



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 04:17 pm GMT

PDB ID : 1O9B  
Title : QUINATE/SHIKIMATE DEHYDROGENASE YDIB COMPLEXED WITH NADH  
Authors : Michel, G.; Cygler, M.  
Deposited on : 2002-12-12  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

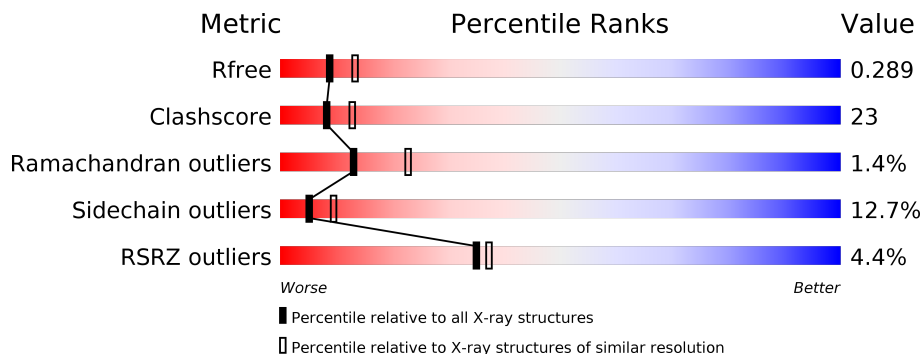
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	288	<div> <div>7%</div> <div>58%</div> <div>34%</div> <div>5% ..</div> </div>
1	B	288	<div> <div>2%</div> <div>58%</div> <div>34%</div> <div>6% .</div> </div>

## 2 Entry composition [i](#)

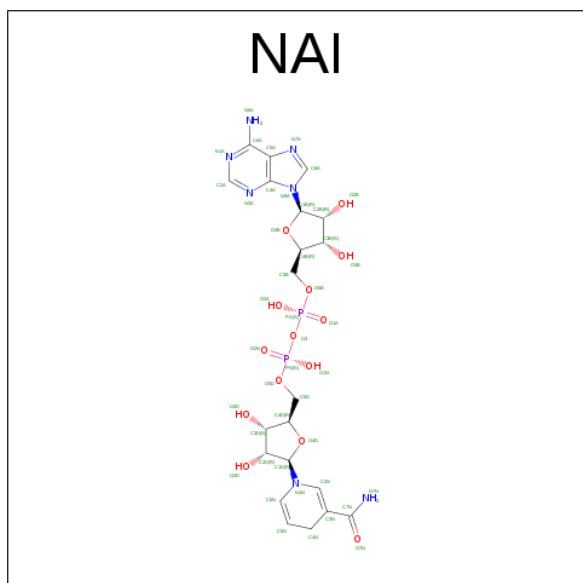
There are 4 unique types of molecules in this entry. The entry contains 4541 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HYPOTHETICAL SHIKIMATE 5-DEHYDROGENASE-LIKE PROTEIN YDIB.

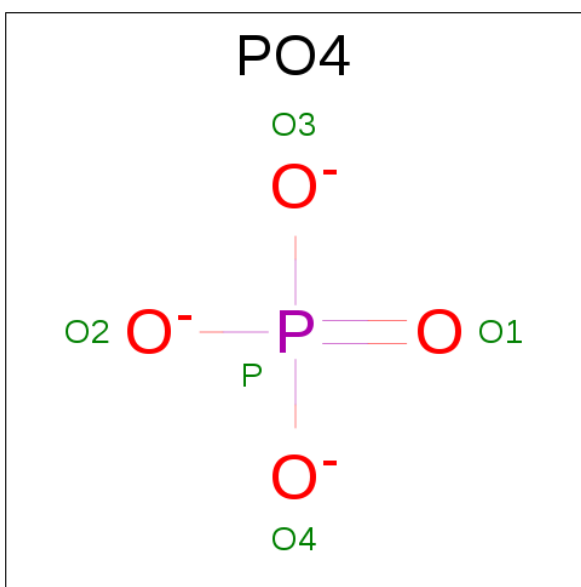
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	Se	58	0	1
			2137	1357	356	410	4	10			
1	B	281	Total	C	N	O	S	Se	16	0	1
			2137	1357	356	410	4	10			

