



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:55 AM GMT

PDB ID : 1PS9  
Title : The Crystal Structure and Reaction Mechanism of E. coli 2,4-Dienoyl CoA Reductase  
Authors : Hubbard, P.A.; Liang, X.; Schulz, H.; Kim, J.J.  
Deposited on : 2003-06-20  
Resolution : 2.20 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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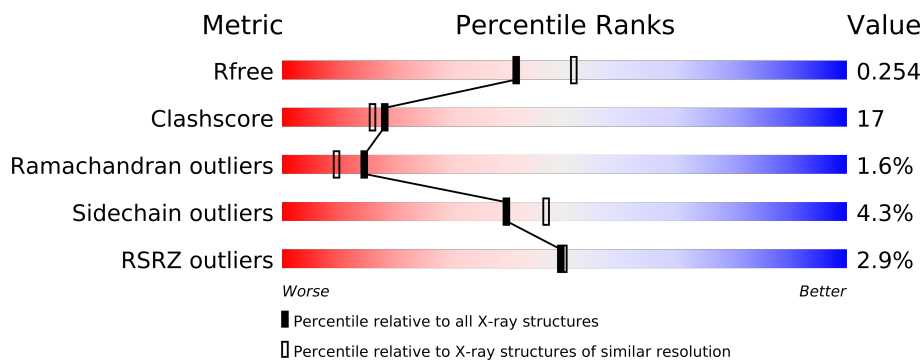
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.20 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	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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	671	

## 2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 5676 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.

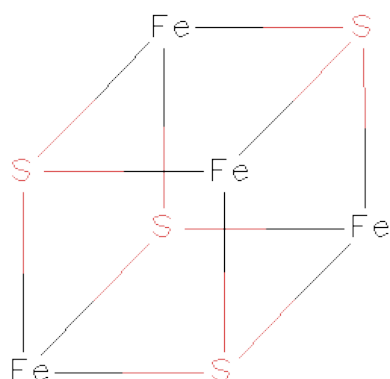
- Molecule 1 is a protein called 2,4-dienoyl-CoA reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	671	Total	C	N	O	S	0	0	0
			5097	3198	916	957	26			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Cl	0	0
			3	3		

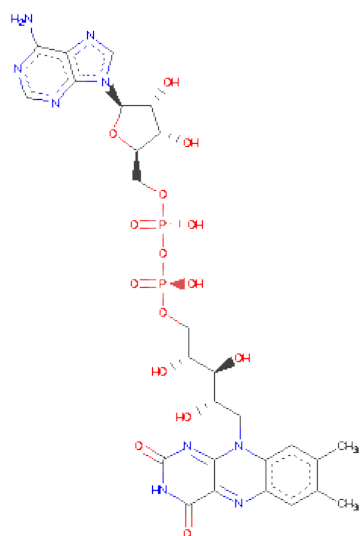
- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		

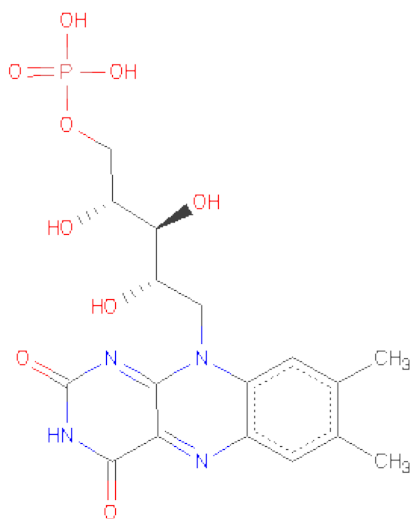
- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:

C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

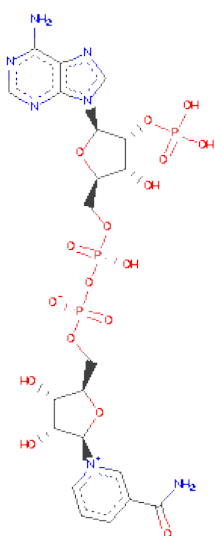
- Molecule 5 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

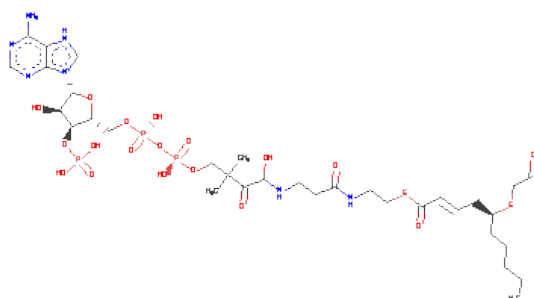
- Molecule 6 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-

letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 7 is 5-MERCAPTOETHANOL-2-DECENOYL-COENZYMEA (three-letter code: MDE) (formula:  $C_{33}H_{55}N_7O_{18}P_3S_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P S	0	0
			63	33	7	18	3 2		

