



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:52 AM GMT

PDB ID : 3F4B  
Title : Crystal structure of Plasmodium berghei Enoyl-acyl-carrier-protein reductase with TRICLOSAN  
Authors : Sacchettini, J.C.; Tsai, H.-C.  
Deposited on : 2008-10-31  
Resolution : 2.49 Å (reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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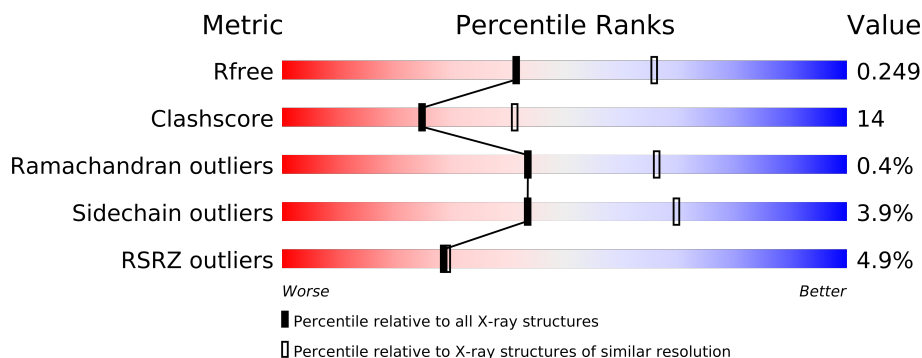
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.49 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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	323	
1	B	323	
1	C	323	
1	D	323	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9407 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

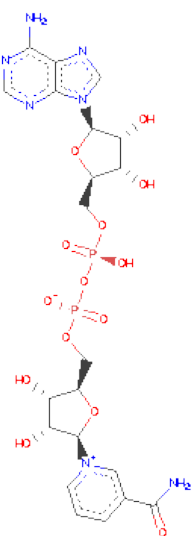
- Molecule 1 is a protein called Enoyl-acyl carrier protein reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2208	1406	367	426	9			
1	B	289	Total	C	N	O	S	0	0	0
			2250	1430	374	437	9			
1	C	282	Total	C	N	O	S	0	0	0
			2191	1396	363	423	9			
1	D	289	Total	C	N	O	S	0	0	0
			2250	1430	374	437	9			

There are 4 discrepancies between the modelled and reference sequences:

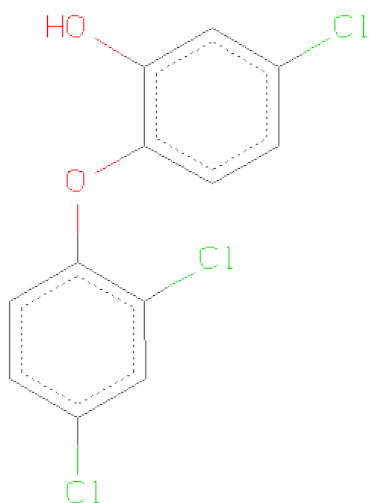
Chain	Residue	Modelled	Actual	Comment	Reference
A	74	MET	-	EXPRESSION TAG	UNP Q6TEI5
B	74	MET	-	EXPRESSION TAG	UNP Q6TEI5
C	74	MET	-	EXPRESSION TAG	UNP Q6TEI5
D	74	MET	-	EXPRESSION TAG	UNP Q6TEI5

- 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	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	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<sub>12</sub>H<sub>7</sub>Cl<sub>3</sub>O<sub>2</sub>).



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

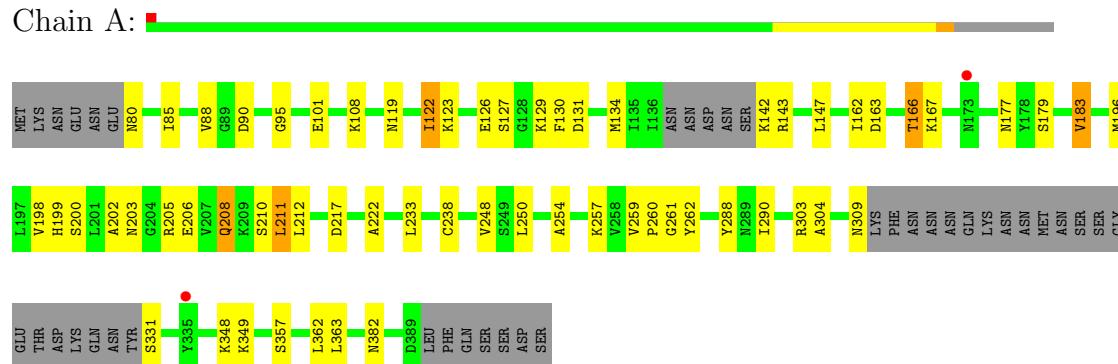
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	79	Total	O	0	0
			79	79		
4	B	54	Total	O	0	0
			54	54		
4	C	66	Total	O	0	0
			66	66		
4	D	65	Total	O	0	0
			65	65		