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C<sub>21</sub>H<sub>29</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

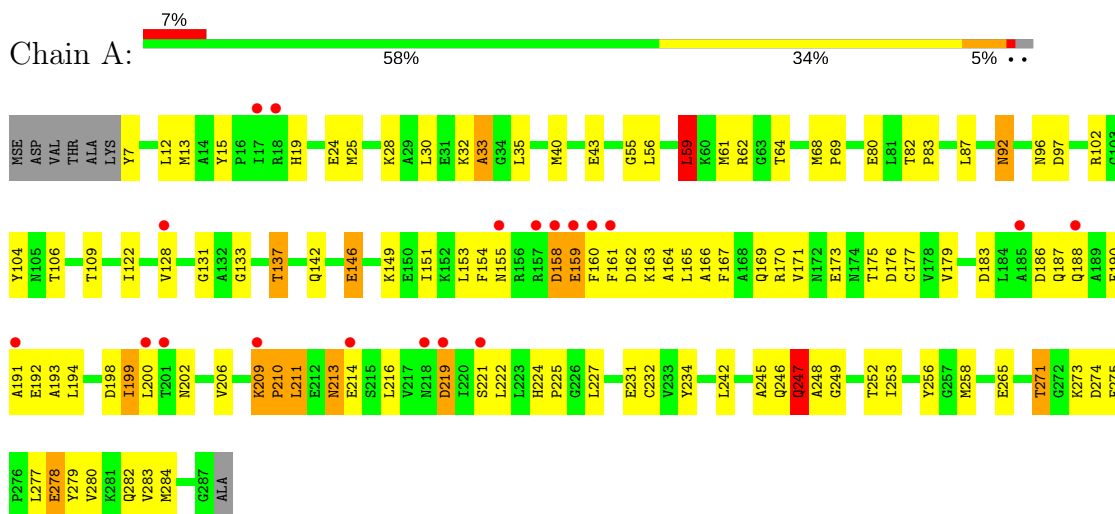
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	88	Total	O	0	0
			88	88		
4	B	66	Total	O	0	0
			66	66		

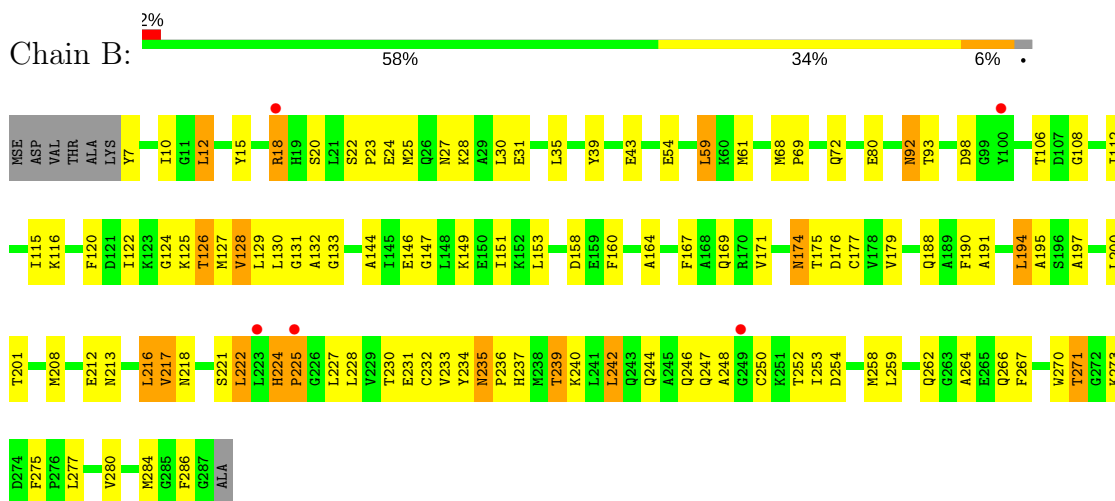
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: HYPOTHETICAL SHIKIMATE 5-DEHYDROGENASE-LIKE PROTEIN YDIB



