



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:08 PM GMT

PDB ID : 1VCF  
Title : Crystal Structure of IPP isomerase at I422  
Authors : Wada, T.; Park, S.-Y.; Tame, R.H.; Kuramitsu, S.; Yokoyama, S.; RIKEN  
Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2004-03-08  
Resolution : 2.60 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.

---

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

MolProbity : 4.02b-467  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

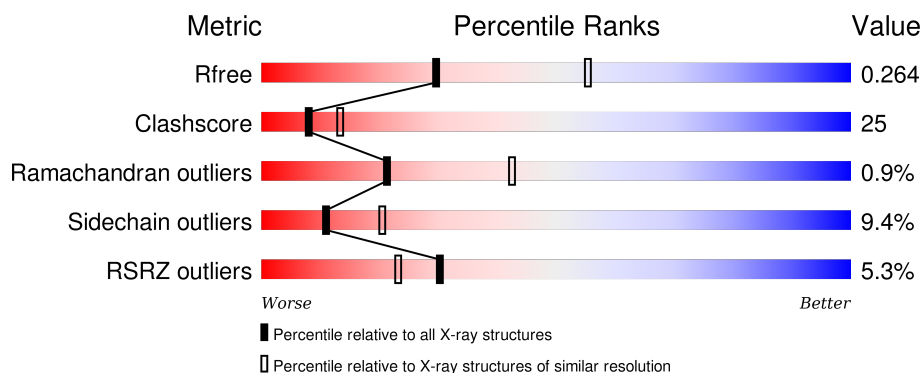
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	332	<div> <div>5%</div> <div>52%</div> <div>34%</div> <div>5%</div> <div>10%</div> </div>
1	B	332	<div> <div>5%</div> <div>50%</div> <div>34%</div> <div>5%</div> <div>10%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4569 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 isopentenyl-diphosphate delta-isomerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	Se	0	0	0
			2264	1441	409	408	1	5			
1	B	298	Total	C	N	O	S	Se	0	0	0
			2242	1424	407	405	1	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
A	66	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
A	91	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
A	92	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
A	143	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
A	185	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
B	66	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
B	91	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
B	92	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
B	143	MSE	MET	MODIFIED RESIDUE	UNP Q746I8
B	185	MSE	MET	MODIFIED RESIDUE	UNP Q746I8

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cd	0	0
			1	1		

- Molecule 3 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).