### 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 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.

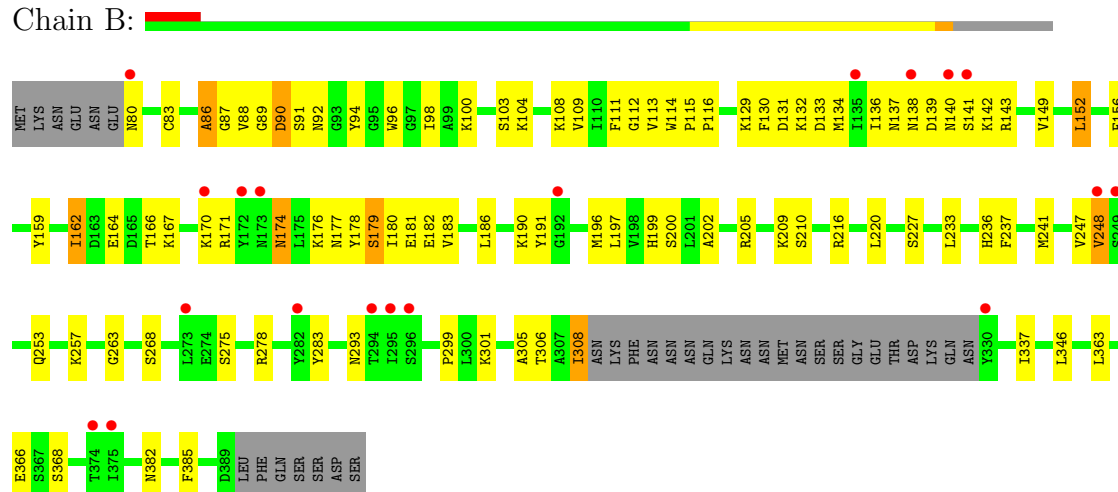
- Molecule 1: Enoyl-acyl carrier protein reductase

Chain A:



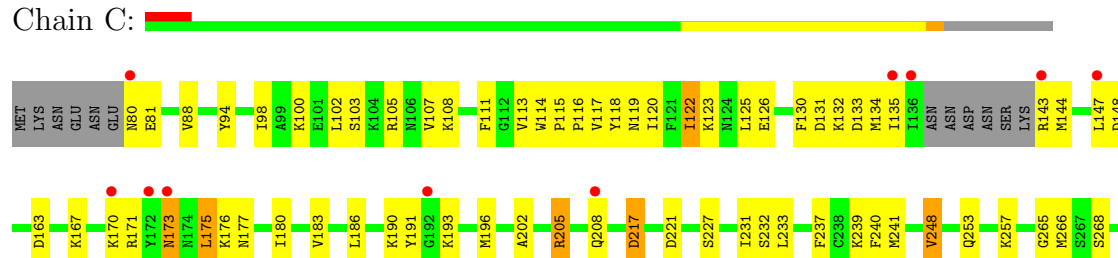
- Molecule 1: Enoyl-acyl carrier protein reductase

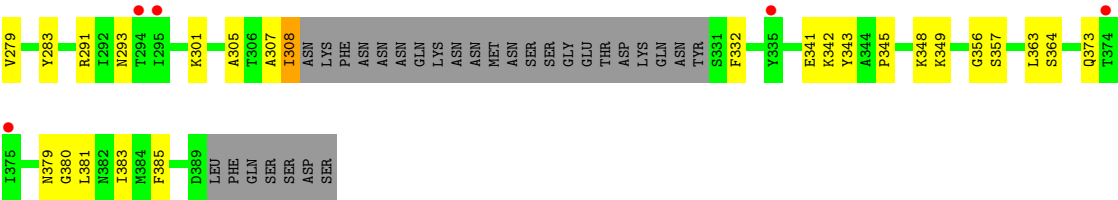
Chain B:



- Molecule 1: Enoyl-acyl carrier protein reductase

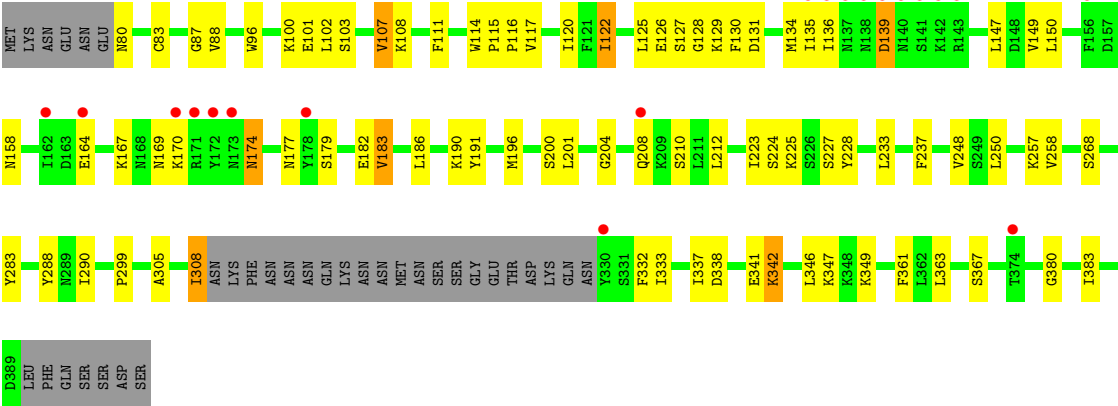
Chain C:





● Molecule 1: Enoyl-acyl carrier protein reductase

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.34Å 121.20Å 87.83Å 90.00° 108.97° 90.00°	Depositor
Resolution (Å)	36.33 – 2.49 36.33 – 2.49	Depositor EDS
% Data completeness (in resolution range)	92.2 (36.33-2.49) 92.2 (36.33-2.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 2.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.183 , 0.254 0.180 , 0.249	Depositor DCC
$R_{free}$ test set	2074 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.7	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 50.2	EDS
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 41336 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9407	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.