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	157.87Å 157.87Å 40.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.80 – 2.50 19.80 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.80-2.50) 99.9 (19.80-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.03 (at 2.50Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.226 , 0.294 0.220 , 0.289	Depositor DCC
$R_{free}$ test set	973 reflections (5.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.6	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 64.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.036 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4541	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, NAI

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	0.54	0/2165	0.82	2/2911 (0.1%)
1	B	0.51	0/2165	0.73	0/2911
All	All	0.52	0/4330	0.78	2/5822 (0.0%)

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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	209	LYS	O-C-N	-10.62	100.92	121.10
1	A	59	LEU	CA-CB-CG	5.71	128.44	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	209	LYS	Mainchain

### 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	2137	0	2129	109	0
1	B	2137	0	2129	94	0
2	A	44	0	27	4	0
2	B	44	0	27	2	0
3	A	15	0	0	0	0
3	B	10	0	0	0	0
4	A	88	0	0	2	0
4	B	66	0	0	3	0
All	All	4541	0	4312	199	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 23.

All (199) 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:271:THR:HG22	1:B:273:LYS:H	1.15	1.06
1:B:175:THR:HG22	1:B:177:CYS:H	1.21	1.04
1:A:271:THR:HG22	1:A:273:LYS:H	1.27	0.98
1:B:191:ALA:HA	1:B:222:LEU:HD21	1.46	0.95
1:A:122:ILE:HD11	1:A:146:GLU:HB3	1.50	0.92
1:B:267:PHE:O	1:B:271:THR:HB	1.77	0.85
1:B:271:THR:CG2	1:B:273:LYS:H	1.87	0.85
1:B:231:GLU:HG2	1:B:239:THR:HG21	1.58	0.85
1:A:56:LEU:HA	1:A:61:MSE:HE3	1.60	0.81
1:B:112:ILE:HG21	1:B:146:GLU:OE1	1.80	0.81
1:A:153:LEU:HD12	1:A:154:PHE:N	1.97	0.80
1:A:151:ILE:HB	1:A:179:VAL:HG22	1.63	0.80
1:B:190:PHE:O	1:B:194:LEU:HB2	1.82	0.80
1:A:175:THR:HG22	1:A:176:ASP:H	1.47	0.79
1:A:92:ASN:HD21	1:A:106:THR:H	1.32	0.77
1:B:127:MSE:HE2	1:B:201:THR:OG1	1.84	0.77
1:B:131:GLY:O	1:B:153:LEU:HD11	1.86	0.76
1:B:116:LYS:HD2	4:B:2043:HOH:O	1.85	0.75
1:A:169:GLN:O	1:A:173:GLU:HG3	1.87	0.74
1:B:175:THR:HG22	1:B:176:ASP:N	2.04	0.72
1:B:129:LEU:O	1:B:153:LEU:HD12	1.90	0.71
1:B:175:THR:HG22	1:B:176:ASP:H	1.54	0.71
1:A:131:GLY:O	1:A:153:LEU:HD11	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ALA:HB1	1:B:175:THR:HG21	1.71	0.71
