYS:HB2	2.15	0.47
1:A:207:VAL:O	1:A:207:VAL:HG12	2.14	0.47
1:A:211:ARG:O	1:A:211:ARG:HG3	2.12	0.47
1:A:124:THR:HG22	1:A:126:THR:H	1.81	0.46
1:A:55:VAL:HG11	1:A:68:ILE:HD11	1.97	0.46
1:A:32:ASN:ND2	1:A:32:ASN:C	2.67	0.46
1:A:236:VAL:O	1:A:239:LEU:HB3	2.15	0.46
1:A:85:ALA:HB3	1:A:88:GLU:HG3	1.97	0.46
1:A:18:VAL:HG12	1:A:19:GLN:OE1	2.16	0.45
1:A:84:LYS:HA	1:A:149:TYR:CE1	2.52	0.45
1:A:124:THR:CG2	4:A:341:UPG:H6'2	2.47	0.45
1:A:84:LYS:HA	1:A:149:TYR:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:VAL:O	1:A:231:ARG:HD3	2.17	0.45
1:A:38:ARG:C	1:A:40:VAL:H	2.20	0.45
1:A:134:ILE:N	1:A:134:ILE:HD12	2.32	0.44
1:A:1:MET:HG3	1:A:25:HIS:CE1	2.52	0.44
1:A:89:SER:O	1:A:148:PRO:HG2	2.17	0.44
1:A:124:THR:HG22	4:A:341:UPG:H6'2	2.00	0.44
1:A:194:GLN:O	6:A:579:HOH:O	2.21	0.44
1:A:22:GLN:NE2	1:A:47:LEU:O	2.49	0.44
1:A:7:GLY:HA2	1:A:31:ASP:OD2	2.18	0.43
1:A:314:VAL:O	1:A:314:VAL:CG2	2.66	0.43
1:A:38:ARG:C	1:A:40:VAL:N	2.71	0.43
1:A:177:TYR:CE1	1:A:243:HIS:CE1	3.07	0.43
1:A:289:ALA:HB1	1:A:290:PRO:HD2	1.99	0.43
1:A:231:ARG:HH11	1:A:231:ARG:HD3	1.32	0.43
1:A:32:ASN:HD22	1:A:33:LEU:N	2.17	0.42
1:A:11:TYR:HB3	3:A:340:NAD:O2N	2.19	0.42
1:A:131:ASN:HA	1:A:132:PRO:HD3	1.83	0.42
1:A:180:PRO:HA	1:A:234:ILE:O	2.19	0.42
1:A:93:PRO:O	1:A:96:TYR:N	2.41	0.42
1:A:45:GLU:OE2	1:A:51:HIS:HB2	2.20	0.42
1:A:190:GLY:HA3	1:A:328:TRP:CD1	2.55	0.42
1:A:39:SER:OG	1:A:337:PRO:O	2.33	0.42
1:A:32:ASN:HB3	1:A:57:GLY:O	2.20	0.41
1:A:163:LEU:O	1:A:164:GLN:C	2.57	0.41
1:A:219:GLY:HA2	6:A:602:HOH:O	2.19	0.41
1:A:177:TYR:CE1	1:A:243:HIS:HE1	2.37	0.41
1:A:200:LEU:HD11	1:A:204:ILE:HD11	2.03	0.41
1:A:204:ILE:CG1	1:A:215:LEU:HD22	2.51	0.41
1:A:237:MET:HB3	1:A:316:ARG:CZ	2.51	0.41
1:A:222:TYR:CZ	1:A:291:ARG:HG2	2.56	0.41
1:A:110:ALA:O	1:A:111:MET:C	2.58	0.41
1:A:277:SER:OG	1:A:284:VAL:HG23	2.21	0.41
1:A:239:LEU:HA	1:A:239:LEU:HD12	1.79	0.40
1:A:124:THR:CG2	1:A:126:THR:H	2.33	0.40
1:A:245:VAL:O	1:A:246:ALA:C	2.58	0.40
1:A:280:CYS:SG	1:A:282:LYS:HG2	2.62	0.40
1:A:310:LEU:O	1:A:311:ASN:CB	2.69	0.40

