



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:32 PM UTC

PDB ID : 1O5I / pdb_00001o5i
Title : Crystal structure of 3-oxoacyl-(acyl carrier protein) reductase (TM1169) from *Thermotoga maritima* at 2.50 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2003-09-17
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

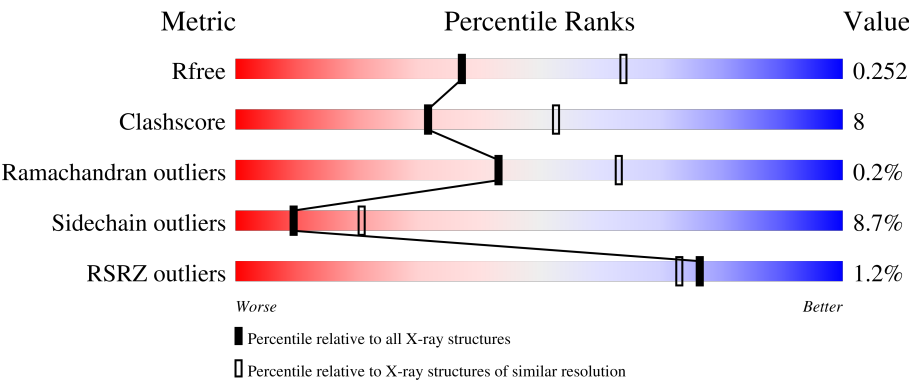
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	249	% 70% 22% • 6%
1	B	249	% 70% 22% • 6%
1	C	249	2% 68% 22% • 6%
1	D	249	75% 17% • 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7361 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 3-oxoacyl-(acyl carrier protein) reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	0	0
			1787	1142	301	335	9			
1	B	234	Total	C	N	O	S	1	0	0
			1791	1142	303	337	9			
1	C	234	Total	C	N	O	S	0	0	0
			1788	1140	302	337	9			
1	D	234	Total	C	N	O	S	4	0	0
			1799	1148	305	337	9			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q9X0Q1
A	-10	GLY	-	expression tag	UNP Q9X0Q1
A	-9	SER	-	expression tag	UNP Q9X0Q1
A	-8	ASP	-	expression tag	UNP Q9X0Q1
A	-7	LYS	-	expression tag	UNP Q9X0Q1
A	-6	ILE	-	expression tag	UNP Q9X0Q1
A	-5	HIS	-	expression tag	UNP Q9X0Q1
A	-4	HIS	-	expression tag	UNP Q9X0Q1
A	-3	HIS	-	expression tag	UNP Q9X0Q1
A	-2	HIS	-	expression tag	UNP Q9X0Q1
A	-1	HIS	-	expression tag	UNP Q9X0Q1
A	0	HIS	-	expression tag	UNP Q9X0Q1
B	-11	MET	-	expression tag	UNP Q9X0Q1
B	-10	GLY	-	expression tag	UNP Q9X0Q1
B	-9	SER	-	expression tag	UNP Q9X0Q1
B	-8	ASP	-	expression tag	UNP Q9X0Q1
B	-7	LYS	-	expression tag	UNP Q9X0Q1
B	-6	ILE	-	expression tag	UNP Q9X0Q1
B	-5	HIS	-	expression tag	UNP Q9X0Q1
B	-4	HIS	-	expression tag	UNP Q9X0Q1
B	-3	HIS	-	expression tag	UNP Q9X0Q1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP Q9X0Q1
B	-1	HIS	-	expression tag	UNP Q9X0Q1
B	0	HIS	-	expression tag	UNP Q9X0Q1
C	-11	MET	-	expression tag	UNP Q9X0Q1
C	-10	GLY	-	expression tag	UNP Q9X0Q1
C	-9	SER	-	expression tag	UNP Q9X0Q1
C	-8	ASP	-	expression tag	UNP Q9X0Q1
C	-7	LYS	-	expression tag	UNP Q9X0Q1
C	-6	ILE	-	expression tag	UNP Q9X0Q1
C	-5	HIS	-	expression tag	UNP Q9X0Q1
C	-4	HIS	-	expression tag	UNP Q9X0Q1
C	-3	HIS	-	expression tag	UNP Q9X0Q1
C	-2	HIS	-	expression tag	UNP Q9X0Q1
C	-1	HIS	-	expression tag	UNP Q9X0Q1
C	0	HIS	-	expression tag	UNP Q9X0Q1
D	-11	MET	-	expression tag	UNP Q9X0Q1
D	-10	GLY	-	expression tag	UNP Q9X0Q1
D	-9	SER	-	expression tag	UNP Q9X0Q1
D	-8	ASP	-	expression tag	UNP Q9X0Q1
D	-7	LYS	-	expression tag	UNP Q9X0Q1
D	-6	ILE	-	expression tag	UNP Q9X0Q1
D	-5	HIS	-	expression tag	UNP Q9X0Q1
D	-4	HIS	-	expression tag	UNP Q9X0Q1
D	-3	HIS	-	expression tag	UNP Q9X0Q1
D	-2	HIS	-	expression tag	UNP Q9X0Q1
D	-1	HIS	-	expression tag	UNP Q9X0Q1
D	0	HIS	-	expression tag	UNP Q9X0Q1

