



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:24 pm GMT

PDB ID : 3OIF  
Title : Crystal Structure of Enoyl-ACP Reductases I (FabI) from *B. subtilis* (complex with NAD and TCL)  
Authors : Kim, K.-H.; Ha, B.H.; Kim, S.J.; Hong, S.K.; Hwang, K.Y.; Kim, E.E.  
Deposited on : 2010-08-19  
Resolution : 2.60 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

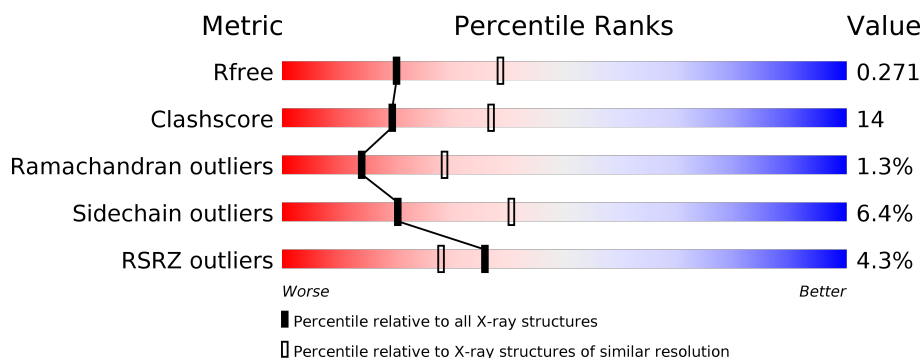
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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	266	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div>• •</div> </div> </div>
1	B	266	<div> <div>3%</div> <div> <div></div> <div>59%</div> <div>24%</div> <div>• 14%</div> </div> </div>
1	C	266	<div> <div>5%</div> <div> <div></div> <div>63%</div> <div>25%</div> <div>• 9%</div> </div> </div>
1	D	266	<div> <div>3%</div> <div> <div></div> <div>65%</div> <div>29%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7703 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 Enoyl-[acyl-carrier-protein] reductase [NADH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			1955	1223	344	378	10			
1	B	228	Total	C	N	O	S	0	0	0
			1723	1075	306	333	9			
1	C	241	Total	C	N	O	S	0	0	0
			1824	1143	318	353	10			
1	D	257	Total	C	N	O	S	0	0	0
			1947	1217	343	377	10			

There are 32 discrepancies between the modelled and reference sequences:

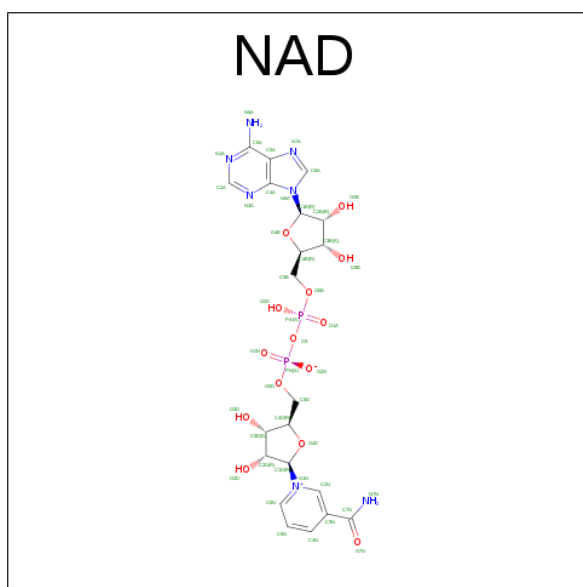
Chain	Residue	Modelled	Actual	Comment	Reference
A	259	LEU	-	EXPRESSION TAG	UNP P54616
A	260	GLU	-	EXPRESSION TAG	UNP P54616
A	261	HIS	-	EXPRESSION TAG	UNP P54616
A	262	HIS	-	EXPRESSION TAG	UNP P54616
A	263	HIS	-	EXPRESSION TAG	UNP P54616
A	264	HIS	-	EXPRESSION TAG	UNP P54616
A	265	HIS	-	EXPRESSION TAG	UNP P54616
A	266	HIS	-	EXPRESSION TAG	UNP P54616
B	259	LEU	-	EXPRESSION TAG	UNP P54616
B	260	GLU	-	EXPRESSION TAG	UNP P54616
B	261	HIS	-	EXPRESSION TAG	UNP P54616
B	262	HIS	-	EXPRESSION TAG	UNP P54616
B	263	HIS	-	EXPRESSION TAG	UNP P54616
B	264	HIS	-	EXPRESSION TAG	UNP P54616
B	265	HIS	-	EXPRESSION TAG	UNP P54616
B	266	HIS	-	EXPRESSION TAG	UNP P54616
C	259	LEU	-	EXPRESSION TAG	UNP P54616
C	260	GLU	-	EXPRESSION TAG	UNP P54616
C	261	HIS	-	EXPRESSION TAG	UNP P54616
C	262	HIS	-	EXPRESSION TAG	UNP P54616
C	263	HIS	-	EXPRESSION TAG	UNP P54616

