



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 04:03 pm GMT

PDB ID : 2NQ8  
Title : Malarial enoyl acyl ACP reductase bound with INH-NAD adduct  
Authors : Freundlich, J.S.; Yu, M.; Lucumi, E.; Kuo, M.; Tsai, H.C.; Valderramos, J.C.; Karagyoov, L.; Jacobs Jr., W.R.; Schiehser, G.A.; Fidock, D.A.; Jacobus, D.P.; Sacchettini, J.C.  
Deposited on : 2006-10-30  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

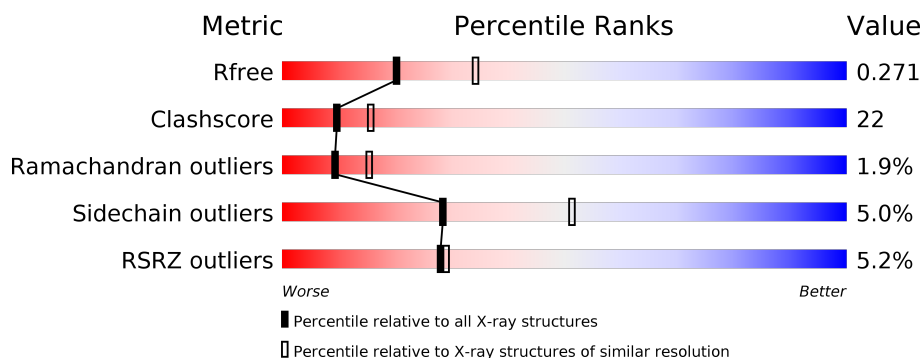
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	229	<div> <div>4%</div> <div> <div></div> <div>62%</div> <div>34%</div> <div>•</div> </div> </div>
1	B	229	<div> <div>5%</div> <div> <div></div> <div>61%</div> <div>36%</div> <div>•</div> </div> </div>
2	C	60	<div> <div>8%</div> <div> <div></div> <div>60%</div> <div>37%</div> <div>•</div> </div> </div>
2	D	60	<div> <div>7%</div> <div> <div></div> <div>67%</div> <div>27%</div> <div>7%</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4842 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.

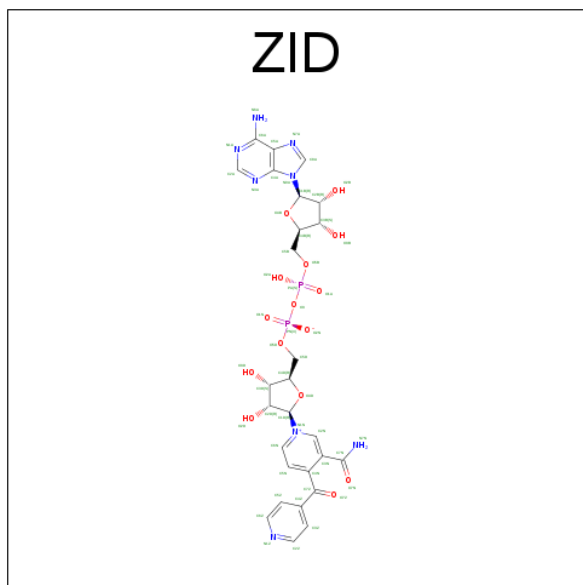
- Molecule 1 is a protein called Enoyl-acyl carrier reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1807	1148	309	340	10			
1	B	229	Total	C	N	O	S	0	0	0
			1807	1148	309	340	10			

- Molecule 2 is a protein called Enoyl-acyl carrier reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	60	Total	C	N	O	S	0	0	0
			482	310	75	96	1			
2	D	60	Total	C	N	O	S	0	0	0
			482	310	75	96	1			

- Molecule 3 is ISONICOTINIC-ACETYL-NICOTINAMIDE-ADENINE DINUCLEOTIDE (three-letter code: ZID) (formula:  $C_{27}H_{30}N_8O_{15}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			52	27	8	15	2		
3	A	1	Total	C	N	O	P	0	0
			52	27	8	15	2		

