



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:15 PM GMT

PDB ID : 1O5I  
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](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 (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

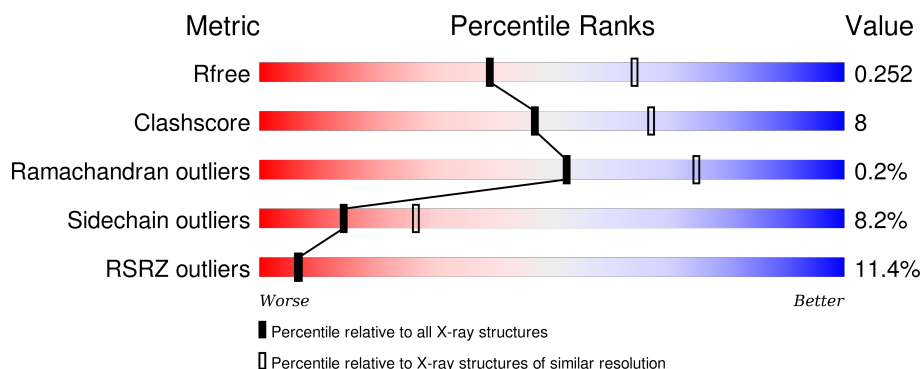
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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	249	<div> <div>8%</div> <div>71%</div> <div>22%</div> <div>6%</div> </div>
1	B	249	<div> <div>8%</div> <div>69%</div> <div>21%</div> <div>6%</div> </div>
1	C	249	<div> <div>16%</div> <div>68%</div> <div>23%</div> <div>6%</div> </div>
1	D	249	<div> <div>10%</div> <div>76%</div> <div>16%</div> <div>6%</div> </div>

## 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	-	LEADER SEQUENCE	UNP Q9X0Q1
A	-10	GLY	-	LEADER SEQUENCE	UNP Q9X0Q1
A	-9	SER	-	LEADER SEQUENCE	UNP Q9X0Q1
A	-8	ASP	-	LEADER SEQUENCE	UNP Q9X0Q1
A	-7	LYS	-	LEADER SEQUENCE	UNP Q9X0Q1
A	-6	ILE	-	LEADER SEQUENCE	UNP Q9X0Q1
A	-5	HIS	-	LEADER SEQUENCE	UNP Q9X0Q1
A	-4	HIS	-	LEADER SEQUENCE	UNP Q9X0Q1
A	-3	HIS	-	LEADER SEQUENCE	UNP Q9X0Q1
A	-2	HIS	-	LEADER SEQUENCE	UNP Q9X0Q1
A	-1	HIS	-	LEADER SEQUENCE	UNP Q9X0Q1
A	0	HIS	-	LEADER SEQUENCE	UNP Q9X0Q1
B	-11	MET	-	LEADER SEQUENCE	UNP Q9X0Q1
B	-10	GLY	-	LEADER SEQUENCE	UNP Q9X0Q1
B	-9	SER	-	LEADER SEQUENCE	UNP Q9X0Q1
B	-8	ASP	-	LEADER SEQUENCE	UNP Q9X0Q1
B	-7	LYS	-	LEADER SEQUENCE	UNP Q9X0Q1
B	-6	ILE	-	LEADER SEQUENCE	UNP Q9X0Q1
B	-5	HIS	-	LEADER SEQUENCE	UNP Q9X0Q1
B	-4	HIS	-	LEADER SEQUENCE	UNP Q9X0Q1
B	-3	HIS	-	LEADER SEQUENCE	UNP Q9X0Q1

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

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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

