W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:33 PM GMT

PDB ID	:	4Y9J
Title	:	Crystal Structure of Caenorhabditis elegans ACDH-11 in complex with C11-CoA
Authors	:	Li, Z.J.; Sun, F.
Deposited on	:	2015-02-17
Resolution	:	1.80 Å(reported)

The following versions of software and data (see references (i)) 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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.
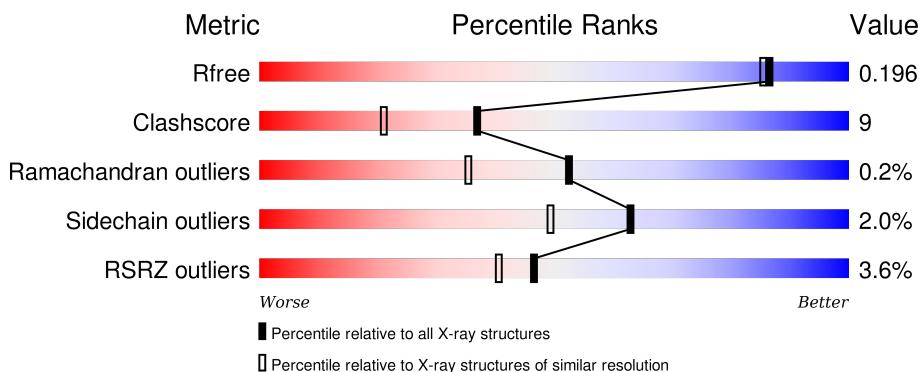
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 >=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 <=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	593	4% / 85% / 13% / •
1	B	593	3% / 87% / 12% / •
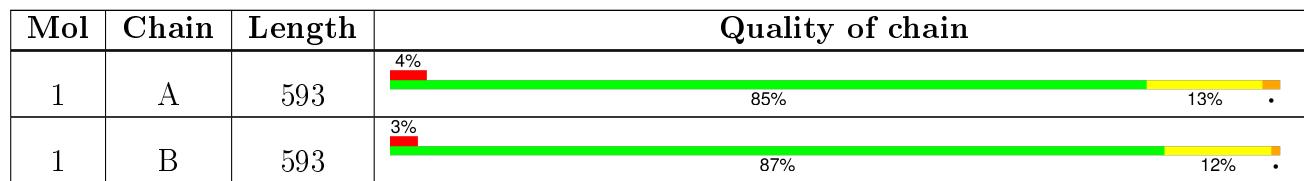
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	UCC	A	702	-	-	X	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10680 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 Protein ACDH-11, isoform b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	592	Total 4697	C 2951	N 834	O 890	S 22	0	11	0
1	B	593	Total 4637	C 2916	N 823	O 877	S 21	0	3	0

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).
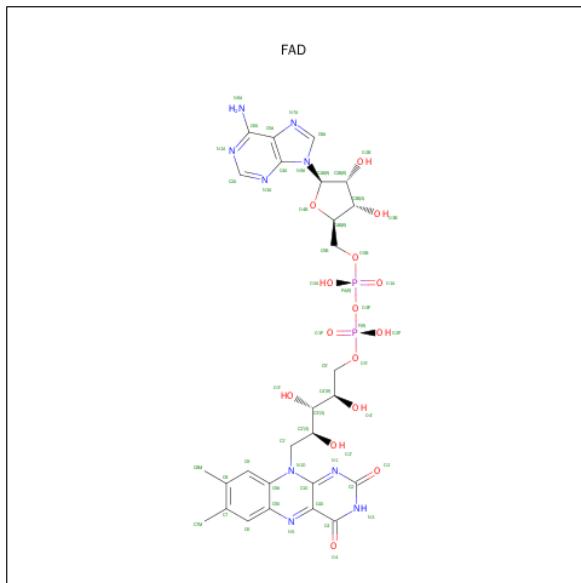
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 3 is S-{(3S,5R,9R)-1-[(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-4-hydroxy-3-(phos phonooxy)tetrahydrofuran-2-yl]-3,5,9-trihydroxy-8,8-dimethyl-3,5-dioxido-10,14-dioxo-2,4, 6-trioxa-11,15-diaza-3lambda 5 ,5lambda 5 -diphosphaheptadecan-17-yl} undecanethioate

(three-letter code: UCC) (formula: $C_{32}H_{56}N_7O_{17}P_3S$).
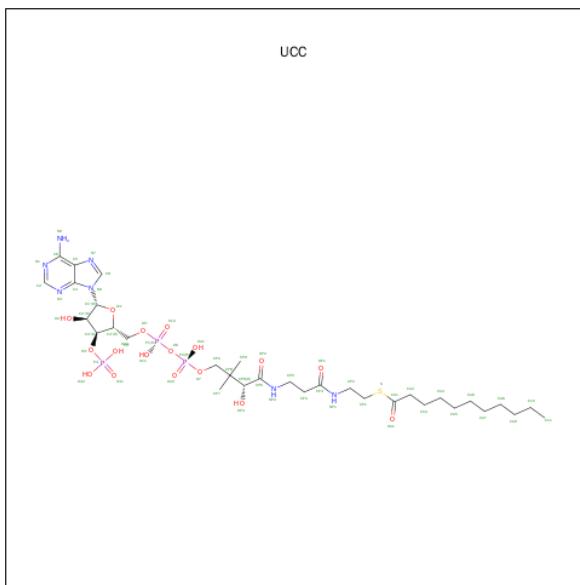
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			60	32	7	17	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			60	32	7	17	3	1		