All (27) 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:A:308:ARG:NH2	1:A:308:ARG:NH2[5_675]	0.89	1.31
1:A:94:LEU:CD1	1:A:105:LEU:CD1[6_765]	1.03	1.17
6:A:714:HOH:O	6:A:714:HOH:O[5_675]	1.04	1.16
6:A:715:HOH:O	6:A:788:HOH:O[5_675]	1.20	1.00
1:A:210:GLY:O	6:A:696:HOH:O[5_565]	1.33	0.87
1:A:133:LYS:CD	6:A:516:HOH:O[5_675]	1.56	0.64
1:A:137:VAL:CG2	6:A:517:HOH:O[5_675]	1.62	0.58
1:A:307:ASP:CB	6:A:523:HOH:O[5_675]	1.65	0.55
1:A:133:LYS:CG	6:A:516:HOH:O[5_675]	1.65	0.55
1:A:139:SER:OG	1:A:304:SER:CB[5_675]	1.76	0.44
1:A:139:SER:CB	1:A:304:SER:CB[5_675]	1.81	0.39
6:A:520:HOH:O	6:A:524:HOH:O[5_675]	1.84	0.36
1:A:94:LEU:CG	1:A:105:LEU:CD1[6_765]	1.87	0.33
1:A:304:SER:O	6:A:523:HOH:O[5_675]	1.91	0.29
1:A:133:LYS:CE	6:A:516:HOH:O[5_675]	1.93	0.27
5:A:410:PEG:O4	5:A:410:PEG:O4[5_675]	1.98	0.22
6:A:521:HOH:O	6:A:521:HOH:O[5_675]	2.00	0.20
1:A:94:LEU:CD2	1:A:105:LEU:CD1[6_765]	2.01	0.19
1:A:106:ARG:NH2	6:A:785:HOH:O[6_765]	2.01	0.19
1:A:137:VAL:CG2	1:A:302:ASP:OD2[5_675]	2.02	0.18
1:A:308:ARG:NH1	6:A:802:HOH:O[5_675]	2.07	0.13
1:A:139:SER:OG	1:A:304:SER:OG[5_675]	2.09	0.11
1:A:165:LYS:CE	6:A:490:HOH:O[6_765]	2.11	0.09
6:A:790:HOH:O	6:A:792:HOH:O[5_675]	2.15	0.05
1:A:134:ILE:O	1:A:134:ILE:O[5_675]	2.16	0.04
1:A:134:ILE:O	6:A:711:HOH:O[5_675]	2.17	0.03
1:A:162:ASP:OD2	6:A:705:HOH:O[6_765]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	336/338 (99%)	319 (95%)	16 (5%)	1 (0%)	46	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	SER

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	282/282 (100%)	264 (94%)	18 (6%)	22	15

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	32	ASN
1	A	50	LYS
1	A	65	MET
1	A	76	THR
1	A	88	GLU
1	A	94	LEU
1	A	95	GLU
1	A	124	THR
1	A	146	GLN
1	A	209	VAL
1	A	211	ARG
1	A	236	VAL
1	A	239	LEU
1	A	261	LEU
1	A	293	GLU
1	A	308	ARG
1	A	313	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN

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Mol	Chain	Res	Type
1	A	146	GLN
1	A	158	GLN
1	A	194	GLN
1	A	274	ASN
1	A	285	ASN
1	A	323	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 ⓘ