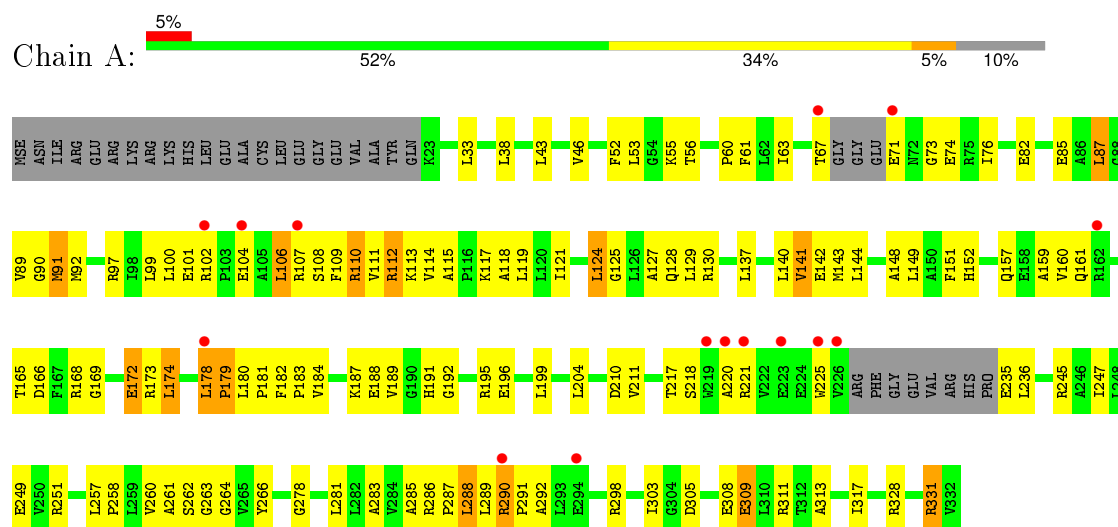


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

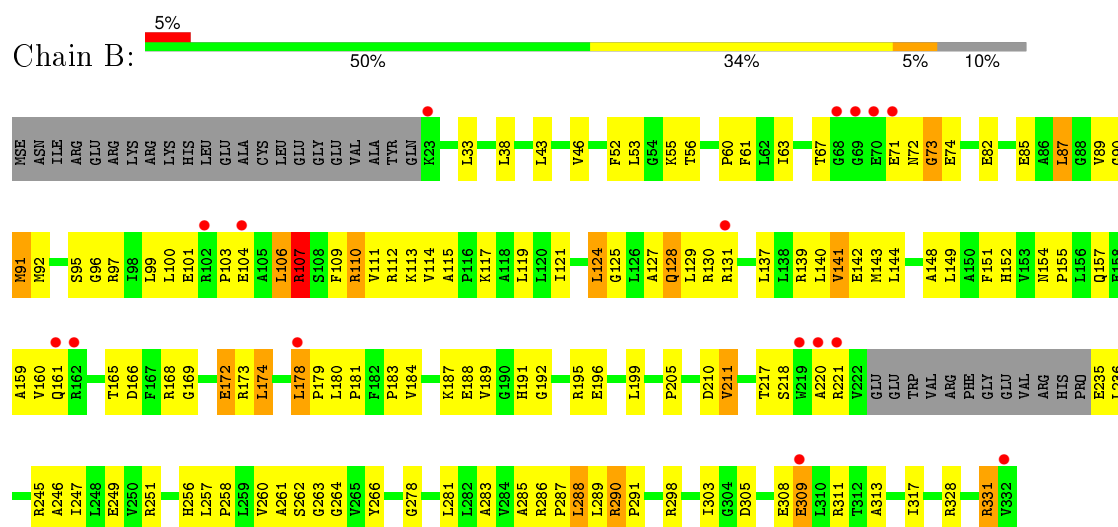
### 3 Residue-property plots [i](#)

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: isopentenyl-diphosphate delta-isomerase



- Molecule 1: isopentenyl-diphosphate delta-isomerase



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.43 Å   144.43 Å   169.82 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	19.94 – 2.60 19.94 – 2.60	Depositor EDS
% Data completeness (in resolution range)	92.3 (19.94-2.60) 92.3 (19.94-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.55 (at 2.59 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.242   ,   0.260 0.246   ,   0.264	Depositor DCC
$R_{free}$ test set	1237 reflections (4.81%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.1	Xtriage
Anisotropy	0.920	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 37.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 25755 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4569	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% 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: FMN, CD

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	0.46	0/2292	0.75	7/3095 (0.2%)
1	B	0.47	0/2269	0.75	6/3063 (0.2%)
All	All	0.47	0/4561	0.75	13/6158 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	ARG	NE-CZ-NH1	-6.69	116.95	120.30
1	B	110	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	112	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	110	ARG	NE-CZ-NH2	6.66	123.63	120.30
1	A	112	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	B	107	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	B	110	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	107	ARG	NE-CZ-NH1	-6.37	117.12	120.30
1	B	107	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	A	107	ARG	NE-CZ-NH2	5.77	123.18	120.30
1	B	112	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	A	298	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	B	298	ARG	NE-CZ-NH1	-5.25	117.67	120.30

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	2264	0	2358	113	0
1	B	2242	0	2340	117	2
2	A	1	0	0	0	0
3	A	31	0	19	3	0
3	B	31	0	19	3	0
All	All	4569	0	4736	230	2

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 25.

All (230) 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:85:GLU:HG3	1:B:115:ALA:HA	1.28	1.12
1:A:85:GLU:HG3	1:A:115:ALA:HA	1.30	1.07
1:A:188:GLU:HG3	1:A:189:VAL:H	1.21	1.04
1:B:188:GLU:HG3	1:B:189:VAL:H	1.20	1.04
1:B:188:GLU:HG3	1:B:189:VAL:N	1.85	0.92
1:A:188:GLU:HG3	1:A:189:VAL:N	1.87	0.90
1:B:33:LEU:HB3	1:B:317:ILE:HD11	1.56	0.88
1:A:218:SER:HB3	1:A:221:ARG:HD3	1.56	0.87
1:B:218:SER:HB3	1:B:221:ARG:HD3	1.57	0.84
1:A:33:LEU:HB3	1:A:317:ILE:HD11	1.61	0.82
1:B:43:LEU:O	1:B:46:VAL:HG12	1.80	0.80
1:B:245:ARG:HH22	1:B:331:ARG:HH22	1.30	0.79
1:B:188:GLU:CG	1:B:189:VAL:H	1.95	0.78
1:B:290:ARG:HD2	1:B:290:ARG:H	1.47	0.78
1:A:290:ARG:H	1:A:290:ARG:HD2	1.47	0.78
1:B:106:LEU:HD12	1:B:110:ARG:HH11	1.48	0.77
1:A:245:ARG:HH22	1:A:331:ARG:HH22	1.31	0.77
1:A:97:ARG:HH11	1:A:125:GLY:H	1.30	0.77
1:B:97:ARG:HH11	1:B:125:GLY:H	1.31	0.76
1:A:188:GLU:CG	1:A:189:VAL:H	1.97	0.76
1:B:317:ILE:HG22	1:B:328:ARG:HD3	1.67	0.75
1:A:43:LEU:O	1:A:46:VAL:HG12	1.85	0.75
1:A:221:ARG:HB2	1:A:221:ARG:NH1	2.03	0.74
1:B:221:ARG:HB2	1:B:221:ARG:NH1	2.03	0.74
1:B:221:ARG:HB2	1:B:221:ARG:HH11	1.52	0.73
1:B:85:GLU:HG3	1:B:115:ALA:CA	2.14	0.73