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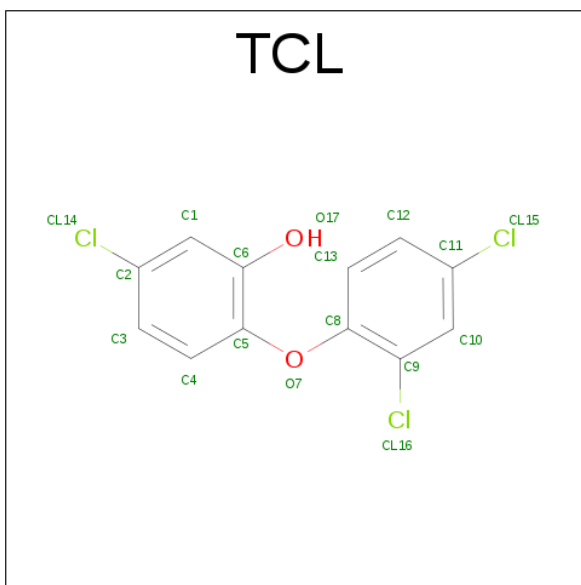
Chain	Residue	Modelled	Actual	Comment	Reference
C	264	HIS	-	EXPRESSION TAG	UNP P54616
C	265	HIS	-	EXPRESSION TAG	UNP P54616
C	266	HIS	-	EXPRESSION TAG	UNP P54616
D	259	LEU	-	EXPRESSION TAG	UNP P54616
D	260	GLU	-	EXPRESSION TAG	UNP P54616
D	261	HIS	-	EXPRESSION TAG	UNP P54616
D	262	HIS	-	EXPRESSION TAG	UNP P54616
D	263	HIS	-	EXPRESSION TAG	UNP P54616
D	264	HIS	-	EXPRESSION TAG	UNP P54616
D	265	HIS	-	EXPRESSION TAG	UNP P54616
D	266	HIS	-	EXPRESSION TAG	UNP P54616

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



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

- Molecule 3 is TRICLOSAN (three-letter code: TCL) (formula:  $C_{12}H_7Cl_3O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	O	0	0
			17	12	3	2		
3	D	1	Total	C	Cl	O	0	0
			17	12	3	2		

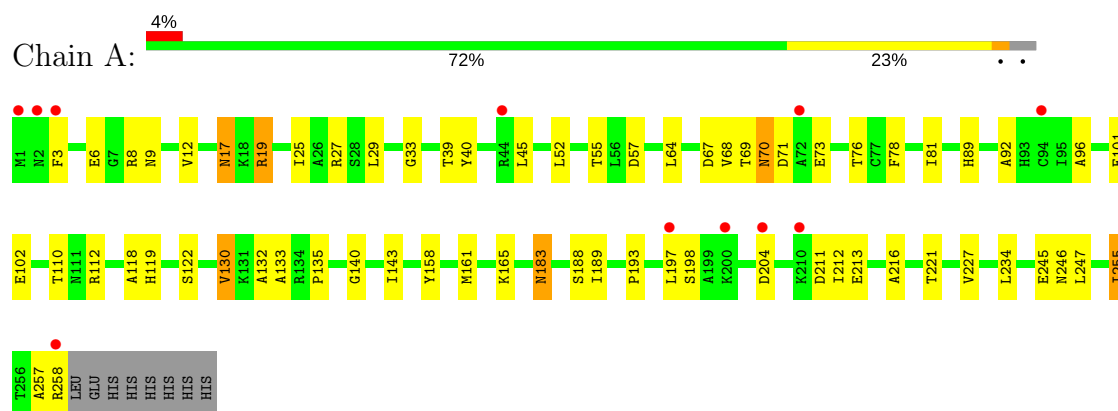
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total	O	0	0
			30	30		
4	B	38	Total	O	0	0
			38	38		
4	C	35	Total	O	0	0
			35	35		
4	D	29	Total	O	0	0
			29	29		

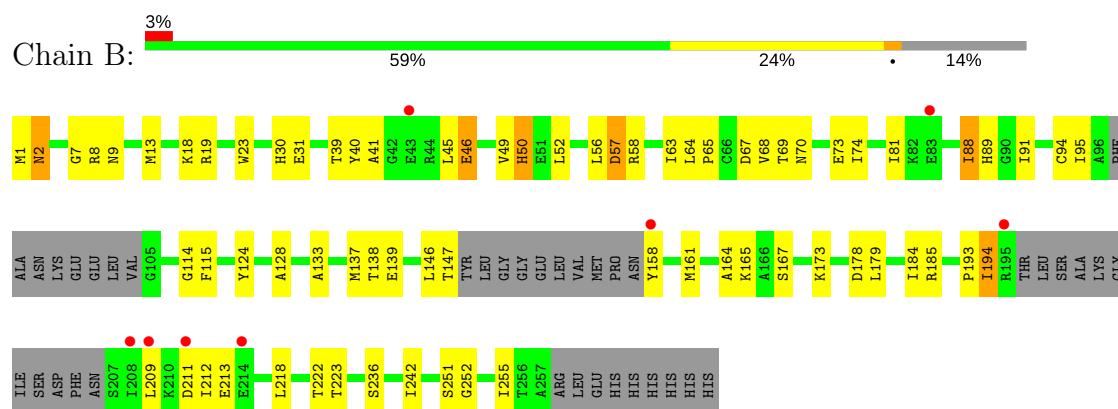
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