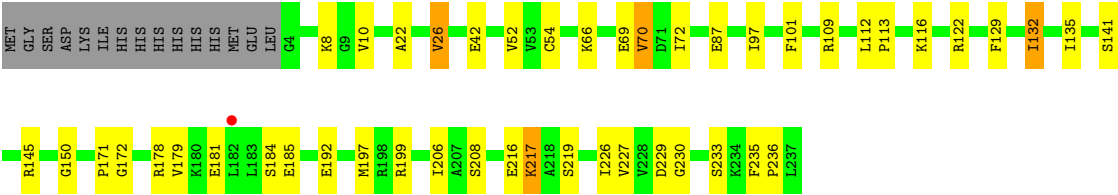
- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			35	15	5	13	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	49	Total	O	0	0
			49	49		
3	B	39	Total	O	0	0
			39	39		
3	C	31	Total	O	0	0
			31	31		
3	D	42	Total	O	0	0
			42	42		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.52Å 117.12Å 140.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.17 – 2.50 41.17 – 2.50	Depositor EDS
% Data completeness (in resolution range)	85.0 (41.17-2.50) 85.0 (41.17-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
R, R_{free}	0.194 , 0.247 0.203 , 0.252	Depositor DCC
R_{free} test set	1562 reflections (4.20%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	1.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7361	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.36% 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, 0.333 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:
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	1.14	3/1814 (0.2%)	1.16	3/2450 (0.1%)
1	B	1.11	1/1818 (0.1%)	1.11	3/2456 (0.1%)
1	C	1.02	1/1815 (0.1%)	1.08	1/2453 (0.0%)
1	D	1.12	3/1826 (0.2%)	1.11	2/2463 (0.1%)
All	All	1.09	8/7273 (0.1%)	1.11	9/9822 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	226	ILE	CA-CB	-7.45	1.45	1.54
1	B	69	GLU	CA-CB	7.01	1.67	1.54
1	D	226	ILE	CA-CB	-6.29	1.46	1.54
1	C	123	ILE	CA-CB	-6.26	1.46	1.54
1	D	227	VAL	CA-CB	6.10	1.61	1.54
1	A	228	VAL	CA-CB	5.41	1.59	1.53
1	D	135	ILE	CA-CB	5.24	1.61	1.54
1	A	104	MET	SD-CE	-5.04	1.67	1.79

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	26	VAL	CB-CA-C	-6.47	103.54	112.02
1	A	108	VAL	CB-CA-C	-6.44	103.76	111.81
1	D	52	VAL	CB-CA-C	-6.03	101.21	110.50
1	C	84	PHE	CB-CA-C	-5.89	98.03	109.76
1	B	69	GLU	N-CA-CB	-5.79	101.61	111.69
1	B	191	VAL	CB-CA-C	-5.73	104.63	111.97
1	B	67	VAL	CB-CA-C	-5.37	105.13	111.09
1	A	26	VAL	CB-CA-C	-5.36	104.96	111.87
1	A	26	VAL	N-CA-CB	5.34	116.68	110.65

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	1787	0	1822	34	0
1	B	1791	0	1822	40	0
1	C	1788	0	1813	35	0
1	D	1799	0	1841	25	0
2	B	35	0	19	2	0
3	A	49	0	0	2	0
3	B	39	0	0	4	1
3	C	31	0	0	1	0
3	D	42	0	0	3	1
All	All	7361	0	7317	117	1

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 8.