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:LEU:HD22	1:A:178:LEU:HG	1.71	0.72
1:A:286:ARG:HB3	1:A:287:PRO:HD3	1.70	0.72
1:A:85:GLU:HG3	1:A:115:ALA:CA	2.15	0.72
1:A:317:ILE:HG22	1:A:328:ARG:HD3	1.70	0.72
1:A:97:ARG:HH12	1:A:152:HIS:CE1	2.08	0.72
1:A:130:ARG:HB3	1:A:173:ARG:NH1	2.05	0.71
1:A:188:GLU:HG2	1:A:192:GLY:N	2.06	0.70
1:A:221:ARG:HB2	1:A:221:ARG:HH11	1.55	0.70
1:A:251:ARG:NH2	1:A:257:LEU:O	2.24	0.70
1:A:264:GLY:HA2	1:A:266:TYR:CZ	2.27	0.70
1:A:218:SER:H	1:A:221:ARG:NH1	1.88	0.69
1:B:286:ARG:HH11	1:B:286:ARG:HG2	1.59	0.68
1:B:97:ARG:HH12	1:B:152:HIS:CE1	2.11	0.68
1:B:196:GLU:HA	1:B:199:LEU:HD12	1.75	0.68
1:B:130:ARG:HB3	1:B:173:ARG:NH1	2.09	0.67
1:A:286:ARG:HH11	1:A:286:ARG:HG2	1.58	0.67
1:A:157:GLN:HE21	1:A:161:GLN:HE22	1.44	0.66
1:A:196:GLU:HA	1:A:199:LEU:HD12	1.76	0.66
1:B:187:LYS:HB3	1:B:210:ASP:HB3	1.76	0.66
1:B:251:ARG:NH2	1:B:257:LEU:O	2.28	0.65
1:B:262:SER:HB3	1:B:283:ALA:HB3	1.78	0.65
1:B:218:SER:H	1:B:221:ARG:NH1	1.94	0.65
1:B:188:GLU:HG2	1:B:192:GLY:N	2.12	0.65
1:B:286:ARG:HB3	1:B:287:PRO:HD3	1.77	0.65
1:B:180:LEU:HD12	1:B:184:VAL:HG21	1.79	0.65
1:A:85:GLU:OE1	1:A:117:LYS:N	2.26	0.64
1:A:178:LEU:O	1:A:180:LEU:N	2.30	0.64
1:B:178:LEU:O	1:B:180:LEU:N	2.31	0.64
1:B:61:PHE:O	1:B:89:VAL:HG13	1.98	0.64
1:A:180:LEU:HD12	1:A:184:VAL:HG21	1.80	0.64
1:B:157:GLN:HE21	1:B:161:GLN:HE22	1.45	0.64
1:B:290:ARG:N	1:B:290:ARG:HD2	2.13	0.63
1:A:290:ARG:N	1:A:290:ARG:HD2	2.14	0.63
1:B:85:GLU:OE1	1:B:117:LYS:N	2.29	0.62
1:A:257:LEU:HD12	1:A:258:PRO:HD2	1.81	0.62
1:A:148:ALA:HB2	1:A:183:PRO:HG2	1.81	0.61
1:B:257:LEU:HD12	1:B:258:PRO:HD2	1.83	0.61
1:A:245:ARG:NH2	1:A:331:ARG:HH22	1.99	0.61
1:A:187:LYS:HB3	1:A:210:ASP:HB3	1.81	0.61
1:B:174:LEU:HD22	1:B:178:LEU:HG	1.83	0.60
1:A:217:THR:HG21	1:A:286:ARG:HG2	1.84	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:GLU:HG2	1:A:192:GLY:H	1.66	0.59
1:B:217:THR:HG21	1:B:286:ARG:HG2	1.85	0.59
1:B:157:GLN:HG3	1:B:161:GLN:NE2	2.17	0.59
1:A:61:PHE:O	1:A:89:VAL:HG13	2.03	0.59
1:B:187:LYS:CB	1:B:210:ASP:HB3	2.33	0.58
1:B:264:GLY:HA2	1:B:266:TYR:CZ	2.38	0.58
1:A:262:SER:HB3	1:A:283:ALA:HB3	1.85	0.58
1:B:97:ARG:HH11	1:B:125:GLY:N	2.00	0.57
1:A:288:LEU:HD21	1:A:303:ILE:HD11	1.87	0.57
1:A:157:GLN:HG3	1:A:161:GLN:NE2	2.19	0.57