1:A:61:MSE:HE1	1:B:59:LEU:HD21	1.74	0.69
1:A:153:LEU:HD12	1:A:154:PHE:H	1.58	0.68
1:A:232:CYS:SG	1:A:258:MSE:HE1	2.33	0.68
1:B:271:THR:HG22	1:B:273:LYS:N	1.99	0.68
1:B:242:LEU:HD21	1:B:252:THR:HB	1.73	0.68
1:B:212:GLU:HG2	1:B:213:ASN:N	2.07	0.68
1:B:217:VAL:HG22	1:B:244:GLN:OE1	1.92	0.68
1:A:167:PHE:O	1:A:171:VAL:HG23	1.94	0.67
1:A:219:ASP:OD2	1:A:221:SER:HB2	1.95	0.66
1:B:240:LYS:O	1:B:244:GLN:HG3	1.95	0.66
1:B:128:VAL:HG12	1:B:200:LEU:HD12	1.76	0.66
1:A:234:TYR:HB2	1:A:256:TYR:CE1	2.30	0.65
1:A:56:LEU:CA	1:A:61:MSE:HE3	2.26	0.65
1:B:230:THR:HG22	1:B:253:ILE:HB	1.79	0.65
1:B:115:ILE:HA	1:B:253:ILE:CD1	2.27	0.65
1:B:175:THR:HG22	1:B:177:CYS:N	2.04	0.62
1:A:175:THR:HG22	1:A:176:ASP:N	2.14	0.62
1:A:155:ASN:HD21	1:A:160:PHE:HB2	1.65	0.61
1:A:35:LEU:HD21	1:A:273:LYS:HG3	1.82	0.61
1:A:232:CYS:HA	1:A:258:MSE:CE	2.31	0.60
1:A:206:VAL:HG21	1:A:216:LEU:HD11	1.83	0.60
1:A:188:GLN:HE21	1:A:188:GLN:HA	1.65	0.60
1:B:126:THR:HG22	1:B:197:ALA:HA	1.83	0.60
1:B:242:LEU:CD2	1:B:252:THR:HB	2.31	0.60
1:A:128:VAL:O	1:A:200:LEU:HD12	2.02	0.59
1:A:224:HIS:HB2	1:A:225:PRO:HD2	1.84	0.59
1:B:175:THR:CG2	1:B:176:ASP:H	2.15	0.59
1:B:128:VAL:HG12	1:B:200:LEU:CD1	2.31	0.59
1:B:259:LEU:O	1:B:262:GLN:HG3	2.02	0.59
1:A:188:GLN:NE2	1:A:188:GLN:HA	2.18	0.59
1:A:279:TYR:O	1:A:283:VAL:HG23	2.03	0.59
1:A:166:ALA:O	1:A:169:GLN:HB2	2.03	0.59
1:B:92:ASN:HD21	1:B:106:THR:H	1.49	0.59
1:A:55:GLY:O	1:A:59:LEU:HB2	2.03	0.59
1:A:82:THR:HB	1:A:83:PRO:HD2	1.85	0.59
1:A:161:PHE:O	1:A:164:ALA:HB3	2.03	0.58
1:B:191:ALA:CA	1:B:222:LEU:HD21	2.26	0.58
1:A:133:GLY:O	1:A:137:THR:OG1	2.22	0.58
1:A:234:TYR:HB2	1:A:256:TYR:CD1	2.38	0.58
1:A:199:ILE:HG13	1:A:200:LEU:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ASN:HD22	1:A:92:ASN:H	1.50	0.57
1:A:59:LEU:HD23	1:A:61:MSE:HE2	1.86	0.57
1:B:115:ILE:HA	1:B:253:ILE:HD11	1.86	0.57
1:A:186:ASP:O	1:A:188:GLN:N	2.38	0.56
1:A:232:CYS:O	2:A:301:NAI:H2N	2.04	0.56
1:B:108:GLY:O	1:B:112:ILE:HG12	2.04	0.56
1:A:97:ASP:OD2	1:A:102:ARG:NH1	2.39	0.56
1:A:15:TYR:HD1	1:A:43:GLU:HG2	1.70	0.56
1:B:174:ASN:HD22	1:B:174:ASN:N	2.04	0.56
1:B:24:GLU:O	1:B:28:LYS:HG2	2.06	0.55
1:A:211:LEU:C	1:A:213:ASN:H	2.07	0.55
1:A:232:CYS:CB	1:A:258:MSE:HE1	2.37	0.55
1:B:258:MSE:HE2	2:B:301:NAI:H4N	1.88	0.55
1:A:188:GLN:C	1:A:190:PHE:H	2.10	0.55
1:A:202:ASN:ND2	1:A:231:GLU:OE1	2.40	0.55
1:B:175:THR:CG2	1:B:176:ASP:N	2.70	0.54
1:A:275:PHE:O	1:A:277:LEU:N	2.39	0.54
1:A:206:VAL:HG11	1:A:216:LEU:CD1	2.38	0.54
1:B:224:HIS:CD2	1:B:227:LEU:HD13	2.43	0.54
1:B:225:PRO:HA	1:B:248:ALA:O	2.08	0.54