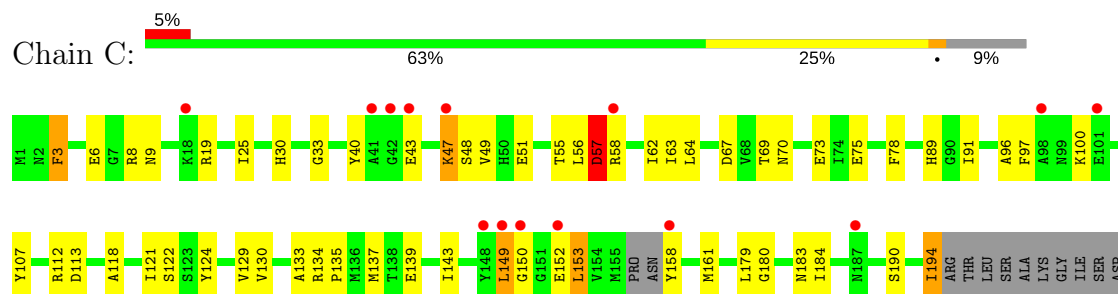
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

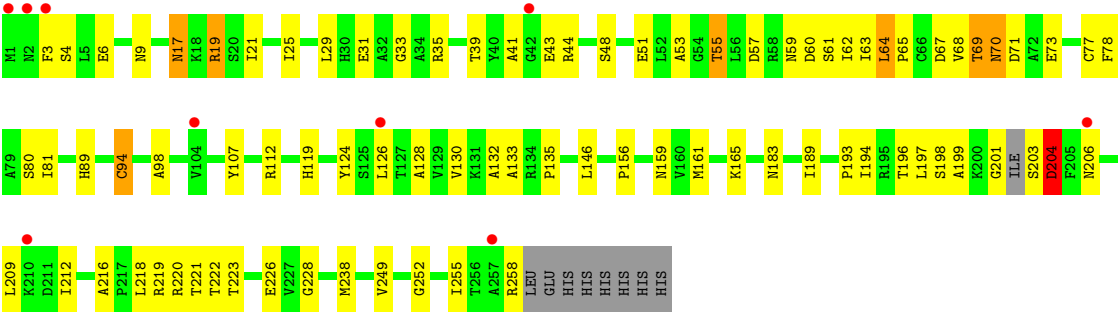


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]





● Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.10Å 83.66Å 203.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 2.60 29.98 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.4 (29.98-2.60) 95.5 (29.98-2.60)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.203 , 0.276 0.202 , 0.271	Depositor DCC
$R_{free}$ test set	1670 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.9	Xtriage
Anisotropy	0.600	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 43.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7703	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 3.97% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.71	0/1984	0.76	0/2683
1	B	0.70	0/1745	0.76	0/2356
1	C	0.67	0/1849	0.77	2/2498 (0.1%)
1	D	0.63	0/1975	0.73	0/2669
All	All	0.68	0/7553	0.75	2/10206 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	219	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	C	153	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	1955	0	1960	54	0
1	B	1723	0	1726	52	0
1	C	1824	0	1824	65	0
1	D	1947	0	1948	67	0
2	A	44	0	26	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	44	0	26	4	0
3	A	17	0	6	2	0
3	D	17	0	6	2	0
4	A	30	0	0	3	0
4	B	38	0	0	3	0
4	C	35	0	0	1	0
4	D	29	0	0	2	0
All	All	7703	0	7522	218	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 14.