1:A:187:LYS:CB	1:A:210:ASP:HB3	2.36	0.56
1:B:124:LEU:O	1:B:151:PHE:HA	2.05	0.56
1:A:97:ARG:HH11	1:A:125:GLY:N	2.01	0.56
1:A:313:ALA:O	1:A:317:ILE:HG12	2.07	0.55
1:A:266:TYR:CD2	1:A:287:PRO:HG2	2.42	0.55
1:B:266:TYR:CD2	1:B:287:PRO:HG2	2.41	0.55
1:A:97:ARG:NH1	1:A:152:HIS:CE1	2.75	0.55
1:B:82:GLU:HB2	1:B:114:VAL:HG21	1.87	0.55
1:B:188:GLU:CG	1:B:189:VAL:N	2.58	0.54
1:B:61:PHE:HD2	1:B:89:VAL:HG11	1.72	0.54
1:B:148:ALA:HB2	1:B:183:PRO:HG2	1.88	0.54
1:B:245:ARG:NH2	1:B:331:ARG:HH22	2.01	0.53
1:B:263:GLY:HA2	3:B:502:FMN:O2P	2.08	0.53
1:A:129:LEU:O	1:A:173:ARG:HD3	2.09	0.53
1:A:61:PHE:HD2	1:A:89:VAL:HG11	1.72	0.53
1:B:180:LEU:HB3	1:B:181:PRO:HD2	1.91	0.53
1:B:188:GLU:HG2	1:B:192:GLY:H	1.74	0.53
1:A:285:ALA:HB3	3:A:501:FMN:O5'	2.09	0.52
1:A:99:LEU:HD21	1:A:106:LEU:HA	1.91	0.52
1:B:172:GLU:CD	1:B:172:GLU:H	2.12	0.52
1:A:172:GLU:CD	1:A:172:GLU:H	2.13	0.52
1:A:55:LYS:HD3	1:A:56:THR:H	1.75	0.52
1:B:217:THR:HG21	1:B:286:ARG:HH11	1.75	0.51
1:A:82:GLU:HB2	1:A:114:VAL:HG21	1.91	0.51
1:A:106:LEU:HD12	1:A:110:ARG:HH11	1.75	0.51
1:B:308:GLU:OE2	1:B:311:ARG:HD2	2.10	0.51
1:B:288:LEU:HD21	1:B:303:ILE:HD11	1.93	0.51
1:A:286:ARG:HD2	1:A:289:LEU:HD12	1.92	0.51
1:A:124:LEU:O	1:A:151:PHE:HA	2.11	0.51
1:A:85:GLU:CG	1:A:115:ALA:HA	2.21	0.51
1:B:313:ALA:O	1:B:317:ILE:HG12	2.11	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:GLY:HA2	1:B:172:GLU:CG	2.40	0.50
1:A:195:ARG:HB3	1:A:249:GLU:HB3	1.94	0.50
1:B:99:LEU:HD11	1:B:144:LEU:HD21	1.92	0.50
1:B:99:LEU:HD21	1:B:106:LEU:HA	1.92	0.50
1:A:217:THR:HG21	1:A:286:ARG:HH11	1.75	0.50
1:B:85:GLU:CG	1:B:115:ALA:HA	2.21	0.50
1:B:251:ARG:NH1	1:B:278:GLY:O	2.41	0.50
1:B:63:ILE:HB	1:B:91:MSE:HG3	1.93	0.50
1:B:195:ARG:HB3	1:B:249:GLU:HB3	1.94	0.50
1:A:218:SER:H	1:A:221:ARG:HH11	1.58	0.50
1:B:89:VAL:CG1	1:B:90:GLY:N	2.74	0.50
1:A:235:GLU:HG3	1:A:236:LEU:HD22	1.94	0.49
1:A:286:ARG:NH1	1:A:286:ARG:HG2	2.25	0.49
1:B:317:ILE:CG2	1:B:328:ARG:HD3	2.39	0.49
1:A:127:ALA:O	1:A:130:ARG:HG2	2.13	0.49
1:B:285:ALA:HB3	3:B:502:FMN:O5'	2.11	0.49
1:B:106:LEU:HD21	1:B:143:MSE:HB3	1.95	0.49
1:B:97:ARG:NH1	1:B:152:HIS:CE1	2.79	0.48
1:A:61:PHE:CE2	1:A:303:ILE:HD12	2.49	0.48
1:A:140:LEU:HA	1:A:143:MSE:HE3	1.95	0.48
1:A:97:ARG:NH1	1:A:125:GLY:H	2.05	0.48