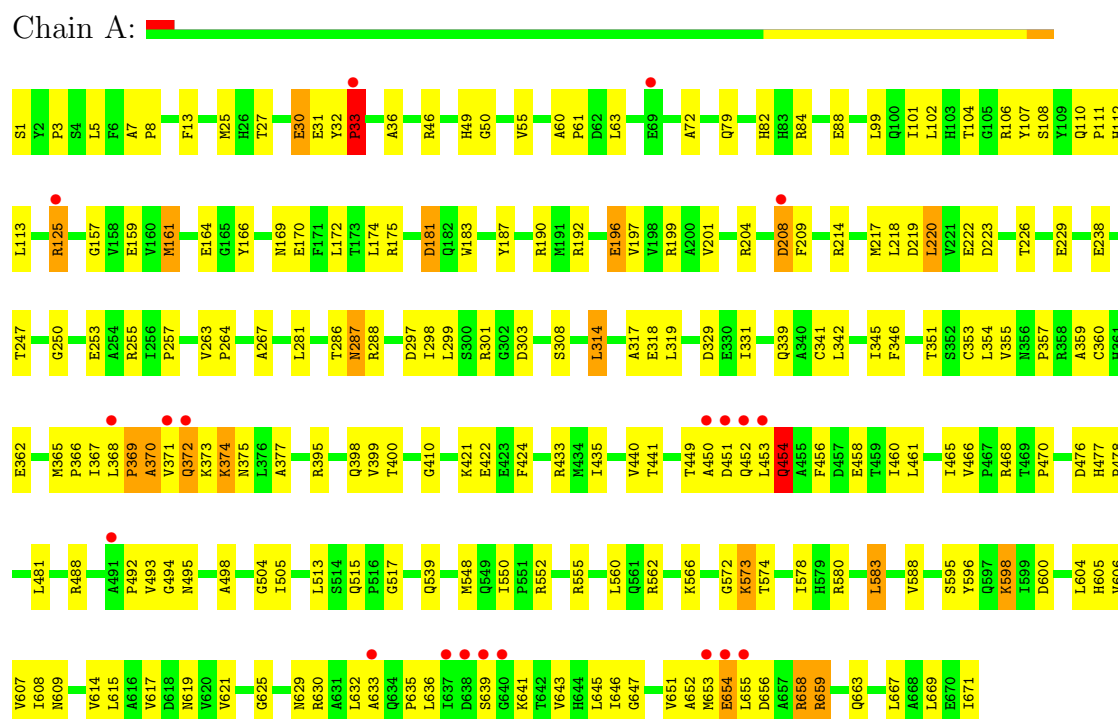
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	373	Total 373	O 373	0	0

### 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: 2,4-dienoyl-CoA reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.60Å 109.23Å 110.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 27.66 – 2.19	Depositor EDS
% Data completeness (in resolution range)	93.7 (30.00-2.20) 95.4 (27.66-2.19)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.20 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.203 , 0.243 0.220 , 0.254	Depositor DCC
$R_{free}$ test set	1918 reflections (4.88%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.5	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 34.4	EDS
Estimated twinning fraction	0.027 for -h,l,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 74790 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5676	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 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: CL, SF4, MDE, FMN, NAP, FAD

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	0.32	0/5192	0.61	1/7044 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	50	GLY	N-CA-C	5.30	126.35	113.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 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	5097	0	5107	177	0
2	A	3	0	0	0	0
3	A	8	0	0	0	0
4	A	53	0	31	1	0
5	A	31	0	19	0	0
6	A	48	0	25	6	0
7	A	63	0	49	2	0
8	A	373	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5676	0	5231	179	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 17.