1:A:242:LEU:HD22	1:A:252:THR:HG23	1.89	0.53
1:B:127:MSE:HE2	1:B:201:THR:CB	2.38	0.53
1:A:210:PRO:HD2	1:A:211:LEU:H	1.73	0.53
1:A:188:GLN:C	1:A:190:PHE:N	2.62	0.53
1:A:232:CYS:HA	1:A:258:MSE:HE1	1.91	0.52
1:A:151:ILE:HG13	1:A:177:CYS:SG	2.49	0.52
1:A:271:THR:HG22	1:A:273:LYS:N	2.11	0.52
1:B:115:ILE:HG12	1:B:253:ILE:HD12	1.90	0.52
1:B:235:ASN:HB3	4:B:2056:HOH:O	2.09	0.52
1:A:191:ALA:HB1	1:A:222:LEU:CD2	2.40	0.52
1:A:206:VAL:HG12	1:A:214:GLU:O	2.09	0.52
1:A:245:ALA:C	1:A:247:GLN:N	2.60	0.52
1:B:231:GLU:HG2	1:B:239:THR:CG2	2.33	0.52
1:B:235:ASN:HA	1:B:236:PRO:C	2.28	0.52
1:B:191:ALA:HA	1:B:222:LEU:CD2	2.30	0.52
1:B:217:VAL:CG2	1:B:217:VAL:O	2.58	0.52
1:A:278:GLU:HG3	4:A:2084:HOH:O	2.09	0.52
1:A:252:THR:CG2	1:A:253:ILE:N	2.74	0.51
1:B:151:ILE:HB	1:B:179:VAL:HG22	1.92	0.51
1:A:15:TYR:CD1	1:A:43:GLU:HG2	2.46	0.50
1:A:258:MSE:HE3	2:A:301:NAI:C7N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:MSE:HE3	1:A:64:THR:HG21	1.94	0.50
1:A:165:LEU:O	1:A:169:GLN:N	2.40	0.50
1:B:188:GLN:NE2	1:B:188:GLN:HA	2.26	0.49
1:A:35:LEU:CD2	1:A:271:THR:HG23	2.42	0.49
1:B:128:VAL:HG12	1:B:128:VAL:O	2.12	0.49
1:A:33:ALA:CB	1:A:35:LEU:CD1	2.91	0.49
1:A:24:GLU:O	1:A:28:LYS:HG3	2.13	0.48
1:B:10:ILE:O	1:B:39:TYR:HA	2.13	0.48
1:A:194:LEU:HD21	1:A:200:LEU:HD22	1.95	0.48
1:B:174:ASN:ND2	1:B:174:ASN:N	2.62	0.48
1:B:264:ALA:HA	1:B:275:PHE:CG	2.48	0.48
1:A:190:PHE:O	1:A:193:ALA:N	2.46	0.48
1:A:198:ASP:O	1:A:227:LEU:HD12	2.14	0.48
1:A:59:LEU:HD21	1:B:61:MSE:HE1	1.95	0.47
1:B:208:MSE:HB2	1:B:233:VAL:HG13	1.96	0.47
1:B:92:ASN:H	1:B:92:ASN:HD22	1.62	0.47
1:A:191:ALA:HB1	1:A:222:LEU:HD22	1.94	0.47
1:B:158:ASP:OD1	1:B:160:PHE:N	2.37	0.47
1:A:61:MSE:CE	1:B:59:LEU:HD21	2.42	0.47
1:B:149:LYS:HD3	4:B:2040:HOH:O	2.14	0.47
1:A:161:PHE:CD1	1:A:161:PHE:C	2.88	0.47
1:B:92:ASN:ND2	1:B:93:THR:OG1	2.47	0.47
1:B:158:ASP:C	1:B:158:ASP:OD1	2.53	0.47
1:A:87:LEU:HD22	1:A:170:ARG:HB3	1.97	0.47
1:A:245:ALA:C	1:A:247:GLN:H	2.17	0.47
1:A:87:LEU:CD2	1:A:170:ARG:HB3	2.45	0.47
1:A:277:LEU:C	1:A:277:LEU:HD23	2.36	0.46
1:A:28:LYS:CD	1:A:283:VAL:HG11	2.45	0.46
1:B:122:ILE:O	1:B:125:LYS:HB2	2.16	0.46
1:A:40:MSE:HB3	1:A:40:MSE:HE2	1.89	0.46
1:B:130:LEU:HD13	1:B:216:LEU:HD23	1.98	0.46
1:A:252:THR:HG22	1:A:253:ILE:N	2.31	0.45
1:A:133:GLY:N	2:A:301:NAI:O3B	2.49	0.45
1:A:32:LYS:HD2	1:A:279:TYR:CZ	2.50	0.45
1:B:126:THR:CG2	1:B:197:ALA:HA	2.46	0.45
1:B:25:MSE:HG3	1:B:284:MSE:HE2	1.98	0.45
1:B:224:HIS:HB2	1:B:225:PRO:CD	2.46	0.45
1:A:211:LEU:C	1:A:213:ASN:N	2.70	0.45
1:B:124:GLY:N	1:B:147:GLY:O	2.46	0.45