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	591	Total	O	0	0
			591	591		
4	B	529	Total	O	0	0
			529	529		

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: Protein ACDH-11, isoform b

Chain A:
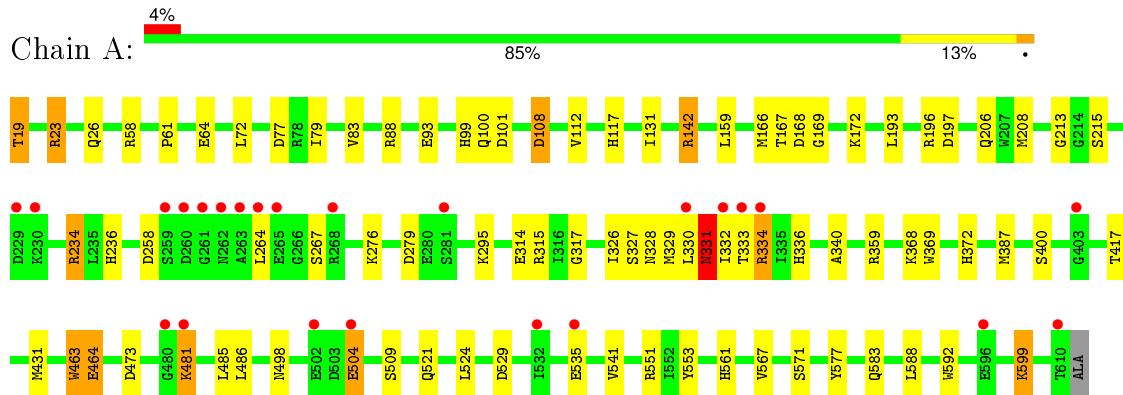
• Molecule 1: Protein ACDH-11, isoform b

Chain B:
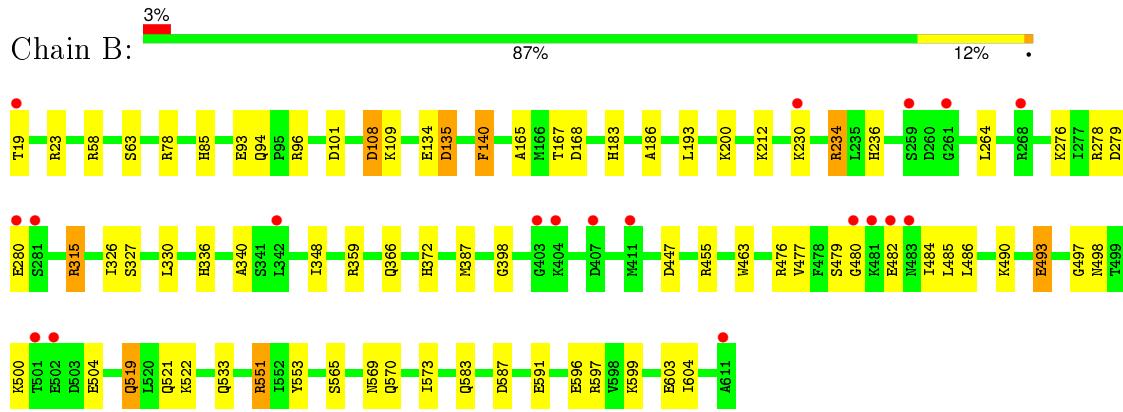
4　Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	138.56Å　　116.68Å　　115.29Å 90.00°　　124.02°　　90.00°	Depositor
Resolution (Å)	50.00　–　1.80 34.84　–　1.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-1.80) 99.6 (34.84-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.78 (at 1.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.145　,　0.186 0.157　,　0.196	Depositor DCC
R_{free} test set	6857 reflections (5.16%)	DCC
Wilson B-factor (Å^2)	33.2	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.7	EDS
Estimated twinning fraction	0.010 for h,-k,-h-l	Xtriage
L-test for twinning [2]	$<|L|> = 0.50, <L^2> = 0.33$	Xtriage
Outliers	0 of 139776 reflections	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	10680	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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: UCC, 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	0.97	3/4780 (0.1%)	1.04	25/6454 (0.4%)
1	B	0.93	1/4723 (0.0%)	0.99	20/6377 (0.3%)
All	All	0.95	4/9503 (0.0%)	1.01	45/12831 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	213	GLY	C-O	7.71	1.35	1.23
1	A	464	GLU	CD-OE2	6.06	1.32	1.25
1	B	134	GLU	CD-OE2	5.80	1.32	1.25
1	A	369	TRP	CB-CG	-5.39	1.40	1.50

