



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:51 AM GMT

PDB ID : 2IX5  
Title : SHORT CHAIN SPECIFIC ACYL-COA OXIDASE FROM ARABIDOPSIS  
THALIANA, ACX4 IN COMPLEX WITH ACETOACETYL-COA  
Authors : Mackenzie, J.; Pedersen, L.; Arent, S.; Henriksen, A.  
Deposited on : 2006-07-07  
Resolution : 2.70 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

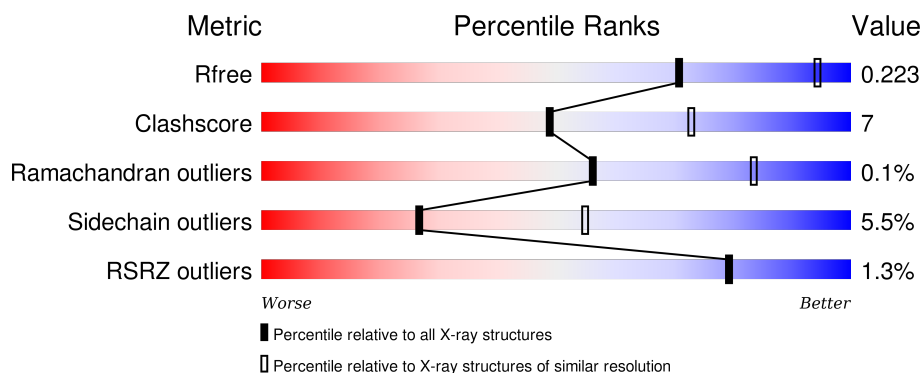
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	436	<div> <div>3%</div> <div>78%</div> <div>16%</div> <div>5%</div> </div>
1	B	436	<div> <div>%</div> <div>79%</div> <div>14%</div> <div>5%</div> </div>
1	C	436	<div> <div>80%</div> <div>14%</div> <div>5%</div> </div>
1	D	436	<div> <div>78%</div> <div>16%</div> <div>5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CAA	A	1432	-	-	-	X
2	CAA	C	1432	-	-	-	X

## 2 Entry composition [i](#)

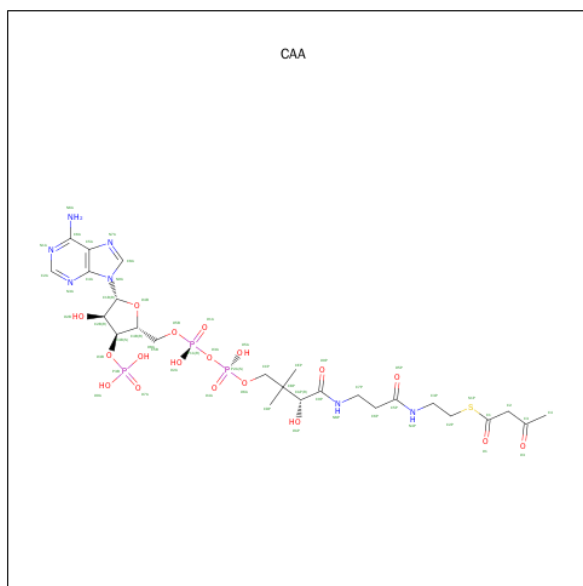
There are 4 unique types of molecules in this entry. The entry contains 13234 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACYL-COENZYME A OXIDASE 4, PEROXISOMAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	1	1
			3166	2022	531	590	23			
1	B	416	Total	C	N	O	S	0	1	1
			3179	2030	534	592	23			
1	C	416	Total	C	N	O	S	0	0	1
			3162	2021	534	584	23			
1	D	416	Total	C	N	O	S	0	0	1
			3159	2017	530	590	22			

- Molecule 2 is ACETOACETYL-COENZYME A (three-letter code: CAA) (formula: C<sub>25</sub>H<sub>40</sub>N<sub>7</sub>O<sub>18</sub>P<sub>3</sub>S).



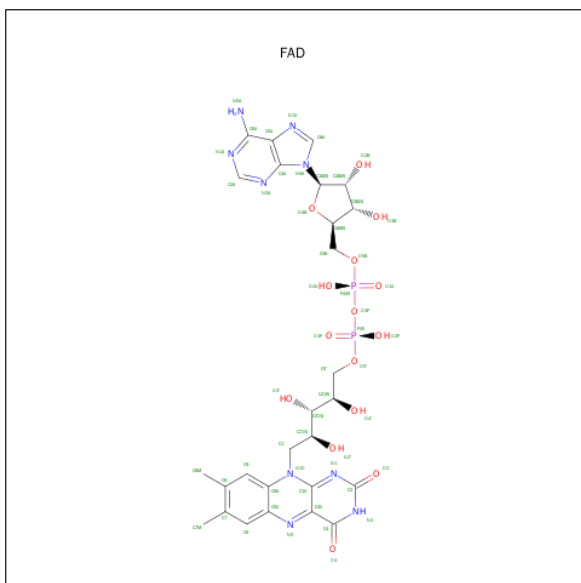
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P S	0	0
			48	21	7	16	3 1		
2	B	1	Total	C	N	O	P S	0	0
			48	21	7	16	3 1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	24	Total	O	0	0
			24	24		
4	B	48	Total	O	0	0
			48	48		
4	C	48	Total	O	0	0
			48	48		