All (218) 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:C:152:GLU:O	1:C:153:LEU:HD23	1.39	1.22
1:C:3:PHE:CD1	1:C:238:MET:HG3	1.93	1.04
1:A:52:LEU:O	1:A:55:THR:HG22	1.56	1.03
1:B:9:ASN:H	1:B:89:HIS:HD2	1.05	1.00
1:C:9:ASN:H	1:C:89:HIS:HD2	1.18	0.91
1:B:173:LYS:CD	1:C:153:LEU:HD22	2.03	0.89
1:C:152:GLU:O	1:C:153:LEU:CD2	2.22	0.87
1:D:59:ASN:HB2	4:D:305:HOH:O	1.74	0.87
1:B:67:ASP:OD1	1:B:69:THR:HB	1.74	0.86
1:B:173:LYS:HD2	1:C:153:LEU:HD22	1.58	0.84
1:A:96:ALA:HB3	3:A:502:TCL:CL16	2.16	0.83
1:C:3:PHE:CE1	1:C:238:MET:HG3	2.15	0.81
1:B:81:ILE:HG21	1:B:88:ILE:HD11	1.61	0.81
1:A:119:HIS:CD2	1:D:119:HIS:CD2	2.70	0.79
1:D:94:CYS:HB3	1:D:146:LEU:HD12	1.65	0.79
1:D:126:LEU:O	1:D:130:VAL:HG23	1.81	0.78
1:C:183:ASN:HD21	1:D:220:ARG:HH12	1.32	0.78
1:B:9:ASN:H	1:B:89:HIS:CD2	1.97	0.77
1:C:96:ALA:HB1	1:C:161:MET:CE	2.14	0.77
1:B:81:ILE:HG21	1:B:88:ILE:CD1	2.13	0.77
1:D:17:ASN:ND2	1:D:19:ARG:H	1.83	0.77
1:A:19:ARG:HH11	1:A:19:ARG:HG3	1.50	0.76
1:A:68:VAL:HG22	2:A:501:NAD:N1A	2.01	0.75
1:A:19:ARG:HH11	1:A:19:ARG:CG	2.01	0.73
1:D:17:ASN:HD22	1:D:17:ASN:C	1.89	0.73
1:B:9:ASN:N	1:B:89:HIS:HD2	1.85	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:ASN:OD1	1:C:73:GLU:HG2	1.90	0.71
1:D:9:ASN:H	1:D:89:HIS:HD2	1.39	0.71
1:A:67:ASP:OD1	1:A:69:THR:HG22	1.91	0.71
1:C:96:ALA:HB1	1:C:161:MET:HE3	1.75	0.69
1:D:64:LEU:HD23	1:D:65:PRO:HD2	1.76	0.68
1:A:102:GLU:HG2	1:A:110:THR:HA	1.77	0.67
1:B:94:CYS:SG	1:B:146:LEU:HD12	2.35	0.67
1:A:119:HIS:HD2	1:D:119:HIS:CD2	2.13	0.66
1:C:57:ASP:OD2	1:C:57:ASP:N	2.26	0.66
1:A:130:VAL:CG2	1:A:143:ILE:HD13	2.26	0.65
1:D:9:ASN:H	1:D:89:HIS:CD2	2.15	0.65
1:C:96:ALA:HB1	1:C:161:MET:HE1	1.79	0.64
1:A:3:PHE:HE2	4:A:280:HOH:O	1.79	0.64
1:D:223:THR:OG1	1:D:226:GLU:HG3	1.97	0.64
1:D:161:MET:CE	1:D:165:LYS:HE2	2.28	0.64
1:B:30:HIS:HE1	1:B:58:ARG:H	1.47	0.63
1:C:245:GLU:HG3	1:C:247:LEU:HD12	1.80	0.63
1:C:3:PHE:HE2	1:D:238:MET:HE3	1.62	0.63
1:B:124:TYR:CE2	1:B:128:ALA:HB2	2.33	0.63
1:B:41:ALA:O	1:B:45:LEU:HD12	1.99	0.63
1:C:3:PHE:HD1	1:C:238:MET:HG3	1.58	0.62
1:D:107:TYR:HA	1:D:159:ASN:HB3	1.81	0.62
1:B:2:ASN:H	1:B:2:ASN:HD22	1.46	0.62
1:D:193:PRO:HG2	1:D:212:ILE:HD11	1.79	0.62
1:B:8:ARG:HA	1:B:89:HIS:CD2	2.34	0.62
1:B:236:SER:HB2	4:B:302:HOH:O	1.99	0.61
1:B:68:VAL:HA	1:B:74:ILE:HD11	1.81	0.61
1:B:70:ASN:HD22	1:B:73:GLU:HB2	1.64	0.61
1:A:245:GLU:HG3	1:A:246:ASN:N	2.17	0.60
1:C:40:TYR:HB3	1:C:49:VAL:HG21	1.84	0.60
1:C:183:ASN:ND2	1:D:220:ARG:HH12	2.00	0.59
1:A:212:ILE:O	1:A:216:ALA:HB3	2.02	0.59
1:B:252:GLY:O	1:B:255:ILE:HG12	2.02	0.59
1:B:2:ASN:N	1:B:2:ASN:HD22	2.00	0.59
1:C:78:PHE:CZ	1:C:129:VAL:HG13	2.38	0.58
1:A:17:ASN:N	1:A:17:ASN:HD22	2.00	0.58
1:A:17:ASN:HD21	1:A:197:LEU:HG	1.68	0.58
1:C:133:ALA:O	1:C:137:MET:HG3	2.04	0.58
1:C:9:ASN:H	1:C:89:HIS:CD2	2.09	0.58
1:D:69:THR:O	1:D:70:ASN:HB3	2.03	0.58
1:D:39:THR:HA	1:D:64:LEU:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:ILE:HD13	1:B:223:THR:HA	1.85	0.58
1:B:40:TYR:CE2	1:B:65:PRO:HB3	2.39	0.57
1:C:78:PHE:CE1	1:C:133:ALA:HB2	2.39	0.57
1:C:212:ILE:H	1:C:212:ILE:HD12	1.68	0.57
1:B:218:LEU:HD12	1:B:251:SER:HA	1.87	0.57
1:D:35:ARG:HG3	1:D:60:ASP:HB3	1.85	0.57
1:A:17:ASN:ND2	1:A:197:LEU:HG	2.18	0.57