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	387	MET	CG-SD-CE	-12.95	79.49	100.20
1	B	234	ARG	NE-CZ-NH1	8.29	124.45	120.30
1	B	108	ASP	CB-CG-OD2	8.12	125.61	118.30
1	A	551	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	A	88	ARG	NE-CZ-NH2	-7.89	116.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	447	ASP	CB-CG-OD2	-7.45	111.60	118.30
1	A	142	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	A	101	ASP	CB-CG-OD1	7.07	124.66	118.30
1	A	551	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	A	332[A]	ILE	O-C-N	-6.90	111.66	122.70
1	A	332[B]	ILE	O-C-N	-6.90	111.66	122.70
1	A	88	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	B	597	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	B	23	ARG	NE-CZ-NH2	6.57	123.58	120.30
1	B	315	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	A	529	ASP	CB-CG-OD1	6.48	124.13	118.30
1	B	78	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	58	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	B	58	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	A	77	ASP	CB-CG-OD1	6.03	123.73	118.30
1	B	551	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	B	101	ASP	CB-CG-OD1	5.64	123.38	118.30
1	B	476	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	142	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	B	23	ARG	NE-CZ-NH1	-5.49	117.56	120.30
1	B	359	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	23	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	264	LEU	CA-CB-CG	5.47	127.89	115.30
1	B	587	ASP	CB-CG-OD1	5.44	123.19	118.30
1	A	279	ASP	CB-CG-OD1	5.43	123.18	118.30
1	A	108	ASP	CB-CG-OD1	5.36	123.13	118.30
1	B	455	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	334[A]	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	A	334[B]	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	A	234	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	278	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	A	258	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	72	LEU	CB-CG-CD1	-5.26	102.06	111.00
1	B	279	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	197	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	A	431	MET	CG-SD-CE	-5.19	91.89	100.20
1	B	476	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	A	359	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	A	529	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	B	278	ARG	NE-CZ-NH1	5.09	122.84	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	331[B]	ASN	Peptide
1	B	480	GLY	Peptide