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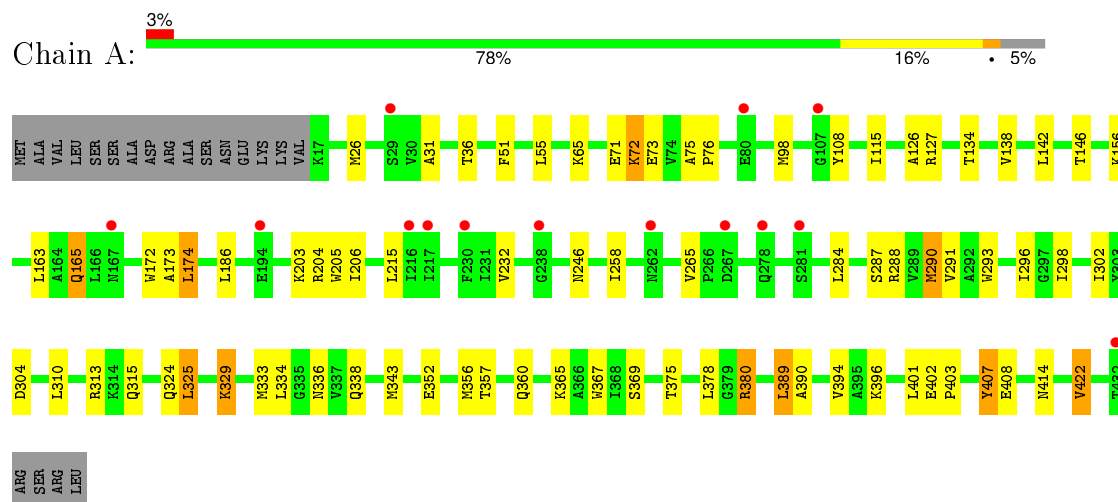
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	44	Total	O	0	0
			44	44		

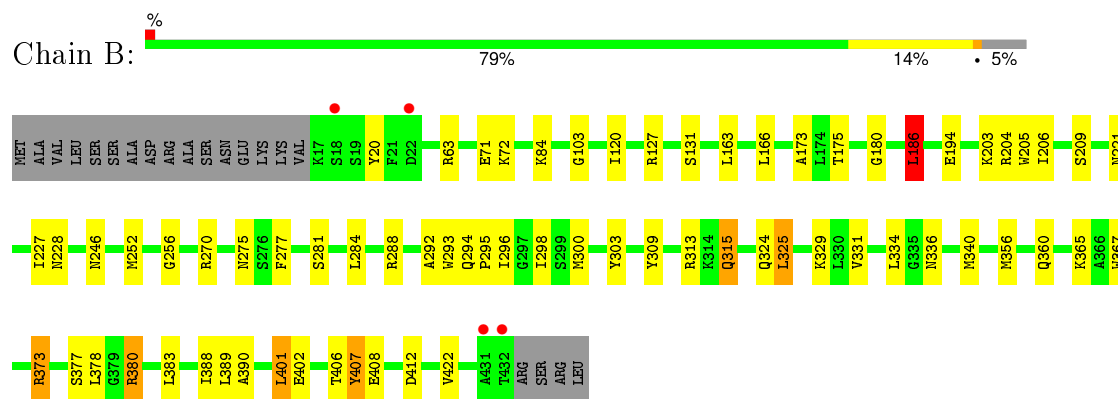
### 3 Residue-property plots

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.

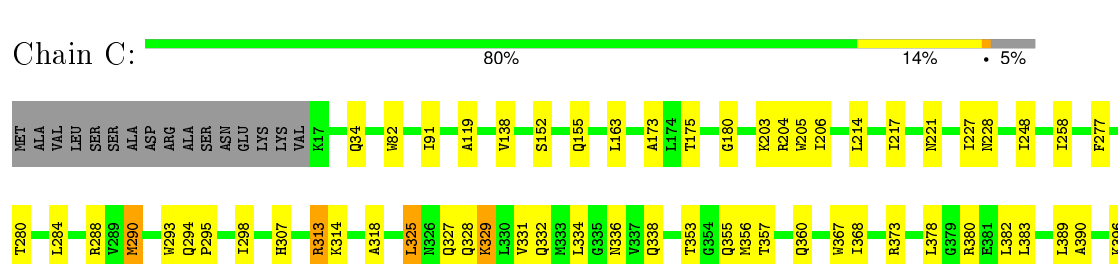
- Molecule 1: ACYL-COENZYME A OXIDASE 4, PEROXISOMAL