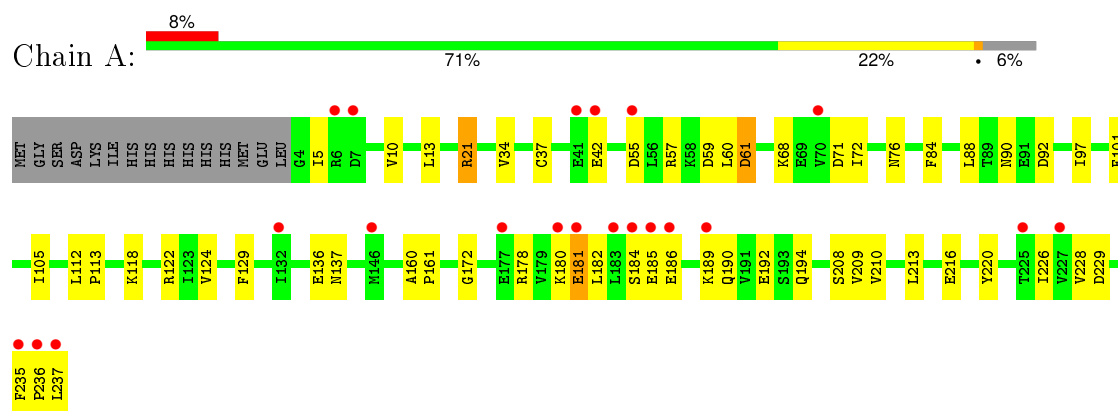
- Molecule 3 is water.

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		

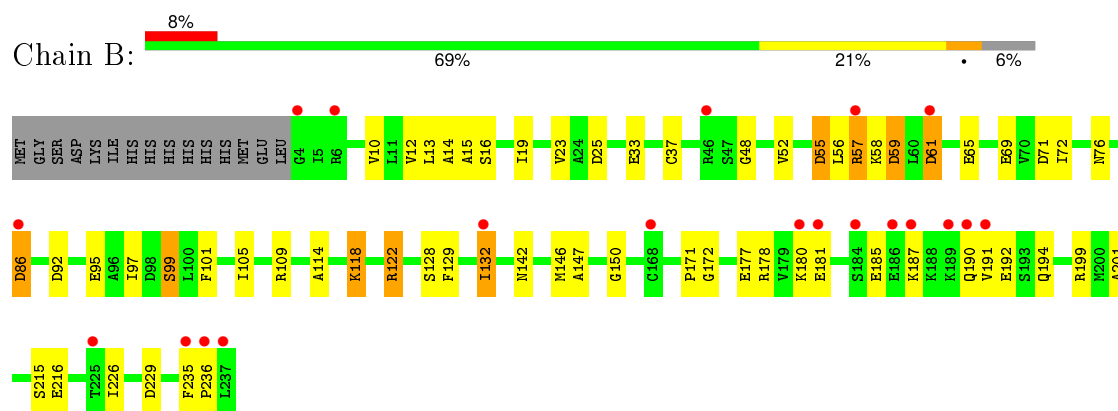
### 3 Residue-property plots [i](#)

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

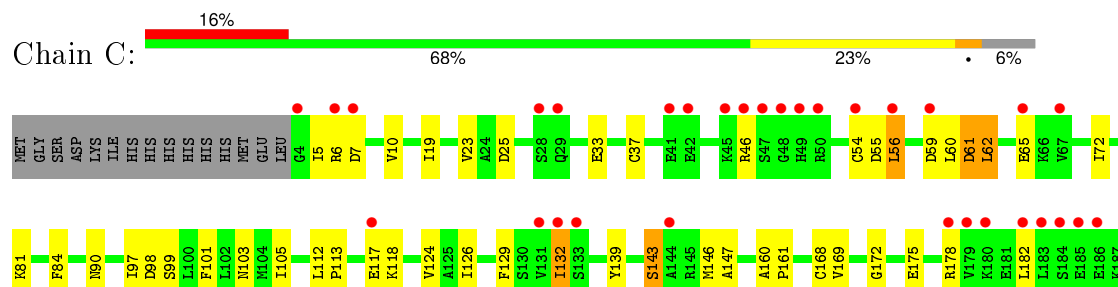
- Molecule 1: 3-oxoacyl-(acyl carrier protein) reductase



