Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 06:52 PM GMT

PDB ID	:	3UE6
Title	:	The dark structure of the blue-light photoreceptor Aureochrome1 LOV
Authors	:	Mitra, D.; Yang, X.; Moffat, K.
Deposited on	:	2011-10-28
Resolution	:	2.75 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

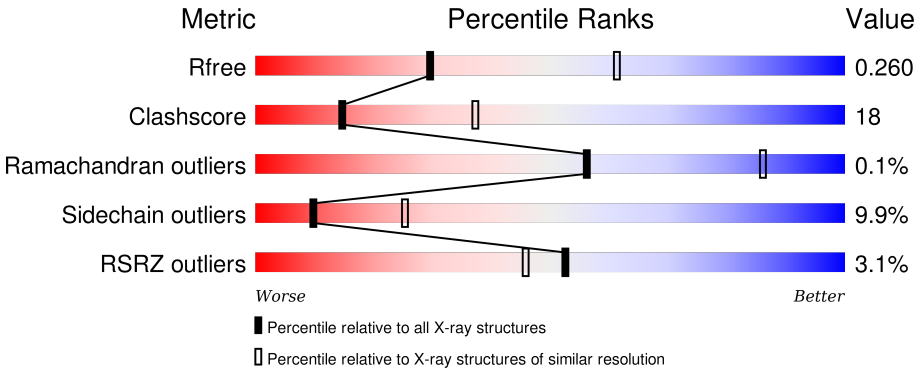
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.75 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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	166	60% 19% • 19%
1	B	166	2% 52% 20% 5% 23%
1	C	166	2% 52% 15% 5% 28%
1	D	166	3% 51% 24% • 22%
1	E	166	5% 55% 24% • 17%

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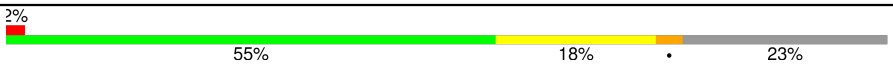
Mol	Chain	Length	Quality of chain
1	F	166	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6392 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 Aureochrome1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	135	Total	C	N	O	S	0	0	0
			1067	675	181	208	3			
1	B	128	Total	C	N	O	S	0	0	0
			1002	634	174	191	3			
1	C	120	Total	C	N	O	S	0	0	0
			946	597	164	183	2			
1	D	130	Total	C	N	O	S	0	0	0
			1023	648	176	196	3			
1	E	138	Total	C	N	O	S	0	0	0
			1094	693	187	211	3			
1	F	127	Total	C	N	O	S	0	0	0
			996	631	173	189	3			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	172	GLY	-	EXPRESSION TAG	UNP A8QW55
A	173	SER	-	EXPRESSION TAG	UNP A8QW55
A	174	HIS	-	EXPRESSION TAG	UNP A8QW55
A	175	MET	-	EXPRESSION TAG	UNP A8QW55
B	172	GLY	-	EXPRESSION TAG	UNP A8QW55
B	173	SER	-	EXPRESSION TAG	UNP A8QW55
B	174	HIS	-	EXPRESSION TAG	UNP A8QW55
B	175	MET	-	EXPRESSION TAG	UNP A8QW55
C	172	GLY	-	EXPRESSION TAG	UNP A8QW55
C	173	SER	-	EXPRESSION TAG	UNP A8QW55
C	174	HIS	-	EXPRESSION TAG	UNP A8QW55
C	175	MET	-	EXPRESSION TAG	UNP A8QW55
D	172	GLY	-	EXPRESSION TAG	UNP A8QW55
D	173	SER	-	EXPRESSION TAG	UNP A8QW55
D	174	HIS	-	EXPRESSION TAG	UNP A8QW55
D	175	MET	-	EXPRESSION TAG	UNP A8QW55
E	172	GLY	-	EXPRESSION TAG	UNP A8QW55