1:A:180:LEU:HB3	1:A:181:PRO:HD2	1.96	0.48
1:A:264:GLY:HA2	1:A:266:TYR:CE1	2.49	0.48
1:B:286:ARG:HD2	1:B:289:LEU:HD12	1.95	0.48
1:A:63:ILE:HB	1:A:91:MSE:HG3	1.96	0.48
1:B:129:LEU:O	1:B:173:ARG:HD3	2.14	0.48
1:A:106:LEU:HD21	1:A:143:MSE:HB3	1.97	0.47
1:B:305:ASP:O	1:B:309:GLU:HB2	2.14	0.47
1:A:178:LEU:HA	1:A:178:LEU:HD23	1.64	0.47
1:A:188:GLU:OE1	1:A:191:HIS:HB2	2.14	0.47
1:A:92:MSE:HG2	1:A:121:ILE:HD12	1.96	0.47
1:B:92:MSE:HG2	1:B:121:ILE:HD12	1.96	0.47
1:B:169:GLY:HA2	1:B:172:GLU:HG2	1.96	0.47
1:B:104:GLU:C	1:B:106:LEU:H	2.17	0.47
1:B:60:PRO:HA	1:B:281:LEU:HD13	1.97	0.47
1:A:245:ARG:NH2	1:A:331:ARG:NH2	2.62	0.47
1:B:99:LEU:CD1	1:B:144:LEU:HD21	2.45	0.47
1:A:181:PRO:HG2	1:A:182:PHE:CD2	2.50	0.47
1:A:245:ARG:HH22	1:A:331:ARG:NH2	2.07	0.46
1:B:286:ARG:NH1	1:B:286:ARG:HG2	2.26	0.46
1:B:178:LEU:HD23	1:B:178:LEU:HA	1.65	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LEU:HD11	1:A:144:LEU:HD21	1.96	0.46
1:A:308:GLU:OE2	1:A:311:ARG:HD2	2.15	0.46
1:B:61:PHE:CE2	1:B:303:ILE:HD12	2.50	0.46
1:B:235:GLU:HG3	1:B:236:LEU:HD22	1.98	0.46
1:B:290:ARG:HB2	1:B:291:PRO:CD	2.46	0.46
1:A:263:GLY:HA2	3:A:501:FMN:O2P	2.15	0.46
1:B:245:ARG:HH22	1:B:331:ARG:NH2	2.06	0.46
1:A:169:GLY:HA2	1:A:172:GLU:HG2	1.97	0.46
1:A:247:ILE:HD11	1:A:261:ALA:HB1	1.98	0.46
1:A:305:ASP:O	1:A:309:GLU:HB2	2.16	0.46
1:A:67:THR:H	3:A:501:FMN:H6	1.80	0.45
1:A:60:PRO:HA	1:A:281:LEU:HD13	1.98	0.45
1:B:169:GLY:O	1:B:172:GLU:HG2	2.16	0.45
1:B:128:GLN:HA	1:B:131:ARG:NH1	2.32	0.45
1:B:290:ARG:HG2	1:B:290:ARG:HH11	1.82	0.45
1:A:317:ILE:CG2	1:A:328:ARG:HD3	2.43	0.45
1:B:137:LEU:O	1:B:141:VAL:HG13	2.16	0.45
1:B:245:ARG:NH2	1:B:331:ARG:NH2	2.64	0.45
1:B:96:GLY:O	1:B:99:LEU:HB2	2.17	0.45
1:A:89:VAL:CG1	1:A:90:GLY:N	2.80	0.45
1:A:137:LEU:O	1:A:141:VAL:HG13	2.16	0.45
1:A:74:GLU:HB2	1:A:108:SER:HA	1.98	0.44
1:B:166:ASP:OD1	1:B:168:ARG:HD3	2.17	0.44
1:A:104:GLU:C	1:A:106:LEU:H	2.20	0.44
1:B:218:SER:H	1:B:221:ARG:HH11	1.64	0.44
1:B:139:ARG:O	1:B:143:MSE:HG3	2.18	0.44
1:A:166:ASP:OD1	1:A:168:ARG:HD3	2.17	0.44
1:B:159:ALA:HA	1:B:165:THR:HG22	2.00	0.44
1:B:140:LEU:HA	1:B:143:MSE:HE3	1.99	0.44
1:B:67:THR:H	3:B:502:FMN:H6	1.83	0.44
1:A:174:LEU:HD13	1:A:204:LEU:HD23	1.99	0.43