All (117) 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:132:ILE:HD11	1:C:227:VAL:HG21	1.37	1.04
1:A:190:GLN:OE1	1:A:194:GLN:NE2	2.10	0.85
1:A:129:PHE:CD2	1:A:172:GLY:HA2	2.23	0.74
1:C:10:VAL:HG22	1:C:72:ILE:HB	1.75	0.69
1:A:182:LEU:HD23	1:A:182:LEU:O	1.94	0.67
1:D:87:GLU:OE2	3:D:277:HOH:O	2.12	0.67
1:A:213:LEU:HD11	1:A:226:ILE:HD13	1.76	0.66
1:A:146:MET:HE2	1:D:150:GLY:CA	2.27	0.65
1:C:213:LEU:HD11	1:C:226:ILE:HD13	1.78	0.64
1:C:112:LEU:HB3	1:C:113:PRO:HD3	1.79	0.63
1:A:71:ASP:OD1	1:A:118:LYS:NZ	2.32	0.61
1:B:95:GLU:O	1:B:99:SER:OG	2.19	0.60
1:B:129:PHE:O	1:B:132:ILE:HD12	2.02	0.60
1:B:13:LEU:HD13	1:B:56:LEU:HD21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ARG:O	1:A:181:GLU:HG3	2.02	0.59
1:A:146:MET:HE2	1:D:150:GLY:HA2	1.86	0.58
1:B:147:ALA:HB2	1:C:147:ALA:HB2	1.87	0.57
1:A:136:GLU:HG3	3:A:266:HOH:O	2.03	0.56
1:B:177:GLU:O	1:B:181:GLU:HG3	2.06	0.56
1:B:146:MET:HE2	1:C:150:GLY:HA2	1.86	0.56
1:C:129:PHE:CD1	1:C:172:GLY:HA2	2.40	0.56
1:B:129:PHE:CD1	1:B:172:GLY:HA2	2.41	0.56
1:B:86:ASP:OD2	3:B:289:HOH:O	2.18	0.55
1:B:187:LYS:O	1:B:191:VAL:HG23	2.06	0.55
1:B:114:ALA:O	1:B:118:LYS:HD3	2.07	0.55
1:A:235:PHE:CE2	1:A:237:LEU:O	2.59	0.54
1:B:16:SER:OG	2:B:256:NAD:O3B	2.22	0.54
1:C:19:ILE:CG2	1:C:126:ILE:HD13	2.37	0.54
1:D:129:PHE:CD1	1:D:172:GLY:HA2	2.42	0.54
1:C:61:ASP:OD1	1:C:61:ASP:N	2.32	0.54
1:C:229:ASP:OD2	1:C:233:SER:OG	2.25	0.54
1:B:192:GLU:CG	1:B:199:ARG:HA	2.38	0.53
1:B:146:MET:HE2	1:C:150:GLY:CA	2.39	0.53
1:D:10:VAL:HG22	1:D:72:ILE:HB	1.91	0.53
1:A:182:LEU:O	1:A:182:LEU:CD2	2.57	0.53
1:B:55:ASP:HB3	1:B:58:LYS:HG3	1.90	0.52
1:A:90:ASN:OD1	1:D:109:ARG:NH2	2.42	0.52
1:A:209:VAL:HG21	1:A:228:VAL:HG21	1.91	0.52