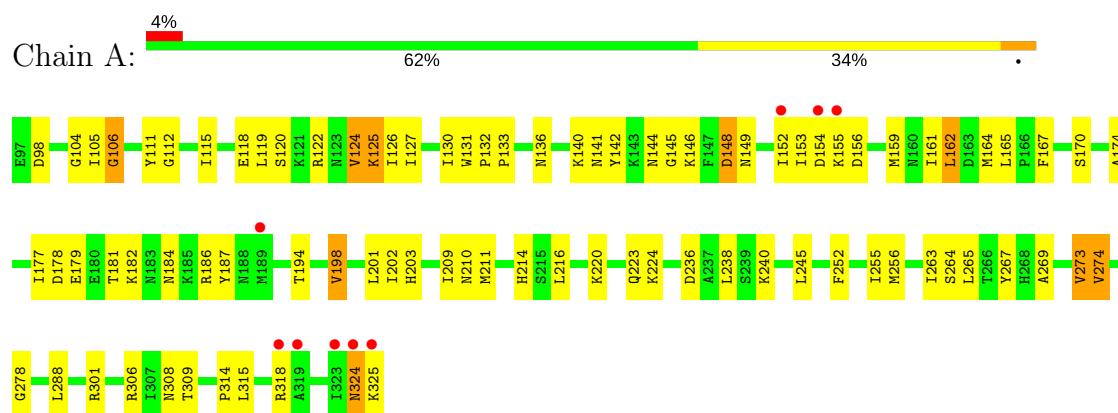
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total	O	0	0
			52	52		
4	B	58	Total	O	0	0
			58	58		
4	C	26	Total	O	0	0
			26	26		
4	D	24	Total	O	0	0
			24	24		

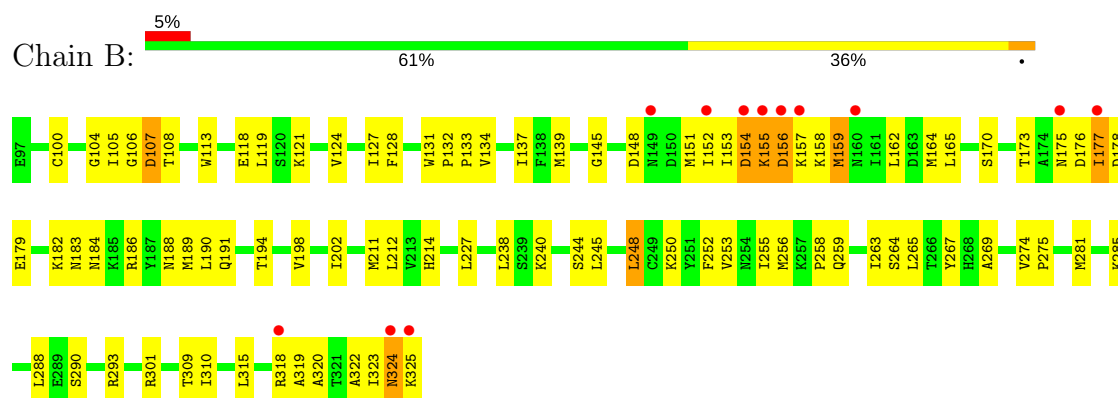
### 3 Residue-property plots

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.

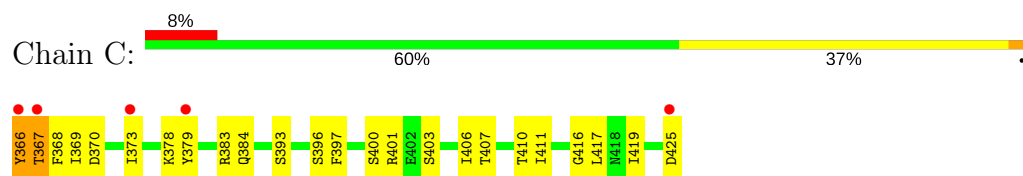
#### • Molecule 1: Enoyl-acyl carrier reductase



#### • Molecule 1: Enoyl-acyl carrier reductase

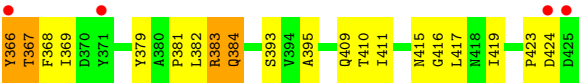


#### • Molecule 2: Enoyl-acyl carrier reductase



#### • Molecule 2: Enoyl-acyl carrier reductase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.90Å 131.90Å 82.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.15 – 2.50 70.15 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.5 (70.15-2.50) 93.3 (70.15-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.50 (at 2.48Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.216 , 0.272 0.215 , 0.271	Depositor DCC
$R_{free}$ test set	2379 reflections (9.84%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.0	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 52.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4842	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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:  
ZID

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	0.36	0/1840	0.59	0/2477
1	B	0.36	0/1840	0.60	0/2477
2	C	0.38	0/491	0.63	0/664
2	D	0.41	0/491	0.63	0/664
All	All	0.37	0/4662	0.60	0/6282

There are no bond length outliers.

There are no bond angle outliers.