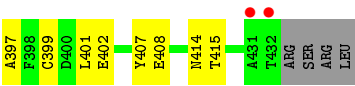


- Molecule 1: ACYL-COENZYME A OXIDASE 4, PEROXISOMAL

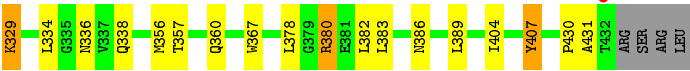
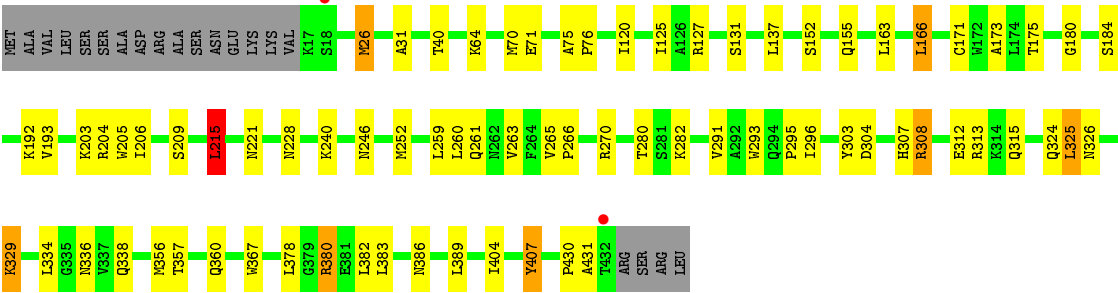
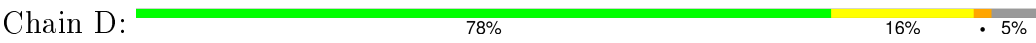


- Molecule 1: ACYL-COENZYME A OXIDASE 4, PEROXISOMAL





● Molecule 1: ACYL-COENZYME A OXIDASE 4, PEROXISOMAL



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.75Å 144.75Å 149.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.70) 99.7 (20.00-2.70)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.186 , 0.232 0.181 , 0.223	Depositor DCC
$R_{free}$ test set	2525 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.0	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 39.6	EDS
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 49727 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13234	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CAA, 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	0.40	0/3238	0.54	0/4393
1	B	0.42	0/3251	0.56	1/4407 (0.0%)
1	C	0.41	0/3231	0.54	0/4381
1	D	0.40	0/3228	0.56	1/4381 (0.0%)
All	All	0.41	0/12948	0.55	2/17562 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	186	LEU	CA-CB-CG	7.45	132.44	115.30
1	D	215	LEU	CA-CB-CG	5.06	126.94	115.30

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	3166	0	3169	61	0
1	B	3179	0	3196	51	0
1	C	3162	0	3180	49	0
1	D	3159	0	3149	51	0
2	A	48	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	48	0	31	0	0
2	C	48	0	31	2	0
2	D	48	0	31	1	0
3	A	53	0	31	1	0
3	B	53	0	31	5	0
3	C	53	0	31	2	0
3	D	53	0	31	3	0
4	A	24	0	0	0	0
4	B	48	0	0	0	0
4	C	48	0	0	1	0
4	D	44	0	0	1	0
All	All	13234	0	12942	187	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 7.