1:A:290:ARG:HH11	1:A:290:ARG:HG2	1.83	0.43
1:A:290:ARG:HB2	1:A:291:PRO:CD	2.47	0.43
1:A:181:PRO:HG2	1:A:182:PHE:CE2	2.53	0.43
1:B:97:ARG:NH1	1:B:125:GLY:N	2.66	0.43
1:B:82:GLU:HB2	1:B:114:VAL:CG2	2.48	0.43
1:B:74:GLU:OE2	1:B:107:ARG:HD3	2.18	0.43
1:A:251:ARG:NH1	1:A:278:GLY:O	2.47	0.43
1:B:157:GLN:HB2	1:B:220:ALA:HB2	1.99	0.43
1:A:169:GLY:HA2	1:A:172:GLU:CG	2.49	0.43
1:A:101:GLU:HG3	1:A:102:ARG:HD2	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLU:N	1:A:71:GLU:OE1	2.51	0.43
1:B:188:GLU:OE1	1:B:191:HIS:HB2	2.19	0.43
1:A:157:GLN:HB2	1:A:220:ALA:HB2	1.99	0.42
1:B:109:PHE:O	1:B:110:ARG:C	2.57	0.42
1:A:210:ASP:HA	1:A:260:VAL:HB	2.00	0.42
1:A:109:PHE:O	1:A:110:ARG:C	2.58	0.42
1:A:159:ALA:HA	1:A:165:THR:HG22	2.01	0.42
1:A:99:LEU:CD1	1:A:144:LEU:HD21	2.49	0.42
1:B:154:ASN:O	1:B:155:PRO:C	2.57	0.42
1:B:72:ASN:O	1:B:73:GLY:C	2.58	0.42
1:A:97:ARG:NH1	1:A:125:GLY:N	2.67	0.42
1:B:55:LYS:HD3	1:B:56:THR:H	1.84	0.42
1:A:76:ILE:HG23	1:A:292:ALA:HB1	2.02	0.42
1:B:101:GLU:O	1:B:103:PRO:HD3	2.19	0.42
1:A:100:LEU:N	1:A:100:LEU:HD22	2.35	0.42
1:B:317:ILE:HG23	1:B:328:ARG:HB3	2.01	0.41
1:B:210:ASP:HA	1:B:260:VAL:HB	2.01	0.41
1:B:46:VAL:HG11	1:B:311:ARG:HG3	2.02	0.41
1:A:99:LEU:CD2	1:A:106:LEU:HA	2.50	0.41
1:A:52:PHE:CE2	1:A:53:LEU:HD22	2.54	0.41
1:B:127:ALA:O	1:B:130:ARG:HG2	2.21	0.41
1:A:112:ARG:NH2	1:A:118:ALA:O	2.44	0.41
1:A:218:SER:CB	1:A:221:ARG:HD3	2.39	0.41
1:A:188:GLU:CG	1:A:189:VAL:N	2.61	0.41
1:B:264:GLY:HA2	1:B:266:TYR:CE1	2.56	0.41
1:B:52:PHE:CE2	1:B:53:LEU:HD22	2.55	0.41
1:B:247:ILE:HD11	1:B:261:ALA:HB1	2.02	0.41
1:B:71:GLU:OE1	1:B:71:GLU:N	2.53	0.41
1:B:95:SER:OG	1:B:97:ARG:HB2	2.21	0.40
1:B:87:LEU:HD23	1:B:303:ILE:HB	2.03	0.40
1:B:100:LEU:HD22	1:B:100:LEU:N	2.36	0.40
1:B:99:LEU:CD2	1:B:106:LEU:HA	2.52	0.40
1:A:148:ALA:CB	1:A:183:PRO:HG2	2.49	0.40
1:A:87:LEU:HD23	1:A:303:ILE:HB	2.02	0.40
1:A:178:LEU:O	1:A:179:PRO:C	2.58	0.40
1:B:178:LEU:O	1:B:179:PRO:C	2.59	0.40
1:B:211:VAL:HG22	1:B:246:ALA:HB1	2.03	0.40
1:A:317:ILE:HG23	1:A:328:ARG:HB3	2.02	0.40
1:B:178:LEU:HD13	1:B:205:PRO:CD	2.52	0.40
1:B:106:LEU:HD12	1:B:110:ARG:NH1	2.24	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:HIS:CE1	1:B:256:HIS:CE1[8_666]	1.93	0.27
1:B:235:GLU:OE2	1:B:309:GLU:OE2[4_665]	2.19	0.01