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	1807	0	1824	89	0
1	B	1807	0	1824	85	0
2	C	482	0	473	25	0
2	D	482	0	473	28	0
3	A	52	0	27	4	0
3	B	52	0	27	7	0
4	A	52	0	0	3	0
4	B	58	0	0	5	0
4	C	26	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	24	0	0	2	0
All	All	4842	0	4648	201	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 22.

All (201) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:LEU:H	3:B:450:ZID:H72N	1.22	0.86
1:B:183:ASN:C	1:B:188:ASN:HD21	1.79	0.85
1:B:325:LYS:H	2:D:367:THR:HA	1.49	0.77
2:D:383:ARG:HH11	2:D:383:ARG:HG3	1.51	0.76
1:A:252:PHE:O	1:A:256:MET:HG3	1.87	0.75
1:B:127:ILE:HD13	1:B:202:ILE:HD12	1.68	0.75
1:B:212:LEU:HD21	1:B:248:LEU:HD13	1.68	0.74
1:B:177:ILE:HD11	1:B:182:LYS:HD2	1.69	0.73
1:A:184:ASN:HD22	1:A:187:TYR:HD1	1.37	0.72
2:C:366:TYR:O	2:C:370:ASP:HB2	1.90	0.71
1:A:127:ILE:HD11	1:A:162:LEU:HD13	1.72	0.71
1:B:139:MET:SD	1:B:164:MET:HE2	2.31	0.70
1:A:136:ASN:HD22	1:A:186:ARG:HH21	1.38	0.69
1:A:132:PRO:HB2	1:A:133:PRO:HD3	1.74	0.68
1:A:174:ALA:O	1:A:177:ILE:HG22	1.92	0.68
1:B:274:VAL:O	1:B:274:VAL:HG23	1.94	0.68
1:A:324:ASN:HD22	2:C:367:THR:HG22	1.59	0.67
2:C:383:ARG:HD3	4:C:140:HOH:O	1.95	0.67
1:B:183:ASN:CA	1:B:188:ASN:HD21	2.09	0.65
1:A:153:ILE:HD11	1:A:159:MET:HB2	1.79	0.65
1:B:170:SER:OG	1:B:240:LYS:HE2	1.95	0.65
1:B:131:TRP:HB2	3:B:450:ZID:N3A	2.11	0.65
1:A:325:LYS:HB3	2:C:368:PHE:HB2	1.77	0.65
1:B:318:ARG:HH11	1:B:318:ARG:HG2	1.60	0.65
1:B:119:LEU:HB3	1:B:124:VAL:CG2	2.26	0.64
1:A:136:ASN:HD22	1:A:186:ARG:NH2	1.96	0.63
1:B:301:ARG:NH2	2:C:379:TYR:HA	2.14	0.63
2:C:416:GLY:O	2:C:419:ILE:HG12	1.99	0.62
1:B:288:LEU:HA	4:B:456:HOH:O	1.99	0.62
1:B:301:ARG:HH21	2:C:379:TYR:HA	1.64	0.62
2:D:424:ASP:HB2	4:D:126:HOH:O	1.99	0.62
1:A:149:ASN:O	1:A:152:ILE:HG12	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:407:THR:HG21	2:D:382:LEU:CD2	2.29	0.61
1:A:127:ILE:CD1	1:A:162:LEU:HB3	2.31	0.61
1:A:274:VAL:O	1:A:274:VAL:HG22	2.02	0.60
1:A:98:ASP:HB3	1:A:211:MET:HE3	1.82	0.60
1:A:131:TRP:HB2	3:A:550:ZID:N3A	2.17	0.59
1:B:267:TYR:HB2	3:B:450:ZID:H5N	1.83	0.59
2:D:416:GLY:O	2:D:419:ILE:HG12	2.02	0.59
1:A:159:MET:HE2	1:A:161:ILE:HD11	1.83	0.59
1:B:244:SER:O	1:B:248:LEU:HB2	2.02	0.59
1:B:145:GLY:HA2	1:B:148:ASP:OD1	2.03	0.59
1:B:173:THR:O	1:B:176:ASP:HB2	2.03	0.58
1:A:130:ILE:HD12	1:A:130:ILE:N	2.18	0.58