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	4697	0	4758	113	0
1	B	4637	0	4701	60	1
2	A	53	0	31	7	0
2	B	53	0	31	0	0
3	A	60	0	52	23	0
3	B	60	0	52	2	0
4	A	591	0	0	57	0
4	B	529	0	0	37	0
All	All	10680	0	9625	181	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (181) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:LYS:HG2	4:B:1121:HOH:O	1.44	1.14
1:A:521:GLN:HG2	4:A:1095:HOH:O	1.49	1.12
1:A:330[B]:LEU:HD22	3:A:702:UCC:H23	1.28	1.07
1:A:330[B]:LEU:O	1:A:331[B]:ASN:HB2	1.64	0.97
3:A:702:UCC:H28	4:A:803:HOH:O	1.64	0.97
1:A:330[B]:LEU:HD21	3:A:702:UCC:CP3	1.96	0.95
1:A:330[B]:LEU:HD11	1:A:334[B]:ARG:NH2	1.81	0.95
1:A:314:GLU:HG3	4:A:1228:HOH:O	1.68	0.94
1:A:330[B]:LEU:CD2	3:A:702:UCC:H23	1.99	0.92
1:A:330[B]:LEU:HD22	3:A:702:UCC:CP2	1.99	0.92
1:A:61:PRO:HB2	4:A:808:HOH:O	1.72	0.89
1:B:330:LEU:HB2	4:B:844:HOH:O	1.72	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:LEU:HB3	4:A:1310:HOH:O	1.73	0.88
1:A:330[B]:LEU:HD13	1:A:464:GLU:OE1	1.75	0.86
1:A:330[B]:LEU:HD21	3:A:702:UCC:OP1	1.76	0.85
1:A:196:ARG:HD2	4:A:1221:HOH:O	1.76	0.83
1:A:93:GLU:HG2	4:A:819:HOH:O	1.77	0.83
1:A:330[A]:LEU:HD13	3:A:702:UCC:N6	1.95	0.82
1:B:183:HIS:HD2	1:B:186:ALA:H	1.28	0.82
1:A:206:GLN:HB2	1:A:329[B]:MET:HE1	1.61	0.81
1:A:588:LEU:HD12	4:A:1204:HOH:O	1.81	0.80
1:B:519:GLN:HA	1:B:519:GLN:HE21	1.46	0.80
1:A:331[A]:ASN:HA	1:A:417:THR:HG21	1.62	0.80
1:A:400:SER:HB3	4:A:837:HOH:O	1.83	0.79
1:B:108:ASP:OD1	4:B:801:HOH:O	2.00	0.79
2:A:701:FAD:H4'	4:A:813:HOH:O	1.82	0.79
1:A:330[B]:LEU:HD11	1:A:334[B]:ARG:HH21	1.46	0.78
1:A:93:GLU:CG	4:A:819:HOH:O	2.31	0.77
1:A:19:THR:N	4:A:804:HOH:O	2.17	0.77
1:A:206:GLN:HB2	1:A:329[B]:MET:CE	2.16	0.76
1:A:330[B]:LEU:HD11	1:A:334[B]:ARG:CZ	2.15	0.76
1:A:334[B]:ARG:NH2	4:A:803:HOH:O	2.18	0.76
2:A:701:FAD:C4'	4:A:813:HOH:O	2.33	0.75
1:A:541:VAL:HG11	4:A:1204:HOH:O	1.85	0.75
1:A:215:SER:O	4:A:801:HOH:O	2.08	0.72
1:B:504:GLU:HG3	4:B:1156:HOH:O	1.90	0.71
1:B:490:LYS:O	1:B:493:GLU:HG3	1.90	0.71
1:B:519:GLN:HG2	4:B:1260:HOH:O	1.90	0.71
4:A:1179:HOH:O	1:B:603:GLU:HB3	1.91	0.71
1:B:63:SER:HB2	4:B:938:HOH:O	1.90	0.70
1:B:569:ASN:O	4:B:802:HOH:O	2.09	0.70
1:B:479:SER:HB2	4:B:912:HOH:O	1.92	0.70
1:B:486:LEU:HD12	4:B:955:HOH:O	1.92	0.69
1:A:330[A]:LEU:CD1	3:A:702:UCC:C6	2.71	0.68
1:A:334[A]:ARG:CD	1:A:417:THR:HG22	2.23	0.68
1:A:331[B]:ASN:ND2	4:A:806:HOH:O	2.27	0.68
1:B:234:ARG:HH11	1:B:236:HIS:CE1	2.12	0.68
1:A:108:ASP:OD2	4:A:802:HOH:O	2.10	0.68
1:A:334[A]:ARG:HD3	1:A:417:THR:HG22	1.77	0.67
3:A:702:UCC:OP2	4:A:803:HOH:O	2.12	0.67
1:A:330[B]:LEU:CD2	3:A:702:UCC:CP2	2.66	0.66
1:B:583:GLN:NE2	4:B:807:HOH:O	2.28	0.66
1:A:400:SER:CB	4:A:837:HOH:O	2.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ARG:HH11	1:A:236:HIS:CE1	2.15	0.65
1:A:330[A]:LEU:HD13	3:A:702:UCC:C6	2.26	0.65