All (179) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:659:ARG:HB2	1:A:659:ARG:HH11	1.15	1.09
1:A:646:ILE:HA	1:A:663:GLN:HE21	1.19	1.07
1:A:646:ILE:HA	1:A:663:GLN:NE2	1.91	0.85
1:A:107:TYR:OH	1:A:253:GLU:HG3	1.76	0.85
1:A:102:LEU:HD13	1:A:161:MET:HG2	1.59	0.82
1:A:465:ILE:HD11	1:A:652:ALA:HB2	1.62	0.80
1:A:656:ASP:HB3	6:A:703:NAP:H1D	1.65	0.79
1:A:658:ARG:HH11	1:A:658:ARG:HB3	1.50	0.76
1:A:659:ARG:CB	1:A:659:ARG:HH11	1.99	0.74
1:A:572:GLY:HA2	1:A:573:LYS:HZ2	1.51	0.73
1:A:513:LEU:HD22	1:A:555:ARG:NH1	2.03	0.72
1:A:654:GLU:CD	1:A:654:GLU:H	1.92	0.72
1:A:263:VAL:O	1:A:288:ARG:HD3	1.89	0.72
1:A:505:ILE:HG13	6:A:703:NAP:H52N	1.70	0.72
1:A:104:THR:OG1	1:A:108:SER:HB3	1.90	0.71
1:A:636:LEU:HB3	1:A:643:VAL:HG21	1.71	0.71
1:A:461:LEU:HB2	1:A:645:LEU:HD23	1.71	0.70
1:A:30:GLU:HB2	1:A:72:ALA:HB2	1.73	0.69
1:A:371:VAL:O	1:A:372:GLN:HG2	1.91	0.69
1:A:630:ARG:HB3	1:A:633:ALA:HB2	1.74	0.68
1:A:400:THR:HA	1:A:441:THR:HG23	1.75	0.68
1:A:218:LEU:HG	1:A:220:LEU:HD13	1.76	0.67
1:A:573:LYS:HE2	8:A:1009:HOH:O	1.92	0.67
1:A:264:PRO:HG2	1:A:267:ALA:HB2	1.75	0.67
1:A:494:GLY:H	1:A:619:ASN:HD22	1.44	0.65
1:A:422:GLU:CD	1:A:422:GLU:H	2.00	0.65
1:A:286:THR:O	1:A:287:ASN:HB2	1.97	0.65
1:A:646:ILE:CA	1:A:663:GLN:HE21	2.04	0.63
1:A:658:ARG:HH11	1:A:658:ARG:CB	2.12	0.63
1:A:466:VAL:HG23	1:A:629:ASN:HB2	1.82	0.62
1:A:659:ARG:HB2	1:A:659:ARG:NH1	2.00	0.62
1:A:102:LEU:HD13	1:A:161:MET:CG	2.27	0.62
1:A:238:GLU:HG3	1:A:281:LEU:HD13	1.82	0.62
1:A:562:ARG:HD3	6:A:703:NAP:O3X	1.99	0.61
1:A:498:ALA:HB2	1:A:617:VAL:HG11	1.83	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:226:THR:OG1	1:A:229:GLU:HG3	2.01	0.60
1:A:345:ILE:HB	1:A:351:THR:HG22	1.83	0.59
1:A:298:ILE:HG23	1:A:303:ASP:HB2	1.83	0.59
1:A:399:VAL:O	1:A:441:THR:HG22	2.02	0.59
1:A:166:TYR:O	1:A:170:GLU:HG3	2.04	0.57
1:A:465:ILE:HD11	1:A:652:ALA:CB	2.34	0.57
1:A:32:TYR:CG	1:A:33:PRO:HD2	2.39	0.57
1:A:319:LEU:HD12	1:A:331:ILE:HD13	1.86	0.57
1:A:513:LEU:HD22	1:A:555:ARG:HH12	1.70	0.56
1:A:548:MET:HB3	1:A:550:ILE:CD1	2.34	0.56
1:A:458:GLU:OE2	1:A:671:ILE:HD11	2.05	0.56
1:A:238:GLU:HG3	1:A:281:LEU:CD1	2.35	0.56
1:A:36:ALA:HB2	1:A:82:HIS:ND1	2.20	0.56
1:A:494:GLY:H	1:A:619:ASN:ND2	2.02	0.55
1:A:468:ARG:O	1:A:470:PRO:HD3	2.06	0.55
1:A:460:ILE:HD12	1:A:460:ILE:N	2.21	0.55
1:A:13:PHE:HB2	1:A:208:ASP:OD1	2.06	0.55
1:A:125:ARG:H	1:A:125:ARG:HD2	1.71	0.55
1:A:493:VAL:HB	1:A:555:ARG:HH12	1.72	0.55
1:A:600:ASP:CG	1:A:605:HIS:HE2	2.09	0.55
1:A:371:VAL:O	1:A:372:GLN:CG	2.54	0.55
1:A:651:VAL:HA	8:A:1027:HOH:O	2.07	0.54
1:A:647:GLY:H	1:A:663:GLN:NE2	2.06	0.54
1:A:654:GLU:CD	1:A:654:GLU:N	2.62	0.53