2:D:383:ARG:HG3	2:D:383:ARG:NH1	2.19	0.58
1:A:105:ILE:HD11	1:A:112:GLY:HA3	1.85	0.58
1:B:177:ILE:HD13	1:B:177:ILE:O	2.03	0.58
2:C:369:ILE:O	2:C:373:ILE:HG22	2.04	0.58
1:A:178:ASP:O	1:A:182:LYS:HG3	2.04	0.57
2:C:383:ARG:HG3	4:C:124:HOH:O	2.05	0.57
1:B:134:VAL:HG12	4:B:489:HOH:O	2.04	0.57
1:B:324:ASN:HA	2:D:367:THR:OG1	2.04	0.57
1:A:301:ARG:NH2	2:D:379:TYR:HA	2.19	0.56
1:A:301:ARG:HH21	2:D:379:TYR:HA	1.71	0.56
1:B:119:LEU:HB3	1:B:124:VAL:HG22	1.87	0.56
1:B:184:ASN:ND2	1:B:186:ARG:H	2.04	0.56
2:D:367:THR:HG22	2:D:369:ILE:H	1.70	0.55
1:A:273:VAL:HA	4:A:566:HOH:O	2.05	0.55
1:A:181:THR:HA	1:A:184:ASN:HB2	1.89	0.55
1:B:105:ILE:HD12	1:B:128:PHE:CD1	2.42	0.55
1:A:154:ASP:O	1:A:156:ASP:N	2.40	0.54
1:A:301:ARG:HH21	2:D:379:TYR:C	2.11	0.54
1:A:198:VAL:O	1:A:202:ILE:HG12	2.08	0.54
1:B:275:PRO:HA	4:B:477:HOH:O	2.07	0.53
1:B:131:TRP:CG	1:B:133:PRO:HD2	2.44	0.53
1:B:155:LYS:C	1:B:157:LYS:H	2.12	0.53
1:A:209:ILE:O	1:A:256:MET:HA	2.08	0.53
1:B:252:PHE:O	1:B:256:MET:HG3	2.09	0.53
1:B:104:GLY:O	3:B:450:ZID:H52A	2.08	0.53
2:D:367:THR:HG22	2:D:369:ILE:HG22	1.91	0.53
1:B:245:LEU:HD22	1:B:288:LEU:HD11	1.91	0.52
1:B:183:ASN:HA	1:B:188:ASN:HD21	1.73	0.52
1:A:127:ILE:HD13	1:A:162:LEU:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ASP:O	1:B:158:LYS:NZ	2.38	0.52
1:A:263:ILE:HA	1:A:308:ASN:O	2.09	0.52
2:C:401:ARG:HD2	4:C:117:HOH:O	2.10	0.52
1:B:263:ILE:CD1	2:D:395:ALA:HB1	2.40	0.52
1:A:122:ARG:NH2	4:A:560:HOH:O	2.42	0.52
1:B:177:ILE:HD11	1:B:182:LYS:CD	2.36	0.52
1:A:318:ARG:HH11	1:A:318:ARG:HG2	1.75	0.51
1:A:152:ILE:HG13	1:A:152:ILE:O	2.10	0.51
1:A:154:ASP:C	1:A:156:ASP:H	2.13	0.51
1:A:126:ILE:HD12	1:A:126:ILE:N	2.25	0.51
1:A:165:LEU:HD12	1:A:202:ILE:HD11	1.91	0.51
1:A:203:HIS:HB2	1:A:255:ILE:HG21	1.91	0.51
1:B:318:ARG:HG2	1:B:318:ARG:NH1	2.26	0.51
1:A:119:LEU:HB3	1:A:124:VAL:HG22	1.92	0.50
1:B:108:THR:HG22	1:B:113:TRP:CE3	2.47	0.50
1:B:309:THR:HG23	2:D:410:THR:HA	1.93	0.50
1:A:118:GLU:HG3	2:C:393:SER:N	2.27	0.50
1:B:177:ILE:HD11	1:B:182:LYS:NZ	2.26	0.50
2:D:409:GLN:HB2	2:D:411:ILE:HD11	1.93	0.50
1:A:111:TYR:O	1:A:115:ILE:HG13	2.12	0.50
1:B:325:LYS:CB	2:D:368:PHE:HB2	2.41	0.50
1:A:170:SER:HB3	1:A:240:LYS:HE2	1.94	0.49
1:A:127:ILE:HD11	1:A:162:LEU:HB3	1.95	0.48
1:A:127:ILE:HG21	1:A:202:ILE:CD1	2.43	0.48
1:A:98:ASP:HB3	1:A:210:ASN:HD21	1.78	0.48
1:B:267:TYR:CE2	1:B:269:ALA:HB2	2.49	0.48
