



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:15 AM 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
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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

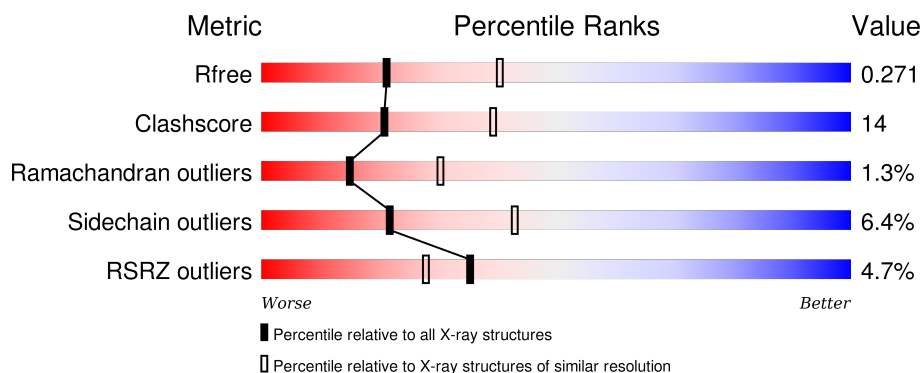
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 ≥ 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>72%</div> <div>23%</div> <div>• •</div> </div>
1	B	266	<div> <div>3%</div> <div>59%</div> <div>24%</div> <div>• 14%</div> </div>
1	C	266	<div> <div>7%</div> <div>63%</div> <div>25%</div> <div>• 9%</div> </div>
1	D	266	<div> <div>3%</div> <div>65%</div> <div>29%</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:

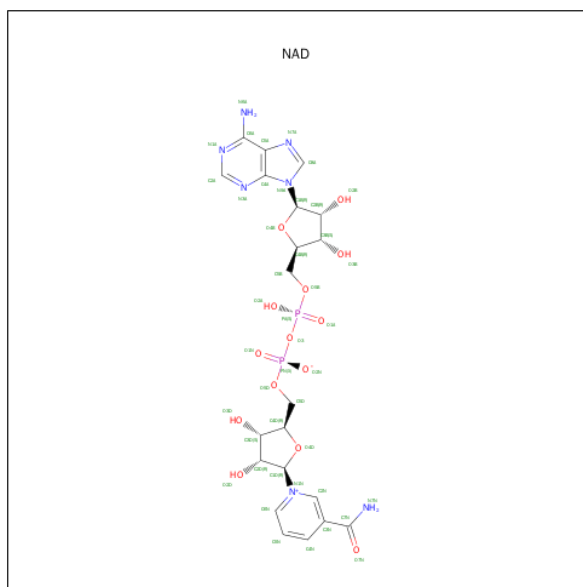
Chain	Residue	Modelled	Actual	Comment	Reference
A	259	LEU	-	EXPRESSION TAG	UNP P54616
A	260	GLU	-	EXPRESSION TAG	UNP P54616
A	261	HIS	-	EXPRESSION TAG	UNP P54616
A	262	HIS	-	EXPRESSION TAG	UNP P54616
A	263	HIS	-	EXPRESSION TAG	UNP P54616
A	264	HIS	-	EXPRESSION TAG	UNP P54616
A	265	HIS	-	EXPRESSION TAG	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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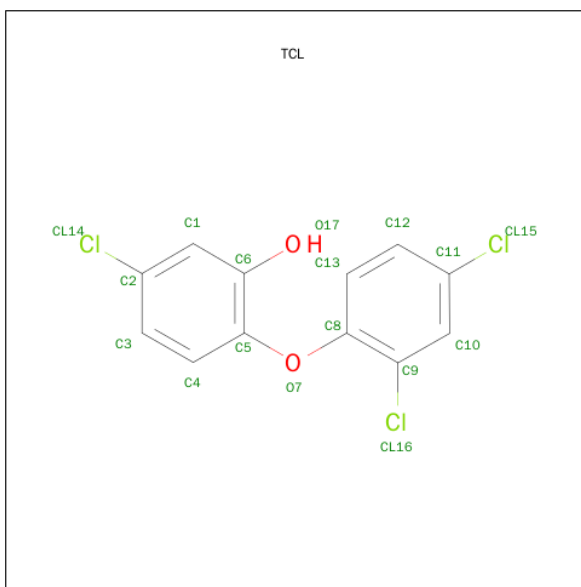
Chain	Residue	Modelled	Actual	Comment	Reference
C	264	HIS	-	EXPRESSION TAG	UNP P54616
C	265	HIS	-	EXPRESSION TAG	UNP P54616
C	266	HIS	-	EXPRESSION TAG	UNP P54616
D	259	LEU	-	EXPRESSION TAG	UNP P54616
D	260	GLU	-	EXPRESSION TAG	UNP P54616
D	261	HIS	-	EXPRESSION TAG	UNP P54616
D	262	HIS	-	EXPRESSION TAG	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: $C_{12}H_7Cl_3O_2$).