1:D:8:LYS:NZ	1:D:216:GLU:OE2	2.42	0.51
1:A:235:PHE:HZ	1:D:235:PHE:HZ	1.59	0.51
1:D:229:ASP:OD2	1:D:233:SER:OG	2.25	0.51
1:A:181:GLU:OE1	1:A:182:LEU:N	2.44	0.51
1:C:19:ILE:HG22	1:C:126:ILE:HD13	1.92	0.51
1:C:19:ILE:O	1:C:23:VAL:HG23	2.11	0.50
1:D:179:VAL:HG21	3:D:261:HOH:O	2.11	0.50
1:B:48:GLY:HA2	3:B:276:HOH:O	2.12	0.50
1:C:124:VAL:HG11	1:C:210:VAL:HG13	1.94	0.50
1:D:22:ALA:O	1:D:26:VAL:HG23	2.12	0.49
1:A:97:ILE:HG21	1:D:97:ILE:HG21	1.94	0.49
1:B:226:ILE:HD12	1:B:226:ILE:N	2.26	0.49
1:B:192:GLU:HG2	1:B:199:ARG:HA	1.94	0.48
1:A:185:GLU:O	1:A:189:LYS:HG2	2.13	0.48
1:B:109:ARG:HD3	3:B:263:HOH:O	2.12	0.48
1:C:101:PHE:CE1	1:C:105:ILE:HD11	2.47	0.48
1:C:101:PHE:CZ	1:C:105:ILE:HD11	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:LEU:HD23	1:C:103:ASN:HD22	1.79	0.47
1:C:175:GLU:HG3	1:C:200:MET:HB2	1.95	0.47
1:C:160:ALA:HB3	1:C:161:PRO:HD3	1.97	0.47
1:C:168:CYS:HB2	1:C:225:THR:OG1	2.15	0.47
1:A:10:VAL:HG22	1:A:72:ILE:HB	1.96	0.47
1:B:235:PHE:CD1	1:D:132:ILE:HG22	2.49	0.47
1:A:101:PHE:CE1	1:A:105:ILE:HD11	2.50	0.46
1:B:10:VAL:HG22	1:B:72:ILE:HB	1.98	0.46
1:A:236:PRO:HB2	1:C:146:MET:HE1	1.97	0.46
1:B:150:GLY:CA	1:C:146:MET:HE3	2.46	0.45
1:B:235:PHE:HZ	1:C:235:PHE:HZ	1.64	0.45
1:D:197:MET:HG3	1:D:230:GLY:O	2.15	0.45
1:A:10:VAL:HB	1:A:34:VAL:HG22	1.97	0.45
1:C:224:GLN:NE2	3:D:266:HOH:O	2.50	0.45
1:D:69:GLU:O	1:D:70:VAL:HG23	2.16	0.45
1:D:217:LYS:N	1:D:217:LYS:HD2	2.32	0.45
1:B:55:ASP:OD1	1:B:57:ARG:HD2	2.16	0.45
1:A:122:ARG:NH2	3:A:275:HOH:O	2.49	0.45
1:B:12:VAL:HG12	1:B:15:ALA:HB2	1.98	0.45
1:B:56:LEU:HD12	2:B:256:NAD:H2A	1.98	0.45
1:A:13:LEU:O	1:A:76:ASN:HB3	2.17	0.45
1:B:128:SER:HA	1:B:171:PRO:HD2	1.99	0.44