## 5 Model quality

### 5.1 Standard geometry

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	0.41	0/2246	0.56	1/3026 (0.0%)
1	B	0.35	0/2290	0.51	0/3088
1	C	0.37	0/2229	0.51	0/3004
1	D	0.37	0/2290	0.51	0/3088
All	All	0.37	0/9055	0.52	1/12206 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	SER	N-CA-C	-5.13	97.15	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2208	0	2210	49	0
1	B	2250	0	2241	74	0
1	C	2191	0	2191	81	0
1	D	2250	0	2241	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	1	0
2	D	44	0	26	1	0
3	A	17	0	6	1	0
3	B	17	0	6	2	0
3	C	17	0	7	0	0
3	D	17	0	6	1	0
4	A	79	0	0	9	0
4	B	54	0	0	3	0
4	C	66	0	0	8	0
4	D	65	0	0	9	0
All	All	9407	0	9012	252	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (252) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:105:ARG:NH1	1:C:364:SER:HB3	1.71	1.04
1:D:88:VAL:HG11	1:D:111:PHE:CD1	2.07	0.90
1:C:202:ALA:HB1	1:C:266:MET:HE1	1.57	0.86
1:C:105:ARG:HH12	1:C:364:SER:HB3	1.39	0.85
1:B:80:ASN:HD22	1:B:108:LYS:HE2	1.42	0.85
1:B:80:ASN:ND2	1:B:108:LYS:HE2	1.92	0.84
1:C:341:GLU:OE2	1:C:349:LYS:HG3	1.80	0.81
1:A:288:TYR:HB2	1:A:290:ILE:HG13	1.61	0.80
1:D:122:ILE:O	1:D:126:GLU:HG2	1.82	0.79
1:D:135:ILE:HG23	1:D:139:ASP:HA	1.66	0.78
1:A:303:ARG:HD3	4:A:58:HOH:O	1.83	0.78
1:C:88:VAL:HG21	1:C:111:PHE:CD1	2.18	0.77
1:C:196:MET:HG2	1:C:363:LEU:HB3	1.64	0.77
1:A:208:GLN:HG3	4:A:439:HOH:O	1.85	0.76
1:A:199:HIS:HD2	1:A:233:LEU:HD12	1.50	0.76
1:B:382:ASN:HD21	1:C:373:GLN:HE22	1.31	0.75
1:D:108:LYS:HE2	1:D:147:LEU:HD22	1.67	0.75
1:A:257:LYS:HE2	1:B:385:PHE:HA	1.70	0.74
1:C:385:PHE:HA	1:D:257:LYS:HE2	1.69	0.73
1:B:91:SER:HA	1:B:96:TRP:CG	2.23	0.73
1:C:122:ILE:O	1:C:126:GLU:HG2	1.89	0.73
1:C:102:LEU:HB3	1:C:107:VAL:CG1	2.18	0.73
1:A:179:SER:O	1:A:183:VAL:HG13	1.89	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:119:ASN:HA	4:C:445:HOH:O	1.89	0.71
1:D:182:GLU:HG3	4:D:423:HOH:O	1.90	0.70
1:A:127:SER:OG	1:A:129:LYS:HE2	1.92	0.70
1:B:237:PHE:O	1:B:241:MET:HG3	1.92	0.69
1:B:190:LYS:HD3	1:B:191:TYR:CE2	2.28	0.69
1:B:139:ASP:HA	1:B:141:SER:HA	1.73	0.69
1:C:102:LEU:O	1:C:107:VAL:HG12	1.92	0.69
1:D:190:LYS:HD3	1:D:191:TYR:CZ	2.27	0.69
1:C:94:TYR:O	1:C:98:ILE:HG13	1.93	0.68
1:A:80:ASN:ND2	1:A:108:LYS:HG3	2.08	0.68
1:B:197:LEU:HB3	1:B:247:VAL:HG22	1.73	0.68
1:B:170:LYS:HG2	1:B:171:ARG:NH1	2.08	0.67
1:A:163:ASP:OD1	1:A:166:THR:HG23	1.95	0.67
1:D:299:PRO:HB2	1:D:337:ILE:HG13	1.77	0.67
1:C:122:ILE:HB	4:C:445:HOH:O	1.95	0.66
1:D:341:GLU:O	1:D:347:LYS:HD3	1.97	0.65
1:A:122:ILE:O	1:A:126:GLU:HG2	1.97	0.65
1:A:254:ALA:HB2	1:A:259:VAL:HG21	1.79	0.65
1:D:150:LEU:HD13	1:D:186:LEU:HD22	1.78	0.64
1:C:105:ARG:NH1	1:C:364:SER:CB	2.57	0.64
1:C:202:ALA:HB1	1:C:266:MET:CE	2.26	0.64
1:C:108:LYS:HB3	1:C:147:LEU:HG	1.80	0.64
1:C:307:ALA:O	1:C:308:ILE:HG12	1.98	0.64
1:A:248:VAL:HG22	1:A:363:LEU:HD21	1.79	0.64
1:C:102:LEU:HD22	1:C:107:VAL:HG11	1.80	0.63
1:B:299:PRO:HB2	1:B:337:ILE:HG13	1.80	0.63
1:C:190:LYS:HD2	1:C:191:TYR:CE2	2.34	0.63
1:D:164:GLU:HA	1:D:167:LYS:HD2	1.81	0.63