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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	NAD	A	340	-	38,48,48	2.03	5 (13%)	47,73,73	2.49	14 (29%)
4	UPG	A	341	-	29,38,38	1.41	5 (17%)	43,58,58	3.20	19 (44%)
5	PEG	A	410	-	6,6,6	0.63	0	5,5,5	1.46	1 (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
3	NAD	A	340	-	-	0/22/62/62	0/5/5/5
4	UPG	A	341	-	-	0/19/59/59	0/3/3/3
5	PEG	A	410	-	-	0/4/4/4	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	340	NAD	C6N-C5N	-2.99	1.31	1.38
4	A	341	UPG	PB-O2B	-2.13	1.45	1.54
4	A	341	UPG	C6-C5	-2.06	1.33	1.38
4	A	341	UPG	C4-N3	2.05	1.36	1.33
3	A	340	NAD	C8A-N7A	2.24	1.38	1.34
4	A	341	UPG	O3C-C3C	2.25	1.48	1.43
4	A	341	UPG	PB-O3B	4.55	1.73	1.60
3	A	340	NAD	C5N-C4N	5.20	1.49	1.38
3	A	340	NAD	C2N-C3N	6.80	1.49	1.39
3	A	340	NAD	C4N-C3N	6.81	1.51	1.39

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	340	NAD	C5N-C4N-C3N	-8.16	110.07	120.33
4	A	341	UPG	O5'-C1'-O3B	-5.38	104.27	111.36
3	A	340	NAD	O3-PN-O5D	-5.31	88.86	102.94
4	A	341	UPG	O5'-C1'-C2'	-4.57	100.91	110.28
4	A	341	UPG	C5-C4-N3	-3.91	113.08	123.12
3	A	340	NAD	O7N-C7N-N7N	-3.87	117.15	122.59
3	A	340	NAD	PN-O3-PA	-3.75	122.19	132.73
3	A	340	NAD	C2N-C3N-C4N	-3.22	114.70	118.29
4	A	341	UPG	O2B-PB-O1B	-2.56	98.64	112.53
3	A	340	NAD	O3-PA-O5B	-2.55	96.17	102.94
4	A	341	UPG	C1'-O5'-C5'	-2.55	108.80	113.75
3	A	340	NAD	O3D-C3D-C2D	-2.27	104.44	111.83
3	A	340	NAD	C2N-C3N-C7N	-2.25	112.76	119.31
4	A	341	UPG	O3A-PA-O5C	-2.23	97.03	102.94
4	A	341	UPG	O3'-C3'-C4'	-2.10	105.61	110.34
4	A	341	UPG	C6-C5-C4	2.03	121.08	117.28
4	A	341	UPG	O2A-PA-O5C	2.13	119.20	108.46
4	A	341	UPG	O2B-PB-O3B	2.21	115.36	106.49
3	A	340	NAD	O3D-C3D-C4D	2.28	117.88	111.05
4	A	341	UPG	O3B-PB-O1B	2.30	118.49	109.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	341	UPG	O5'-C5'-C4'	2.35	114.10	109.68
4	A	341	UPG	O2'-C2'-C1'	2.58	115.68	110.02
3	A	340	NAD	C4A-C5A-N7A	2.76	112.02	109.48
5	A	410	PEG	C3-O2-C2	3.12	126.74	113.31
4	A	341	UPG	O2B-PB-O3A	3.20	119.61	105.09
4	A	341	UPG	C4C-O4C-C1C	3.29	113.33	109.72
4	A	341	UPG	O3A-PB-O3B	3.36	113.30	103.63
4	A	341	UPG	C1'-C2'-C3'	3.39	116.66	109.97
3	A	340	NAD	O5D-PN-O1N	3.46	123.05	109.62
3	A	340	NAD	C3N-C7N-N7N	4.03	122.23	117.82
3	A	340	NAD	C4B-O4B-C1B	4.21	114.34	109.72
4	A	341	UPG	O3B-C1'-C2'	6.87	121.23	108.39
3	A	340	NAD	O4D-C1D-N1N	6.91	115.72	108.13
4	A	341	UPG	C4-N3-C2	14.29	128.29	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	340	NAD	2	0
4	A	341	UPG	3	0
5	A	410	PEG	3	1

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.