All (187) 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:D:357:THR:H	1:D:360:GLN:HE21	1.31	0.78
1:C:204:ARG:HH21	1:D:386:ASN:HD21	1.32	0.77
1:B:194[B]:GLU:H	1:B:194[B]:GLU:CD	1.90	0.75
1:C:288:ARG:HD3	1:C:414:ASN:HD21	1.52	0.74
1:A:146:THR:HG21	1:A:172:TRP:HE1	1.53	0.74
1:A:336:ASN:HD22	1:D:367:TRP:HE1	1.35	0.72
1:A:165:GLN:HA	1:A:165:GLN:HE21	1.57	0.70
1:A:357:THR:H	1:A:360:GLN:HE21	1.38	0.70
1:A:173:ALA:HA	1:A:206:ILE:HD12	1.74	0.70
1:A:422:VAL:O	1:D:307:HIS:HE1	1.75	0.69
1:B:336:ASN:HD22	1:C:367:TRP:HE1	1.41	0.69
1:B:296:ILE:O	1:B:300:MET:HG3	1.93	0.68
1:A:367:TRP:HE1	1:D:336:ASN:ND2	1.93	0.66
1:D:171:CYS:SG	1:D:215:LEU:HD13	2.37	0.64
1:A:333:MET:HG2	1:A:375:THR:HG23	1.79	0.64
1:B:324:GLN:HB3	1:D:325:LEU:HD13	1.79	0.64
1:A:380:ARG:NH2	1:B:406:THR:OG1	2.26	0.64
1:C:204:ARG:HH21	1:D:386:ASN:ND2	1.95	0.64
1:D:329:LYS:HG3	1:D:378:LEU:HD22	1.79	0.64
1:A:291:VAL:HG21	1:A:408:GLU:HG3	1.80	0.64
1:D:131:SER:CB	1:D:252:MET:HB2	2.29	0.63
1:A:367:TRP:HE1	1:D:336:ASN:HD22	1.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:GLY:HA3	3:B:1433:FAD:O2P	2.00	0.62
1:D:240:LYS:HE2	1:D:259:LEU:HD23	1.82	0.61
1:A:287:SER:O	1:A:291:VAL:HG23	2.00	0.61
1:C:329:LYS:HG3	1:C:378:LEU:HD22	1.82	0.61
1:D:356:MET:HA	1:D:360:GLN:NE2	2.15	0.61
1:B:71:GLU:OE1	1:B:127:ARG:NH2	2.34	0.61
1:C:284:LEU:O	1:C:288:ARG:HB2	2.01	0.60
1:D:260:LEU:HD23	1:D:263:VAL:HG21	1.83	0.60
1:B:294:GLN:HB2	1:B:295:PRO:HD3	1.83	0.60
1:D:40:THR:O	1:D:308:ARG:NH2	2.35	0.60
1:A:115:ILE:HG22	1:A:352:GLU:HG3	1.83	0.59
1:A:290:MET:CE	1:A:290:MET:HA	2.33	0.59
1:D:221:ASN:HD22	1:D:228:ASN:HD21	1.50	0.59
1:C:298:ILE:HG23	1:C:397:ALA:HB1	1.85	0.58
1:C:334:LEU:O	1:C:338:GLN:HG2	2.03	0.58
1:A:329:LYS:HG3	1:A:378:LEU:HD22	1.85	0.57
1:C:175:THR:HG23	1:C:180:GLY:HA2	1.86	0.57
1:A:127:ARG:NH1	1:A:304:ASP:OD2	2.38	0.57
1:A:72:LYS:HG3	1:A:73:GLU:HG2	1.87	0.57
1:B:336:ASN:ND2	1:C:367:TRP:HE1	2.03	0.56
1:D:357:THR:H	1:D:360:GLN:NE2	2.03	0.56
1:A:336:ASN:ND2	1:D:367:TRP:HE1	2.03	0.56
1:A:215:LEU:HB2	1:A:232:VAL:HG22	1.88	0.56
1:C:357:THR:H	1:C:360:GLN:HE21	1.54	0.56
1:C:356:MET:HA	1:C:360:GLN:NE2	2.21	0.55
1:B:131:SER:CB	1:B:252:MET:HB2	2.37	0.55
1:C:34:GLN:NE2	1:C:314:LYS:H	2.03	0.55
1:B:175:THR:OG1	3:B:1433:FAD:H1'1	2.07	0.55
1:D:228:ASN:ND2	1:D:270:ARG:HH21	2.05	0.54
1:A:365:LYS:O	1:A:369:SER:HB2	2.07	0.54
1:C:203:LYS:HB2	1:C:258:ILE:HB	1.88	0.54
1:D:204:ARG:O	1:D:205:TRP:HB2	2.08	0.54
1:D:203:LYS:HB3	1:D:206:ILE:HD11	1.89	0.54
1:B:356:MET:HA	1:B:360:GLN:HE22	1.72	0.54
1:B:284:LEU:O	1:B:288:ARG:HG3	2.08	0.54
1:A:357:THR:H	1:A:360:GLN:NE2	2.04	0.54
1:D:334:LEU:O	1:D:338:GLN:HG2	2.08	0.54
1:A:204:ARG:O	1:A:205:TRP:HB2	2.07	0.54
1:B:356:MET:HA	1:B:360:GLN:NE2	2.23	0.53
1:C:34:GLN:HB2	4:C:2004:HOH:O	2.08	0.53
1:A:26:MET:CE	1:A:31:ALA:HA	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:LEU:O	1:A:186:LEU:HD11	2.09	0.53
1:A:293:TRP:HA	1:A:296:ILE:HD12	1.92	0.52
1:B:221:ASN:HB2	1:B:228:ASN:ND2	2.24	0.52
1:B:228:ASN:ND2	1:B:270:ARG:HH11	2.07	0.52
1:A:203:LYS:HB2	1:A:258:ILE:HB	1.93	0.51
1:A:402:GLU:HB2	1:A:403:PRO:HD3	1.93	0.51
1:C:204:ARG:NH2	1:D:386:ASN:HD21	2.05	0.51
1:C:408:GLU:HA	2:C:1432:CAA:H32	1.91	0.51
1:B:221:ASN:HD22	1:B:228:ASN:HD21	1.57	0.51
1:A:65:LYS:HE3	1:A:98:MET:O	2.11	0.51
1:B:173:ALA:HA	1:B:206:ILE:HG12	1.93	0.50
1:D:127:ARG:NH1	1:D:304:ASP:OD2	2.45	0.50
1:A:288:ARG:HD3	1:A:414:ASN:HD21	1.76	0.50
1:D:175:THR:OG1	3:D:1433:FAD:HI1	2.12	0.50
1:C:290:MET:CE	1:C:290:MET:HA	2.42	0.49
1:A:115:ILE:CG2	1:A:352:GLU:HG3	2.42	0.48
1:D:221:ASN:HD22	1:D:228:ASN:ND2	2.11	0.48
1:B:407:TYR:C	1:B:407:TYR:CD1	2.87	0.48
1:C:221:ASN:HD22	1:C:228:ASN:ND2	2.11	0.48
1:B:331:VAL:HG21	1:C:415:THR:HB	1.94	0.48
2:D:1432:CAA:H2A	4:D:2027:HOH:O	2.12	0.48
1:B:204:ARG:O	1:B:205:TRP:HB2	2.13	0.48
1:A:365:LYS:O	1:A:369:SER:CB	2.62	0.48
1:C:204:ARG:O	1:C:205:TRP:HB2	2.14	0.48
1:C:173:ALA:HA	1:C:206:ILE:HG12	1.95	0.48
1:A:108:TYR:CZ	1:A:156:LYS:HD3	2.48	0.48
1:B:407:TYR:C	1:B:407:TYR:HD1	2.16	0.48
1:B:329:LYS:HG2	1:B:378:LEU:HD22	1.96	0.48
1:D:152:SER:H	1:D:155:GLN:HE21	1.61	0.47
1:D:75:ALA:HB3	1:D:76:PRO:HD3	1.97	0.47
1:C:294:GLN:HB2	1:C:295:PRO:HD3	1.97	0.47
1:C:353:THR:HB	1:C:355:GLN:HG2	1.95	0.47
1:A:403:PRO:HG3	1:B:388:ILE:HD13	1.96	0.47
1:C:204:ARG:HG2	1:C:205:TRP:CD1	2.49	0.47
1:B:315:GLN:HA	1:B:315:GLN:HE21	1.80	0.47
1:A:71:GLU:OE1	1:A:127:ARG:NH2	2.48	0.47
1:A:284:LEU:O	1:A:288:ARG:HG3	2.15	0.47