1:B:235:PHE:HA	1:B:236:PRO:HD3	1.86	0.44
1:A:129:PHE:HD2	1:A:172:GLY:HA2	1.75	0.44
1:B:142:ASN:O	1:B:146:MET:HG2	2.18	0.44
1:B:179:VAL:C	1:B:181:GLU:H	2.25	0.43
1:C:197:MET:HG3	1:C:230:GLY:O	2.19	0.43
1:A:88:LEU:O	1:D:109:ARG:NH1	2.51	0.43
1:C:169:VAL:HG21	1:C:210:VAL:HG22	2.00	0.43
1:A:220:TYR:CD2	1:B:201:ALA:HB2	2.53	0.43
1:C:129:PHE:CE2	1:C:232:LEU:HD23	2.53	0.43
1:D:171:PRO:HB3	1:D:206:ILE:HG21	2.00	0.43
1:D:179:VAL:C	1:D:181:GLU:H	2.26	0.43
1:C:199:ARG:HG3	1:C:199:ARG:HH11	1.84	0.43
1:B:97:ILE:HG21	1:C:97:ILE:HG21	2.00	0.42
1:D:235:PHE:CD1	1:D:236:PRO:HD2	2.54	0.42
1:B:19:ILE:O	1:B:23:VAL:HG23	2.19	0.42
1:C:60:LEU:HD23	1:C:60:LEU:HA	1.80	0.42
1:A:179:VAL:C	1:A:181:GLU:H	2.27	0.42
1:B:14:ALA:HB3	1:B:76:ASN:HD22	1.83	0.42
1:B:226:ILE:N	1:B:226:ILE:CD1	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:VAL:HG11	1:A:210:VAL:HG13	2.01	0.42
1:B:122:ARG:NH2	3:B:286:HOH:O	2.51	0.42
1:A:160:ALA:N	1:A:161:PRO:HD2	2.35	0.42
1:A:235:PHE:CD1	1:A:236:PRO:HD2	2.55	0.42
1:A:84:PHE:CE1	1:A:137:ASN:HB3	2.56	0.41
1:B:132:ILE:HG22	1:D:235:PHE:CE1	2.56	0.41
1:C:179:VAL:C	1:C:181:GLU:H	2.28	0.41
1:A:112:LEU:HB3	1:A:113:PRO:HD3	2.02	0.41
1:A:21:ARG:HA	1:A:21:ARG:HD2	1.90	0.41
1:A:61:ASP:OD1	1:A:61:ASP:N	2.53	0.41
1:B:101:PHE:CE1	1:B:105:ILE:HD11	2.55	0.41
1:C:90:ASN:HB3	3:C:255:HOH:O	2.20	0.41
1:D:112:LEU:N	1:D:113:PRO:CD	2.83	0.41
1:B:97:ILE:HD12	1:C:97:ILE:HD12	2.03	0.41
1:D:192:GLU:HG3	1:D:199:ARG:HA	2.02	0.41
1:B:122:ARG:NH1	1:B:215:SER:O	2.54	0.41
1:C:62:LEU:O	1:C:62:LEU:HD12	2.19	0.41
1:C:139:TYR:O	1:C:143:SER:OG	2.40	0.40
1:D:97:ILE:O	1:D:101:PHE:HB3	2.21	0.40
1:B:58:LYS:HB2	1:B:59:ASP:H	1.75	0.40
1:D:141:SER:O	1:D:145:ARG:HG3	2.22	0.40