1:C:380:GLY:O	1:C:383:ILE:HG12	1.98	0.63
1:D:83:CYS:HB2	1:D:196:MET:HB2	1.81	0.63
1:B:202:ALA:HB3	3:B:500:TCL:CL16	2.36	0.63
1:B:209:LYS:O	1:B:263:GLY:HA3	1.99	0.62
1:C:131:ASP:O	1:C:135:ILE:HG23	1.99	0.61
1:C:163:ASP:O	1:C:167:LYS:HG3	2.00	0.61
1:A:259:VAL:O	1:A:259:VAL:HG23	2.00	0.61
1:B:220:LEU:HD11	1:D:224:SER:HB2	1.81	0.61
1:D:174:ASN:N	1:D:174:ASN:OD1	2.32	0.61
1:A:108:LYS:HD2	1:A:147:LEU:HD13	1.81	0.61
1:D:338:ASP:O	1:D:342:LYS:HB2	2.02	0.60
1:B:89:GLY:O	1:B:90:ASP:HB3	2.00	0.60
1:A:205:ARG:HG3	4:A:414:HOH:O	2.01	0.60
1:A:196:MET:HG2	1:A:363:LEU:HB3	1.83	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:109:VAL:HG11	1:B:111:PHE:HE1	1.66	0.60
1:D:101:GLU:HB3	4:D:404:HOH:O	2.01	0.59
1:B:111:PHE:HB2	1:B:149:VAL:HG22	1.84	0.59
1:C:180:ILE:HD13	1:C:232:SER:HB3	1.84	0.59
1:B:91:SER:HA	1:B:96:TRP:CB	2.32	0.58
1:B:109:VAL:CG1	1:B:111:PHE:HE1	2.16	0.58
1:D:127:SER:OG	1:D:129:LYS:HG2	2.03	0.58
1:A:205:ARG:NH2	1:A:217:ASP:OD2	2.35	0.57
1:C:102:LEU:HB3	1:C:107:VAL:HG11	1.86	0.57
1:D:177:ASN:HA	1:D:182:GLU:OE1	2.05	0.57
1:D:196:MET:HG2	1:D:363:LEU:HB3	1.86	0.57
1:B:179:SER:HB2	1:B:182:GLU:OE1	2.04	0.56
1:D:88:VAL:HG11	1:D:111:PHE:CG	2.39	0.56
1:C:301:LYS:O	1:C:301:LYS:HG3	2.05	0.56
1:A:238:CYS:HB2	4:A:55:HOH:O	2.05	0.56
1:C:105:ARG:HH11	1:C:364:SER:HB3	1.68	0.56
1:A:130:PHE:O	1:A:134:MET:HG3	2.06	0.56
1:C:115:PRO:HB2	1:C:116:PRO:HD3	1.87	0.56
1:C:265:GLY:O	1:C:268:SER:HB3	2.05	0.56
1:C:108:LYS:HE3	4:C:427:HOH:O	2.06	0.56
1:B:181:GLU:HB2	1:B:236:HIS:CE1	2.41	0.56
1:D:149:VAL:O	1:D:150:LEU:HD23	2.05	0.55
1:D:102:LEU:O	1:D:107:VAL:HG13	2.06	0.55
1:B:131:ASP:CG	1:B:143:ARG:HH12	2.09	0.55
1:D:342:LYS:O	1:D:347:LYS:HE3	2.08	0.54
1:A:142:LYS:HA	4:A:446:HOH:O	2.06	0.54
1:A:80:ASN:HD21	1:A:108:LYS:HG3	1.71	0.54
1:D:179:SER:HB2	4:D:423:HOH:O	2.08	0.53
1:A:211:LEU:HD22	1:C:231:ILE:HD13	1.89	0.53
1:C:305:ALA:O	1:C:308:ILE:HG13	2.09	0.53
1:C:105:ARG:NH2	1:C:196:MET:SD	2.81	0.53
1:D:258:VAL:HA	4:D:429:HOH:O	2.09	0.53
1:A:288:TYR:CB	1:A:290:ILE:HG13	2.38	0.52
1:C:237:PHE:O	1:C:241:MET:HG3	2.09	0.52
1:B:94:TYR:O	1:B:98:ILE:HG13	2.08	0.52
1:C:88:VAL:HG12	4:C:426:HOH:O	2.10	0.52
1:A:162:ILE:HG22	1:A:167:LYS:HG3	1.92	0.51
1:C:193:LYS:HD3	4:C:421:HOH:O	2.09	0.51
1:B:186:LEU:C	1:B:186:LEU:HD23	2.31	0.51
1:D:204:GLY:N	3:D:500:TCL:CL15	2.80	0.51
1:B:190:LYS:HD3	1:B:191:TYR:CZ	2.45	0.51
1:C:132:LYS:O	1:C:135:ILE:HG12	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:257:LYS:HD2	4:D:435:HOH:O	2.10	0.51
1:B:205:ARG:HD3	4:B:430:HOH:O	2.10	0.51
1:C:125:LEU:HD13	1:C:130:PHE:HD2	1.74	0.51
1:B:205:ARG:CD	4:B:430:HOH:O	2.59	0.51
1:B:210:SER:HB2	1:D:283:TYR:CZ	2.46	0.50
1:C:98:ILE:HG12	1:C:356:GLY:HA2	1.94	0.50
1:B:104:LYS:HB3	1:B:136:ILE:HG21	1.94	0.50
1:B:156:PHE:CE1	1:B:162:ILE:HA	2.47	0.50
1:D:158:ASN:HA	4:D:423:HOH:O	2.12	0.50
1:B:190:LYS:HG2	1:B:191:TYR:CD2	2.47	0.50
1:C:348:LYS:HE3	4:C:430:HOH:O	2.12	0.50
1:B:301:LYS:HE3	1:B:306:THR:OG1	2.12	0.50
1:C:170:LYS:O	1:C:170:LYS:HG2	2.11	0.50