1:D:131:SER:HB3	1:D:252:MET:HB2	1.97	0.46
1:A:389:LEU:HD13	1:B:205:TRP:HH2	1.79	0.46
1:C:357:THR:H	1:C:360:GLN:NE2	2.14	0.46
1:D:180:GLY:HA3	3:D:1433:FAD:O2P	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:TYR:CD1	1:A:407:TYR:C	2.89	0.46
1:A:407:TYR:C	1:A:407:TYR:HD1	2.19	0.46
1:B:373:ARG:HD3	1:B:402:GLU:OE2	2.15	0.46
1:C:203:LYS:HB3	1:C:206:ILE:CD1	2.46	0.46
1:A:380:ARG:HH22	1:B:406:THR:HG1	1.60	0.46
1:C:402:GLU:OE1	1:D:380:ARG:HD3	2.16	0.46
1:D:71:GLU:OE1	1:D:127:ARG:NH2	2.49	0.46
1:C:327:GLN:O	1:C:331:VAL:HG23	2.16	0.46
1:A:204:ARG:HG2	1:A:205:TRP:CD1	2.50	0.45
1:B:63:ARG:HD2	1:B:120:ILE:HG12	1.97	0.45
1:A:51:PHE:HZ	1:A:338:GLN:HA	1.82	0.45
1:A:290:MET:HE2	1:A:290:MET:HA	1.99	0.45
3:B:1433:FAD:C2'	3:B:1433:FAD:H9	2.47	0.45
1:A:26:MET:HE3	1:A:31:ALA:HA	1.99	0.45
1:A:390:ALA:HB3	1:B:246:ASN:HB3	1.99	0.45
1:C:390:ALA:HB3	1:D:246:ASN:HB3	1.98	0.44
1:C:34:GLN:NE2	1:C:313:ARG:HH11	2.16	0.44
1:B:205:TRP:HB3	3:B:1433:FAD:C9A	2.46	0.44
1:B:367:TRP:HE1	1:C:336:ASN:ND2	2.16	0.44
1:B:336:ASN:HB3	1:B:340:MET:HE2	1.99	0.44
1:C:329:LYS:HB3	1:C:382:LEU:HD11	2.00	0.44
1:B:209:SER:OG	1:B:256:GLY:HA3	2.17	0.44
1:B:186:LEU:HD13	1:B:227:ILE:CD1	2.48	0.44
1:C:152:SER:H	1:C:155:GLN:HE21	1.66	0.43
3:C:1433:FAD:H4B	1:D:382:LEU:O	2.18	0.43
1:A:65:LYS:HB3	1:A:65:LYS:HE2	1.88	0.43
1:B:298:ILE:HG21	1:B:401:LEU:HD22	1.99	0.43
1:D:356:MET:HA	1:D:360:GLN:HE22	1.84	0.43
1:D:291:VAL:O	1:D:295:PRO:HD3	2.18	0.43
1:D:173:ALA:HA	1:D:206:ILE:HG12	2.01	0.43
1:A:315:GLN:HA	1:A:315:GLN:NE2	2.34	0.43
1:C:248:ILE:O	1:C:399:CYS:HB3	2.19	0.43
1:B:293:TRP:HA	1:B:296:ILE:HD12	2.01	0.43
1:B:227:ILE:HD12	1:B:277:PHE:HB2	2.01	0.43
1:A:26:MET:HE2	1:A:31:ALA:HA	2.01	0.43
1:C:290:MET:HE2	1:C:290:MET:HA	2.01	0.43
1:C:227:ILE:HD12	1:C:277:PHE:HB2	2.00	0.43
1:B:309:TYR:CD2	1:B:383:LEU:HD22	2.54	0.43
1:D:203:LYS:HB3	1:D:206:ILE:CD1	2.49	0.43
1:D:26:MET:HB3	1:D:31:ALA:HB2	2.01	0.43
1:A:325:LEU:HD23	1:B:412:ASP:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:LEU:HD12	1:D:325:LEU:HD12	2.01	0.43
1:A:324:GLN:NE2	3:D:1433:FAD:N1A	2.67	0.43
1:A:246:ASN:HB3	1:B:390:ALA:HB3	2.00	0.43
1:A:126:ALA:HB1	1:A:298:ILE:HG13	2.01	0.42
1:A:334:LEU:O	1:A:338:GLN:HG2	2.19	0.42
1:C:152:SER:OG	1:C:155:GLN:HG2	2.19	0.42
1:C:119:ALA:HB1	1:C:293:TRP:CE2	2.55	0.42
1:A:134:THR:O	1:A:138:VAL:HG22	2.20	0.42
1:C:356:MET:HA	1:C:360:GLN:HE22	1.84	0.42
1:A:356:MET:HA	1:A:360:GLN:NE2	2.34	0.42
1:C:173:ALA:HB3	1:C:217:ILE:HD13	2.01	0.42
1:D:303:TYR:CZ	1:D:334:LEU:HD13	2.54	0.42
1:B:292:ALA:O	1:B:295:PRO:HD2	2.20	0.42
3:C:1433:FAD:H1B	1:D:326:ASN:HD21	1.85	0.42
1:C:82:TRP:CE2	1:C:396:LYS:HG3	2.55	0.42
3:B:1433:FAD:C9	3:B:1433:FAD:H2'	2.50	0.42
1:C:284:LEU:HD21	2:C:1432:CAA:H31	2.02	0.41
1:D:293:TRP:HA	1:D:296:ILE:HD12	2.02	0.41
1:C:34:GLN:NE2	1:C:313:ARG:HD3	2.35	0.41
1:D:265:VAL:HA	1:D:266:PRO:HD3	1.92	0.41
1:D:308:ARG:HD3	1:D:312:GLU:OE2	2.21	0.41
1:B:203:LYS:HB3	1:B:206:ILE:CD1	2.51	0.41
1:D:166:LEU:HA	1:D:166:LEU:HD13	1.91	0.41
1:A:343:MET:CE	1:D:338:GLN:HB2	2.51	0.41
1:C:295:PRO:HB2	1:C:368:ILE:HG22	2.03	0.41
1:D:404:ILE:HA	1:D:407:TYR:CE1	2.56	0.41
1:B:270:ARG:HH22	1:B:275:ASN:HD21	1.66	0.41
1:B:203:LYS:HB3	1:B:206:ILE:HD13	2.02	0.41
1:B:303:TYR:CZ	1:B:334:LEU:HD13	2.56	0.41
1:C:318:ALA:HB2	1:D:430:PRO:HG3	2.02	0.41
1:A:142:LEU:O	1:A:146:THR:HG23	2.21	0.41
1:B:373:ARG:NH1	1:B:402:GLU:OE1	2.53	0.41
1:A:403:PRO:HB3	3:A:1433:FAD:HM71	2.01	0.40
1:A:402:GLU:OE1	1:B:380:ARG:HD3	2.22	0.40
1:A:75:ALA:HB3	1:A:76:PRO:HD3	2.03	0.40
1:A:302:ILE:HG23	1:A:394[A]:VAL:HG23	2.04	0.40
1:D:206:ILE:HG22	1:D:209:SER:HB3	2.04	0.40
1:A:324:GLN:HB3	1:C:325:LEU:HD13	2.03	0.40
1:B:422:VAL:O	1:C:307:HIS:HE1	2.04	0.40
1:D:70:MET:HG3	1:D:125:ILE:HA	2.03	0.40
1:C:328:GLN:O	1:C:332:GLN:HG3	2.21	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	415/436 (95%)	406 (98%)	9 (2%)	0	100	100
1	B	415/436 (95%)	401 (97%)	13 (3%)	1 (0%)	52	80
1	C	414/436 (95%)	405 (98%)	9 (2%)	0	100	100
1	D	414/436 (95%)	402 (97%)	11 (3%)	1 (0%)	52	80
All	All	1658/1744 (95%)	1614 (97%)	42 (2%)	2 (0%)	56	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	103	GLY
1	D	431	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	336/357 (94%)	318 (95%)	18 (5%)	27	56
1	B	339/357 (95%)	321 (95%)	18 (5%)	28	57
1	C	335/357 (94%)	320 (96%)	15 (4%)	34	65
1	D	333/357 (93%)	310 (93%)	23 (7%)	19	43
All	All	1343/1428 (94%)	1269 (94%)	74 (6%)	27	55