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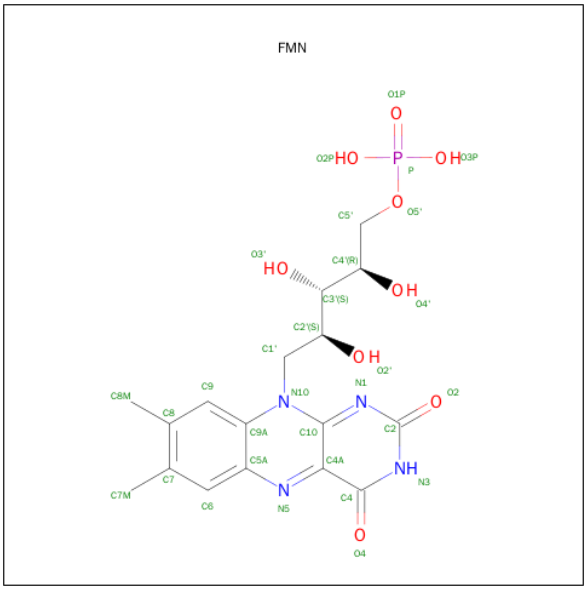
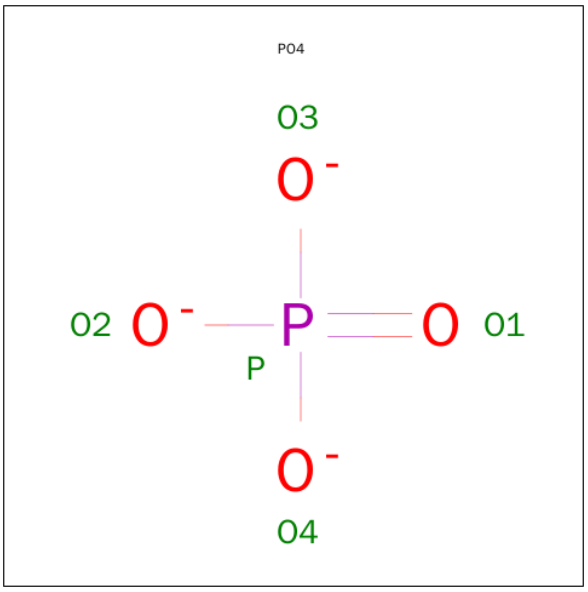
Chain	Residue	Modelled	Actual	Comment	Reference
E	173	SER	-	EXPRESSION TAG	UNP A8QW55
E	174	HIS	-	EXPRESSION TAG	UNP A8QW55
E	175	MET	-	EXPRESSION TAG	UNP A8QW55
F	172	GLY	-	EXPRESSION TAG	UNP A8QW55
F	173	SER	-	EXPRESSION TAG	UNP A8QW55
F	174	HIS	-	EXPRESSION TAG	UNP A8QW55
F	175	MET	-	EXPRESSION TAG	UNP A8QW55

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	E	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	F	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O P 5 4 1	0	0
3	F	1	Total O P 5 4 1	0	0

- Molecule 4 is water.

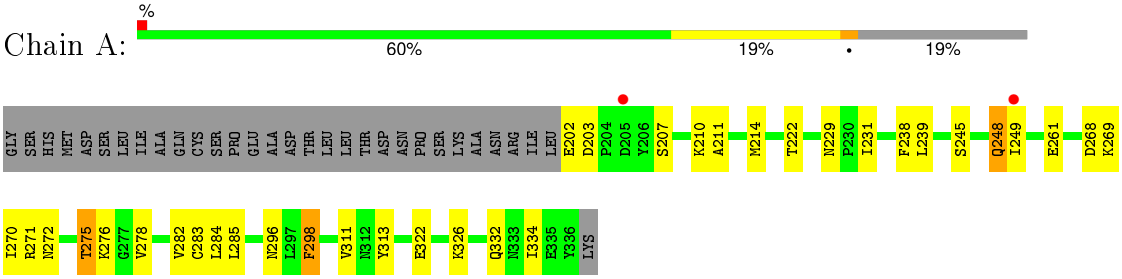
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	23	Total O 23 23	0	0
4	B	19	Total O 19 19	0	0
4	C	1	Total O 1 1	0	0
4	E	9	Total O 9 9	0	0
4	F	16	Total O 16 16	0	0

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.

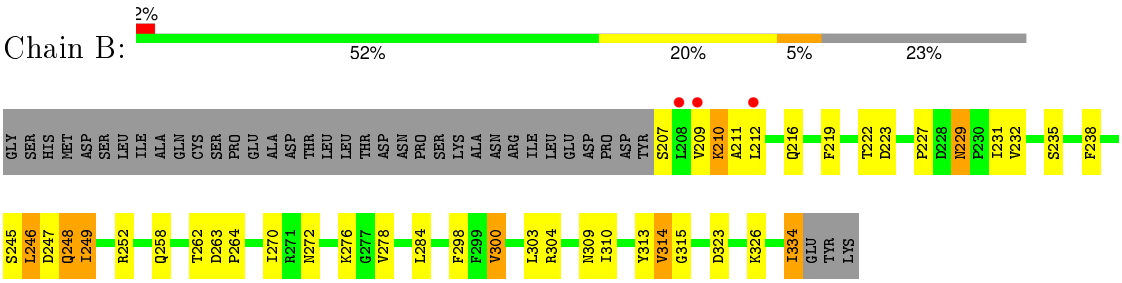
- Molecule 1: Aureochrome1

Chain A:



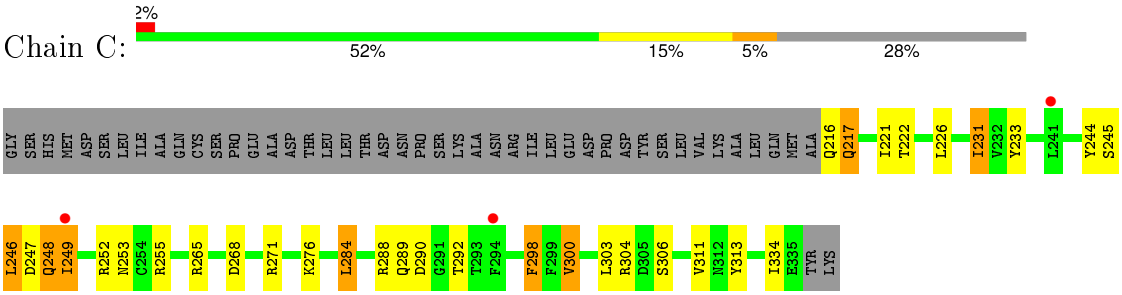
- Molecule 1: Aureochrome1

Chain B:



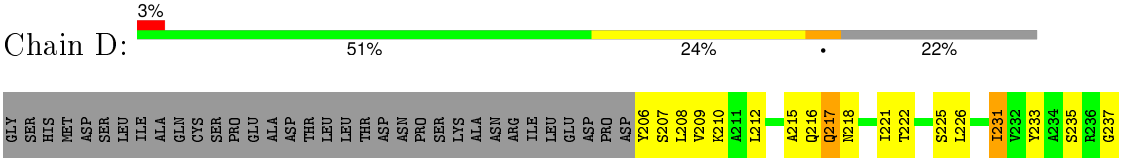
- Molecule 1: Aureochrome1

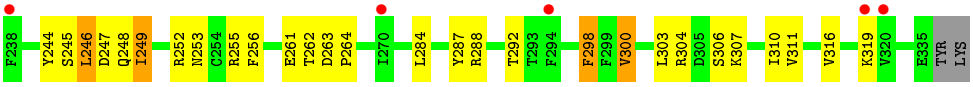
Chain C:



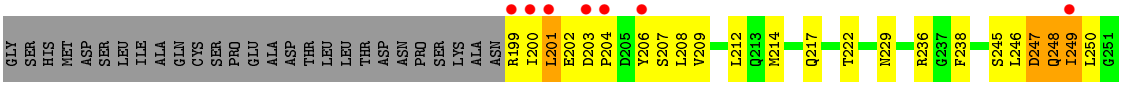
- Molecule 1: Aureochrome1

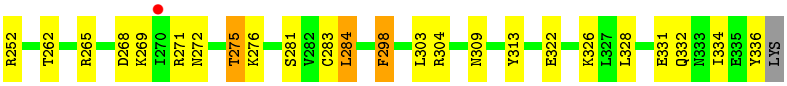
Chain D:



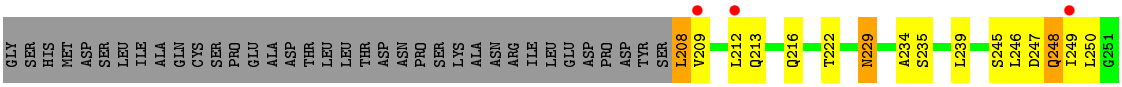


• Molecule 1: Aureochrome1





• Molecule 1: Aureochrome1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	73.99Å 73.99Å 177.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.09 – 2.75 33.09 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.6 (33.09-2.75) 99.8 (33.09-2.75)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.59 (at 2.76Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.192 , 0.256 0.195 , 0.260	Depositor DCC
R_{free} test set	1257 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	77.8	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 60.1	EDS
Estimated twinning fraction	0.488 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Outliers	0 of 24721 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6392	wwPDB-VP
Average B, all atoms (Å^2)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, PO4

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	0.26	0/1086	0.45	0/1475
1	B	0.26	0/1018	0.46	0/1381
1	C	0.26	0/962	0.44	0/1306
1	D	0.25	0/1040	0.44	0/1411
1	E	0.26	0/1113	0.44	0/1511
1	F	0.25	0/1012	0.47	0/1373
All	All	0.26	0/6231	0.45	0/8457

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	1067	0	1049	24	0
1	B	1002	0	1004	37	0
1	C	946	0	934	45	0
1	D	1023	0	1019	50	0
1	E	1094	0	1084	54	0
1	F	996	0	999	41	0
2	A	31	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	31	0	19	0	0
2	C	31	0	19	2	0
2	D	31	0	19	0	0
2	E	31	0	19	1	0
2	F	31	0	19	0	0
3	B	5	0	0	0	0
3	F	5	0	0	0	0
4	A	23	0	0	1	0
4	B	19	0	0	0	0
4	C	1	0	0	0	0
4	E	9	0	0	0	0
4	F	16	0	0	1	0
All	All	6392	0	6203	223	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 18.