All (1) 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)
3:B:263:HOH:O	3:D:279:HOH:O[3_645]	1.97	0.23

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	232/249 (93%)	223 (96%)	8 (3%)	1 (0%)	30	49
1	B	232/249 (93%)	220 (95%)	11 (5%)	1 (0%)	30	49
1	C	232/249 (93%)	219 (94%)	13 (6%)	0	100	100
1	D	232/249 (93%)	222 (96%)	10 (4%)	0	100	100
All	All	928/996 (93%)	884 (95%)	42 (4%)	2 (0%)	43	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	180	LYS
1	A	180	LYS

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	191/212 (90%)	176 (92%)	15 (8%)	11	24
1	B	192/212 (91%)	177 (92%)	15 (8%)	11	24
1	C	191/212 (90%)	167 (87%)	24 (13%)	4	9
1	D	193/212 (91%)	180 (93%)	13 (7%)	15	31
All	All	767/848 (90%)	700 (91%)	67 (9%)	9	21

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	37	CYS
1	A	42	GLU
1	A	53	VAL
1	A	60	LEU
1	A	68	LYS
1	A	70	VAL
1	A	177	GLU
1	A	180	LYS

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Mol	Chain	Res	Type
1	A	181	GLU
1	A	184	SER
1	A	186	GLU
1	A	192	GLU
1	A	208	SER
1	A	216	GLU
1	B	33	GLU
1	B	52	VAL
1	B	57	ARG
1	B	61	ASP
1	B	65	GLU
1	B	99	SER
1	B	117	GLU
1	B	118	LYS
1	B	122	ARG
1	B	132	ILE
1	B	178	ARG
1	B	185	GLU
1	B	194	GLN
1	B	200	MET
1	B	216	GLU
1	C	5	ILE
1	C	6	ARG
1	C	37	CYS
1	C	46	ARG
1	C	54	CYS
1	C	56	LEU
1	C	61	ASP
1	C	62	LEU
1	C	65	GLU
1	C	70	VAL
1	C	81	LYS
1	C	99	SER
1	C	117	GLU
1	C	118	LYS
1	C	132	ILE
1	C	143	SER
1	C	146	MET
1	C	178	ARG
1	C	182	LEU
1	C	190	GLN
1	C	208	SER

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Mol	Chain	Res	Type
1	C	216	GLU
1	C	225	THR
1	C	233	SER
1	D	42	GLU
1	D	54	CYS
1	D	66	LYS
1	D	70	VAL
1	D	116	LYS
1	D	122	ARG
1	D	132	ILE
1	D	178	ARG
1	D	184	SER
1	D	185	GLU
1	D	208	SER
1	D	217	LYS
1	D	219	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	B	194	GLN
1	C	190	GLN
1	C	194	GLN
1	D	76	ASN
1	D	190	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is 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	B	256	-	38,38,48	1.36	5 (13%)	53,58,73	1.88	14 (26%)

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	B	256	-	-	7/22/51/62	0/4/4/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	256	NAD	PN-O3	4.09	1.63	1.59
2	B	256	NAD	PA-O3	2.98	1.62	1.59
2	B	256	NAD	C2A-N1A	2.69	1.38	1.33
2	B	256	NAD	C8A-N7A	2.64	1.36	1.31
2	B	256	NAD	C2A-N3A	2.09	1.37	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	256	NAD	N3A-C2A-N1A	-6.37	118.93	128.58
2	B	256	NAD	C5A-C4A-N3A	-4.10	121.08	126.72
2	B	256	NAD	N9A-C8A-N7A	-3.83	108.50	113.94
2	B	256	NAD	C2A-N3A-C4A	3.59	120.61	111.83
2	B	256	NAD	C2B-C3B-C4B	2.95	108.32	102.61
2	B	256	NAD	C5A-N7A-C8A	2.93	108.05	103.45
2	B	256	NAD	N3A-C4A-N9A	2.80	131.92	127.17
2	B	256	NAD	C1D-C2D-C3D	2.75	106.03	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	256	NAD	O2N-PN-O3	2.41	113.79	107.27
2	B	256	NAD	O3B-C3B-C4B	-2.33	104.39	111.08
2	B	256	NAD	O2A-PA-O5B	2.33	118.11	107.57
2	B	256	NAD	O4D-C4D-C3D	2.17	106.64	104.63
2	B	256	NAD	O5B-C5B-C4B	2.08	116.07	108.99
2	B	256	NAD	C4A-N9A-C8A	2.02	107.86	105.74

There are no chirality outliers.

All (7) torsion outliers are listed below:

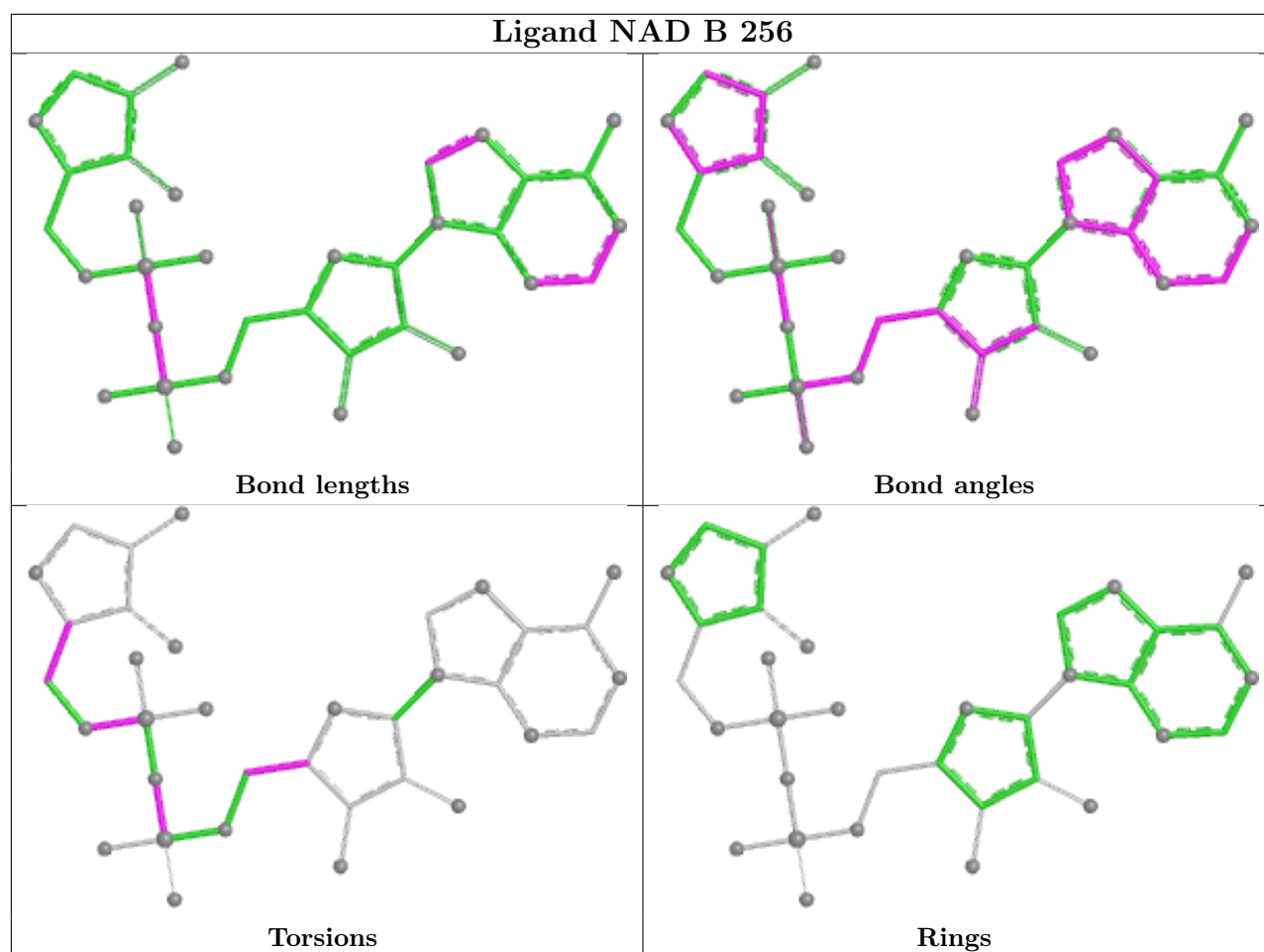
Mol	Chain	Res	Type	Atoms
2	B	256	NAD	C5D-O5D-PN-O1N
2	B	256	NAD	O4D-C4D-C5D-O5D
2	B	256	NAD	C3D-C4D-C5D-O5D
2	B	256	NAD	O4B-C4B-C5B-O5B
2	B	256	NAD	PN-O3-PA-O5B
2	B	256	NAD	C5D-O5D-PN-O3
2	B	256	NAD	C5D-O5D-PN-O2N

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	256	NAD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	234/249 (93%)	-0.21	2 (0%) 81 78	6, 14, 32, 41	0
1	B	234/249 (93%)	0.00	3 (1%) 75 71	6, 15, 31, 38	1 (0%)
1	C	234/249 (93%)	0.13	5 (2%) 63 59	5, 14, 37, 48	0
1	D	234/249 (93%)	-0.09	1 (0%) 88 86	7, 14, 28, 39	1 (0%)
All	All	936/996 (93%)	-0.04	11 (1%) 76 73	5, 14, 32, 48	2 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	4	GLY	4.0
1	B	186	GLU	3.0
1	A	4	GLY	3.0
1	C	182	LEU	2.7
1	D	182	LEU	2.6
1	B	4	GLY	2.6
1	A	54	CYS	2.6
1	C	179	VAL	2.4
1	C	184	SER	2.4
1	C	54	CYS	2.2
1	B	54	CYS	2.1