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	THR
1	A	55	LEU
1	A	72	LYS
1	A	163	LEU
1	A	165	GLN
1	A	174	LEU
1	A	265	VAL
1	A	290	MET
1	A	310	LEU
1	A	313	ARG
1	A	325	LEU
1	A	329	LYS
1	A	380	ARG
1	A	389	LEU
1	A	396	LYS
1	A	401	LEU
1	A	407	TYR
1	A	422	VAL
1	B	20	TYR
1	B	72	LYS
1	B	84	LYS
1	B	163	LEU
1	B	166	LEU
1	B	186	LEU
1	B	281	SER
1	B	313	ARG
1	B	315	GLN
1	B	325	LEU
1	B	365	LYS
1	B	373	ARG
1	B	377	SER
1	B	380	ARG
1	B	389	LEU
1	B	401	LEU
1	B	407	TYR
1	B	408	GLU
1	C	91	ILE
1	C	138	VAL
1	C	163	LEU
1	C	214	LEU
1	C	280	THR
1	C	290	MET

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Mol	Chain	Res	Type
1	C	313	ARG
1	C	325	LEU
1	C	329	LYS
1	C	373	ARG
1	C	380	ARG
1	C	383	LEU
1	C	389	LEU
1	C	401	LEU
1	C	407	TYR
1	D	26	MET
1	D	64	LYS
1	D	120	ILE
1	D	137	LEU
1	D	163	LEU
1	D	166	LEU
1	D	184	SER
1	D	192	LYS
1	D	193	VAL
1	D	215	LEU
1	D	261	GLN
1	D	280	THR
1	D	282	LYS
1	D	308	ARG
1	D	313	ARG
1	D	315	GLN
1	D	324	GLN
1	D	325	LEU
1	D	329	LYS
1	D	380	ARG
1	D	383	LEU
1	D	389	LEU
1	D	407	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	202	GLN
1	A	228	ASN
1	A	261	GLN
1	A	307	HIS
1	A	326	ASN