1:C:100:LYS:HD3	1:C:133:ASP:O	2.11	0.50
1:C:80:ASN:HB2	1:C:108:LYS:NZ	2.28	0.49
1:C:176:LYS:O	1:C:177:ASN:HB2	2.12	0.49
1:D:288:TYR:HB2	1:D:290:ILE:HG13	1.93	0.49
1:D:114:TRP:CD1	1:D:115:PRO:HD2	2.47	0.49
1:D:80:ASN:HB3	1:D:108:LYS:NZ	2.27	0.49
1:A:259:VAL:HG23	1:A:262:TYR:HB3	1.93	0.49
1:B:100:LYS:O	1:B:103:SER:HB2	2.11	0.49
1:D:305:ALA:HB1	1:D:333:ILE:HG12	1.94	0.49
1:D:130:PHE:O	1:D:134:MET:HG3	2.13	0.49
1:B:199:HIS:HD2	1:B:233:LEU:HD12	1.78	0.49
1:B:170:LYS:HG2	1:B:171:ARG:HH12	1.77	0.49
1:B:346:LEU:HD11	1:C:291:ARG:HG2	1.94	0.49
1:B:174:ASN:OD1	1:B:174:ASN:N	2.45	0.49
1:C:248:VAL:HA	1:C:293:ASN:O	2.13	0.49
1:C:81:GLU:HB3	1:C:196:MET:HE1	1.95	0.48
1:C:147:LEU:HD13	1:C:191:TYR:CE1	2.48	0.48
1:C:123:LYS:HB3	1:C:123:LYS:HE2	1.65	0.48
1:B:115:PRO:HB2	1:B:116:PRO:HD3	1.94	0.48
1:B:87:GLY:HA3	1:B:200:SER:O	2.14	0.48
1:B:159:TYR:O	1:B:162:ILE:HG23	2.13	0.48
1:C:117:VAL:HA	1:C:120:ILE:HD12	1.95	0.48
1:A:382:ASN:CG	4:A:429:HOH:O	2.52	0.48
1:D:341:GLU:OE2	1:D:349:LYS:HG3	2.13	0.48
1:B:90:ASP:OD1	1:B:92:ASN:HB2	2.14	0.48
1:C:130:PHE:O	1:C:134:MET:HG3	2.14	0.48
1:B:114:TRP:CE2	1:B:116:PRO:HG2	2.49	0.48
1:D:341:GLU:HA	4:D:422:HOH:O	2.13	0.47
1:A:163:ASP:CG	1:A:166:THR:HG23	2.35	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:135:ILE:HG22	1:C:143:ARG:HH11	1.79	0.47
1:B:205:ARG:HB2	4:B:430:HOH:O	2.14	0.47
1:C:118:TYR:CD2	1:C:175:LEU:HD22	2.50	0.47
1:A:131:ASP:HB3	1:A:143:ARG:HH12	1.80	0.47
1:C:123:LYS:O	1:C:126:GLU:HB2	2.15	0.47
1:C:170:LYS:HA	1:C:173:ASN:ND2	2.30	0.47
1:D:208:GLN:HE21	1:D:308:ILE:HA	1.80	0.47
1:B:109:VAL:CG1	1:B:111:PHE:CE1	2.96	0.46
1:D:170:LYS:HB3	1:D:170:LYS:HE2	1.73	0.46
1:A:382:ASN:OD1	4:A:429:HOH:O	2.20	0.46
1:A:203:ASN:O	1:A:222:ALA:HA	2.14	0.46
1:C:342:LYS:HG2	1:C:343:TYR:CZ	2.50	0.46
1:B:152:LEU:HD23	1:B:178:TYR:O	2.15	0.46
1:D:179:SER:O	1:D:183:VAL:HG13	2.15	0.46
1:B:368:SER:HB2	1:C:348:LYS:NZ	2.31	0.46
1:B:283:TYR:CZ	1:D:210:SER:HB2	2.51	0.46
1:B:139:ASP:HB2	1:B:140:ASN:OD1	2.15	0.46
1:C:134:MET:HE3	1:C:144:MET:HB3	1.97	0.46
1:A:348:LYS:HG2	1:A:349:LYS:N	2.31	0.46
1:C:381:LEU:HD23	4:C:444:HOH:O	2.15	0.46
1:D:200:SER:O	2:D:550:NAD:H52N	2.16	0.46
1:A:206:GLU:HA	1:A:208:GLN:HE21	1.81	0.45
1:D:115:PRO:HB2	1:D:116:PRO:HD3	1.97	0.45
1:A:261:GLY:N	4:A:427:HOH:O	2.23	0.45
1:A:257:LYS:HE3	1:B:257:LYS:HZ3	1.80	0.45
1:D:233:LEU:O	1:D:237:PHE:HB2	2.16	0.45
1:A:254:ALA:CB	1:A:259:VAL:CG2	2.94	0.45
1:B:162:ILE:HG13	1:B:166:THR:CG2	2.47	0.45
1:B:308:ILE:HG13	1:B:308:ILE:H	1.33	0.45
1:A:208:GLN:HG3	1:A:208:GLN:H	1.49	0.44
1:D:380:GLY:O	1:D:383:ILE:HG12	2.16	0.44
1:C:88:VAL:O	1:C:113:VAL:HG22	2.17	0.44
1:A:210:SER:HB2	1:C:283:TYR:CZ	2.52	0.44
1:A:260:PRO:HA	4:A:427:HOH:O	2.17	0.44
1:B:164:GLU:OE1	1:B:167:LYS:HD2	2.18	0.44
1:B:248:VAL:HA	1:B:293:ASN:O	2.18	0.44
1:B:132:LYS:HG3	1:B:133:ASP:OD1	2.17	0.44
1:B:83:CYS:HB2	1:B:196:MET:HB2	2.00	0.44
1:B:130:PHE:O	1:B:134:MET:HG3	2.18	0.43
1:D:87:GLY:HA3	1:D:201:LEU:HB3	2.00	0.43
1:D:288:TYR:CB	1:D:290:ILE:HG13	2.48	0.43