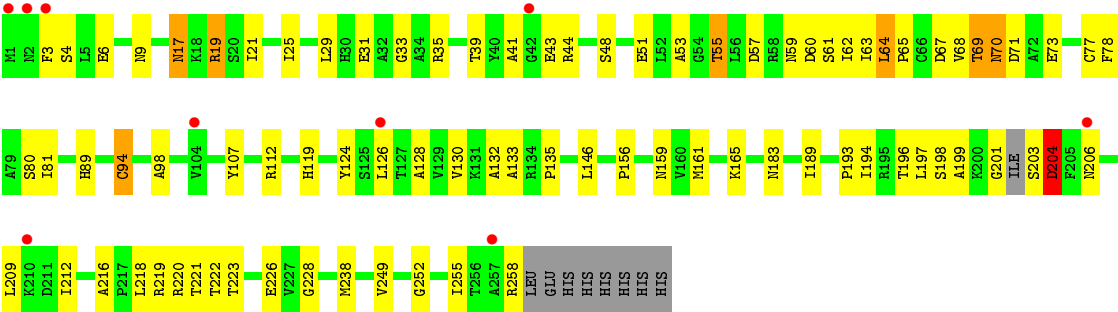
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	O	0	0
			17	12	3	2		
3	D	1	Total	C	Cl	O	0	0
			17	12	3	2		