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](#)

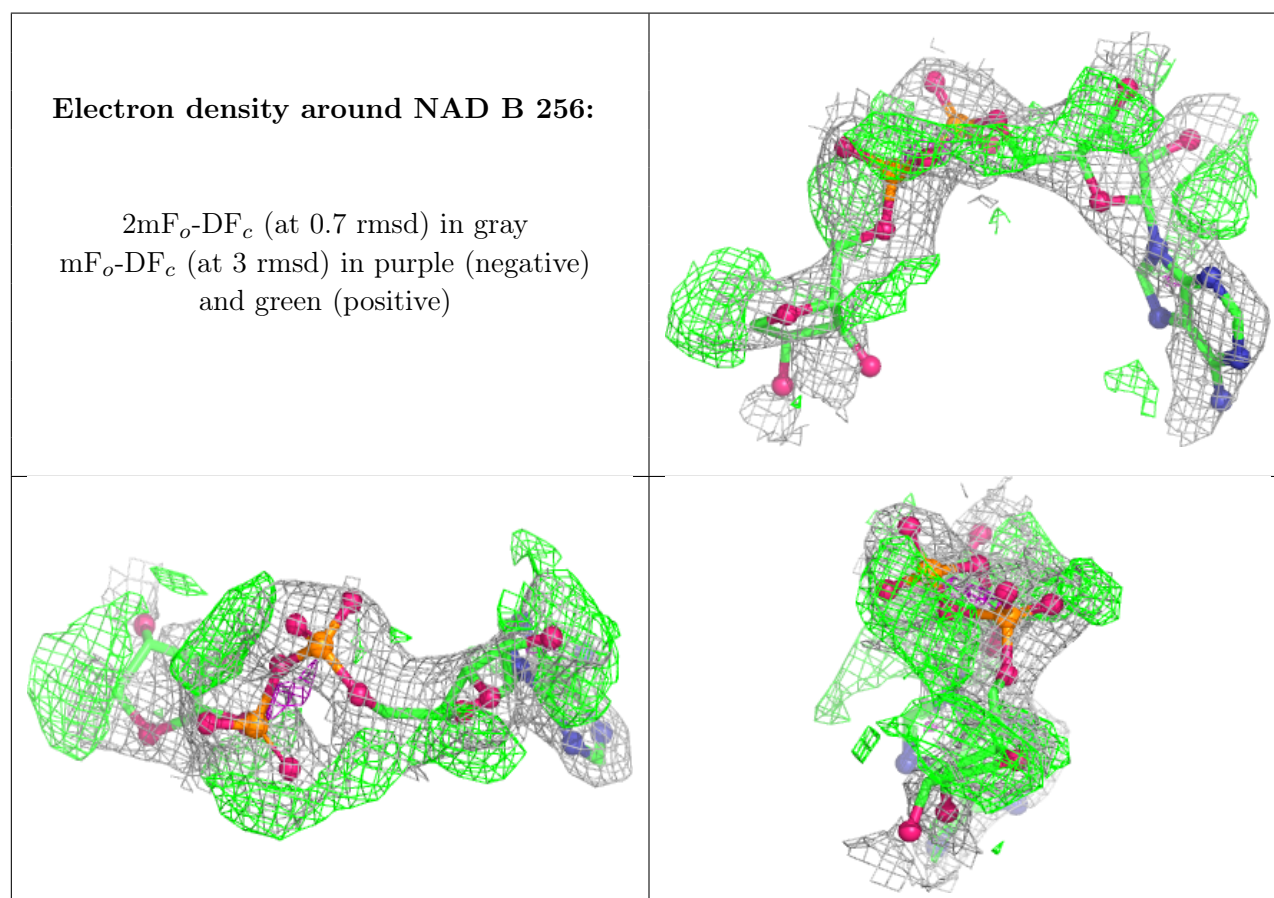
There are no oligosaccharides in this entry.

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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	B	256	35/44	0.75	0.19	15,17,20,20	35

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.