1:A:223:GLN:HB2	4:A:575:HOH:O	2.13	0.48
1:A:314:PRO:HD3	3:A:550:ZID:H6Z	1.95	0.47
1:A:124:VAL:O	1:A:126:ILE:HD12	2.14	0.47
1:B:121:LYS:HG2	1:B:153:ILE:HG21	1.95	0.47
1:B:152:ILE:HG12	1:B:158:LYS:HZ2	1.79	0.47
2:D:367:THR:CG2	2:D:369:ILE:HG22	2.45	0.47
1:A:119:LEU:HB3	1:A:124:VAL:CG2	2.44	0.47
1:A:111:TYR:CE1	1:A:315:LEU:HD22	2.49	0.47
2:C:379:TYR:HE1	2:C:425:ASP:HB3	1.78	0.47
1:A:214:HIS:O	1:A:264:SER:HA	2.15	0.47
2:C:407:THR:HG21	2:D:382:LEU:HD21	1.97	0.47
1:A:194:THR:O	1:A:198:VAL:HG13	2.14	0.47
1:A:105:ILE:CG2	1:A:106:GLY:N	2.77	0.46
1:B:113:TRP:CH2	1:B:151:MET:HG2	2.50	0.46
1:A:224:LYS:O	1:A:278:GLY:HA3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:THR:O	1:B:198:VAL:HG22	2.16	0.46
1:B:252:PHE:CD1	1:B:255:ILE:HD11	2.50	0.46
1:A:141:ASN:HB3	1:A:146:LYS:HB2	1.96	0.46
1:B:325:LYS:HB2	2:D:368:PHE:HB2	1.97	0.46
1:B:191:GLN:HB2	4:B:505:HOH:O	2.14	0.46
1:B:258:PRO:O	1:B:259:GLN:HB2	2.16	0.46
1:B:214:HIS:O	1:B:264:SER:HA	2.14	0.46
2:C:397:PHE:CZ	2:C:403:SER:HB3	2.51	0.46
1:B:198:VAL:O	1:B:202:ILE:HG12	2.16	0.46
1:A:131:TRP:CG	1:A:133:PRO:HD2	2.50	0.46
1:B:118:GLU:HG3	2:D:393:SER:N	2.31	0.46
1:A:122:ARG:NH1	2:C:400:SER:HB3	2.30	0.45
1:B:274:VAL:O	1:B:274:VAL:CG2	2.63	0.45
1:B:165:LEU:HB3	4:B:480:HOH:O	2.15	0.45
1:B:127:ILE:CD1	1:B:202:ILE:HD12	2.43	0.45
1:B:127:ILE:HG21	1:B:202:ILE:CD1	2.46	0.45
1:B:158:LYS:O	1:B:159:MET:C	2.54	0.45
1:B:153:ILE:O	1:B:154:ASP:C	2.55	0.45
2:D:409:GLN:HB2	2:D:411:ILE:CD1	2.47	0.45
1:B:127:ILE:HG21	1:B:202:ILE:HD11	1.98	0.45
1:A:140:LYS:HG2	1:A:144:ASN:ND2	2.32	0.44
1:B:315:LEU:N	3:B:450:ZID:H72N	2.01	0.44
1:B:245:LEU:HD22	1:B:288:LEU:CD1	2.47	0.44
1:A:179:GLU:HA	1:A:182:LYS:HD3	1.99	0.44
2:D:366:TYR:CD2	2:D:366:TYR:N	2.86	0.44
2:D:411:ILE:HD12	2:D:411:ILE:N	2.32	0.44
1:A:127:ILE:HG21	1:A:202:ILE:HD12	1.99	0.44
1:B:127:ILE:HD13	1:B:202:ILE:CD1	2.43	0.44
1:B:189:MET:HG3	1:B:190:LEU:HG	1.99	0.44
1:B:319:ALA:HB2	3:B:450:ZID:O1A	2.17	0.44
1:B:106:GLY:O	1:B:107:ASP:HB3	2.18	0.44
1:B:319:ALA:O	1:B:322:ALA:HB3	2.18	0.44
2:D:381:PRO:HD2	2:D:415:ASN:O	2.17	0.44
1:A:267:TYR:CE2	1:A:269:ALA:HB2	2.52	0.44
1:B:179:GLU:O	1:B:182:LYS:HB3	2.17	0.43
1:B:250:LYS:O	1:B:253:VAL:HG12	2.18	0.43
1:B:290:SER:HA	1:B:293:ARG:NH2	2.33	0.43
1:A:131:TRP:CE2	1:A:133:PRO:HG2	2.54	0.43
1:A:220:LYS:HG3	1:A:236:ASP:OD1	2.18	0.43
1:A:153:ILE:O	1:A:154:ASP:C	2.56	0.43