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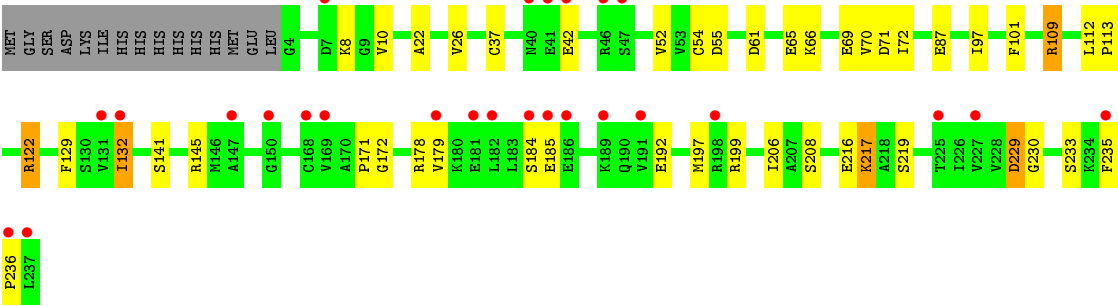
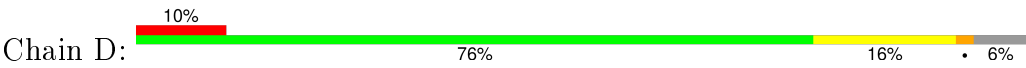


- Molecule 1: 3-oxoacyl-(acyl carrier protein) reductase





● Molecule 1: 3-oxoacyl-(acyl carrier protein) reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 85.1 (41.17-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.7	Xtriage
Anisotropy	1.018	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 49.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 31597 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7361	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.89	0/1814	0.95	6/2450 (0.2%)
1	B	0.86	1/1818 (0.1%)	0.96	9/2456 (0.4%)
1	C	0.79	0/1815	0.92	5/2453 (0.2%)
1	D	0.86	0/1826	0.99	9/2463 (0.4%)
All	All	0.85	1/7273 (0.0%)	0.95	29/9822 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	69	GLU	CA-CB	6.07	1.67	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	229	ASP	CB-CG-OD2	7.78	125.30	118.30
1	B	122	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	B	71	ASP	CB-CG-OD2	7.34	124.91	118.30
1	B	25	ASP	CB-CG-OD2	7.15	124.74	118.30
1	A	61	ASP	CB-CG-OD2	6.90	124.51	118.30
1	D	122	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	D	55	ASP	CB-CG-OD1	6.61	124.25	118.30
1	B	61	ASP	CB-CG-OD2	6.59	124.23	118.30
1	A	59	ASP	CB-CG-OD2	6.48	124.13	118.30
1	D	71	ASP	CB-CG-OD2	6.43	124.09	118.30
1	B	86	ASP	CB-CG-OD2	6.33	123.99	118.30
1	A	55	ASP	CB-CG-OD2	6.19	123.87	118.30
1	C	84	PHE	CB-CA-C	-6.18	98.03	110.40
1	C	7	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	92	ASP	CB-CG-OD2	6.08	123.78	118.30
1	D	109	ARG	NE-CZ-NH1	6.08	123.34	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	55	ASP	CB-CG-OD2	5.81	123.53	118.30
1	B	229	ASP	CB-CG-OD1	5.78	123.50	118.30
1	C	25	ASP	CB-CG-OD2	5.66	123.39	118.30
1	B	92	ASP	CB-CG-OD2	5.63	123.37	118.30
1	B	59	ASP	CB-CG-OD2	5.58	123.33	118.30
1	C	98	ASP	CB-CG-OD2	5.47	123.22	118.30
1	D	229	ASP	CB-CG-OD1	5.45	123.21	118.30
1	D	37	CYS	CA-CB-SG	5.45	123.80	114.00
1	D	52	VAL	CB-CA-C	-5.36	101.21	111.40
1	D	61	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	229	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	21	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	D	55	ASP	OD1-CG-OD2	-5.10	113.62	123.30