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Mol	Chain	Res	Type
1	A	336	ASN
1	A	360	GLN
1	A	414	ASN
1	B	118	ASN
1	B	167	ASN
1	B	228	ASN
1	B	275	ASN
1	B	307	HIS
1	B	326	ASN
1	B	336	ASN
1	B	360	GLN
1	B	414	ASN
1	C	34	GLN
1	C	50	HIS
1	C	60	GLN
1	C	118	ASN
1	C	155	GLN
1	C	202	GLN
1	C	225	ASN
1	C	228	ASN
1	C	261	GLN
1	C	262	ASN
1	C	294	GLN
1	C	307	HIS
1	C	326	ASN
1	C	336	ASN
1	C	360	GLN
1	C	414	ASN
1	D	118	ASN
1	D	155	GLN
1	D	228	ASN
1	D	278	GLN
1	D	307	HIS
1	D	326	ASN
1	D	336	ASN
1	D	360	GLN
1	D	386	ASN
1	D	414	ASN

### 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 ⓘ

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$
2	CAA	A	1432	-	40,50,56	1.01	2 (5%)	50,75,83	1.86	6 (12%)
3	FAD	A	1433	-	48,58,58	0.86	3 (6%)	54,89,89	2.06	7 (12%)
2	CAA	B	1432	-	40,50,56	1.01	2 (5%)	50,75,83	1.94	5 (10%)
3	FAD	B	1433	-	48,58,58	0.95	2 (4%)	54,89,89	2.21	10 (18%)
2	CAA	C	1432	-	40,50,56	1.05	3 (7%)	50,75,83	1.84	5 (10%)
3	FAD	C	1433	-	48,58,58	0.92	2 (4%)	54,89,89	2.00	8 (14%)
2	CAA	D	1432	-	40,50,56	1.04	1 (2%)	50,75,83	1.91	5 (10%)
3	FAD	D	1433	-	48,58,58	0.93	2 (4%)	54,89,89	2.15	9 (16%)

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	CAA	A	1432	-	-	0/44/64/71	0/3/3/3
3	FAD	A	1433	-	-	0/30/50/50	0/6/6/6
2	CAA	B	1432	-	-	0/44/64/71	0/3/3/3
3	FAD	B	1433	-	-	0/30/50/50	0/6/6/6
2	CAA	C	1432	-	-	0/44/64/71	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	C	1433	-	-	0/30/50/50	0/6/6/6
2	CAA	D	1432	-	-	0/44/64/71	0/3/3/3
3	FAD	D	1433	-	-	0/30/50/50	0/6/6/6

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1433	FAD	C10-N10	-3.69	1.34	1.39
3	C	1433	FAD	C10-N10	-3.40	1.35	1.39
3	B	1433	FAD	C9A-N10	-2.95	1.34	1.38
3	A	1433	FAD	C10-N10	-2.71	1.36	1.39
3	B	1433	FAD	C10-N10	-2.35	1.36	1.39
3	D	1433	FAD	C9A-N10	-2.20	1.35	1.38
3	A	1433	FAD	C9A-N10	-2.12	1.35	1.38
3	C	1433	FAD	C9A-N10	-2.07	1.35	1.38
2	C	1432	CAA	P3B-O8A	2.06	1.62	1.54
2	A	1432	CAA	P3B-O8A	2.13	1.62	1.54
3	A	1433	FAD	O4B-C1B	2.24	1.44	1.41
2	B	1432	CAA	P3B-O8A	2.29	1.62	1.54
2	C	1432	CAA	O4B-C1B	2.57	1.44	1.41
2	D	1432	CAA	P3B-O7A	3.18	1.61	1.51
2	C	1432	CAA	P3B-O7A	3.31	1.62	1.51
2	A	1432	CAA	P3B-O7A	3.33	1.62	1.51
2	B	1432	CAA	P3B-O7A	3.42	1.62	1.51