2:D:366:TYR:O	2:D:367:THR:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:VAL:O	1:A:274:VAL:CG2	2.66	0.43
1:B:267:TYR:HB2	3:B:450:ZID:C5N	2.49	0.43
1:B:265:LEU:HD13	1:B:310:ILE:HB	2.01	0.43
1:A:324:ASN:ND2	2:C:367:THR:HG22	2.30	0.43
2:C:366:TYR:N	2:C:366:TYR:CD2	2.86	0.43
1:A:156:ASP:O	1:A:156:ASP:OD1	2.36	0.43
1:A:120:SER:OG	1:A:159:MET:HG3	2.19	0.43
1:A:301:ARG:HH21	2:D:379:TYR:CA	2.31	0.43
1:A:125:LYS:C	1:A:126:ILE:HD12	2.39	0.43
1:A:318:ARG:NH1	1:A:318:ARG:HG2	2.34	0.43
1:A:306:ARG:HD2	2:C:406:ILE:O	2.18	0.42
2:C:379:TYR:CE1	2:C:425:ASP:HB3	2.53	0.42
1:A:104:GLY:HA3	1:A:216:LEU:HB3	2.00	0.42
1:A:216:LEU:HD12	1:A:216:LEU:C	2.39	0.42
1:B:269:ALA:HB1	1:B:274:VAL:HG22	2.01	0.42
2:D:383:ARG:CG	2:D:383:ARG:NH1	2.83	0.42
1:A:105:ILE:HA	1:A:105:ILE:HD13	1.87	0.42
1:A:153:ILE:HD11	1:A:159:MET:CB	2.47	0.42
1:B:293:ARG:HD3	4:D:73:HOH:O	2.18	0.42
1:A:98:ASP:CB	1:A:210:ASN:HD21	2.32	0.42
1:A:142:TYR:CD2	1:A:164:MET:HE1	2.55	0.42
1:A:267:TYR:HB2	3:A:550:ZID:H5N	2.01	0.42
1:B:154:ASP:C	1:B:156:ASP:H	2.23	0.41
1:B:153:ILE:HB	1:B:157:LYS:HB2	2.02	0.41
2:D:384:GLN:HE21	2:D:384:GLN:HB3	1.72	0.41
1:B:269:ALA:HB2	1:B:274:VAL:HG21	2.02	0.41
1:B:281:MET:O	1:B:285:LYS:HG2	2.20	0.41
1:A:177:ILE:HG23	1:A:177:ILE:O	2.21	0.41
1:B:119:LEU:HB3	1:B:124:VAL:HG21	1.98	0.41
1:A:124:VAL:O	1:A:126:ILE:CD1	2.69	0.41
1:A:265:LEU:HB3	3:A:550:ZID:H1D	2.02	0.41
1:A:140:LYS:O	1:A:141:ASN:C	2.58	0.41
1:A:132:PRO:HD3	1:A:167:PHE:O	2.20	0.41
1:A:309:THR:CG2	2:C:410:THR:HA	2.50	0.41
1:B:131:TRP:CD1	1:B:132:PRO:HD2	2.55	0.41
1:B:301:ARG:NH2	2:C:378:LYS:O	2.54	0.41
1:A:122:ARG:CZ	2:C:396:SER:OG	2.69	0.41
1:A:122:ARG:NE	2:C:396:SER:OG	2.54	0.41
1:B:320:ALA:O	1:B:323:ILE:HG12	2.20	0.40
1:A:245:LEU:HD22	1:A:288:LEU:CD1	2.51	0.40
1:A:122:ARG:NH1	2:C:396:SER:O	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ALA:CB	1:A:274:VAL:HG13	2.51	0.40
1:B:100:CYS:HB2	1:B:211:MET:HB2	2.03	0.40
1:A:145:GLY:HA2	1:A:148:ASP:OD1	2.22	0.40
1:B:155:LYS:O	1:B:157:LYS:N	2.52	0.40
1:B:178:ASP:O	1:B:182:LYS:HB2	2.22	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	227/229 (99%)	208 (92%)	16 (7%)	3 (1%)	14	25
1	B	227/229 (99%)	206 (91%)	16 (7%)	5 (2%)	8	12
2	C	58/60 (97%)	53 (91%)	4 (7%)	1 (2%)	11	18
2	D	58/60 (97%)	52 (90%)	4 (7%)	2 (3%)	4	5
All	All	570/578 (99%)	519 (91%)	40 (7%)	11 (2%)	9	15