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	31	0
1	B	1791	0	1822	37	0
1	C	1788	0	1813	32	0
1	D	1799	0	1841	22	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	109	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 (109) 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: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:B:129:PHE:O	1:B:132:ILE:HD12	2.02	0.60
1:B:95:GLU:O	1:B:99:SER:OG	2.19	0.60
1:B:13:LEU:HD13	1:B:56:LEU:HD21	1.83	0.59
1:A:178:ARG:O	1:A:181:GLU:HG3	2.02	0.59
1:B:147:ALA:HB2	1:C:147:ALA:HB2	1.87	0.57
1:B:16:SER:OG	2:B:256:NAD:O3B	2.22	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: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:A:71:ASP:OD1	1:A:118:LYS:NZ	2.32	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: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:N	1:C:61:ASP:OD1	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:D:10:VAL:HG22	1:D:72:ILE:HB	1.91	0.53
1:A:182:LEU:CD2	1:A:182:LEU:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:B:226:ILE:HD12	2.26	0.49
1:B:192:GLU:HG2	1:B:199:ARG:HA	1.94	0.48
1:B:150:GLY:CA	1:C:146:MET:HE3	2.43	0.48
1:C:101:PHE:CE1	1:C:105:ILE:HD11	2.47	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:CZ	1:C:105:ILE:HD11	2.49	0.47
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: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:D:69:GLU:O	1:D:70:VAL:HG23	2.16	0.45
1:C:224:GLN:NE2	3:D:266:HOH:O	2.50	0.45
1:D:217:LYS:HD2	1:D:217:LYS:N	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: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:A:236:PRO:HB2	1:C:146:MET:HE1	2.00	0.43
1:C:199:ARG:HH11	1:C:199:ARG:HG3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:C:60:LEU:HD23	1.80	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
1:B:122:ARG:NH2	3:B:286:HOH:O	2.51	0.42
1:A:124:VAL:HG11	1:A:210:VAL:HG13	2.01	0.42
1:A:235:PHE:CD1	1:A:236:PRO:HD2	2.55	0.42
1:A:160:ALA:N	1:A:161:PRO:HD2	2.35	0.42
1:B:132:ILE:HG22	1:D:235:PHE:CE1	2.56	0.41
1:A:84:PHE:CE1	1:A:137:ASN:HB3	2.56	0.41
1:A:112:LEU:HB3	1:A:113:PRO:HD3	2.02	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:A:21:ARG:HD2	1:A:21:ARG:HA	1.90	0.41
1:A:61:ASP:N	1:A:61:ASP:OD1	2.53	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:D:97:ILE:O	1:D:101:PHE:HB3	2.21	0.40
1:C:139:TYR:O	1:C:143:SER:OG	2.40	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%)	39	61
1	B	232/249 (93%)	220 (95%)	11 (5%)	1 (0%)	39	61
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%)	52	75

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%)	179 (94%)	12 (6%)	22	40
1	B	192/212 (91%)	178 (93%)	14 (7%)	17	32
1	C	191/212 (90%)	166 (87%)	25 (13%)	5	9
1	D	193/212 (91%)	181 (94%)	12 (6%)	23	41
All	All	767/848 (90%)	704 (92%)	63 (8%)	14	27

All (63) 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	57	ARG
1	A	60	LEU
1	A	68	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	37	CYS
1	B	52	VAL
1	B	57	ARG
1	B	61	ASP
1	B	65	GLU
1	B	99	SER
1	B	118	LYS
1	B	132	ILE
1	B	178	ARG
1	B	185	GLU
1	B	190	GLN
1	B	194	GLN
1	B	216	GLU
1	C	5	ILE
1	C	6	ARG
1	C	33	GLU
1	C	37	CYS
1	C	46	ARG
1	C	54	CYS
1	C	55	ASP
1	C	56	LEU
1	C	59	ASP
1	C	61	ASP
1	C	62	LEU
1	C	65	GLU
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	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	65	GLU
1	D	66	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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	190	GLN
1	A	194	GLN
1	A	224	GLN
1	B	194	GLN
1	C	190	GLN
1	C	194	GLN
1	C	224	GLN
1	D	49	HIS
1	D	194	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

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	-	31,38,48	1.10	2 (6%)	39,58,73	2.47	5 (12%)

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	-	-	0/18/51/62	0/4/4/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	256	NAD	C2A-N1A	2.53	1.38	1.33
2	B	256	NAD	C2A-N3A	3.09	1.37	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	256	NAD	N3A-C2A-N1A	-13.01	118.93	128.89
2	B	256	NAD	C1B-N9A-C4A	-2.46	123.22	126.94
2	B	256	NAD	O3B-C3B-C4B	-2.22	104.39	111.05
2	B	256	NAD	C1D-C2D-C3D	2.72	106.03	101.64
2	B	256	NAD	C2B-C3B-C4B	2.78	108.32	102.61

There are no chirality outliers.

There are no torsion outliers.