1:B:15:TYR:HE1	1:B:43:GLU:OE1	2.00	0.45
1:A:104:TYR:CD1	1:A:104:TYR:N	2.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:CYS:O	2:B:301:NAI:H2N	2.16	0.45
1:A:92:ASN:ND2	1:A:106:THR:H	2.09	0.45
1:B:234:TYR:O	1:B:235:ASN:HB2	2.16	0.44
1:A:80:GLU:HB3	1:A:102:ARG:HG2	1.99	0.44
1:A:68:MSE:HA	1:A:69:PRO:HA	1.82	0.44
1:B:120:PHE:CE2	1:B:125:LYS:HE2	2.52	0.44
1:A:188:GLN:O	1:A:190:PHE:N	2.51	0.44
1:B:18:ARG:O	1:B:18:ARG:HG2	2.15	0.44
1:A:188:GLN:HE21	1:A:188:GLN:CA	2.26	0.44
1:A:33:ALA:HB3	1:A:35:LEU:CD1	2.48	0.44
1:A:159:GLU:CD	1:A:159:GLU:H	2.21	0.43
1:A:232:CYS:CA	1:A:258:MSE:HE1	2.48	0.43
1:B:225:PRO:O	1:B:250:CYS:HA	2.18	0.43
1:B:266:GLN:HB3	1:B:270:TRP:CZ3	2.53	0.43
1:A:92:ASN:N	1:A:92:ASN:HD22	2.12	0.43
1:B:18:ARG:HB3	1:B:18:ARG:HE	1.35	0.43
1:B:271:THR:CG2	1:B:273:LYS:N	2.70	0.43
1:B:271:THR:CG2	1:B:273:LYS:HB2	2.48	0.43
1:A:109:THR:HA	1:A:142:GLN:HG2	2.00	0.43
1:A:186:ASP:C	1:A:188:GLN:H	2.23	0.42
1:B:224:HIS:CB	1:B:225:PRO:CD	2.97	0.42
1:A:109:THR:HG22	1:A:142:GLN:NE2	2.34	0.42
1:B:27:ASN:O	1:B:31:GLU:HG3	2.19	0.42
1:A:56:LEU:N	1:A:61:MSE:HE3	2.35	0.42
1:B:228:LEU:HD12	1:B:228:LEU:HA	1.76	0.42
1:A:33:ALA:CB	1:A:35:LEU:HD12	2.49	0.42
1:A:59:LEU:HD21	1:B:61:MSE:CE	2.48	0.42
1:B:133:GLY:HA2	1:B:160:PHE:CE1	2.55	0.42
1:A:175:THR:CG2	1:A:176:ASP:H	2.27	0.42
1:B:112:ILE:HG23	1:B:122:ILE:HD13	2.02	0.42
1:B:240:LYS:HB3	1:B:240:LYS:HE3	1.78	0.42
1:B:195:ALA:HA	1:B:224:HIS:HE1	1.85	0.41
1:B:280:VAL:O	1:B:284:MSE:HG2	2.20	0.41
1:A:25:MSE:HG3	1:A:280:VAL:HG11	2.02	0.41
1:B:132:ALA:CB	1:B:164:ALA:HB2	2.51	0.41
1:A:33:ALA:HB1	1:A:35:LEU:CD1	2.50	0.41
1:B:271:THR:HG23	1:B:273:LYS:HG2	2.01	0.41
1:B:194:LEU:HD13	1:B:222:LEU:HD22	2.03	0.41
1:B:194:LEU:HD21	1:B:200:LEU:HD22	2.02	0.41
1:A:258:MSE:HB2	4:A:2049:HOH:O	2.20	0.41
1:A:258:MSE:HE3	2:A:301:NAI:N7N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LEU:O	1:A:277:LEU:HD23	2.20	0.41
1:A:247:GLN:C	1:A:249:GLY:H	2.24	0.41
1:A:62:ARG:NH1	1:A:96:ASN:O	2.54	0.41
1:A:25:MSE:HE3	1:A:25:MSE:HB2	1.98	0.41
1:A:163:LYS:HD2	1:A:163:LYS:HA	1.75	0.41
1:B:22:SER:N	1:B:23:PRO:CD	2.84	0.41
1:B:284:MSE:HB3	1:B:286:PHE:CZ	2.56	0.40
1:A:137:THR:HG22	1:A:167:PHE:CD2	2.56	0.40
1:B:12:LEU:HG	1:B:39:TYR:OH	2.21	0.40
1:B:167:PHE:O	1:B:171:VAL:HG23	2.21	0.40
1:A:24:GLU:HG2	1:A:284:MSE:SE	2.71	0.40
1:A:158:ASP:HB2	1:A:159:GLU:OE2	2.20	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	279/288 (97%)	252 (90%)	21 (8%)	6 (2%)	8	12
1	B	279/288 (97%)	252 (90%)	25 (9%)	2 (1%)	25	43
All	All	558/576 (97%)	504 (90%)	46 (8%)	8 (1%)	13	23