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	LYS
1	A	324	ASN
2	C	367	THR
2	D	367	THR
1	B	159	MET
1	B	324	ASN
2	D	423	PRO
1	A	106	GLY
1	B	107	ASP
1	B	155	LYS

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Mol	Chain	Res	Type
1	B	154	ASP

### 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	197/197 (100%)	188 (95%)	9 (5%)	31	55
1	B	197/197 (100%)	189 (96%)	8 (4%)	35	61
2	C	53/53 (100%)	49 (92%)	4 (8%)	16	29
2	D	53/53 (100%)	49 (92%)	4 (8%)	16	29
All	All	500/500 (100%)	475 (95%)	25 (5%)	28	51

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	VAL
1	A	125	LYS
1	A	148	ASP
1	A	162	LEU
1	A	198	VAL
1	A	201	LEU
1	A	238	LEU
1	A	273	VAL
1	A	274	VAL
1	B	137	ILE
1	B	156	ASP
1	B	162	LEU
1	B	175	ASN
1	B	177	ILE
1	B	227	LEU
1	B	238	LEU
1	B	248	LEU
2	C	366	TYR
2	C	384	GLN
2	C	411	ILE

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Mol	Chain	Res	Type
2	C	417	LEU
2	D	366	TYR
2	D	383	ARG
2	D	384	GLN
2	D	417	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	ASN
1	A	160	ASN
1	A	188	ASN
1	A	200	ASN
1	A	203	HIS
1	A	210	ASN
1	A	228	ASN
1	A	254	ASN
1	A	302	ASN
1	A	324	ASN
1	B	183	ASN
1	B	184	ASN
1	B	188	ASN
1	B	200	ASN
1	B	259	GLN
1	B	302	ASN
2	C	384	GLN
2	D	384	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

2 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
3	ZID	A	550	-	50,57,57	2.24	14 (28%)	55,86,86	3.59	20 (36%)
3	ZID	B	450	-	50,57,57	2.09	15 (30%)	55,86,86	3.46	18 (32%)

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
3	ZID	A	550	-	-	0/30/70/70	0/6/6/6
3	ZID	B	450	-	-	0/30/70/70	0/6/6/6

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	450	ZID	C6A-N6A	-4.15	1.17	1.34
3	A	550	ZID	C6A-N6A	-3.97	1.17	1.34
3	B	450	ZID	C5A-N7A	-2.81	1.29	1.39
3	A	550	ZID	C5A-N7A	-2.76	1.30	1.39
3	B	450	ZID	C2D-C1D	-2.16	1.50	1.53
3	A	550	ZID	C5N-C4N	2.00	1.43	1.39
3	A	550	ZID	C2A-N3A	2.15	1.35	1.32
3	B	450	ZID	O7Z-C7Z	2.22	1.26	1.22
3	B	450	ZID	C2A-N3A	2.34	1.36	1.32
3	B	450	ZID	C5Z-C4Z	2.34	1.43	1.39
3	B	450	ZID	C3Z-C4Z	2.36	1.43	1.39
3	A	550	ZID	C5Z-C4Z	2.50	1.43	1.39
3	A	550	ZID	C3Z-C4Z	2.50	1.43	1.39
3	B	450	ZID	O4D-C1D	2.52	1.44	1.41
3	B	450	ZID	C2N-C3N	2.61	1.42	1.38
3	B	450	ZID	C4Z-C7Z	2.72	1.54	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	550	ZID	C4Z-C7Z	2.83	1.54	1.49
3	A	550	ZID	C4N-C3N	2.96	1.45	1.40
3	A	550	ZID	C2N-C3N	2.98	1.42	1.38
3	B	450	ZID	C6N-N1N	2.99	1.43	1.35
3	B	450	ZID	C4N-C3N	3.06	1.45	1.40
3	A	550	ZID	C6N-N1N	3.08	1.43	1.35
3	A	550	ZID	O4D-C1D	3.44	1.46	1.41
3	A	550	ZID	C4N-C7Z	3.92	1.58	1.50
3	B	450	ZID	C4N-C7Z	3.99	1.58	1.50
3	B	450	ZID	C3N-C7N	4.72	1.56	1.50
3	A	550	ZID	C3N-C7N	5.88	1.58	1.50
3	B	450	ZID	C4A-N3A	8.17	1.47	1.35
3	A	550	ZID	C4A-N3A	8.36	1.47	1.35