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

## 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	234/249 (93%)	0.53	21 (8%)	12 12	6, 14, 32, 41	0
1	B	234/249 (93%)	0.55	20 (8%)	13 14	6, 15, 31, 38	1 (0%)
1	C	234/249 (93%)	1.01	40 (17%)	2 2	5, 14, 37, 48	0
1	D	234/249 (93%)	0.67	26 (11%)	7 7	7, 14, 28, 39	1 (0%)
All	All	936/996 (93%)	0.69	107 (11%)	7 6	5, 14, 32, 48	2 (0%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	179	VAL	6.6
1	B	237	LEU	5.5
1	C	237	LEU	5.3
1	C	132	ILE	4.9
1	B	186	GLU	4.7
1	D	42	GLU	4.7
1	A	180	LYS	4.6
1	C	186	GLU	4.5
1	C	178	ARG	4.5
1	A	181	GLU	4.2
1	A	183	LEU	4.2
1	A	177	GLU	4.1
1	D	182	LEU	4.1
1	A	185	GLU	4.0
1	C	184	SER	4.0
1	D	46	ARG	4.0
1	C	185	GLU	4.0
1	C	235	PHE	4.0
1	C	47	SER	4.0
1	C	236	PRO	3.9
1	B	57	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	190	GLN	3.9
1	B	61	ASP	3.8
1	D	179	VAL	3.7
1	C	182	LEU	3.7
1	B	184	SER	3.6
1	C	29	GLN	3.5
1	A	132	ILE	3.4
1	C	59	ASP	3.4
1	C	6	ARG	3.3
1	B	180	LYS	3.3
1	A	235	PHE	3.3
1	C	131	VAL	3.2
1	C	65	GLU	3.2
1	C	56	LEU	3.1
1	A	42	GLU	3.1
1	C	54	CYS	3.1
1	C	42	GLU	3.0
1	A	237	LEU	3.0
1	D	198	ARG	3.0
1	C	45	LYS	2.9
1	C	4	GLY	2.9
1	A	236	PRO	2.9
1	D	235	PHE	2.8
1	A	227	VAL	2.8
1	D	150	GLY	2.7
1	D	47	SER	2.7
1	C	225	THR	2.7
1	C	117	GLU	2.7
1	C	41	GLU	2.7
1	B	236	PRO	2.7
1	A	55	ASP	2.6
1	D	185	GLU	2.6
1	C	183	LEU	2.6
1	A	7	ASP	2.6
1	C	50	ARG	2.6
1	C	227	VAL	2.6
1	D	40	ASN	2.5
1	C	28	SER	2.5
1	D	236	PRO	2.5
1	B	190	GLN	2.5
1	D	131	VAL	2.5
1	B	132	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	49	HIS	2.5
1	D	184	SER	2.5
1	D	7	ASP	2.5
1	A	189	LYS	2.5
1	C	226	ILE	2.5
1	D	189	LYS	2.5
1	D	132	ILE	2.5
1	B	86	ASP	2.4
1	D	227	VAL	2.4
1	B	181	GLU	2.4
1	D	225	THR	2.4
1	C	180	LYS	2.3
1	D	237	LEU	2.3
1	C	7	ASP	2.3
1	D	168	CYS	2.3
1	A	146	MET	2.3
1	D	186	GLU	2.3
1	B	189	LYS	2.3
1	B	235	PHE	2.3
1	D	147	ALA	2.2
1	C	133	SER	2.2
1	B	4	GLY	2.2
1	B	46	ARG	2.2
1	C	67	VAL	2.2
1	A	186	GLU	2.2
1	C	46	ARG	2.2
1	D	181	GLU	2.2
1	A	6	ARG	2.2
1	C	193	SER	2.2
1	A	70	VAL	2.2
1	A	184	SER	2.2
1	D	191	VAL	2.1
1	B	168	CYS	2.1
1	D	169	VAL	2.1
1	B	191	VAL	2.1
1	A	41	GLU	2.1
1	C	188	LYS	2.1
1	A	225	THR	2.1
1	C	48	GLY	2.1
1	D	41	GLU	2.1
1	B	187	LYS	2.1
1	B	6	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	144	ALA	2.0
1	B	225	THR	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( $\text{\AA}^2$ )	Q<0.9
2	NAD	B	256	35/44	0.77	0.30	1.50	15,17,20,20	35

## 6.5 Other polymers [i](#)

There are no such residues in this entry.