1:A:573:LYS:NZ	1:A:573:LYS:H	2.07	0.53
1:A:214:ARG:HH21	1:A:286:THR:HG21	1.73	0.53
1:A:572:GLY:HA2	1:A:573:LYS:NZ	2.24	0.53
1:A:451:ASP:O	1:A:454:GLN:HG3	2.09	0.53
1:A:187:TYR:CZ	1:A:229:GLU:HB3	2.44	0.52
1:A:377:ALA:HB2	1:A:456:PHE:CG	2.44	0.52
1:A:583:LEU:HB3	1:A:588:VAL:HG21	1.92	0.52
1:A:573:LYS:HZ3	1:A:573:LYS:H	1.56	0.52
1:A:636:LEU:CB	1:A:643:VAL:HG21	2.39	0.52
1:A:357:PRO:HG3	8:A:960:HOH:O	2.09	0.52
1:A:63:LEU:HG	8:A:754:HOH:O	2.09	0.51
1:A:1:SER:C	1:A:3:PRO:HD3	2.29	0.51
1:A:61:PRO:HG3	1:A:101:ILE:CG2	2.40	0.51
1:A:410:GLY:HA2	4:A:701:FAD:O3B	2.10	0.51
1:A:192:ARG:HD3	8:A:915:HOH:O	2.10	0.51
1:A:192:ARG:HH11	1:A:192:ARG:HG3	1.75	0.51
1:A:441:THR:HA	8:A:1012:HOH:O	2.10	0.51
1:A:192:ARG:O	1:A:196:GLU:HB2	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:172:LEU:O	1:A:190:ARG:HD2	2.10	0.50
1:A:222:GLU:O	1:A:223:ASP:HB2	2.10	0.50
1:A:181:ASP:OD2	1:A:183:TRP:HD1	1.94	0.50
1:A:488:ARG:HD3	8:A:1021:HOH:O	2.11	0.50
1:A:550:ILE:HD12	1:A:550:ILE:N	2.26	0.50
1:A:61:PRO:HG3	1:A:101:ILE:HG22	1.93	0.50
1:A:630:ARG:HB3	1:A:633:ALA:CB	2.39	0.50
1:A:552:ARG:HD3	8:A:971:HOH:O	2.12	0.49
1:A:362:GLU:CD	1:A:362:GLU:H	2.15	0.49
1:A:36:ALA:HB2	1:A:82:HIS:CE1	2.46	0.49
1:A:164:GLU:HA	1:A:250:GLY:O	2.13	0.49
1:A:562:ARG:HD2	1:A:596:TYR:HE1	1.75	0.49
1:A:573:LYS:CD	1:A:573:LYS:H	2.26	0.49
1:A:495:ASN:O	1:A:555:ARG:HB3	2.13	0.48
1:A:197:VAL:O	1:A:201:VAL:HG23	2.13	0.48
1:A:598:LYS:HE3	1:A:605:HIS:CG	2.48	0.48
1:A:421:LYS:HD3	1:A:424:PHE:HE2	1.78	0.48
1:A:106:ARG:HA	1:A:113:LEU:HD12	1.95	0.48
1:A:55:VAL:HG11	1:A:159:GLU:OE1	2.14	0.48
1:A:370:ALA:O	1:A:371:VAL:C	2.51	0.47
1:A:608:ILE:HG22	1:A:609:ASN:ND2	2.29	0.47
1:A:493:VAL:HB	1:A:555:ARG:NH1	2.29	0.47
1:A:550:ILE:HD12	1:A:550:ILE:H	1.78	0.47
1:A:199:ARG:HG3	8:A:869:HOH:O	2.13	0.47
1:A:32:TYR:CD2	1:A:33:PRO:HD2	2.50	0.47
1:A:49:HIS:CE1	1:A:318:GLU:HG2	2.49	0.47
1:A:605:HIS:ND1	1:A:614:VAL:HG22	2.28	0.47
1:A:583:LEU:HB3	1:A:588:VAL:CG2	2.45	0.47
1:A:372:GLN:O	1:A:374:LYS:HD3	2.14	0.47
1:A:639:SER:HB3	1:A:641:LYS:HE3	1.95	0.47
1:A:257:PRO:HG3	1:A:578:ILE:HG23	1.96	0.47
1:A:286:THR:HB	1:A:308:SER:HB3	1.97	0.47
1:A:238:GLU:OE1	1:A:281:LEU:HD13	2.15	0.46
1:A:454:GLN:HG2	1:A:641:LYS:HZ1	1.79	0.46
1:A:339:GLN:O	1:A:658:ARG:NH2	2.49	0.46
1:A:604:LEU:HG	1:A:606:VAL:HG13	1.97	0.46
1:A:99:LEU:C	1:A:99:LEU:HD23	2.36	0.46
1:A:368:LEU:O	1:A:395:ARG:NH1	2.48	0.46
1:A:595:SER:HB2	1:A:607:VAL:HB	1.98	0.46
1:A:5:LEU:HA	1:A:299:LEU:CD1	2.44	0.46
1:A:319:LEU:CD1	1:A:331:ILE:HD13	2.45	0.45
1:A:600:ASP:OD2	1:A:605:HIS:NE2	2.49	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:329:ASP:OD2	1:A:433:ARG:HD3	2.16	0.45