1:A:119:HIS:CD2	1:D:119:HIS:HD2	2.23	0.57
1:A:255:ILE:HA	1:C:153:LEU:HD13	1.87	0.57
1:C:190:SER:HB2	1:C:246:ASN:HD21	1.69	0.57
1:C:149:LEU:HD11	1:C:254:HIS:HA	1.86	0.57
1:D:69:THR:O	1:D:70:ASN:CB	2.51	0.57
1:D:17:ASN:HD21	1:D:19:ARG:HB2	1.69	0.56
1:C:3:PHE:HE2	1:D:238:MET:CE	2.18	0.56
1:A:71:ASP:OD1	1:D:112:ARG:NH1	2.38	0.56
1:D:17:ASN:HD22	1:D:19:ARG:H	1.54	0.56
1:A:78:PHE:CE1	1:A:133:ALA:HB2	2.40	0.56
1:A:69:THR:O	1:A:70:ASN:HB2	2.06	0.56
1:D:17:ASN:ND2	1:D:17:ASN:C	2.59	0.55
1:D:41:ALA:HB2	2:D:601:NAD:C2A	2.35	0.55
1:A:9:ASN:H	1:A:89:HIS:HD2	1.54	0.55
1:D:94:CYS:HB3	1:D:146:LEU:CD1	2.36	0.55
1:D:198:SER:HB3	3:D:602:TCL:C9	2.37	0.55
1:A:68:VAL:O	1:D:112:ARG:NH2	2.39	0.55
1:B:88:ILE:O	1:B:137:MET:HG2	2.07	0.55
1:D:21:ILE:HD11	1:D:194:ILE:HD12	1.89	0.55
1:D:161:MET:HE1	1:D:165:LYS:HE2	1.90	0.54
1:C:69:THR:O	1:C:70:ASN:HB3	2.07	0.54
1:A:255:ILE:HA	1:C:153:LEU:CD1	2.38	0.54
1:C:180:GLY:HA2	1:D:218:LEU:HD23	1.90	0.53
1:C:97:PHE:O	1:C:118:ALA:HA	2.08	0.53
1:A:193:PRO:HA	2:A:501:NAD:O7N	2.09	0.53
1:A:39:THR:HA	1:A:64:LEU:O	2.08	0.53
1:D:161:MET:HE3	1:D:165:LYS:HE2	1.90	0.52
1:C:8:ARG:HA	1:C:89:HIS:CD2	2.45	0.52
1:B:23:TRP:CH2	1:B:52:LEU:HB3	2.45	0.52
1:D:70:ASN:ND2	1:D:73:GLU:OE1	2.42	0.52
1:B:89:HIS:HE1	1:B:139:GLU:OE1	1.93	0.51
1:C:243:THR:CG2	1:D:252:GLY:HA3	2.41	0.51
1:C:254:HIS:HD2	4:C:297:HOH:O	1.94	0.51
1:D:6:GLU:HA	1:D:33:GLY:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:PHE:HB3	1:C:121:ILE:HG21	1.92	0.51
1:A:130:VAL:HG22	1:A:143:ILE:HD13	1.93	0.51
1:A:27:ARG:HD2	4:A:288:HOH:O	2.11	0.51
2:A:501:NAD:H2N	2:A:501:NAD:O1N	2.10	0.51
1:B:81:ILE:HG21	1:B:88:ILE:HD12	1.91	0.51
1:D:189:ILE:HG23	1:D:249:VAL:HG23	1.92	0.51
1:D:132:ALA:O	1:D:135:PRO:HD2	2.10	0.51
1:A:25:ILE:O	1:A:29:LEU:HG	2.12	0.50
1:C:3:PHE:CD1	1:C:238:MET:CG	2.82	0.50
1:A:118:ALA:O	1:A:122:SER:HB2	2.11	0.50
1:B:2:ASN:H	1:B:2:ASN:ND2	2.09	0.49
1:D:59:ASN:O	1:D:61:SER:N	2.34	0.49
1:D:62:ILE:C	1:D:63:ILE:HG12	2.33	0.49
1:D:124:TYR:CE2	1:D:128:ALA:HB2	2.48	0.49
1:C:63:ILE:O	1:C:64:LEU:HD23	2.13	0.48
1:B:161:MET:HE1	1:B:165:LYS:HE2	1.95	0.48
1:C:130:VAL:HG22	1:C:143:ILE:HD13	1.94	0.48
1:A:12:VAL:HA	1:A:92:ALA:HB3	1.95	0.48
1:C:62:ILE:O	1:C:63:ILE:HD13	2.13	0.48
1:D:252:GLY:O	1:D:255:ILE:HG12	2.14	0.47
1:B:158:TYR:O	1:B:161:MET:HB2	2.15	0.47
1:C:118:ALA:O	1:C:122:SER:HB2	2.14	0.47
1:C:150:GLY:HA3	1:C:158:TYR:CD2	2.49	0.47
1:B:193:PRO:CG	1:B:212:ILE:CD1	2.93	0.47
1:A:19:ARG:HG3	1:A:19:ARG:NH1	2.25	0.47
1:C:152:GLU:O	1:C:153:LEU:CG	2.63	0.47
1:C:243:THR:HG23	1:D:252:GLY:HA3	1.97	0.47
1:D:98:ALA:HB2	1:D:161:MET:HG2	1.96	0.47
1:C:210:LYS:O	1:C:214:GLU:HG2	2.15	0.46
1:D:51:GLU:O	1:D:55:THR:HG22	2.15	0.46
1:C:30:HIS:CE1	1:C:56:LEU:HB3	2.50	0.46
1:B:39:THR:HA	1:B:64:LEU:O	2.15	0.46
1:A:198:SER:HB3	3:A:502:TCL:C9	2.45	0.46
1:C:209:LEU:HA	1:C:212:ILE:HD13	1.98	0.46
1:A:188:SER:OG	1:A:246:ASN:ND2	2.49	0.46
1:B:91:ILE:HD11	1:B:133:ALA:CB	2.46	0.46
1:B:56:LEU:O	1:B:57:ASP:C	2.54	0.46
1:B:161:MET:CE	1:B:165:LYS:HE2	2.46	0.46
1:B:173:LYS:HD3	1:C:153:LEU:HD22	1.96	0.46
1:B:49:VAL:HG12	1:B:63:ILE:HD12	1.97	0.46
1:A:6:GLU:HA	1:A:33:GLY:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:PHE:CE2	4:A:280:HOH:O	2.56	0.46