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	450	ZID	C4B-O4B-C1B	-14.91	93.90	109.77
3	A	550	ZID	C4B-O4B-C1B	-14.18	94.68	109.77
3	B	450	ZID	C1B-N9A-C4A	-10.87	107.86	126.64
3	A	550	ZID	C1B-N9A-C4A	-10.25	108.92	126.64
3	B	450	ZID	C3N-C4N-C7Z	-9.08	107.50	122.94
3	A	550	ZID	C3N-C4N-C7Z	-9.01	107.62	122.94
3	B	450	ZID	N3A-C2A-N1A	-8.74	121.25	128.86
3	A	550	ZID	N3A-C2A-N1A	-8.61	121.36	128.86
3	A	550	ZID	O5D-PN-O1N	-6.49	83.08	109.25
3	A	550	ZID	C5N-C4N-C7Z	-4.92	107.58	118.64
3	B	450	ZID	C5N-C4N-C7Z	-4.71	108.06	118.64
3	A	550	ZID	O2N-PN-O5D	-4.40	87.35	108.14
3	A	550	ZID	C3N-C7N-N7N	-2.79	113.88	118.16
3	A	550	ZID	C5Z-C6Z-N1Z	-2.75	118.83	123.63
3	B	450	ZID	C5Z-C6Z-N1Z	-2.72	118.87	123.63
3	B	450	ZID	O4B-C4B-C3B	-2.71	99.78	105.17
3	B	450	ZID	C3N-C7N-N7N	-2.51	114.32	118.16
3	A	550	ZID	O4B-C4B-C3B	-2.50	100.19	105.17
3	B	450	ZID	C5A-C6A-N6A	-2.16	116.06	120.47
3	B	450	ZID	C3Z-C2Z-N1Z	-2.01	120.11	123.63
3	B	450	ZID	C2A-N1A-C6A	2.07	122.38	118.77
3	B	450	ZID	O7N-C7N-C3N	2.17	122.88	120.28
3	A	550	ZID	C2A-N1A-C6A	2.26	122.72	118.77
3	A	550	ZID	O7N-C7N-C3N	2.33	123.06	120.28
3	B	450	ZID	O4B-C4B-C5B	2.34	117.31	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	550	ZID	O2N-PN-O1N	2.47	125.08	112.28
3	A	550	ZID	C4N-C7Z-C4Z	2.55	123.79	119.47
3	B	450	ZID	C6Z-N1Z-C2Z	2.67	123.27	116.83
3	A	550	ZID	C6Z-N1Z-C2Z	2.68	123.29	116.83
3	B	450	ZID	N6A-C6A-N1A	3.16	125.03	118.77
3	A	550	ZID	N6A-C6A-N1A	3.21	125.12	118.77
3	A	550	ZID	C4A-C5A-N7A	3.36	112.66	109.41
3	B	450	ZID	C4A-C5A-N7A	3.48	112.77	109.41
3	A	550	ZID	O5B-C5B-C4B	3.61	121.79	109.00
3	A	550	ZID	O2D-C2D-C3D	3.73	123.77	111.83
3	B	450	ZID	O2D-C2D-C3D	3.87	124.22	111.83
3	B	450	ZID	O5B-C5B-C4B	4.13	123.66	109.00
3	A	550	ZID	O2A-PA-O1A	5.28	139.61	112.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	550	ZID	4	0
3	B	450	ZID	7	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	229/229 (100%)	0.20	9 (3%) 40 42	8, 22, 65, 85	0
1	B	229/229 (100%)	0.12	12 (5%) 28 29	7, 23, 60, 96	0
2	C	60/60 (100%)	0.41	5 (8%) 12 12	9, 17, 66, 83	0
2	D	60/60 (100%)	0.29	4 (6%) 19 19	7, 18, 60, 82	0
All	All	578/578 (100%)	0.20	30 (5%) 28 29	7, 22, 65, 96	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	366	TYR	10.2
1	A	155	LYS	9.5
1	A	154	ASP	7.8
1	A	325	LYS	7.5
2	D	366	TYR	6.8
1	B	155	LYS	6.8
2	D	425	ASP	6.3
1	A	324	ASN	5.5
2	C	425	ASP	5.4
1	B	325	LYS	5.1
1	B	154	ASP	4.2
1	B	152	ILE	4.0
1	A	318	ARG	3.9
1	B	157	LYS	3.7
1	A	319	ALA	3.1
1	A	189	MET	3.0
1	B	156	ASP	2.9
2	D	371	TYR	2.8
1	B	175	ASN	2.6
1	B	324	ASN	2.6
2	D	424	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	318	ARG	2.3
1	A	323	ILE	2.2
2	C	367	THR	2.2
2	C	373	ILE	2.1
1	B	160	ASN	2.1
1	A	152	ILE	2.1
1	B	149	ASN	2.1
2	C	379	TYR	2.0
1	B	177	ILE	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	ZID	B	450	52/52	0.89	0.23	1.52	2,25,31,40	52
3	ZID	A	550	52/52	0.81	0.25	1.01	2,25,31,40	52

## 6.5 Other polymers [i](#)

There are no such residues in this entry.