1:A:202:ALA:HB3	3:A:400:TCL:CL16	2.55	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:205:ARG:NH2	1:C:217:ASP:OD2	2.50	0.43
1:C:103:SER:OG	1:C:144:MET:HG3	2.18	0.43
1:D:204:GLY:HA2	4:D:426:HOH:O	2.19	0.43
1:A:119:ASN:O	1:A:123:LYS:HG3	2.18	0.43
1:D:117:VAL:HA	1:D:120:ILE:HD12	2.01	0.43
1:B:142:LYS:HG3	1:B:142:LYS:O	2.19	0.43
1:D:128:GLY:HA2	1:D:131:ASP:OD1	2.18	0.43
1:D:83:CYS:HB2	1:D:196:MET:CB	2.48	0.43
1:B:366:GLU:O	1:C:357:SER:OG	2.37	0.43
1:A:85:ILE:HG12	1:A:198:VAL:HB	1.99	0.43
1:A:88:VAL:HG22	1:A:95:GLY:HA3	2.01	0.43
1:C:107:VAL:O	1:C:107:VAL:HG13	2.17	0.43
1:C:345:PRO:HD2	1:C:379:ASN:O	2.19	0.43
1:D:96:TRP:O	1:D:100:LYS:HG3	2.19	0.43
1:B:275:SER:HA	1:B:278:ARG:NH2	2.33	0.42
1:C:253:GLN:O	1:C:253:GLN:HG2	2.20	0.42
1:C:81:GLU:HB3	1:C:196:MET:CE	2.48	0.42
1:A:177:ASN:O	1:A:183:VAL:HG12	2.19	0.42
1:C:308:ILE:HB	1:C:332:PHE:HB3	2.01	0.42
1:C:193:LYS:HA	1:C:240:PHE:O	2.20	0.42
2:C:450:NAD:O2N	2:C:450:NAD:N7N	2.48	0.42
1:C:186:LEU:HD23	1:C:186:LEU:C	2.40	0.42
1:D:201:LEU:C	1:D:201:LEU:HD12	2.39	0.42
1:C:257:LYS:CE	4:D:408:HOH:O	2.67	0.42
1:D:223:ILE:O	1:D:227:SER:HB2	2.20	0.42
1:B:196:MET:HG2	1:B:363:LEU:HB3	2.02	0.42
1:B:382:ASN:ND2	1:C:373:GLN:HE22	2.07	0.42
1:A:362:LEU:HA	1:A:362:LEU:HD23	1.88	0.42
1:A:257:LYS:NZ	1:B:257:LYS:NZ	2.67	0.42
1:B:86:ALA:O	1:B:112:GLY:O	2.37	0.42
1:B:216:ARG:HB2	1:D:228:TYR:CE2	2.55	0.42
1:C:239:LYS:HG2	4:C:67:HOH:O	2.20	0.42
1:B:171:ARG:HA	1:B:171:ARG:HD3	1.96	0.41
1:D:248:VAL:HG23	1:D:363:LEU:HD21	2.02	0.41
1:A:200:SER:CB	1:A:250:LEU:HD23	2.50	0.41
1:B:88:VAL:O	1:B:113:VAL:HG22	2.20	0.41
1:C:114:TRP:CG	1:C:116:PRO:HD2	2.55	0.41
1:D:361:PHE:CZ	1:D:367:SER:HB3	2.55	0.41
1:C:205:ARG:HD3	1:C:221:ASP:OD2	2.20	0.41
1:D:248:VAL:HG23	1:D:363:LEU:CD2	2.50	0.41
1:D:169:ASN:OD1	1:D:170:LYS:N	2.52	0.41
1:B:180:ILE:O	1:B:183:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:101:GLU:HG3	1:A:357:SER:N	2.36	0.41
1:D:117:VAL:HG12	1:D:120:ILE:HD12	2.02	0.41
1:B:137:ASN:HA	1:B:138:ASN:C	2.40	0.41
1:B:253:GLN:OE1	1:B:257:LYS:HE3	2.21	0.41
1:C:170:LYS:HE3	1:C:171:ARG:HD2	2.03	0.41
1:D:125:LEU:CD1	1:D:134:MET:HE1	2.51	0.41
1:B:114:TRP:CG	1:B:116:PRO:HD2	2.56	0.41
1:C:233:LEU:HD23	1:C:233:LEU:HA	1.84	0.41
1:B:176:LYS:O	1:B:177:ASN:HB2	2.21	0.41
1:C:307:ALA:C	1:C:308:ILE:HG12	2.41	0.41
1:A:211:LEU:HD12	1:C:279:VAL:HB	2.03	0.41
1:A:303:ARG:HG3	1:A:304:ALA:N	2.36	0.40
1:C:114:TRP:CD1	1:C:116:PRO:HD2	2.56	0.40
1:B:301:LYS:HG3	1:B:301:LYS:O	2.21	0.40
1:D:100:LYS:O	1:D:103:SER:HB2	2.20	0.40
1:B:305:ALA:HB2	3:B:500:TCL:H41	2.03	0.40
1:B:139:ASP:HA	1:B:140:ASN:HA	1.64	0.40
1:D:103:SER:HB3	1:D:136:ILE:HD13	2.03	0.40
1:D:200:SER:HA	1:D:250:LEU:HD23	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	278/323 (86%)	266 (96%)	11 (4%)	1 (0%)	43	66
1	B	285/323 (88%)	270 (95%)	13 (5%)	2 (1%)	30	50
1	C	276/323 (85%)	258 (94%)	17 (6%)	1 (0%)	43	66
1	D	285/323 (88%)	266 (93%)	19 (7%)	0	100	100
All	All	1124/1292 (87%)	1060 (94%)	60 (5%)	4 (0%)	43	66