All (223) 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:F:246:LEU:CD2	1:F:249:ILE:HD11	1.44	1.46
1:F:246:LEU:HD22	1:F:249:ILE:HD11	1.15	1.14
1:F:246:LEU:HD23	1:F:249:ILE:HD11	1.27	1.07
1:D:217:GLN:HG2	1:D:237:GLY:H	1.17	1.05
1:D:246:LEU:O	1:D:246:LEU:HD22	1.57	1.02
1:F:246:LEU:CD2	1:F:249:ILE:CD1	2.40	0.98
1:F:246:LEU:HD22	1:F:249:ILE:CD1	1.92	0.98
1:C:217:GLN:HE21	1:C:217:GLN:H	1.02	0.94
1:E:283:CYS:H	1:E:332:GLN:HE22	1.13	0.94
1:E:199:ARG:HA	1:E:200:ILE:HG13	1.48	0.94
1:A:283:CYS:H	1:A:332:GLN:HE22	1.15	0.89
1:B:238:PHE:HE2	1:B:249:ILE:CD1	1.88	0.87
1:C:246:LEU:O	1:C:246:LEU:HD22	1.74	0.85
1:E:238:PHE:HE2	1:E:249:ILE:CD1	1.90	0.83
1:D:217:GLN:HG2	1:D:237:GLY:N	1.94	0.82
1:C:304:ARG:O	1:D:216:GLN:HB2	1.80	0.81
1:D:231:ILE:HD11	1:D:249:ILE:CG2	2.10	0.81
1:E:207:SER:HB3	1:F:216:GLN:HE22	1.46	0.81
1:E:283:CYS:H	1:E:332:GLN:NE2	1.78	0.80
1:E:238:PHE:HE2	1:E:249:ILE:HD13	1.45	0.78
1:E:200:ILE:HB	1:F:209:VAL:HB	1.63	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:ILE:HD11	1:C:249:ILE:HG22	1.66	0.77
1:C:246:LEU:CD2	1:C:246:LEU:O	2.33	0.76
1:E:272:ASN:HD21	1:E:276:LYS:HE2	1.51	0.74
1:C:217:GLN:N	1:C:217:GLN:HE21	1.82	0.74
1:B:298:PHE:CZ	1:B:300:VAL:HG13	2.22	0.73
1:F:246:LEU:O	1:F:249:ILE:CG1	2.35	0.73
1:C:288:ARG:HH11	1:C:292:THR:HG23	1.53	0.73
1:E:271:ARG:O	1:E:275:THR:HG23	1.88	0.72
1:B:238:PHE:CE2	1:B:249:ILE:CD1	2.73	0.71
1:F:246:LEU:HD23	1:F:249:ILE:CD1	2.16	0.71
1:E:283:CYS:N	1:E:332:GLN:HE22	1.86	0.71
1:B:212:LEU:HD13	1:E:331:GLU:HB2	1.71	0.71
1:E:199:ARG:CA	1:E:200:ILE:HG13	2.20	0.71
1:C:244:TYR:CB	1:C:249:ILE:HD11	2.21	0.71
1:E:245:SER:O	1:E:248:GLN:HG3	1.90	0.71
1:F:246:LEU:O	1:F:249:ILE:HG13	1.92	0.70
1:B:238:PHE:HE2	1:B:249:ILE:HD13	1.57	0.68
1:C:246:LEU:C	1:C:246:LEU:HD22	2.13	0.68
1:D:216:GLN:HB3	1:D:217:GLN:HA	1.75	0.68
1:B:272:ASN:HD21	1:B:276:LYS:NZ	1.91	0.68
1:D:246:LEU:C	1:D:246:LEU:HD22	2.12	0.68
1:D:217:GLN:HG3	1:D:217:GLN:O	1.94	0.68
1:A:245:SER:O	1:A:248:GLN:HG3	1.94	0.68
1:A:283:CYS:N	1:A:332:GLN:HE22	1.88	0.68
1:A:283:CYS:H	1:A:332:GLN:NE2	1.90	0.68
1:D:231:ILE:HD11	1:D:249:ILE:HG22	1.76	0.67
1:A:269:LYS:HD3	1:A:282:VAL:HG22	1.76	0.67
1:A:238:PHE:HE2	1:A:249:ILE:HD13	1.60	0.67
1:C:253:ASN:HD21	2:C:500:FMN:H3'	1.60	0.67
1:E:238:PHE:CE2	1:E:249:ILE:CD1	2.77	0.66
1:F:246:LEU:HA	1:F:249:ILE:HG12	1.78	0.65
1:C:244:TYR:CG	1:C:249:ILE:HD11	2.32	0.65
1:E:202:GLU:HG2	1:F:281:SER:HB2	1.78	0.64
1:A:239:LEU:CD2	1:A:249:ILE:HD12	2.28	0.64