- 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		



• 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, α , β , γ	64.10 Å 83.66 Å 203.55 Å 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
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.61 Å)	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	1678 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.600	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 32958 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7703	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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:D:223:THR:OG1	1:D:226:GLU:HG3	1.97	0.64
1:A:3:PHE:HE2	4:A:280:HOH:O	1.79	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:3:PHE:HE2	1:D:238:MET:HE3	1.62	0.63
1:C:245:GLU:HG3	1:C:247:LEU:HD12	1.80	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:C:9:ASN:H	1:C:89:HIS:CD2	2.09	0.58
1:C:133:ALA:O	1:C:137:MET:HG3	2.04	0.58
1:A:17:ASN:HD21	1:A:197:LEU:HG	1.68	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:D:35:ARG:HG3	1:D:60:ASP:HB3	1.85	0.57
1:B:218:LEU:HD12	1:B:251:SER:HA	1.87	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:D:69:THR:O	1:D:70:ASN:CB	2.51	0.57
1:C:149:LEU:HD11	1:C:254:HIS:HA	1.86	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:69:THR:O	1:A:70:ASN:HB2	2.06	0.56
1:A:78:PHE:CE1	1:A:133:ALA:HB2	2.40	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:D:94:CYS:HB3	1:D:146:LEU:CD1	2.36	0.55
1:A:9:ASN:H	1:A:89:HIS:HD2	1.54	0.55
1:D:198:SER:HB3	3:D:602:TCL:C9	2.37	0.55
1:B:88:ILE:O	1:B:137:MET:HG2	2.07	0.55
1:A:68:VAL:O	1:D:112:ARG:NH2	2.39	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
2:A:501:NAD:H2N	2:A:501:NAD:O1N	2.10	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
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:C:3:PHE:CD1	1:C:238:MET:CG	2.82	0.50
1:A:25:ILE:O	1:A:29:LEU:HG	2.12	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:C:152:GLU:O	1:C:153:LEU:CG	2.63	0.47
1:A:19:ARG:HG3	1:A:19:ARG:NH1	2.25	0.47
1:D:98:ALA:HB2	1:D:161:MET:HG2	1.96	0.47
1:C:243:THR:HG23	1:D:252:GLY:HA3	1.97	0.47
1:D:51:GLU:O	1:D:55:THR:HG22	2.15	0.46
1:C:210:LYS:O	1:C:214:GLU:HG2	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:56:LEU:O	1:B:57:ASP:C	2.54	0.46
1:B:91:ILE:HD11	1:B:133:ALA:CB	2.46	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:3:PHE:CE2	4:A:280:HOH:O	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:ILE:HG12	1:D:228:GLY:HA2	1.97	0.46
1:A:6:GLU:HA	1:A:33:GLY:O	2.16	0.46
1:D:222:THR:HG22	1:D:223:THR:H	1.81	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:B:179:LEU:HB3	1:B:184:ILE:HB	1.97	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:A:258:ARG:HG2	1:C:153:LEU:HG	1.98	0.45
1:B:40:TYR:CE2	1:B:46:GLU:HB2	2.52	0.45
1:C:78:PHE:HZ	1:C:129:VAL:HG13	1.82	0.44
1:A:17:ASN:N	1:A:17:ASN:ND2	2.65	0.44
1:B:30:HIS:CE1	1:B:58:ARG:H	2.30	0.44
1:C:69:THR:O	1:C:70:ASN:CB	2.64	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:B:164:ALA:O	1:B:167:SER:HB3	2.17	0.44
1:B:46:GLU:O	1:B:50:HIS:HB2	2.17	0.44
1:A:161:MET:O	1:A:165:LYS:HG2	2.17	0.44
1:C:134:ARG:N	1:C:135:PRO:CD	2.79	0.44
2:D:601:NAD:H3D	3:D:602:TCL:CL16	2.55	0.44
1:B:193:PRO:HG3	1:B:212:ILE:CD1	2.48	0.44
1:D:212:ILE:HG23	1:D:216:ALA:HB2	1.99	0.43
1:A:70:ASN:ND2	1:A:73:GLU:HG3	2.34	0.43
1:A:40:TYR:HB2	1:A:45:LEU:HB2	2.00	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:78:PHE:HA	1:A:81:ILE:HD12	2.02	0.42
1:A:158:TYR:CZ	1:A:161:MET:HG3	2.55	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: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:C:179:LEU:HB3	1:C:184:ILE:HB	2.01	0.41
1:D:222:THR:HG22	1:D:223:THR:N	2.35	0.41
1:C:47:LYS:HG2	1:C:51:GLU:OE1	2.19	0.41
1:B:185:ARG:HD2	1:B:242:ILE:O	2.20	0.41
1:D:67:ASP:OD2	1:D:69:THR:HG23	2.20	0.41
1:A:140:GLY:HA2	1:A:183:ASN:HB3	2.02	0.41
1:D:203:SER:O	1:D:204:ASP:C	2.59	0.41
1:C:233:PHE:CZ	1:C:239:SER:HB3	2.55	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:D:64:LEU:HD11	1:D:80:SER:HB3	2.02	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: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:D:6:GLU:HG2	4:D:295:HOH:O	2.20	0.40
1:B:115:PHE:CE1	1:C:124:TYR:HB2	2.56	0.40
1:D:17:ASN:ND2	1:D:19:ARG:N	2.62	0.40
1:A:213:GLU:HG3	1:A:221:THR:HG23	2.02	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%)	16	33
1	B	220/266 (83%)	203 (92%)	16 (7%)	1 (0%)	34	60
1	C	235/266 (88%)	215 (92%)	16 (7%)	4 (2%)	11	22
1	D	253/266 (95%)	225 (89%)	23 (9%)	5 (2%)	9	18
All	All	964/1064 (91%)	879 (91%)	72 (8%)	13 (1%)	15	30

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%)	35	64
1	B	184/217 (85%)	171 (93%)	13 (7%)	18	36
1	C	194/217 (89%)	182 (94%)	12 (6%)	23	45
1	D	208/217 (96%)	191 (92%)	17 (8%)	14	27
All	All	795/868 (92%)	744 (94%)	51 (6%)	22	43

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	-	38,48,48	1.62	3 (7%)	47,73,73	2.35	9 (19%)
3	TCL	A	502	-	18,18,18	2.06	3 (16%)	25,25,25	1.12	3 (12%)
2	NAD	D	601	-	38,48,48	1.71	3 (7%)	47,73,73	2.37	9 (19%)
3	TCL	D	602	-	18,18,18	1.79	2 (11%)	25,25,25	1.04	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	2.35	1.38	1.33
3	A	502	TCL	C9-CL16	2.37	1.79	1.73
2	A	501	NAD	C2A-N1A	2.49	1.38	1.33
2	D	601	NAD	C2A-N3A	3.95	1.39	1.32
2	A	501	NAD	C2A-N3A	3.99	1.39	1.32
3	D	602	TCL	C8-C9	4.44	1.47	1.39
3	A	502	TCL	C8-C9	5.17	1.49	1.39
3	D	602	TCL	C6-C5	5.37	1.48	1.40
3	A	502	TCL	C6-C5	5.40	1.49	1.40
2	A	501	NAD	O7N-C7N	7.64	1.40	1.24
2	D	601	NAD	O7N-C7N	8.29	1.41	1.24