1:B:570:GLN:HA	4:B:802:HOH:O	1.96	0.65
1:A:592:TRP:HB2	4:A:1204:HOH:O	1.97	0.64
1:B:234:ARG:HH11	1:B:236:HIS:HE1	1.45	0.64
1:B:497:GLY:O	1:B:498:ASN:CG	2.36	0.64
1:A:481:LYS:HB3	4:A:900:HOH:O	1.96	0.64
1:A:168:ASP:OD2	1:A:336:HIS:HE1	1.81	0.62
1:B:276:LYS:CE	4:B:1080:HOH:O	2.46	0.62
1:A:330[B]:LEU:CD2	3:A:702:UCC:CP3	2.74	0.62
1:A:330[B]:LEU:HD12	1:A:330[B]:LEU:C	2.20	0.62
1:B:168:ASP:OD2	1:B:336:HIS:HE1	1.83	0.61
1:B:200:LYS:HE3	4:B:1194:HOH:O	1.99	0.61
1:A:169:GLY:HA3	1:A:329[B]:MET:HG3	1.83	0.61
1:A:571:SER:HB3	4:A:1179:HOH:O	2.02	0.60
1:A:330[B]:LEU:CD1	1:A:334[B]:ARG:NE	2.65	0.60
1:A:340:ALA:CB	3:A:702:UCC:H18	2.32	0.59
1:A:100:GLN:HG2	4:A:1025:HOH:O	2.03	0.59
4:A:1043:HOH:O	1:B:372:HIS:HD2	1.85	0.59
1:B:551:ARG:HD2	4:B:807:HOH:O	2.03	0.59
1:A:208[B]:MET:SD	1:A:330[B]:LEU:HD23	2.43	0.58
1:A:108:ASP:CG	4:A:802:HOH:O	2.41	0.58
1:A:561:HIS:CE1	4:A:859:HOH:O	2.55	0.58
1:A:571:SER:CB	4:A:1179:HOH:O	2.51	0.57
1:B:85:HIS:HB2	4:B:1217:HOH:O	2.03	0.57
1:A:330[A]:LEU:HD12	3:A:702:UCC:C6	2.34	0.57
1:A:583:GLN:HG3	4:A:902:HOH:O	2.05	0.57
1:A:485:LEU:HB3	4:A:1095:HOH:O	2.04	0.56
1:A:276:LYS:NZ	4:A:814:HOH:O	2.39	0.56
1:A:330[B]:LEU:HD11	1:A:334[B]:ARG:NE	2.21	0.55
1:A:131:ILE:O	1:A:142:ARG:HB2	2.06	0.55
1:A:330[B]:LEU:HA	1:A:333[B]:THR:OG1	2.06	0.55
1:B:583:GLN:OE1	4:B:803:HOH:O	2.18	0.55
1:B:596:GLU:HG2	4:B:1152:HOH:O	2.07	0.55
1:A:234:ARG:HH11	1:A:236:HIS:HE1	1.55	0.55
1:A:330[B]:LEU:CD1	1:A:334[B]:ARG:CZ	2.83	0.54
1:A:64:GLU:HG2	4:A:808:HOH:O	2.07	0.54
1:A:336:HIS:HD2	4:A:1066:HOH:O	1.90	0.54
1:A:463:TRP:CE3	3:A:702:UCC:H4	2.43	0.54
1:A:330[B]:LEU:CD2	3:A:702:UCC:OP1	2.53	0.54
1:A:368:LYS:NZ	4:A:809:HOH:O	2.31	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:ALA:CB	3:B:702:UCC:H18	2.38	0.53
1:B:140:PHE:HA	1:B:398:GLY:HA3	1.91	0.53
1:A:372:HIS:HD2	4:B:927:HOH:O	1.91	0.53
1:B:276:LYS:HE3	4:B:1080:HOH:O	2.08	0.53
1:A:567:VAL:HG23	4:A:859:HOH:O	2.09	0.53
1:A:206:GLN:NE2	1:A:330[B]:LEU:HB2	2.24	0.52
1:A:166:MET:HB3	1:A:329[B]:MET:CE	2.40	0.52
1:B:183:HIS:CD2	1:B:186:ALA:H	2.19	0.52
1:A:326[B]:ILE:HG13	1:A:326[B]:ILE:O	2.09	0.52
1:A:330[A]:LEU:CD1	3:A:702:UCC:C5	2.88	0.52
1:A:334[A]:ARG:NH2	3:A:702:UCC:H52	2.06	0.52
1:B:276:LYS:NZ	4:B:819:HOH:O	2.43	0.52
1:B:63:SER:C	4:B:938:HOH:O	2.48	0.52
1:A:315:ARG:NH1	1:A:317:GLY:O	2.41	0.52
1:A:93:GLU:HG3	4:A:819:HOH:O	2.05	0.51
1:B:485:LEU:HD21	1:B:521:GLN:HA	1.93	0.51
1:B:482:GLU:O	1:B:484:ILE:HD12	2.11	0.51
1:B:573:ILE:HD12	4:B:802:HOH:O	2.10	0.51
1:A:583:GLN:CG	4:A:902:HOH:O	2.58	0.50
1:B:591:GLU:OE1	4:B:804:HOH:O	2.20	0.50
1:A:588:LEU:CD1	4:A:1204:HOH:O	2.51	0.49
1:A:334[A]:ARG:HH22	3:A:702:UCC:H52	1.61	0.49
1:B:276:LYS:HE2	4:B:1080:HOH:O	2.12	0.49
1:B:336:HIS:HD2	4:B:1031:HOH:O	1.96	0.49
1:A:485:LEU:HD11	1:A:524:LEU:HD13	1.96	0.48