1:B:246:LEU:O	1:B:246:LEU:HD22	1.98	0.64
1:C:231:ILE:CD1	1:C:249:ILE:HG22	2.28	0.64
1:E:246:LEU:O	1:E:246:LEU:HD13	1.98	0.63
1:C:246:LEU:CD2	1:C:246:LEU:C	2.67	0.63
1:A:238:PHE:CE2	1:A:249:ILE:HD13	2.34	0.63
1:C:245:SER:O	1:C:248:GLN:HG3	1.98	0.63
1:F:246:LEU:O	1:F:249:ILE:HG12	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ILE:HD13	1:B:249:ILE:HG23	1.80	0.62
1:D:262:THR:HG23	1:D:284:LEU:HD22	1.81	0.62
1:E:199:ARG:N	1:E:200:ILE:HA	2.14	0.62
1:A:238:PHE:HE2	1:A:249:ILE:CD1	2.14	0.61
1:A:211:ALA:O	1:A:214:MET:HG3	2.00	0.61
1:D:245:SER:O	1:D:248:GLN:CG	2.49	0.61
1:A:272:ASN:OD1	1:A:276:LYS:HE2	2.01	0.60
1:E:246:LEU:HD13	1:E:250:LEU:HG	1.83	0.60
1:E:272:ASN:ND2	1:E:276:LYS:HE2	2.16	0.60
1:F:239:LEU:HD21	1:F:249:ILE:HD13	1.84	0.60
1:E:199:ARG:O	1:E:199:ARG:HG2	2.01	0.60
1:C:303:LEU:HD22	1:D:212:LEU:O	2.01	0.60
1:B:212:LEU:HD13	1:E:331:GLU:CB	2.31	0.59
1:D:215:ALA:HB1	1:D:316:VAL:HG13	1.84	0.59
1:C:222:THR:HG22	1:C:231:ILE:HA	1.84	0.59
1:A:222:THR:OG1	1:A:313:TYR:HB2	2.02	0.59
1:F:298:PHE:CZ	1:F:300:VAL:HG13	2.37	0.59
1:E:248:GLN:O	1:E:252:ARG:HD3	2.03	0.59
1:F:272:ASN:HD21	1:F:276:LYS:NZ	2.01	0.59
1:F:246:LEU:HD22	1:F:249:ILE:CG1	2.33	0.58
1:B:231:ILE:CD1	1:B:249:ILE:HG23	2.34	0.58
1:C:231:ILE:HD11	1:C:249:ILE:CG2	2.33	0.57
1:B:238:PHE:HE2	1:B:249:ILE:HD11	1.70	0.57
1:B:207:SER:HB2	1:B:211:ALA:HB2	1.88	0.56
1:A:207:SER:HB3	1:B:216:GLN:HE22	1.70	0.56
1:D:288:ARG:HH11	1:D:292:THR:HG23	1.70	0.56
1:D:298:PHE:CZ	1:D:300:VAL:HG13	2.41	0.56
1:D:245:SER:O	1:D:248:GLN:HG2	2.06	0.56
1:F:245:SER:O	1:F:248:GLN:HG3	2.06	0.56
1:D:216:GLN:CB	1:D:217:GLN:HA	2.34	0.55
1:B:238:PHE:CE2	1:B:249:ILE:HD13	2.40	0.55
1:E:204:PRO:HD2	1:F:281:SER:OG	2.06	0.55
1:C:231:ILE:CD1	1:C:249:ILE:CG2	2.84	0.54
1:B:303:LEU:HD11	1:B:314:VAL:HG22	1.90	0.54
1:D:231:ILE:CD1	1:D:249:ILE:CG2	2.84	0.54
1:A:239:LEU:HD23	1:A:249:ILE:HD12	1.89	0.54
1:B:245:SER:O	1:B:248:GLN:HG3	2.07	0.54
1:C:233:TYR:CE2	1:D:221:ILE:HD11	2.43	0.54
1:D:206:TYR:O	1:D:209:VAL:HG12	2.08	0.53
1:D:245:SER:O	1:D:248:GLN:HG3	2.09	0.53
4:A:611:HOH:O	1:B:235:SER:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:247:ASP:OD1	1:E:247:ASP:N	2.39	0.53
1:F:272:ASN:HD21	1:F:276:LYS:HZ1	1.56	0.53
1:E:206:TYR:HB3	1:F:216:GLN:OE1	2.09	0.52
1:B:207:SER:N	1:B:210:LYS:HZ2	2.08	0.52
1:F:249:ILE:HG13	1:F:250:LEU:N	2.24	0.52
1:E:262:THR:HG23	1:E:284:LEU:CD2	2.39	0.52
1:F:246:LEU:CA	1:F:249:ILE:HG12	2.40	0.51