## 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	293/332 (88%)	273 (93%)	17 (6%)	3 (1%)	19	39
1	B	294/332 (89%)	271 (92%)	21 (7%)	2 (1%)	26	51
All	All	587/664 (88%)	544 (93%)	38 (6%)	5 (1%)	21	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	GLY
1	A	178	LEU
1	B	73	GLY
1	B	178	LEU
1	A	179	PRO

### 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	225/246 (92%)	204 (91%)	21 (9%)	11	21

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	222/246 (90%)	201 (90%)	21 (10%)	11	20
All	All	447/492 (91%)	405 (91%)	42 (9%)	11	20

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	87	LEU
1	A	91	MSE
1	A	106	LEU
1	A	111	VAL
1	A	113	LYS
1	A	119	LEU
1	A	124	LEU
1	A	128	GLN
1	A	141	VAL
1	A	142	GLU
1	A	149	LEU
1	A	160	VAL
1	A	172	GLU
1	A	174	LEU
1	A	211	VAL
1	A	225	TRP
1	A	288	LEU
1	A	290	ARG
1	A	309	GLU
1	A	331	ARG
1	B	38	LEU
1	B	87	LEU
1	B	91	MSE
1	B	106	LEU
1	B	107	ARG
1	B	111	VAL
1	B	113	LYS
1	B	119	LEU
1	B	124	LEU
1	B	128	GLN
1	B	141	VAL
1	B	142	GLU
1	B	149	LEU
1	B	160	VAL
1	B	172	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	174	LEU
1	B	211	VAL
1	B	288	LEU
1	B	290	ARG
1	B	309	GLU
1	B	331	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	152	HIS
1	A	161	GLN
1	B	128	GLN
1	B	161	GLN

### 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](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	FMN	A	501	-	32,33,33	2.62	9 (28%)	34,50,50	4.21	17 (50%)
3	FMN	B	502	-	32,33,33	2.63	10 (31%)	34,50,50	4.23	17 (50%)

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	FMN	A	501	-	-	0/18/18/18	0/3/3/3
3	FMN	B	502	-	-	0/18/18/18	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	FMN	C2-N1	-2.08	1.33	1.38
3	B	502	FMN	C8-C7	2.15	1.46	1.41
3	A	501	FMN	C8-C7	2.40	1.47	1.41
3	B	502	FMN	C6-C7	2.88	1.45	1.37
3	B	502	FMN	C5'-C4'	3.00	1.56	1.51
3	A	501	FMN	C6-C7	3.14	1.46	1.37
3	B	502	FMN	C9A-C5A	3.33	1.49	1.42
3	A	501	FMN	C9A-C5A	3.38	1.49	1.42
3	A	501	FMN	C5'-C4'	3.61	1.57	1.51
3	B	502	FMN	C9-C9A	4.17	1.49	1.40
3	A	501	FMN	C9-C9A	4.32	1.50	1.40
3	A	501	FMN	C2-N3	4.50	1.47	1.38
3	B	502	FMN	C5A-N5	4.90	1.43	1.35
3	A	501	FMN	C5A-N5	4.91	1.43	1.35
3	B	502	FMN	C2-N3	5.00	1.48	1.38
3	A	501	FMN	C4-N3	5.86	1.43	1.33
3	B	502	FMN	C4-N3	6.03	1.43	1.33
3	A	501	FMN	C4A-C10	7.26	1.54	1.40
3	B	502	FMN	C4A-C10	7.32	1.54	1.40