1:B:108:ASP:CG	4:B:801:HOH:O	2.45	0.48
1:B:477:VAL:HG12	1:B:484:ILE:HG12	1.95	0.48
1:B:212:LYS:HD3	4:B:1284:HOH:O	2.14	0.47
1:A:206:GLN:CB	1:A:329[B]:MET:HE1	2.40	0.47
1:A:334[A]:ARG:HB2	1:A:417:THR:CG2	2.45	0.47
1:A:19:THR:CA	4:A:804:HOH:O	2.59	0.47
1:A:334[A]:ARG:HB2	1:A:417:THR:HG23	1.95	0.47
2:A:701:FAD:H1B	4:A:995:HOH:O	2.13	0.47
1:A:167:THR:HG23	1:A:193:LEU:HD22	1.98	0.46
4:A:995:HOH:O	1:B:366:GLN:HG2	2.15	0.46
1:A:334[A]:ARG:HD2	1:A:417:THR:HG22	1.95	0.46
1:A:535:GLU:O	1:A:535:GLU:HG3	2.16	0.46
1:A:19:THR:HA	4:A:804:HOH:O	2.16	0.46
1:A:498:ASN:HB2	4:A:1062:HOH:O	2.17	0.45
1:A:166:MET:O	1:A:329[B]:MET:HE3	2.16	0.45
1:A:206:GLN:HE22	1:A:330[B]:LEU:HB2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330[A]:LEU:CD1	3:A:702:UCC:N6	2.75	0.45
1:B:96:ARG:NH1	4:B:815:HOH:O	2.40	0.45
1:A:481:LYS:HB2	4:A:816:HOH:O	2.17	0.45
1:B:500:LYS:HG3	4:B:1196:HOH:O	2.16	0.45
1:B:479:SER:CB	4:B:912:HOH:O	2.61	0.44
1:A:327[B]:SER:O	1:A:331[B]:ASN:CB	2.65	0.44
3:A:702:UCC:CP5	4:A:803:HOH:O	2.42	0.44
1:A:334[A]:ARG:NH1	3:A:702:UCC:H53	2.15	0.44
1:A:172:LYS:HG3	1:A:328[B]:ASN:HB3	2.00	0.44
1:A:79:ILE:HA	1:A:83:VAL:HB	1.99	0.44
1:A:169:GLY:CA	1:A:329[B]:MET:HA	2.48	0.43
1:A:99:HIS:HD2	4:A:802:HOH:O	1.99	0.43
1:A:504:GLU:HG2	4:A:1109:HOH:O	2.18	0.43
1:A:196:ARG:CD	4:A:1221:HOH:O	2.50	0.43
1:B:326:ILE:HA	1:B:326:ILE:HD12	1.89	0.43
2:A:701:FAD:C4A	4:A:995:HOH:O	2.67	0.43
1:A:599:LYS:HG2	4:A:1311:HOH:O	2.19	0.43
1:B:93:GLU:HG2	4:B:834:HOH:O	2.17	0.43
1:A:473:ASP:HB2	4:A:917:HOH:O	2.18	0.43
1:A:314:GLU:CG	4:A:1228:HOH:O	2.47	0.43
1:B:135:ASP:N	1:B:135:ASP:OD1	2.37	0.43
1:B:63:SER:CB	4:B:938:HOH:O	2.59	0.43
1:B:327:SER:HB3	4:B:831:HOH:O	2.19	0.43
1:B:372:HIS:HE1	4:B:977:HOH:O	2.02	0.42
1:A:509:SER:OG	1:A:577:TYR:HA	2.20	0.42
1:A:112:VAL:CG2	1:A:117:HIS:NE2	2.83	0.42
1:A:334[A]:ARG:HD2	1:A:417:THR:CG2	2.50	0.42
1:A:535:GLU:HB3	4:A:1281:HOH:O	2.19	0.42
1:B:109:LYS:NZ	4:B:818:HOH:O	2.43	0.41
1:B:604:ILE:HG21	1:B:604:ILE:HD13	1.80	0.41
1:B:165:ALA:HB2	3:B:702:UCC:H56	2.02	0.41
1:A:334[A]:ARG:NH2	3:A:702:UCC:N6	2.69	0.41
1:A:535:GLU:O	1:A:535:GLU:CG	2.68	0.41
1:B:94:GLN:OE1	4:B:805:HOH:O	2.22	0.41
1:B:167:THR:HG23	1:B:193:LEU:HD22	2.03	0.41
1:A:23:ARG:NH2	1:A:26:GLN:HG3	2.35	0.41
1:B:500:LYS:HG2	4:B:1202:HOH:O	2.21	0.41
1:B:599:LYS:NZ	1:B:603:GLU:OE2	2.48	0.41
2:A:701:FAD:C1B	4:A:995:HOH:O	2.69	0.41
1:A:215:SER:HB2	2:A:701:FAD:O1A	2.21	0.41
1:A:571:SER:CA	4:A:1179:HOH:O	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:LYS:HB3	1:B:212:LYS:HE2	1.90	0.41
1:A:295:LYS:HD2	2:A:701:FAD:HM72	2.01	0.40
1:A:330[B]:LEU:CD1	1:A:334[B]:ARG:HE	2.34	0.40
1:A:387:MET:HG3	4:A:1152:HOH:O	2.20	0.40
1:B:348:ILE:HD12	1:B:348:ILE:HA	1.96	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:565:SER:OG	1:B:565:SER:OG[2_555]	1.95	0.25