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	GLN
1	A	211	LEU
1	B	225	PRO
1	A	33	ALA
1	A	248	ALA
1	A	247	GLN

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Mol	Chain	Res	Type
1	B	235	ASN
1	A	210	PRO

### 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	224/218 (103%)	200 (89%)	24 (11%)	8	15
1	B	224/218 (103%)	191 (85%)	33 (15%)	3	6
All	All	448/436 (103%)	391 (87%)	57 (13%)	5	9

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	TYR
1	A	12	LEU
1	A	19	HIS
1	A	30	LEU
1	A	59	LEU
1	A	92	ASN
1	A	137	THR
1	A	146	GLU
1	A	149	LYS
1	A	158	ASP
1	A	159	GLU
1	A	162	ASP
1	A	183	ASP
1	A	192	GLU
1	A	199	ILE
1	A	213	ASN
1	A	219	ASP
1	A	246	GLN
1	A	247	GLN
1	A	265	GLU
1	A	271	THR

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Mol	Chain	Res	Type
1	A	274	ASP
1	A	278	GLU
1	A	282	GLN
1	B	7	TYR
1	B	12	LEU
1	B	18	ARG
1	B	20	SER
1	B	30	LEU
1	B	35	LEU
1	B	54	GLU
1	B	59	LEU
1	B	68	MSE
1	B	69	PRO
1	B	72	GLN
1	B	80	GLU
1	B	92	ASN
1	B	98	ASP
1	B	126	THR
1	B	128	VAL
1	B	169	GLN
1	B	174	ASN
1	B	194	LEU
1	B	216	LEU
1	B	217	VAL
1	B	218	ASN
1	B	221	SER
1	B	222	LEU
1	B	224	HIS
1	B	237	HIS
1	B	239	THR
1	B	242	LEU
1	B	246	GLN
1	B	247	GLN
1	B	254	ASP
1	B	271	THR
1	B	277	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	92	ASN

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Mol	Chain	Res	Type
1	A	155	ASN
1	A	188	GLN
1	A	246	GLN
1	A	262	GLN
1	B	46	ASN
1	B	92	ASN
1	B	142	GLN
1	B	174	ASN
1	B	187	GLN
1	B	188	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 ⓘ

7 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	NAI	A	301	-	40,48,48	1.23	5 (12%)	41,73,73	1.38	5 (12%)
3	PO4	A	302	-	4,4,4	1.42	1 (25%)	6,6,6	0.61	0
3	PO4	A	303	-	4,4,4	0.98	0	6,6,6	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PO4	A	304	-	4,4,4	0.88	0	6,6,6	0.46	0
2	NAI	B	301	-	40,48,48	1.34	5 (12%)	41,73,73	1.33	4 (9%)
3	PO4	B	302	-	4,4,4	1.25	0	6,6,6	0.66	0
3	PO4	B	303	-	4,4,4	1.35	1 (25%)	6,6,6	0.50	0