1:B:304:ARG:HA	1:B:309:ASN:O	2.09	0.51
1:B:248:GLN:O	1:B:252:ARG:HD3	2.10	0.51
1:C:298:PHE:CZ	1:C:300:VAL:HG13	2.46	0.51
1:C:304:ARG:O	1:D:216:GLN:CB	2.54	0.51
1:E:217:GLN:NE2	1:F:311:VAL:HG22	2.25	0.51
1:E:262:THR:HG23	1:E:284:LEU:HD21	1.93	0.50
1:F:246:LEU:C	1:F:249:ILE:HG12	2.32	0.50
1:E:212:LEU:HD12	1:F:314:VAL:HG11	1.94	0.50
1:C:244:TYR:HB3	1:C:249:ILE:HD11	1.93	0.50
1:E:246:LEU:CD1	1:E:250:LEU:HG	2.41	0.50
1:E:204:PRO:HG3	1:F:212:LEU:CD2	2.42	0.49
1:C:290:ASP:OD1	1:C:292:THR:HG22	2.11	0.49
1:C:268:ASP:OD2	1:C:271:ARG:NH2	2.43	0.49
1:B:223:ASP:HB2	1:B:232:VAL:HG11	1.95	0.49
1:D:210:LYS:HD3	1:D:210:LYS:C	2.33	0.49
1:E:248:GLN:O	1:E:252:ARG:CD	2.61	0.49
1:F:283:CYS:HA	1:F:296:ASN:O	2.11	0.49
1:B:272:ASN:HD21	1:B:276:LYS:HZ1	1.61	0.49
1:F:235:SER:HB2	4:F:511:HOH:O	2.12	0.49
1:C:216:GLN:HE21	1:D:208:LEU:HB2	1.77	0.49
1:C:221:ILE:HD11	1:D:233:TYR:CZ	2.48	0.48
1:A:238:PHE:CE2	1:A:249:ILE:CD1	2.95	0.48
1:D:244:TYR:CB	1:D:249:ILE:HD11	2.42	0.48
1:C:231:ILE:HG23	1:C:252:ARG:O	2.13	0.48
1:C:288:ARG:HH11	1:C:292:THR:CG2	2.22	0.48
1:B:298:PHE:HZ	1:B:300:VAL:HG13	1.74	0.48
1:D:222:THR:HG22	1:D:231:ILE:HA	1.96	0.48
1:C:245:SER:OG	1:C:248:GLN:HG2	2.14	0.48
1:A:271:ARG:O	1:A:275:THR:HG23	2.13	0.48
1:D:225:SER:HB2	1:D:226:LEU:HD22	1.96	0.48
1:D:253:ASN:HD22	1:D:255:ARG:HG2	1.79	0.48
1:F:234:ALA:HB3	1:F:249:ILE:CD1	2.44	0.47
1:F:246:LEU:HA	1:F:249:ILE:CG1	2.43	0.47
1:A:261:GLU:HB3	1:A:285:LEU:HD23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:THR:OG1	1:E:313:TYR:HB2	2.13	0.47
1:E:281:SER:HA	1:E:298:PHE:O	2.15	0.47
1:A:270:ILE:HD13	1:A:298:PHE:HE2	1.79	0.47
1:A:270:ILE:HD13	1:A:298:PHE:CE2	2.49	0.47
1:B:310:ILE:HG21	1:B:313:TYR:CZ	2.50	0.47
1:E:202:GLU:HB3	1:E:203:ASP:HA	1.97	0.47
1:E:201:LEU:HD22	1:F:331:GLU:CG	2.46	0.46
1:A:322:GLU:O	1:A:326:LYS:HG3	2.15	0.46
1:F:246:LEU:HA	1:F:249:ILE:CD1	2.45	0.46
1:D:217:GLN:HG3	1:D:235:SER:HB2	1.97	0.46
1:D:222:THR:HA	1:D:231:ILE:HA	1.98	0.46
1:D:288:ARG:HH11	1:D:292:THR:CG2	2.27	0.46
1:B:209:VAL:O	1:B:209:VAL:HG12	2.16	0.46
1:C:271:ARG:NH1	2:C:500:FMN:O3P	2.50	0.45
1:D:244:TYR:HD1	1:D:248:GLN:NE2	2.14	0.45
1:B:222:THR:OG1	1:B:229:ASN:ND2	2.50	0.45
1:B:258:GLN:HG2	1:B:262:THR:HG21	1.98	0.45
1:D:209:VAL:HG13	1:D:210:LYS:N	2.32	0.45
1:C:222:THR:HG22	1:C:231:ILE:CA	2.48	0.44
1:E:201:LEU:HD22	1:F:331:GLU:HG2	1.98	0.44
1:E:304:ARG:HA	1:E:309:ASN:O	2.18	0.44
1:E:199:ARG:O	1:E:199:ARG:CG	2.64	0.44
1:F:304:ARG:HA	1:F:309:ASN:O	2.17	0.44