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	601/593 (101%)	588 (98%)	10 (2%)	3 (0%)	34	17
1	B	594/593 (100%)	583 (98%)	11 (2%)	0	100	100
All	All	1195/1186 (101%)	1171 (98%)	21 (2%)	3 (0%)	52	29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	331[A]	ASN
1	A	331[B]	ASN
1	A	481	LYS

5.3.2 Protein sidechains (i)

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	508/497 (102%)	501 (99%)	7 (1%)	74	65
1	B	500/497 (101%)	487 (97%)	13 (3%)	54	37
All	All	1008/994 (101%)	988 (98%)	20 (2%)	63	49

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	A	159	LEU
1	A	267	SER
1	A	463	TRP
1	A	504	GLU
1	A	553	TYR
1	A	599	LYS
1	B	19	THR
1	B	135	ASP
1	B	140	PHE
1	B	230	LYS
1	B	264	LEU
1	B	280	GLU
1	B	315	ARG
1	B	463	TRP
1	B	493	GLU
1	B	519	GLN
1	B	522	LYS
1	B	533	GLN
1	B	553	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	GLN
1	A	236	HIS
1	A	336	HIS
1	A	372	HIS
1	A	458	GLN
1	B	99	HIS

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Mol	Chain	Res	Type
1	B	100	GLN
1	B	183	HIS
1	B	206	GLN
1	B	236	HIS
1	B	328	ASN
1	B	336	HIS
1	B	372	HIS
1	B	458	GLN
1	B	519	GLN
1	B	608	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 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	FAD	A	701	-	48,58,58	1.63	9 (18%)	54,89,89	3.09	19 (35%)
3	UCC	A	702	-	52,62,62	1.26	4 (7%)	64,88,88	1.82	10 (15%)
2	FAD	B	701	-	48,58,58	1.85	9 (18%)	54,89,89	2.80	18 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	UCC	B	702	-	52,62,62	1.35	6 (11%)	64,88,88	3.33	18 (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
2	FAD	A	701	-	-	0/30/50/50	0/6/6/6
3	UCC	A	702	-	-	0/57/77/77	0/3/3/3
2	FAD	B	701	-	-	0/30/50/50	0/6/6/6
3	UCC	B	702	-	-	0/57/77/77	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	FAD	C1'-N10	-5.80	1.42	1.48
3	B	702	UCC	CA1-S	-4.11	1.67	1.76
3	A	702	UCC	CA1-S	-3.82	1.68	1.76
2	B	701	FAD	C4X-C10	2.04	1.44	1.41
3	B	702	UCC	OP3-CP8	2.10	1.46	1.42
2	A	701	FAD	C2A-N3A	2.17	1.36	1.32
2	B	701	FAD	O3B-C3B	2.18	1.48	1.43
2	A	701	FAD	C8-C7	2.21	1.46	1.41
2	B	701	FAD	C6-C7	2.25	1.44	1.37
2	A	701	FAD	C4X-N5	2.39	1.37	1.33
3	A	702	UCC	C5-C4	2.55	1.46	1.40
2	B	701	FAD	C10-N10	2.55	1.42	1.39
3	B	702	UCC	CA2-CA1	2.63	1.53	1.50
3	B	702	UCC	CP9-CPB	2.69	1.59	1.53
3	B	702	UCC	C5-C4	2.70	1.46	1.40
2	B	701	FAD	C5A-C4A	2.80	1.46	1.40
2	A	701	FAD	C8A-N7A	2.82	1.40	1.34
2	A	701	FAD	C4X-C10	2.87	1.46	1.41
3	A	702	UCC	CA2-CA1	3.35	1.54	1.50
2	A	701	FAD	C5A-C4A	3.37	1.48	1.40
2	A	701	FAD	C9A-C5X	3.97	1.50	1.42
2	A	701	FAD	C4-C4X	4.00	1.49	1.41
2	A	701	FAD	O4B-C1B	4.41	1.46	1.41
2	B	701	FAD	C5X-N5	4.61	1.42	1.35
2	B	701	FAD	C4X-N5	4.92	1.41	1.33
2	B	701	FAD	C4-C4X	4.96	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	UCC	OA1-CA1	5.32	1.29	1.21
3	B	702	UCC	OA1-CA1	5.39	1.29	1.21