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	NAI	A	301	-	-	0/25/72/72	0/5/5/5
3	PO4	A	302	-	-	0/0/0/0	0/0/0/0
3	PO4	A	303	-	-	0/0/0/0	0/0/0/0
3	PO4	A	304	-	-	0/0/0/0	0/0/0/0
2	NAI	B	301	-	-	0/25/72/72	0/5/5/5
3	PO4	B	302	-	-	0/0/0/0	0/0/0/0
3	PO4	B	303	-	-	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)
2	B	301	NAI	C4N-C5N	-3.06	1.42	1.49
2	B	301	NAI	C2B-C1B	-3.05	1.48	1.53
2	A	301	NAI	C4N-C5N	-2.87	1.42	1.49
2	A	301	NAI	C2N-C3N	2.06	1.40	1.34
3	A	302	PO4	P-O1	2.41	1.55	1.50
2	B	301	NAI	C6N-N1N	2.43	1.44	1.37
2	A	301	NAI	C6N-N1N	2.44	1.44	1.37
3	B	303	PO4	P-O1	2.50	1.55	1.50
2	A	301	NAI	C6N-C5N	2.64	1.38	1.33
2	B	301	NAI	C2A-N1A	3.00	1.39	1.33
2	A	301	NAI	C2A-N1A	3.11	1.39	1.33
2	B	301	NAI	C6N-C5N	3.44	1.39	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	NAI	C3N-C2N-N1N	-4.43	116.66	123.08
2	A	301	NAI	C3N-C2N-N1N	-4.33	116.80	123.08
2	A	301	NAI	C1D-N1N-C2N	-4.22	113.93	121.09
2	B	301	NAI	C1D-N1N-C2N	-3.83	114.59	121.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	NAI	O4B-C4B-C5B	-2.36	101.45	109.40
2	A	301	NAI	O5D-PN-O2N	2.03	117.42	109.25
2	A	301	NAI	C4A-C5A-N7A	2.52	111.84	109.41
2	A	301	NAI	C4B-O4B-C1B	2.71	112.65	109.77
2	B	301	NAI	C4A-C5A-N7A	2.80	112.12	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NAI	4	0
2	B	301	NAI	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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	271/288 (94%)	0.22	19 (7%) <span>17</span> <span>17</span>	19, 46, 86, 106	41 (15%)
1	B	271/288 (94%)	0.00	5 (1%) <span>69</span> <span>70</span>	19, 44, 81, 104	20 (7%)
All	All	542/576 (94%)	0.11	24 (4%) <span>35</span> <span>37</span>	19, 45, 84, 106	61 (11%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	249	GLY	6.4
1	A	188	GLN	4.4
1	A	155	ASN	4.4
1	A	219	ASP	4.0
1	A	18	ARG	3.8
1	A	161	PHE	3.7
1	A	160	PHE	3.7
1	A	159	GLU	3.5
1	A	218	ASN	3.5
1	A	128	VAL	3.0
1	A	191	ALA	2.7
1	A	185	ALA	2.6
1	A	214	GLU	2.6
1	A	200	LEU	2.6
1	B	18	ARG	2.5
1	A	158	ASP	2.4
1	A	201	THR	2.2
1	B	223	LEU	2.2
1	B	225	PRO	2.2
1	B	100	TYR	2.1
1	A	17	ILE	2.1
1	A	157	ARG	2.1
1	A	221	SER	2.1
1	A	209	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	PO4	B	303	5/5	0.96	0.16	1.60	71,71,82,86	0
3	PO4	B	302	5/5	0.88	0.18	1.52	77,77,85,86	0
2	NAI	B	301	44/44	0.95	0.15	0.03	26,43,51,58	0
2	NAI	A	301	44/44	0.88	0.18	-0.02	37,61,74,77	0
3	PO4	A	304	5/5	0.93	0.12	-0.74	87,88,92,95	0
3	PO4	A	303	5/5	0.92	0.22	-	78,84,85,86	0
3	PO4	A	302	5/5	0.87	0.20	-	78,80,82,87	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.