1:A:477:HIS:ND1	1:A:478:PRO:HD2	2.32	0.45
1:A:375:ASN:ND2	1:A:398:GLN:OE1	2.48	0.45
1:A:371:VAL:O	1:A:372:GLN:NE2	2.49	0.45
1:A:79:GLN:O	1:A:82:HIS:HB3	2.17	0.45
1:A:435:ILE:HG23	1:A:440:VAL:HB	1.97	0.45
1:A:632:LEU:HD12	1:A:632:LEU:N	2.31	0.45
1:A:346:PHE:CD1	7:A:704:MDE:H9'1	2.52	0.45
1:A:286:THR:OG1	1:A:287:ASN:N	2.49	0.45
1:A:27:THR:O	1:A:351:THR:HG23	2.17	0.45
1:A:365:MET:N	1:A:366:PRO:HD3	2.32	0.44
1:A:217:MET:HE3	1:A:247:THR:HA	2.00	0.44
1:A:548:MET:HB3	1:A:550:ILE:HD12	1.99	0.44
1:A:481:LEU:O	1:A:621:VAL:HA	2.17	0.44
1:A:27:THR:N	1:A:30:GLU:OE1	2.47	0.44
1:A:625:GLY:CA	6:A:703:NAP:H52A	2.47	0.44
1:A:639:SER:O	1:A:641:LYS:HG3	2.18	0.44
1:A:60:ALA:HA	1:A:61:PRO:HD3	1.75	0.43
1:A:604:LEU:HD23	1:A:615:LEU:HD12	1.99	0.43
1:A:219:ASP:O	1:A:220:LEU:HB2	2.18	0.43
1:A:157:GLY:HA2	1:A:209:PHE:CZ	2.52	0.43
1:A:566:LYS:HE2	1:A:580:ARG:HD2	2.00	0.43
1:A:454:GLN:HG2	1:A:641:LYS:NZ	2.33	0.43
1:A:655:LEU:HD22	1:A:659:ARG:HB3	1.99	0.43
1:A:174:LEU:HG	1:A:190:ARG:NH1	2.33	0.43
1:A:255:ARG:HA	1:A:255:ARG:NE	2.33	0.43
1:A:450:ALA:HB2	1:A:635:PRO:HB2	2.00	0.43
1:A:573:LYS:HD3	1:A:573:LYS:N	2.34	0.43
1:A:110:GLN:HA	1:A:111:PRO:HD3	1.87	0.43
1:A:505:ILE:HD12	6:A:703:NAP:O2N	2.19	0.43
1:A:46:ARG:CZ	1:A:317:ALA:HB2	2.49	0.43
1:A:647:GLY:N	1:A:663:GLN:NE2	2.66	0.42
1:A:492:PRO:HD2	8:A:1079:HOH:O	2.19	0.42
1:A:598:LYS:HE3	1:A:605:HIS:CD2	2.54	0.42
1:A:353:CYS:SG	1:A:355:VAL:HG22	2.59	0.42
1:A:84:ARG:HG2	1:A:88:GLU:OE2	2.19	0.42
1:A:354:LEU:C	1:A:354:LEU:HD23	2.39	0.42
1:A:651:VAL:O	1:A:655:LEU:HG	2.19	0.42
1:A:359:ALA:O	1:A:360:CYS:HB2	2.19	0.42
1:A:655:LEU:HD22	1:A:659:ARG:HG2	2.01	0.42
1:A:368:LEU:O	1:A:369:PRO:C	2.57	0.42
1:A:377:ALA:HB2	1:A:456:PHE:CD2	2.55	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:369:PRO:O	1:A:395:ARG:O	2.38	0.42
1:A:449:THR:HG22	1:A:450:ALA:N	2.34	0.42
1:A:247:THR:HB	1:A:286:THR:HG22	2.02	0.42
1:A:297:ASP:O	1:A:301:ARG:HG3	2.19	0.42
1:A:573:LYS:CD	1:A:573:LYS:N	2.82	0.41
6:A:703:NAP:H6N	6:A:703:NAP:H2D	1.89	0.41
1:A:7:ALA:HA	1:A:8:PRO:HD3	1.96	0.41
1:A:341:CYS:SG	1:A:342:LEU:N	2.91	0.41
1:A:175:ARG:HB2	1:A:223:ASP:HB2	2.03	0.41
1:A:196:GLU:OE1	1:A:196:GLU:HA	2.21	0.41
1:A:452:GLN:OE1	1:A:452:GLN:HA	2.20	0.41
7:A:704:MDE:H5'1	7:A:704:MDE:H8	2.03	0.41
1:A:367:ILE:HG12	1:A:669:LEU:HD22	2.03	0.41
1:A:25:MET:HE1	1:A:314:LEU:HD13	2.03	0.41
1:A:658:ARG:NH1	1:A:658:ARG:CB	2.82	0.41
1:A:515:GLN:HG3	1:A:517:GLY:O	2.21	0.40
1:A:342:LEU:HG	1:A:574:THR:HG21	2.03	0.40
1:A:110:GLN:HG2	1:A:112:HIS:H	1.86	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	669/671 (100%)	620 (93%)	38 (6%)	11 (2%)	14 9