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1433	FAD	N3A-C2A-N1A	-10.71	120.69	128.89
3	D	1433	FAD	N3A-C2A-N1A	-10.32	121.00	128.89
3	B	1433	FAD	N3A-C2A-N1A	-9.91	121.31	128.89
2	C	1432	CAA	N3A-C2A-N1A	-9.82	121.37	128.89
2	A	1432	CAA	N3A-C2A-N1A	-9.75	121.43	128.89
3	C	1433	FAD	N3A-C2A-N1A	-9.59	121.55	128.89
2	B	1432	CAA	N3A-C2A-N1A	-9.52	121.60	128.89
2	D	1432	CAA	N3A-C2A-N1A	-8.83	122.14	128.89
2	B	1432	CAA	C4B-O4B-C1B	-6.19	102.92	109.72
2	D	1432	CAA	C4B-O4B-C1B	-5.25	103.95	109.72
2	C	1432	CAA	C4B-O4B-C1B	-4.63	104.64	109.72
3	C	1433	FAD	P-O3P-PA	-4.23	120.84	132.73
3	B	1433	FAD	C4X-C4-N3	-4.23	117.80	123.59
2	D	1432	CAA	P2A-O3A-P1A	-3.79	122.08	132.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1433	FAD	P-O3P-PA	-3.71	122.30	132.73
2	A	1432	CAA	C4B-O4B-C1B	-3.66	105.69	109.72
3	B	1433	FAD	P-O3P-PA	-3.58	122.66	132.73
3	D	1433	FAD	C2B-C1B-N9A	-3.35	109.17	114.29
2	A	1432	CAA	C6P-C7P-N8P	-3.31	104.62	111.88
3	D	1433	FAD	P-O3P-PA	-3.19	123.77	132.73
3	C	1433	FAD	C4X-C4-N3	-3.10	119.35	123.59
3	B	1433	FAD	C4X-C10-N10	-2.93	118.79	120.52
2	B	1432	CAA	P2A-O3A-P1A	-2.92	124.52	132.73
3	D	1433	FAD	C4X-C4-N3	-2.89	119.63	123.59
3	A	1433	FAD	C4A-C5A-N7A	-2.74	106.96	109.48
3	A	1433	FAD	C4X-C4-N3	-2.72	119.87	123.59
3	C	1433	FAD	C4A-C5A-N7A	-2.72	106.98	109.48
2	C	1432	CAA	P2A-O3A-P1A	-2.71	125.12	132.73
2	D	1432	CAA	C2B-C1B-N9A	-2.63	110.28	114.29
2	A	1432	CAA	P2A-O3A-P1A	-2.36	126.11	132.73
3	D	1433	FAD	O3P-P-O5'	-2.32	96.78	102.94
3	B	1433	FAD	C2B-C1B-N9A	-2.28	110.80	114.29
3	B	1433	FAD	O4'-C4'-C5'	-2.23	105.34	110.19
3	D	1433	FAD	O4'-C4'-C5'	-2.13	105.55	110.19
2	A	1432	CAA	O8A-P3B-O7A	-2.08	103.87	110.58
2	C	1432	CAA	O8A-P3B-O7A	-2.06	103.94	110.58
3	C	1433	FAD	C1'-N10-C9A	2.06	121.17	118.86
2	B	1432	CAA	C2B-C1B-N9A	2.20	117.65	114.29
3	D	1433	FAD	C4X-N5-C5X	2.57	119.72	116.76
2	C	1432	CAA	O4B-C1B-N9A	2.68	113.71	108.10
3	C	1433	FAD	C5X-C9A-N10	2.69	119.66	117.62
3	B	1433	FAD	C4-C4X-C10	2.70	121.67	119.94
3	C	1433	FAD	C4X-N5-C5X	2.71	119.88	116.76
3	B	1433	FAD	C4X-N5-C5X	2.74	119.91	116.76
3	A	1433	FAD	C4X-N5-C5X	2.76	119.94	116.76
2	B	1432	CAA	O4B-C1B-N9A	2.76	113.89	108.10
2	A	1432	CAA	O6A-CCP-CBP	2.86	115.15	110.55
3	A	1433	FAD	C5X-C9A-N10	2.95	119.86	117.62
3	D	1433	FAD	C5X-C9A-N10	3.28	120.11	117.62
3	B	1433	FAD	C5X-C9A-N10	3.97	120.64	117.62
2	D	1432	CAA	O4B-C1B-N9A	4.36	117.22	108.10
3	A	1433	FAD	C4-N3-C2	5.84	120.30	115.25
3	C	1433	FAD	C4-N3-C2	6.05	120.48	115.25
3	D	1433	FAD	C4-N3-C2	6.35	120.74	115.25
3	B	1433	FAD	C4-N3-C2	6.66	121.00	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1433	FAD	1	0
3	B	1433	FAD	5	0
2	C	1432	CAA	2	0
3	C	1433	FAD	2	0
2	D	1432	CAA	1	0
3	D	1433	FAD	3	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	416/436 (95%)	-0.07	14 (3%) 49 49	28, 36, 47, 52	0
1	B	416/436 (95%)	-0.41	4 (0%) 84 85	28, 35, 47, 52	0
1	C	416/436 (95%)	-0.38	2 (0%) 91 93	28, 35, 44, 54	0
1	D	416/436 (95%)	-0.36	2 (0%) 91 93	29, 35, 45, 48	0
All	All	1664/1744 (95%)	-0.31	22 (1%) 79 79	28, 35, 46, 54	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	432	THR	8.3
1	B	432	THR	5.6
1	D	432	THR	5.6
1	C	432	THR	5.2
1	B	22	ASP	3.9
1	A	194	GLU	3.2
1	C	431	ALA	3.1
1	A	281	SER	3.0
1	A	267	ASP	2.9
1	A	216	ILE	2.7
1	D	18	SER	2.6
1	A	107	GLY	2.6
1	A	238	GLY	2.5
1	A	80	GLU	2.4
1	B	18	SER	2.4
1	B	431	ALA	2.2
1	A	167	ASN	2.2
1	A	230	PHE	2.2
1	A	262	ASN	2.1
1	A	217	ILE	2.1
1	A	278	GLN	2.0
1	A	29	SER	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
2	CAA	C	1432	48/54	0.84	0.25	3.33	42,52,56,56	48
2	CAA	A	1432	48/54	0.74	0.32	2.30	33,41,45,46	48
2	CAA	B	1432	48/54	0.91	0.18	1.70	29,36,50,50	0
2	CAA	D	1432	48/54	0.94	0.16	0.92	32,41,45,46	0
3	FAD	A	1433	53/53	0.95	0.14	-0.40	43,45,53,53	0
3	FAD	D	1433	53/53	0.97	0.11	-0.96	23,27,32,32	0
3	FAD	C	1433	53/53	0.97	0.11	-1.17	29,31,32,33	0
3	FAD	B	1433	53/53	0.97	0.10	-1.34	20,24,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.