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	FAD	N3A-C2A-N1A	-12.54	119.29	128.89
3	B	702	UCC	CP9-CPB-CPA	-10.97	94.28	108.50
3	A	702	UCC	N3-C2-N1	-9.28	121.79	128.89
3	B	702	UCC	CA2-CA1-S	-8.33	105.86	113.36
3	B	702	UCC	CP7-CPB-CP9	-8.29	92.63	109.28
3	B	702	UCC	N3-C2-N1	-7.85	122.88	128.89
2	A	701	FAD	C4-C4X-C10	-7.38	115.22	119.94
2	B	701	FAD	C4X-C4-N3	-7.01	114.00	123.59
2	B	701	FAD	N3A-C2A-N1A	-6.57	123.86	128.89
2	A	701	FAD	C4B-O4B-C1B	-5.86	103.28	109.72
2	A	701	FAD	C4X-C10-N10	-5.09	117.52	120.52
3	B	702	UCC	CP9-CPB-CP8	-5.03	100.17	109.34
2	B	701	FAD	C4X-N5-C5X	-4.24	111.88	116.76
2	B	701	FAD	C6-C5X-N5	-4.05	113.75	118.96
3	B	702	UCC	CP4-CP5-NP2	-3.89	103.34	111.88
2	B	701	FAD	C4-C4X-C10	-3.80	117.51	119.94
2	A	701	FAD	C4X-C4-N3	-3.80	118.40	123.59
3	B	702	UCC	CA6-CA7-CA8	-3.36	97.16	114.53
3	B	702	UCC	C1'-N9-C4	-3.30	121.96	126.94
2	A	701	FAD	C1B-N9A-C4A	-3.23	122.07	126.94
3	A	702	UCC	C1'-N9-C4	-3.01	122.41	126.94
3	A	702	UCC	C2'-C1'-N9	-2.93	109.82	114.29
3	A	702	UCC	O3'-P3-O31	-2.82	100.06	107.11
3	B	702	UCC	CP2-NP1-CP3	-2.77	117.34	122.79
2	B	701	FAD	P-O3P-PA	-2.77	124.96	132.73
2	A	701	FAD	C9A-C5X-N5	-2.75	118.29	122.36
3	B	702	UCC	C4-C5-N7	-2.62	107.06	109.48
3	A	702	UCC	CP2-NP1-CP3	-2.56	117.77	122.79
2	A	701	FAD	C1'-C2'-C3'	-2.46	102.80	109.82
2	B	701	FAD	C4A-C5A-N7A	-2.43	107.25	109.48
2	B	701	FAD	O3B-C3B-C2B	-2.25	104.51	111.83
2	B	701	FAD	C1B-N9A-C4A	-2.24	123.56	126.94
2	A	701	FAD	C2B-C1B-N9A	-2.23	110.88	114.29
2	B	701	FAD	C4B-O4B-C1B	-2.04	107.48	109.72
3	A	702	UCC	O21-P2-O6	2.02	114.24	105.09
2	B	701	FAD	O4B-C4B-C3B	2.07	109.32	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	UCC	CP9-CPB-CPA	2.07	111.19	108.50
2	B	701	FAD	C2A-N1A-C6A	2.12	122.56	118.77
3	B	702	UCC	O21-P2-O22	2.16	124.23	112.53
2	A	701	FAD	O4'-C4'-C5'	2.18	114.94	110.19
3	B	702	UCC	O32-P3-O31	2.21	117.69	110.58
3	B	702	UCC	O33-P3-O31	2.22	117.72	110.58
2	B	701	FAD	O4B-C1B-N9A	2.29	112.88	108.10
2	B	701	FAD	C7M-C7-C8	2.40	126.01	120.73
2	A	701	FAD	O4B-C4B-C3B	2.41	110.01	105.15
3	A	702	UCC	CP7-CPB-CP8	2.42	113.76	109.34
2	A	701	FAD	O4B-C1B-N9A	2.42	113.17	108.10
2	B	701	FAD	C6-C5X-C9A	2.54	122.32	118.98
2	A	701	FAD	N6A-C6A-N1A	2.60	124.78	119.20
2	A	701	FAD	C6-C5X-N5	2.76	122.51	118.96
3	A	702	UCC	O33-P3-O31	2.82	119.65	110.58
2	B	701	FAD	C1'-N10-C9A	2.99	122.22	118.86
2	A	701	FAD	C2A-N1A-C6A	3.06	124.23	118.77
2	A	701	FAD	O2'-C2'-C3'	3.19	117.05	109.02
3	B	702	UCC	OA1-CA1-S	3.32	125.47	122.83
3	A	702	UCC	OA1-CA1-CA2	4.02	126.71	123.94
2	A	701	FAD	C4-C4X-N5	4.06	123.64	118.72
2	A	701	FAD	C4X-N5-C5X	4.15	121.54	116.76
3	B	702	UCC	CA3-CA2-CA1	4.49	119.75	113.12
3	B	702	UCC	CP7-CPB-CP8	5.40	119.21	109.34
2	B	701	FAD	C5X-C9A-N10	5.63	121.89	117.62
3	B	702	UCC	OA1-CA1-CA2	6.85	128.65	123.94
2	A	701	FAD	C4-N3-C2	9.21	123.21	115.25
3	B	702	UCC	CP7-CPB-CPA	11.65	123.60	108.50
2	B	701	FAD	C4-N3-C2	12.07	125.68	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	FAD	7	0
3	A	702	UCC	23	0
3	B	702	UCC	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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(Å²)	Q<0.9
1	A	592/593 (99%)	-0.22	24 (4%)	41	35	25, 40, 68, 96	0
1	B	593/593 (100%)	-0.19	19 (3%)	51	45	23, 45, 79, 116	0
All	All	1185/1186 (99%)	-0.21	43 (3%)	46	40	23, 43, 74, 116	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	259	SER	4.5
1	B	611	ALA	4.5
1	A	260	ASP	4.4
1	A	330[A]	LEU	4.1
1	A	268	ARG	3.6
1	A	263	ALA	3.6
1	A	229	ASP	3.3
1	B	501	THR	3.3
1	A	480	GLY	3.2
1	B	261	GLY	3.2
1	A	264	LEU	3.2
1	A	610	THR	3.1
1	B	19	THR	3.0
1	B	407	ASP	2.9
1	B	403	GLY	2.9
1	B	281	SER	2.8
1	B	483	ASN	2.7
1	B	482	GLU	2.7
1	A	481	LYS	2.7
1	A	502	GLU	2.6
1	B	280	GLU	2.6
1	B	411	MET	2.6
1	A	332[A]	ILE	2.6
1	B	230	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	333[A]	THR	2.5
1	A	262	ASN	2.5
1	A	265	GLU	2.4
1	A	596	GLU	2.4
1	B	481	LYS	2.4
1	A	261	GLY	2.4
1	B	502	GLU	2.4
1	A	230	LYS	2.3
1	A	504	GLU	2.3
1	A	535	GLU	2.2
1	A	281	SER	2.2
1	A	334[A]	ARG	2.2
1	B	342	LEU	2.1
1	B	259	SER	2.1
1	A	403	GLY	2.1
1	A	532	ILE	2.1
1	B	268	ARG	2.1
1	B	480	GLY	2.0
1	B	404	LYS	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, 95th 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^2)	Q<0.9
3	UCC	A	702	60/60	0.76	0.31	2.76	41,53,57,59	48
2	FAD	A	701	53/53	0.90	0.13	1.06	31,49,58,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	UCC	B	702	60/60	0.91	0.12	0.23	43,53,61,65	0
2	FAD	B	701	53/53	0.96	0.08	-0.52	29,37,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.