1:E:271:ARG:HD3	2:E:500:FMN:O3P	2.17	0.43
1:C:233:TYR:CZ	1:D:221:ILE:HD11	2.53	0.43
1:B:219:PHE:HA	1:B:315:GLY:O	2.17	0.43
1:C:284:LEU:HD23	1:C:284:LEU:HA	1.79	0.43
1:C:244:TYR:CZ	1:C:289:GLN:HB2	2.53	0.43
1:A:231:ILE:HD12	1:A:249:ILE:HG23	2.00	0.43
1:E:265:ARG:O	1:E:268:ASP:HB2	2.17	0.43
1:E:334:ILE:HA	1:E:334:ILE:HD13	1.92	0.43
1:D:304:ARG:HD3	1:D:310:ILE:HG12	2.01	0.43
1:D:206:TYR:HA	1:D:209:VAL:HG12	2.01	0.43
1:C:222:THR:OG1	1:C:313:TYR:HB2	2.19	0.42
1:C:253:ASN:HD22	1:C:255:ARG:HG2	1.84	0.42
1:C:216:GLN:HE22	1:D:207:SER:HB3	1.84	0.42
1:D:298:PHE:CE1	1:D:300:VAL:HG13	2.53	0.42
1:B:309:ASN:HD21	1:C:276:LYS:NZ	2.17	0.42
1:B:263:ASP:HA	1:B:264:PRO:HD2	1.88	0.42
1:F:266:ALA:HA	1:F:269:LYS:HD2	2.00	0.42
1:C:311:VAL:HG13	1:D:217:GLN:NE2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:246:LEU:HD13	1:E:246:LEU:C	2.39	0.42
1:A:268:ASP:OD1	1:A:271:ARG:NH2	2.53	0.42
1:D:263:ASP:HA	1:D:264:PRO:HD2	1.90	0.42
1:C:246:LEU:O	1:C:246:LEU:HD23	2.15	0.42
1:D:208:LEU:O	1:D:212:LEU:HG	2.18	0.42
1:D:210:LYS:HD3	1:D:210:LYS:O	2.19	0.42
1:D:231:ILE:HD11	1:D:249:ILE:HG21	1.94	0.42
1:E:208:LEU:HD13	1:E:303:LEU:HD11	2.02	0.42
1:B:272:ASN:HD21	1:B:276:LYS:HZ2	1.67	0.42
1:C:216:GLN:O	1:C:216:GLN:HG2	2.19	0.42
1:B:278:VAL:HG11	1:C:304:ARG:HD2	2.02	0.42
1:D:226:LEU:HD22	1:D:226:LEU:N	2.35	0.42
1:E:238:PHE:CE2	1:E:249:ILE:HD13	2.37	0.42
1:D:215:ALA:HB1	1:D:316:VAL:CG1	2.49	0.42
1:E:204:PRO:HB2	1:E:206:TYR:CE2	2.55	0.41
1:E:203:ASP:HA	1:E:204:PRO:HD3	1.94	0.41
1:C:221:ILE:HG12	1:C:233:TYR:HB3	2.02	0.41
1:B:247:ASP:N	1:B:247:ASP:OD1	2.53	0.41
1:F:222:THR:HB	1:F:229:ASN:ND2	2.35	0.41
1:A:283:CYS:HA	1:A:296:ASN:O	2.20	0.41
1:F:265:ARG:O	1:F:269:LYS:HD2	2.20	0.41
1:B:270:ILE:HD12	1:B:284:LEU:HD11	2.03	0.41
1:D:231:ILE:HG23	1:D:252:ARG:O	2.20	0.41
1:E:322:GLU:O	1:E:326:LYS:HG3	2.21	0.41
1:E:328:LEU:O	1:E:332:GLN:HG3	2.20	0.41
1:E:201:LEU:HD23	1:E:202:GLU:OE2	2.21	0.41
1:E:199:ARG:N	1:E:200:ILE:HG13	2.35	0.41
1:C:244:TYR:CE1	1:C:289:GLN:HB2	2.56	0.41
1:A:231:ILE:CD1	1:A:249:ILE:HG23	2.51	0.41
1:B:334:ILE:HG12	1:D:319:LYS:HE2	2.03	0.41
1:E:199:ARG:HE	1:F:208:LEU:HD21	1.86	0.41
1:C:288:ARG:HD2	1:C:292:THR:CG2	2.51	0.41
1:E:209:VAL:HG21	1:F:299:PHE:HE1	1.87	0.40
1:E:203:ASP:OD1	1:F:299:PHE:CE2	2.74	0.40
1:B:231:ILE:HD13	1:B:249:ILE:CG2	2.48	0.40
1:B:323:ASP:N	1:B:323:ASP:OD1	2.51	0.40
1:D:253:ASN:O	1:D:256:PHE:CD2	2.75	0.40
1:D:261:GLU:HG2	1:D:287:TYR:OH	2.22	0.40