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	NAD	N3A-C2A-N1A	-12.21	119.54	128.89
2	A	501	NAD	N3A-C2A-N1A	-11.94	119.75	128.89
2	A	501	NAD	C4B-O4B-C1B	-3.79	105.56	109.72
2	D	601	NAD	C1B-N9A-C4A	-3.48	121.70	126.94
2	D	601	NAD	C4B-O4B-C1B	-3.37	106.02	109.72
3	D	602	TCL	C10-C11-CL15	-2.90	115.54	119.14
2	A	501	NAD	C2B-C1B-N9A	-2.83	109.96	114.29
2	D	601	NAD	PN-O3-PA	-2.53	125.62	132.73
3	A	502	TCL	C10-C11-CL15	-2.47	116.07	119.14
2	A	501	NAD	O7N-C7N-N7N	-2.24	119.45	122.59
2	D	601	NAD	O3B-C3B-C4B	-2.15	104.61	111.05
2	D	601	NAD	O3-PA-O5B	2.08	108.45	102.94
3	A	502	TCL	C8-O7-C5	2.09	122.82	117.75
2	D	601	NAD	O7N-C7N-C3N	2.25	122.04	119.59
2	A	501	NAD	O4B-C4B-C5B	2.31	117.57	109.32
2	A	501	NAD	O4B-C1B-N9A	2.50	113.34	108.10
2	A	501	NAD	O3-PA-O5B	2.58	109.77	102.94
3	A	502	TCL	C8-C9-CL16	2.61	122.63	119.42
2	D	601	NAD	O4D-C1D-N1N	4.14	112.67	108.13
2	A	501	NAD	O4D-C1D-N1N	4.23	112.78	108.13
2	A	501	NAD	C3N-C7N-N7N	4.43	122.67	117.82
2	D	601	NAD	O4B-C1B-N9A	4.88	118.32	108.10

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 [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, 95th 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 ²)	Q<0.9
1	A	258/266 (96%)	-0.06	11 (4%) 39 31	24, 44, 75, 91	0
1	B	228/266 (85%)	-0.07	8 (3%) 48 40	22, 43, 71, 87	0
1	C	241/266 (90%)	0.04	18 (7%) 17 12	27, 46, 74, 84	0
1	D	257/266 (96%)	0.13	9 (3%) 48 40	26, 51, 81, 95	0
All	All	984/1064 (92%)	0.01	46 (4%) 35 28	22, 46, 78, 95	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	208	ILE	6.9
1	B	211	ASP	4.9
1	A	204	ASP	4.8
1	D	3	PHE	4.2
1	A	3	PHE	4.2
1	A	197	LEU	4.0
1	D	42	GLY	3.8
1	C	148	TYR	3.8
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	3.2
1	C	101	GLU	3.1
1	C	158	TYR	3.1
1	D	2	ASN	3.0
1	A	72	ALA	2.9
1	A	258	ARG	2.8
1	B	43	GLU	2.8
1	B	195	ARG	2.8
1	D	210	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	43	GLU	2.5
1	C	58	ARG	2.4
1	B	214	GLU	2.4
1	A	44	ARG	2.3
1	A	1	MET	2.3
1	A	200	LYS	2.3
1	B	209	LEU	2.3
1	A	210	LYS	2.3
1	C	150	GLY	2.3
1	B	83	GLU	2.3
1	C	187	ASN	2.2
1	A	94	CYS	2.2
1	C	18	LYS	2.2
1	C	41	ALA	2.2
1	C	98	ALA	2.1
1	D	206	ASN	2.1
1	C	47	LYS	2.1
1	D	1	MET	2.1
1	D	104	VAL	2.1
1	D	126	LEU	2.1
1	C	152	GLU	2.1
1	C	155	MET	2.1
1	C	145	THR	2.0
1	C	188	SER	2.0
1	C	144	VAL	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, 95th 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(\AA^2)	Q<0.9
3	TCL	A	502	17/17	0.91	0.17	-0.09	43,50,63,70	0
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.