1:D:25:ILE:HG12	1:D:228:GLY:HA2	1.97	0.46
1:D:222:THR:HG22	1:D:223:THR:H	1.81	0.45
1:B:179:LEU:HB3	1:B:184:ILE:HB	1.97	0.45
1:B:2:ASN:N	1:B:2:ASN:ND2	2.64	0.45
1:D:193:PRO:HA	2:D:601:NAD:O7N	2.16	0.45
1:C:25:ILE:HG12	1:C:228:GLY:HA2	1.98	0.45
1:D:77:CYS:O	1:D:81:ILE:HG13	2.15	0.45
1:A:247:LEU:HD12	1:A:247:LEU:N	2.32	0.45
1:B:114:GLY:HA3	4:B:283:HOH:O	2.16	0.45
1:C:47:LYS:O	1:C:51:GLU:HG3	2.17	0.45
1:C:194:ILE:CG2	1:C:194:ILE:O	2.64	0.45
1:B:40:TYR:CE2	1:B:46:GLU:HB2	2.52	0.45
1:A:258:ARG:HG2	1:C:153:LEU:HG	1.98	0.45
1:A:17:ASN:N	1:A:17:ASN:ND2	2.65	0.44
1:C:78:PHE:HZ	1:C:129:VAL:HG13	1.82	0.44
1:B:30:HIS:CE1	1:B:58:ARG:H	2.30	0.44
1:A:8:ARG:HA	1:A:89:HIS:CD2	2.52	0.44
1:B:13:MET:HB3	1:B:95:ILE:HD11	2.00	0.44
1:C:69:THR:O	1:C:70:ASN:CB	2.64	0.44
1:B:164:ALA:O	1:B:167:SER:HB3	2.17	0.44
1:A:161:MET:O	1:A:165:LYS:HG2	2.17	0.44
1:B:46:GLU:O	1:B:50:HIS:HB2	2.17	0.44
1:C:134:ARG:N	1:C:135:PRO:CD	2.79	0.44
1:B:193:PRO:HG3	1:B:212:ILE:CD1	2.48	0.44
2:D:601:NAD:H3D	3:D:602:TCL:CL16	2.55	0.44
1:D:212:ILE:HG23	1:D:216:ALA:HB2	1.99	0.43
1:A:40:TYR:HB2	1:A:45:LEU:HB2	2.00	0.43
1:A:70:ASN:ND2	1:A:73:GLU:HG3	2.34	0.43
1:A:212:ILE:HG23	1:A:216:ALA:HB2	2.00	0.43
1:B:7:GLY:HA2	4:B:290:HOH:O	2.18	0.43
1:B:209:LEU:O	1:B:213:GLU:HG3	2.18	0.43
1:A:112:ARG:NH1	1:D:71:ASP:OD1	2.52	0.43
1:A:70:ASN:ND2	1:A:73:GLU:OE1	2.51	0.43
1:B:193:PRO:HG2	1:B:212:ILE:CD1	2.49	0.43
1:C:6:GLU:HA	1:C:33:GLY:O	2.18	0.43
1:D:206:ASN:HA	1:D:209:LEU:HD12	2.01	0.43
1:C:91:ILE:HD11	1:C:133:ALA:CB	2.49	0.43
1:A:189:ILE:HG21	1:A:227:VAL:HG13	2.00	0.42
1:C:89:HIS:HE1	1:C:139:GLU:OE2	2.02	0.42
1:A:132:ALA:O	1:A:135:PRO:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:ASP:O	1:C:69:THR:O	2.37	0.42
1:D:201:GLY:O	1:D:203:SER:N	2.52	0.42
1:A:158:TYR:CZ	1:A:161:MET:HG3	2.55	0.42
1:A:78:PHE:HA	1:A:81:ILE:HD12	2.02	0.42
1:B:45:LEU:O	1:B:46:GLU:C	2.58	0.42
1:B:178:ASP:OD2	1:C:107:TYR:HB3	2.19	0.42
1:C:179:LEU:HB3	1:C:184:ILE:HB	2.01	0.41
1:D:68:VAL:HG22	2:D:601:NAD:N1A	2.35	0.41
1:D:53:ALA:HB2	1:D:63:ILE:HD11	2.01	0.41
1:B:185:ARG:HD2	1:B:242:ILE:O	2.20	0.41
1:C:47:LYS:HG2	1:C:51:GLU:OE1	2.19	0.41
1:D:222:THR:HG22	1:D:223:THR:N	2.35	0.41
1:A:140:GLY:HA2	1:A:183:ASN:HB3	2.02	0.41
1:D:67:ASP:OD2	1:D:69:THR:HG23	2.20	0.41
1:C:233:PHE:CZ	1:C:239:SER:HB3	2.55	0.41
1:D:203:SER:O	1:D:204:ASP:C	2.59	0.41
1:C:91:ILE:HD13	1:C:129:VAL:HG12	2.02	0.41
1:A:245:GLU:HG3	1:A:246:ASN:H	1.85	0.41
1:C:180:GLY:CA	1:D:218:LEU:HD23	2.51	0.41
1:D:25:ILE:O	1:D:29:LEU:HG	2.20	0.41
1:D:64:LEU:HD11	1:D:80:SER:HB3	2.02	0.41
1:A:234:LEU:HD23	1:A:234:LEU:HA	1.93	0.41
1:D:78:PHE:CE1	1:D:133:ALA:HB2	2.56	0.41
1:B:115:PHE:CE1	1:C:124:TYR:HB2	2.56	0.40
1:D:6:GLU:HG2	4:D:295:HOH:O	2.20	0.40
1:A:213:GLU:HG3	1:A:221:THR:HG23	2.02	0.40
1:D:17:ASN:ND2	1:D:19:ARG:N	2.62	0.40
1:D:196:THR:H	1:D:199:ALA:HB3	1.86	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	256/266 (96%)	236 (92%)	17 (7%)	3 (1%)	15	32
1	B	220/266 (83%)	203 (92%)	16 (7%)	1 (0%)	32	58
1	C	235/266 (88%)	215 (92%)	16 (7%)	4 (2%)	11	21
1	D	253/266 (95%)	225 (89%)	23 (9%)	5 (2%)	9	17
All	All	964/1064 (91%)	879 (91%)	72 (8%)	13 (1%)	14	29