All (4) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	B	90	ASP
1	A	90	ASP
1	C	173	ASN
1	B	86	ALA

### 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	242/280 (86%)	235 (97%)	7 (3%)	55	81
1	B	247/280 (88%)	238 (96%)	9 (4%)	47	73
1	C	240/280 (86%)	230 (96%)	10 (4%)	40	66
1	D	247/280 (88%)	235 (95%)	12 (5%)	35	59
All	All	976/1120 (87%)	938 (96%)	38 (4%)	43	70

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	ILE
1	A	166	THR
1	A	183	VAL
1	A	208	GLN
1	A	211	LEU
1	A	212	LEU
1	A	309	ASN
1	B	129	LYS
1	B	152	LEU
1	B	162	ILE
1	B	174	ASN
1	B	179	SER
1	B	227	SER
1	B	248	VAL
1	B	268	SER
1	B	308	ILE
1	C	122	ILE
1	C	148	ASP
1	C	175	LEU

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Mol	Chain	Res	Type
1	C	183	VAL
1	C	205	ARG
1	C	208	GLN
1	C	217	ASP
1	C	227	SER
1	C	248	VAL
1	C	308	ILE
1	D	107	VAL
1	D	122	ILE
1	D	139	ASP
1	D	174	ASN
1	D	183	VAL
1	D	212	LEU
1	D	225	LYS
1	D	268	SER
1	D	308	ILE
1	D	332	PHE
1	D	342	LYS
1	D	346	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	208	GLN
1	B	169	ASN
1	B	236	HIS
1	B	253	GLN
1	C	119	ASN
1	C	174	ASN
1	C	253	GLN
1	C	373	GLN
1	D	208	GLN
1	D	242	ASN
1	D	382	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

8 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	TCL	A	400	-	18,18,18	1.03	1 (5%)	25,25,25	0.82	0
2	NAD	A	450	-	48,48,48	0.77	1 (2%)	73,73,73	1.81	11 (15%)
3	TCL	B	500	-	18,18,18	1.13	2 (11%)	25,25,25	0.95	2 (8%)
2	NAD	B	550	-	48,48,48	0.75	2 (4%)	73,73,73	1.72	10 (13%)
3	TCL	C	400	-	18,18,18	1.00	1 (5%)	25,25,25	0.77	0
2	NAD	C	450	-	48,48,48	0.84	1 (2%)	73,73,73	1.70	11 (15%)
3	TCL	D	500	-	18,18,18	1.07	2 (11%)	25,25,25	0.76	1 (4%)
2	NAD	D	550	-	48,48,48	0.77	1 (2%)	73,73,73	1.73	11 (15%)

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	TCL	A	400	-	-	0/4/4/4	0/2/2/2
2	NAD	A	450	-	-	0/30/62/62	0/3/5/5
3	TCL	B	500	-	-	0/4/4/4	0/2/2/2
2	NAD	B	550	-	-	0/30/62/62	0/3/5/5
3	TCL	C	400	-	-	0/4/4/4	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	C	450	-	-	0/30/62/62	0/3/5/5
3	TCL	D	500	-	-	0/4/4/4	0/2/2/2
2	NAD	D	550	-	-	0/30/62/62	0/3/5/5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	450	NAD	C4A-N9A	-3.28	1.33	1.37
3	B	500	TCL	C9-CL16	3.12	1.81	1.73
3	D	500	TCL	C9-CL16	2.81	1.80	1.73
2	A	450	NAD	C4A-N9A	-2.50	1.34	1.37
2	D	550	NAD	C4A-N9A	-2.40	1.34	1.37
3	D	500	TCL	C11-CL15	2.23	1.79	1.74
3	A	400	TCL	C9-CL16	2.21	1.79	1.73
3	C	400	TCL	C9-CL16	2.20	1.79	1.73
2	B	550	NAD	O4D-C1D	2.17	1.44	1.41
3	B	500	TCL	C11-CL15	2.13	1.79	1.74
2	B	550	NAD	C4A-N9A	-2.08	1.34	1.37