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	453	LEU
1	A	504	GLY
1	A	653	MET
1	A	287	ASN
1	A	369	PRO

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Mol	Chain	Res	Type
1	A	373	LYS
1	A	454	GLN
1	A	33	PRO
1	A	372	GLN
1	A	181	ASP
1	A	370	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	537/537 (100%)	514 (96%)	23 (4%)	40	47

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLU
1	A	31	GLU
1	A	33	PRO
1	A	125	ARG
1	A	161	MET
1	A	169	ASN
1	A	196	GLU
1	A	204	ARG
1	A	208	ASP
1	A	220	LEU
1	A	314	LEU
1	A	374	LYS
1	A	454	GLN
1	A	476	ASP
1	A	539	GLN
1	A	560	LEU
1	A	573	LYS
1	A	583	LEU
1	A	598	LYS
1	A	654	GLU
1	A	658	ARG
1	A	659	ARG

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Mol	Chain	Res	Type
1	A	667	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	HIS
1	A	207	ASN
1	A	405	HIS
1	A	538	GLN
1	A	549	GLN
1	A	597	GLN
1	A	609	ASN
1	A	613	GLN
1	A	619	ASN
1	A	634	GLN
1	A	663	GLN

### 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 ⓘ

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 for Mogul analysis.

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	SF4	A	700	1	12,12,12	28.80	7 (58%)	0,24,24	0.00	-
4	FAD	A	701	-	58,58,58	4.05	25 (43%)	85,89,89	2.56	23 (27%)
5	FMN	A	702	-	33,33,33	2.67	10 (30%)	46,50,50	3.47	13 (28%)
6	NAP	A	703	-	52,52,52	2.10	13 (25%)	80,80,80	2.02	17 (21%)
7	MDE	A	704	-	65,65,65	3.65	19 (29%)	91,92,92	2.26	26 (28%)

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	SF4	A	700	1	-	0/0/48/48	0/0/5/5
4	FAD	A	701	-	-	0/34/50/50	0/1/6/6
5	FMN	A	702	-	-	0/18/18/18	0/0/3/3
6	NAP	A	703	-	-	0/35/67/67	0/3/5/5
7	MDE	A	704	-	1/1/13/18	1/64/82/82	0/1/3/3

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	700	SF4	S1-FE4	-55.69	1.95	2.33
3	A	700	SF4	S2-FE4	-54.92	1.96	2.33
3	A	700	SF4	S4-FE3	-44.21	2.03	2.33
3	A	700	SF4	S3-FE4	-42.77	2.04	2.33
7	A	704	MDE	O9P-C9P	-22.21	1.23	1.41
4	A	701	FAD	C1'-C2'	13.36	1.64	1.51
7	A	704	MDE	OAP-CAP	11.64	1.44	1.21
4	A	701	FAD	C9A-N10	10.07	1.53	1.38
5	A	702	FMN	C1'-N10	-9.68	1.37	1.48
4	A	701	FAD	C10-N10	8.83	1.57	1.38
6	A	703	NAP	C4A-N3A	8.82	1.49	1.35
4	A	701	FAD	C2'-C3'	8.02	1.70	1.53
4	A	701	FAD	C4X-C10	7.63	1.54	1.40
4	A	701	FAD	C4-N3	7.24	1.49	1.37
4	A	701	FAD	C6-C5X	7.05	1.50	1.41
4	A	701	FAD	C9A-C5X	6.92	1.56	1.42
4	A	701	FAD	C8-C7	5.95	1.58	1.40
3	A	700	SF4	S2-FE3	-5.65	2.29	2.33
5	A	702	FMN	C9A-N10	5.61	1.47	1.38
5	A	702	FMN	C4-C4A	5.39	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	FAD	C9-C9A	5.23	1.51	1.40
7	A	704	MDE	C2A-N3A	5.16	1.42	1.32
4	A	701	FAD	C2A-N3A	5.05	1.42	1.32
6	A	703	NAP	PA-O3	-4.89	1.51	1.59
7	A	704	MDE	C2A-N1A	4.81	1.43	1.33
6	A	703	NAP	C2N-C3N	4.80	1.45	1.38
4	A	701	FAD	C2A-N1A	4.76	1.43	1.33
5	A	702	FMN	C1'-C2'	4.71	1.56	1.51
4	A	701	FAD	C5'-C4'	4.63	1.59	1.51
7	A	704	MDE	C5A-C4A	4.54	1.47	1.40
6	A	703	NAP	PN-O3	-4.49	1.51	1.60
7	A	704	MDE	C8A-N9A	4.41	1.39	1.34
7	A	704	MDE	C2'-C3'	4.36	1.44	1.31
4	A	701	FAD	C2-N3	4.25	1.45	1.37
4	A	701	FAD	C5X-N5	4.13	1.41	1.35
4	A	701	FAD	C1'-N10	4.13	1.52	1.48
4	A	701	FAD	C4-C4X	4.11	1.47	1.41
7	A	704	MDE	CEP-CBP	3.96	1.62	1.53
4	A	701	FAD	P-O3P	-3.94	1.52	1.59
7	A	704	MDE	O2B-C2B	3.85	1.52	1.43
4	A	701	FAD	C10-N1	3.83	1.42	1.35
7	A	704	MDE	CB-CB1	3.72	1.55	1.49
4	A	701	FAD	O2B-C2B	3.61	1.51	1.43
7	A	704	MDE	OB1-CB1	3.27	1.42	1.19
4	A	701	FAD	C6-C7	3.13	1.46	1.37
6	A	703	NAP	C5A-C4A	3.11	1.47	1.40
4	A	701	FAD	C4X-N5	2.92	1.42	1.36
6	A	703	NAP	C8A-N9A	2.86	1.40	1.36
6	A	703	NAP	C4N-C3N	2.86	1.44	1.39
3	A	700	SF4	S4-FE1	-2.84	2.31	2.33
4	A	701	FAD	C9-C8	2.77	1.45	1.37
4	A	701	FAD	C5A-C4A	2.76	1.46	1.40
6	A	703	NAP	P2B-O1X	2.70	1.60	1.51
7	A	704	MDE	C8A-N7A	2.62	1.38	1.34
5	A	702	FMN	C7M-C7	2.53	1.56	1.51
6	A	703	NAP	C6N-N1N	2.51	1.42	1.35
3	A	700	SF4	S2-FE1	2.51	2.34	2.33
7	A	704	MDE	C2B-C1B	2.48	1.57	1.53
6	A	703	NAP	O4D-C1D	2.41	1.45	1.41
5	A	702	FMN	C10-N1	2.40	1.39	1.35
5	A	702	FMN	C10-N10	2.40	1.44	1.38
4	A	701	FAD	C8A-N7A	2.38	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	704	MDE	O4B-C1B	2.33	1.44	1.41
7	A	704	MDE	C5P-N4P	2.29	1.38	1.33
5	A	702	FMN	C5'-C4'	-2.26	1.48	1.51
6	A	703	NAP	O4B-C1B	2.18	1.44	1.41
6	A	703	NAP	C1D-N1N	2.17	1.55	1.48
7	A	704	MDE	C6A-C5A	2.14	1.49	1.44
6	A	703	NAP	C3N-C7N	2.11	1.54	1.50
5	A	702	FMN	P-O3P	-2.09	1.47	1.54
7	A	704	MDE	CBP-CAP	2.06	1.59	1.52
5	A	702	FMN	C8M-C8	2.06	1.55	1.51
7	A	704	MDE	C4A-N3A	-2.05	1.32	1.35
7	A	704	MDE	C9P-CAP	2.02	1.57	1.53