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	257	ALA
1	B	57	ASP
1	C	58	ARG
1	D	57	ASP
1	D	204	ASP
1	C	55	THR
1	D	70	ASN
1	A	57	ASP
1	C	210	LYS
1	D	219	ARG
1	C	57	ASP
1	D	43	GLU

### 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	209/217 (96%)	200 (96%)	9 (4%)	33	61
1	B	184/217 (85%)	171 (93%)	13 (7%)	17	34
1	C	194/217 (89%)	182 (94%)	12 (6%)	21	42
1	D	208/217 (96%)	191 (92%)	17 (8%)	13	26
All	All	795/868 (92%)	744 (94%)	51 (6%)	20	40

All (51) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	17	ASN
1	A	19	ARG
1	A	76	THR
1	A	101	GLU
1	A	130	VAL
1	A	183	ASN
1	A	204	ASP
1	A	211	ASP
1	A	255	ILE
1	B	1	MET
1	B	2	ASN
1	B	18	LYS
1	B	19	ARG
1	B	31	GLU
1	B	46	GLU
1	B	50	HIS
1	B	88	ILE
1	B	138	THR
1	B	147	THR
1	B	194	ILE
1	B	211	ASP
1	B	222	THR
1	C	3	PHE
1	C	19	ARG
1	C	43	GLU
1	C	47	LYS
1	C	48	SER
1	C	57	ASP
1	C	75	GLU
1	C	100	LYS
1	C	112	ARG
1	C	113	ASP
1	C	149	LEU
1	C	194	ILE
1	D	3	PHE
1	D	4	SER
1	D	17	ASN
1	D	19	ARG
1	D	31	GLU
1	D	44	ARG
1	D	48	SER
1	D	55	THR
1	D	64	LEU

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Mol	Chain	Res	Type
1	D	69	THR
1	D	94	CYS
1	D	156	PRO
1	D	183	ASN
1	D	197	LEU
1	D	204	ASP
1	D	221	THR
1	D	258	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	30	HIS
1	A	89	HIS
1	A	99	ASN
1	A	109	ASN
1	A	183	ASN
1	A	246	ASN
1	B	2	ASN
1	B	30	HIS
1	B	70	ASN
1	B	89	HIS
1	B	109	ASN
1	B	183	ASN
1	B	254	HIS
1	C	2	ASN
1	C	30	HIS
1	C	89	HIS
1	C	109	ASN
1	C	183	ASN
1	C	246	ASN
1	D	17	ASN
1	D	30	HIS
1	D	84	GLN
1	D	89	HIS
1	D	99	ASN
1	D	109	ASN
1	D	183	ASN
1	D	246	ASN