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	FMN	O3P-P-O5'	-8.96	80.56	106.72
3	B	502	FMN	O3P-P-O1P	-8.83	81.82	110.63
3	A	501	FMN	O3P-P-O1P	-8.74	82.12	110.63
3	B	502	FMN	O3P-P-O5'	-8.54	81.80	106.72

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	FMN	C4A-C4-N3	-5.89	115.82	123.52
3	A	501	FMN	N3-C2-N1	-5.73	118.04	127.69
3	B	502	FMN	N3-C2-N1	-5.72	118.06	127.69
3	A	501	FMN	C4A-C4-N3	-5.59	116.22	123.52
3	B	502	FMN	O3P-P-O2P	-5.51	87.22	107.44
3	A	501	FMN	O3P-P-O2P	-5.40	87.61	107.44
3	B	502	FMN	C7M-C7-C6	-4.14	108.63	120.33
3	A	501	FMN	C7M-C7-C6	-4.13	108.67	120.33
3	B	502	FMN	C9A-C5A-N5	-3.23	116.92	122.18
3	A	501	FMN	C9A-C5A-N5	-3.13	117.08	122.18
3	B	502	FMN	O3'-C3'-C4'	-2.25	102.89	108.73
3	A	501	FMN	O3'-C3'-C4'	-2.14	103.18	108.73
3	A	501	FMN	O2P-P-O1P	2.26	118.01	110.63
3	B	502	FMN	O2P-P-O1P	2.51	118.81	110.63
3	A	501	FMN	C4A-N5-C5A	3.15	120.43	116.72
3	A	501	FMN	C6-C5A-N5	3.17	122.86	118.92
3	B	502	FMN	C4A-N5-C5A	3.27	120.57	116.72
3	B	502	FMN	C6-C5A-N5	3.30	123.03	118.92
3	B	502	FMN	O2P-P-O5'	3.36	116.54	106.72
3	A	501	FMN	O2P-P-O5'	3.48	116.87	106.72
3	A	501	FMN	C7M-C7-C8	4.74	130.93	120.73
3	B	502	FMN	C7M-C7-C8	4.77	130.99	120.73
3	B	502	FMN	O5'-P-O1P	5.51	120.93	107.08
3	A	501	FMN	O5'-P-O1P	5.60	121.17	107.08
3	A	501	FMN	C1'-N10-C9A	7.75	127.81	118.83
3	B	502	FMN	C1'-N10-C9A	7.98	128.08	118.83
3	B	502	FMN	C4-N3-C2	8.92	122.60	115.16
3	A	501	FMN	C4-N3-C2	8.93	122.61	115.16
3	A	501	FMN	C5A-C9A-N10	8.99	124.32	117.58
3	B	502	FMN	C5A-C9A-N10	9.00	124.33	117.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	FMN	3	0
3	B	502	FMN	3	0

## 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	294/332 (88%)	-0.06	15 (5%) 32 25	34, 49, 91, 106	0
1	B	293/332 (88%)	-0.02	16 (5%) 29 21	31, 48, 89, 106	0
All	All	587/664 (88%)	-0.04	31 (5%) 30 23	31, 49, 90, 106	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	162	ARG	4.8
1	B	221	ARG	4.4
1	A	162	ARG	4.1
1	A	102	ARG	3.7
1	A	219	TRP	3.6
1	B	70	GLU	3.5
1	A	223	GLU	3.4
1	B	161	GLN	3.4
1	B	219	TRP	3.2
1	B	332	VAL	3.2
1	B	68	GLY	3.1
1	A	221	ARG	2.9
1	B	71	GLU	2.8
1	A	225	TRP	2.7
1	A	104	GLU	2.7
1	B	102	ARG	2.7
1	A	71	GLU	2.6
1	B	131	ARG	2.6
1	A	178	LEU	2.5
1	B	69	GLY	2.5
1	A	290	ARG	2.4
1	A	107	ARG	2.4
1	B	309	GLU	2.3
1	B	178	LEU	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	23	LYS	2.3
1	A	294	GLU	2.2
1	B	220	ALA	2.1
1	A	67	THR	2.1
1	A	220	ALA	2.0
1	B	104	GLU	2.0
1	A	226	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	FMN	A	501	31/31	0.91	0.23	0.73	60,68,70,71	0
3	FMN	B	502	31/31	0.94	0.21	0.30	58,67,69,70	0
2	CD	A	601	1/1	0.99	0.07	-1.55	64,64,64,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.