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	450	NAD	N3A-C2A-N1A	-9.91	120.42	128.71
2	D	550	NAD	N3A-C2A-N1A	-9.10	121.10	128.71
2	B	550	NAD	N3A-C2A-N1A	-8.92	121.25	128.71
2	C	450	NAD	N3A-C2A-N1A	-8.78	121.37	128.71
2	D	550	NAD	O4B-C1B-N9A	5.66	113.70	108.44
2	B	550	NAD	O4B-C1B-N9A	5.61	113.66	108.44
2	A	450	NAD	O4B-C1B-N9A	5.49	113.54	108.44
2	B	550	NAD	N3A-C4A-N9A	4.18	132.98	125.43
2	A	450	NAD	N3A-C4A-N9A	4.02	132.69	125.43
2	C	450	NAD	O4D-C1D-N1N	3.95	112.00	107.95
2	C	450	NAD	C4B-O4B-C1B	-3.90	105.52	109.75
2	C	450	NAD	C8A-N9A-C4A	3.88	109.86	106.90
2	D	550	NAD	N3A-C4A-N9A	3.86	132.41	125.43
2	C	450	NAD	N3A-C4A-N9A	3.57	131.88	125.43
2	B	550	NAD	O4D-C1D-N1N	3.28	111.31	107.95
2	B	550	NAD	C5A-C4A-N3A	-3.05	119.07	125.70
2	A	450	NAD	C5A-C4A-N3A	-2.93	119.32	125.70
2	B	550	NAD	C4A-C5A-N7A	-2.82	107.11	109.52
2	A	450	NAD	C4A-C5A-N7A	-2.79	107.13	109.52
2	B	550	NAD	O4B-C1B-C2B	-2.78	102.51	106.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	550	NAD	C3B-C2B-C1B	2.75	105.21	100.91
2	C	450	NAD	C1B-N9A-C4A	-2.75	121.89	126.64
2	D	550	NAD	C8A-N9A-C4A	2.60	108.88	106.90
2	A	450	NAD	C2A-N3A-C4A	2.56	121.30	114.01
2	D	550	NAD	C4A-C5A-N7A	-2.56	107.33	109.52
2	D	550	NAD	C5A-C4A-N3A	-2.56	120.14	125.70
2	D	550	NAD	O4D-C1D-N1N	2.53	110.54	107.95
2	C	450	NAD	C4A-C5A-N7A	-2.37	107.49	109.52
2	B	550	NAD	PN-O3-PA	-2.35	122.87	132.95
2	D	550	NAD	O4D-C1D-C2D	-2.34	103.18	106.77
2	A	450	NAD	O4D-C1D-N1N	2.34	110.34	107.95
2	C	450	NAD	N7A-C8A-N9A	-2.32	107.79	114.36
2	B	550	NAD	C4B-O4B-C1B	-2.30	107.25	109.75
2	B	550	NAD	C2A-N3A-C4A	2.30	120.55	114.01
2	A	450	NAD	C3N-C7N-N7N	2.28	120.36	117.77
2	C	450	NAD	PN-O3-PA	-2.27	123.21	132.95
2	A	450	NAD	O4B-C1B-C2B	-2.26	103.30	106.77
3	D	500	TCL	O7-C5-C6	2.24	120.89	116.33
3	B	500	TCL	C8-C9-CL16	2.19	122.31	119.45
2	A	450	NAD	O7N-C7N-C3N	-2.17	117.13	119.58
2	D	550	NAD	C2A-N3A-C4A	2.12	120.05	114.01
2	A	450	NAD	C4B-O4B-C1B	-2.07	107.50	109.75
3	B	500	TCL	O7-C5-C6	2.06	120.54	116.33
2	C	450	NAD	O4B-C1B-N9A	2.06	110.36	108.44
2	C	450	NAD	C5A-C4A-N3A	-2.05	121.23	125.70
2	D	550	NAD	N7A-C8A-N9A	-2.02	108.64	114.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	284/323 (87%)	-0.11	2 (0%) 84 86	43, 58, 78, 93	0
1	B	289/323 (89%)	0.31	19 (6%) 18 17	47, 68, 110, 140	0
1	C	282/323 (87%)	0.14	15 (5%) 25 26	46, 66, 90, 109	0
1	D	289/323 (89%)	0.25	20 (6%) 17 16	46, 67, 109, 139	0
All	All	1144/1292 (88%)	0.15	56 (4%) 28 29	43, 64, 98, 140	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	136	ILE	6.0
1	D	330	TYR	5.3
1	B	140	ASN	5.0
1	D	172	TYR	4.6
1	D	135	ILE	4.0
1	B	141	SER	3.9
1	D	142	LYS	3.8
1	D	170	LYS	3.8
1	B	330	TYR	3.6
1	D	140	ASN	3.5
1	C	335	TYR	3.5
1	D	141	SER	3.5
1	D	137	ASN	3.4
1	D	139	ASP	3.3
1	A	173	ASN	3.2
1	B	80	ASN	3.0
1	B	170	LYS	3.0
1	A	335	TYR	2.9
1	D	143	ARG	2.9
1	D	162	ILE	2.9
1	B	374	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	208	GLN	2.9
1	B	295	ILE	2.8
1	C	143	ARG	2.8
1	C	295	ILE	2.8
1	C	294	THR	2.7
1	D	173	ASN	2.7
1	C	375	ILE	2.7
1	B	173	ASN	2.6
1	B	135	ILE	2.6
1	B	375	ILE	2.6
1	D	138	ASN	2.5
1	C	172	TYR	2.5
1	C	192	GLY	2.4
1	C	135	ILE	2.4
1	C	136	ILE	2.4
1	B	172	TYR	2.4
1	C	374	THR	2.4
1	C	80	ASN	2.3
1	C	147	LEU	2.3
1	D	156	PHE	2.3
1	C	170	LYS	2.3
1	B	192	GLY	2.2
1	D	178	TYR	2.2
1	B	273	LEU	2.2
1	D	164	GLU	2.2
1	C	173	ASN	2.1
1	D	374	THR	2.1
1	B	138	ASN	2.1
1	B	296	SER	2.1
1	B	248	VAL	2.1
1	B	282	TYR	2.1
1	B	249	SER	2.1
1	B	294	THR	2.0
1	C	208	GLN	2.0
1	D	171	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	TCL	B	500	17/17	0.18	0.71	57,67,84,90	0
3	TCL	D	500	17/17	0.18	0.64	57,68,79,86	0
3	TCL	C	400	17/17	0.16	0.19	57,65,80,90	0
2	NAD	D	550	44/44	0.15	-0.09	53,71,85,88	0
2	NAD	A	450	44/44	0.12	-0.33	44,56,64,68	0
2	NAD	C	450	44/44	0.13	-0.34	59,69,77,82	0
3	TCL	A	400	17/17	0.12	-0.74	49,58,74,86	0
2	NAD	B	550	44/44	0.12	-0.77	56,72,79,82	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.