### 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$
2	NAD	A	501	-	41,48,48	1.61	3 (7%)	43,73,73	2.13	6 (13%)
3	TCL	A	502	-	18,18,18	2.11	3 (16%)	25,25,25	1.14	2 (8%)
2	NAD	D	601	-	41,48,48	1.71	3 (7%)	43,73,73	1.98	5 (11%)
3	TCL	D	602	-	18,18,18	1.84	2 (11%)	25,25,25	1.05	1 (4%)

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	NAD	A	501	-	-	0/22/62/62	0/5/5/5
3	TCL	A	502	-	-	0/4/4/4	0/2/2/2
2	NAD	D	601	-	-	0/22/62/62	0/5/5/5
3	TCL	D	602	-	-	0/4/4/4	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	NAD	C2A-N1A	2.38	1.38	1.33
3	A	502	TCL	C9-CL16	2.43	1.79	1.73
2	A	501	NAD	C2A-N1A	2.52	1.38	1.33
2	D	601	NAD	C2A-N3A	4.21	1.39	1.32
2	A	501	NAD	C2A-N3A	4.24	1.39	1.32
3	D	602	TCL	C8-C9	4.52	1.47	1.39
3	A	502	TCL	C8-C9	5.27	1.49	1.39
3	D	602	TCL	C6-C5	5.58	1.48	1.40
3	A	502	TCL	C6-C5	5.62	1.49	1.40
2	A	501	NAD	O7N-C7N	7.90	1.40	1.24
2	D	601	NAD	O7N-C7N	8.58	1.41	1.24

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	NAD	N3A-C2A-N1A	-10.70	119.54	128.86
2	A	501	NAD	N3A-C2A-N1A	-10.46	119.75	128.86
2	A	501	NAD	C4B-O4B-C1B	-3.96	105.56	109.77
2	D	601	NAD	C4B-O4B-C1B	-3.52	106.02	109.77
2	A	501	NAD	C5A-C6A-N6A	-3.14	114.07	120.47
3	D	602	TCL	C10-C11-CL15	-2.88	115.54	119.14
2	D	601	NAD	C1B-N9A-C4A	-2.86	121.70	126.64
3	A	502	TCL	C10-C11-CL15	-2.46	116.07	119.14
2	D	601	NAD	O3B-C3B-C4B	-2.22	104.61	111.09
2	A	501	NAD	O7N-C7N-N7N	-2.20	119.45	122.58
2	D	601	NAD	O7N-C7N-C3N	2.07	122.04	119.62
2	A	501	NAD	O4B-C4B-C5B	2.42	117.57	109.40
3	A	502	TCL	C8-C9-CL16	2.78	122.63	119.42
2	A	501	NAD	C3N-C7N-N7N	4.29	122.67	117.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAD	3	0
3	A	502	TCL	2	0
2	D	601	NAD	4	0
3	D	602	TCL	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

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	258/266 (96%)	-0.10	11 (4%) 36 28	24, 44, 75, 91	0
1	B	228/266 (85%)	-0.10	8 (3%) 44 36	22, 43, 71, 87	0
1	C	241/266 (90%)	0.01	14 (5%) 24 18	27, 46, 74, 84	0
1	D	257/266 (96%)	0.09	9 (3%) 44 36	26, 51, 81, 95	0
All	All	984/1064 (92%)	-0.02	42 (4%) 36 28	22, 46, 78, 95	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	208	ILE	6.8
1	B	211	ASP	4.8
1	A	204	ASP	4.7
1	D	3	PHE	4.2
1	A	3	PHE	4.1
1	A	197	LEU	4.0
1	D	42	GLY	3.7
1	C	148	TYR	3.7
1	D	257	ALA	3.5
1	C	149	LEU	3.5
1	B	158	TYR	3.4
1	A	2	ASN	3.2
1	C	42	GLY	3.1
1	C	101	GLU	3.0
1	C	158	TYR	3.0
1	D	2	ASN	3.0
1	A	72	ALA	2.8
1	A	258	ARG	2.8
1	B	195	ARG	2.7
1	B	43	GLU	2.7
1	D	210	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	43	GLU	2.5
1	C	58	ARG	2.3
1	B	214	GLU	2.3
1	A	44	ARG	2.3
1	B	209	LEU	2.2
1	A	200	LYS	2.2
1	C	150	GLY	2.2
1	A	210	LYS	2.2
1	A	1	MET	2.2
1	B	83	GLU	2.2
1	C	187	ASN	2.1
1	C	18	LYS	2.1
1	A	94	CYS	2.1
1	C	41	ALA	2.1
1	C	98	ALA	2.1
1	D	126	LEU	2.1
1	D	206	ASN	2.1
1	D	104	VAL	2.1
1	C	47	LYS	2.1
1	C	152	GLU	2.0
1	D	1	MET	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	TCL	A	502	17/17	0.91	0.17	-0.09	43,50,63,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAD	A	501	44/44	0.94	0.14	-0.52	46,50,55,57	0
3	TCL	D	602	17/17	0.93	0.15	-0.53	46,51,62,67	0
2	NAD	D	601	44/44	0.95	0.14	-0.79	51,55,61,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.