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	702	FMN	C2-N1-C10	12.33	127.41	114.98
4	A	701	FAD	C2'-C1'-N10	-11.05	97.79	112.45
5	A	702	FMN	C4A-C10-N1	-9.85	112.89	122.73
6	A	703	NAP	C8A-N9A-C4A	-9.25	99.84	106.90
4	A	701	FAD	C4X-C10-N10	-9.11	115.96	120.51
4	A	701	FAD	C2-N1-C10	8.25	123.30	114.98
5	A	702	FMN	C9A-N10-C10	-7.71	114.20	121.77
5	A	702	FMN	C1'-N10-C9A	7.50	126.17	118.87
7	A	704	MDE	O9P-C9P-N8P	6.59	120.94	113.12
5	A	702	FMN	C5'-C4'-C3'	-6.58	99.64	112.06
7	A	704	MDE	P2A-O3A-P1A	-5.99	114.12	131.68
6	A	703	NAP	O7N-C7N-N7N	-5.74	114.30	122.59
7	A	704	MDE	C8A-N9A-C1B	5.65	135.04	125.99
4	A	701	FAD	N3A-C2A-N1A	-5.41	124.18	128.71
7	A	704	MDE	OAP-CAP-C9P	-5.30	111.21	118.62
7	A	704	MDE	N3A-C2A-N1A	-5.21	124.35	128.71
4	A	701	FAD	C1'-N10-C9A	5.15	123.88	118.87
4	A	701	FAD	C1B-N9A-C4A	-5.05	117.92	126.64
7	A	704	MDE	C8A-N7A-C5A	-4.88	105.04	108.52
5	A	702	FMN	C4A-C10-N10	4.84	122.92	120.51
6	A	703	NAP	N3A-C4A-N9A	4.78	134.06	125.43
5	A	702	FMN	C5A-C9A-N10	4.75	121.48	116.80
7	A	704	MDE	CBP-CAP-C9P	-4.70	111.61	119.43
4	A	701	FAD	C8A-N9A-C1B	4.69	135.62	126.38
7	A	704	MDE	O9P-C9P-CAP	4.49	120.53	110.26
7	A	704	MDE	C2P-S1P-C1'	4.48	105.36	99.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	703	NAP	O7N-C7N-C3N	4.31	124.44	119.58
7	A	704	MDE	C1B-N9A-C4A	-4.24	119.30	126.64
7	A	704	MDE	CEP-CBP-CCP	-4.24	101.62	109.14
7	A	704	MDE	N7A-C8A-N9A	4.17	113.78	109.18
6	A	703	NAP	C4A-C5A-N7A	4.03	112.97	109.52
5	A	702	FMN	C4-C4A-C10	3.92	123.28	116.95
4	A	701	FAD	C4'-C3'-C2'	3.88	122.02	113.25
6	A	703	NAP	O2N-PN-O1N	-3.84	107.14	118.72
4	A	701	FAD	C4A-C5A-N7A	-3.59	106.44	109.52
5	A	702	FMN	O5'-P-O1P	-3.59	96.19	106.71
7	A	704	MDE	OAP-CAP-CBP	-3.59	115.12	120.98
6	A	703	NAP	C5A-C4A-N3A	-3.50	118.07	125.70
5	A	702	FMN	O4'-C4'-C3'	3.49	117.73	109.05
5	A	702	FMN	C4A-N5-C5A	3.47	120.58	116.69
6	A	703	NAP	PN-O5D-C5D	3.43	132.09	120.24
7	A	704	MDE	O6A-CCP-CBP	3.42	116.29	110.57
4	A	701	FAD	C10-C4X-N5	3.39	124.57	120.45
7	A	704	MDE	CAP-C9P-N8P	3.26	118.53	110.45
7	A	704	MDE	C2'-C1'-S1P	3.20	120.13	112.94
6	A	703	NAP	C8A-N9A-C1B	3.16	132.60	126.38
5	A	702	FMN	N1-C10-N10	3.12	124.18	115.97
6	A	703	NAP	C3N-C7N-N7N	3.07	121.27	117.77
4	A	701	FAD	O4B-C1B-N9A	3.05	111.28	108.44
7	A	704	MDE	O8B-P3B-O3B	-3.05	98.32	107.09
6	A	703	NAP	PN-O3-PA	-3.04	119.89	132.95
7	A	704	MDE	CB1-CB-SG	-3.02	109.31	113.77
4	A	701	FAD	C6-C5X-N5	-2.94	115.55	118.97
6	A	703	NAP	N7A-C8A-N9A	2.90	122.56	114.36
4	A	701	FAD	N3-C2-N1	-2.83	115.16	121.19
6	A	703	NAP	C6N-N1N-C2N	-2.76	118.92	122.04
7	A	704	MDE	O4B-C4B-C5B	2.71	119.03	109.36
7	A	704	MDE	O2A-P1A-O3A	2.62	117.55	105.14
7	A	704	MDE	CB-SG-C5'	2.53	107.20	102.04
4	A	701	FAD	C8M-C8-C9	-2.50	114.36	120.38
7	A	704	MDE	O7B-P3B-O3B	2.46	114.19	107.09
4	A	701	FAD	C3B-C2B-C1B	2.44	104.73	100.91
4	A	701	FAD	N1-C10-N10	2.43	122.35	115.97
4	A	701	FAD	O4B-C4B-C5B	2.39	117.89	109.36
7	A	704	MDE	O3A-P1A-O5B	-2.34	92.96	103.41
4	A	701	FAD	C9-C9A-N10	2.25	126.44	121.59
7	A	704	MDE	C4'-C3'-C2'	-2.21	120.53	125.69
7	A	704	MDE	OB1-CB1-CB	-2.20	113.80	126.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	703	NAP	C8A-N7A-C5A	-2.20	96.76	103.58
6	A	703	NAP	C4D-O4D-C1D	2.17	112.11	109.75
4	A	701	FAD	C4X-N5-C5X	2.15	119.10	116.69
7	A	704	MDE	C4B-O4B-C1B	-2.13	107.44	109.75
4	A	701	FAD	O4B-C4B-C3B	2.12	109.47	105.17
6	A	703	NAP	C3D-C2D-C1D	2.10	104.19	100.91
6	A	703	NAP	C2N-C3N-C7N	2.06	125.48	119.35
4	A	701	FAD	C1'-N10-C10	-2.05	116.26	119.17
4	A	701	FAD	C9A-C5X-N5	2.05	125.50	122.37
4	A	701	FAD	O4B-C1B-C2B	2.03	109.88	106.77
5	A	702	FMN	C6-C5A-C9A	2.02	121.81	119.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	704	MDE	C9P

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	704	MDE	CAP-C9P-N8P-C7P

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	671/671 (100%)	0.16	20 (2%) 48 48	16, 35, 64, 87	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	371	VAL	6.7
1	A	637	ILE	5.3
1	A	640	GLY	4.4
1	A	638	ASP	4.3
1	A	453	LEU	3.8
1	A	368	LEU	3.8
1	A	639	SER	3.4
1	A	653	MET	3.3
1	A	452	GLN	3.2
1	A	451	ASP	3.1
1	A	633	ALA	2.7
1	A	125	ARG	2.7
1	A	655	LEU	2.6
1	A	450	ALA	2.5
1	A	69	GLU	2.3
1	A	33	PRO	2.1
1	A	491	ALA	2.1
1	A	654	GLU	2.1
1	A	208	ASP	2.1
1	A	372	GLN	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
7	MDE	A	704	63/63	0.21	1.75	25,51,94,97	0
6	NAP	A	703	48/48	0.22	1.08	34,67,94,95	0
4	FAD	A	701	53/53	0.18	0.79	24,35,55,56	0
5	FMN	A	702	31/31	0.17	0.59	17,20,23,23	0
2	CL	A	706	1/1	0.16	0.29	55,55,55,55	0
2	CL	A	707	1/1	0.14	0.06	70,70,70,70	0
3	SF4	A	700	8/8	0.10	-0.78	19,20,22,24	0
2	CL	A	705	1/1	0.07	-2.76	69,69,69,69	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.