There are no symmetry-related clashes.

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	133/166 (80%)	132 (99%)	1 (1%)	0	100 100
1	B	126/166 (76%)	121 (96%)	4 (3%)	1 (1%)	24 55
1	C	118/166 (71%)	117 (99%)	1 (1%)	0	100 100
1	D	128/166 (77%)	124 (97%)	4 (3%)	0	100 100
1	E	136/166 (82%)	134 (98%)	2 (2%)	0	100 100
1	F	125/166 (75%)	121 (97%)	4 (3%)	0	100 100
All	All	766/996 (77%)	749 (98%)	16 (2%)	1 (0%)	56 86

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	227	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	118/145 (81%)	107 (91%)	11 (9%)	11 29
1	B	111/145 (77%)	102 (92%)	9 (8%)	15 36
1	C	105/145 (72%)	92 (88%)	13 (12%)	6 15
1	D	113/145 (78%)	101 (89%)	12 (11%)	8 22
1	E	121/145 (83%)	109 (90%)	12 (10%)	10 25
1	F	110/145 (76%)	100 (91%)	10 (9%)	12 30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	678/870 (78%)	611 (90%)	67 (10%)	10 25

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	GLU
1	A	203	ASP
1	A	210	LYS
1	A	229	ASN
1	A	248	GLN
1	A	275	THR
1	A	278	VAL
1	A	284	LEU
1	A	298	PHE
1	A	311	VAL
1	A	334	ILE
1	B	210	LYS
1	B	229	ASN
1	B	246	LEU
1	B	248	GLN
1	B	249	ILE
1	B	300	VAL
1	B	314	VAL
1	B	326	LYS
1	B	334	ILE
1	C	217	GLN
1	C	226	LEU
1	C	231	ILE
1	C	246	LEU
1	C	247	ASP
1	C	248	GLN
1	C	249	ILE
1	C	265	ARG
1	C	284	LEU
1	C	298	PHE
1	C	300	VAL
1	C	306	SER
1	C	334	ILE
1	D	217	GLN
1	D	218	ASN
1	D	231	ILE
1	D	246	LEU

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Mol	Chain	Res	Type
1	D	247	ASP
1	D	249	ILE
1	D	298	PHE
1	D	300	VAL
1	D	303	LEU
1	D	306	SER
1	D	307	LYS
1	D	311	VAL
1	E	201	LEU
1	E	214	MET
1	E	229	ASN
1	E	236	ARG
1	E	247	ASP
1	E	248	GLN
1	E	249	ILE
1	E	269	LYS
1	E	275	THR
1	E	284	LEU
1	E	298	PHE
1	E	336	TYR
1	F	208	LEU
1	F	213	GLN
1	F	229	ASN
1	F	247	ASP
1	F	248	GLN
1	F	252	ARG
1	F	284	LEU
1	F	300	VAL
1	F	314	VAL
1	F	326	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	ASN
1	A	330	ASN
1	A	332	GLN
1	B	229	ASN
1	B	272	ASN
1	B	309	ASN
1	C	216	GLN
1	C	217	GLN

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Mol	Chain	Res	Type
1	C	253	ASN
1	C	309	ASN
1	C	312	ASN
1	D	217	GLN
1	D	253	ASN
1	E	229	ASN
1	E	272	ASN
1	E	330	ASN
1	E	332	GLN
1	F	229	ASN
1	F	272	ASN
1	F	309	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	FMN	A	500	-	32,33,33	1.21	2 (6%)	34,50,50	1.75	6 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	FMN	B	401	-	32,33,33	1.22	3 (9%)	34,50,50	1.70	6 (17%)
3	PO4	B	402	-	4,4,4	0.72	0	6,6,6	0.24	0
2	FMN	C	500	-	32,33,33	1.20	3 (9%)	34,50,50	1.64	5 (14%)
2	FMN	D	500	-	32,33,33	1.19	3 (9%)	34,50,50	1.69	5 (14%)
2	FMN	E	500	-	32,33,33	1.21	4 (12%)	34,50,50	1.67	5 (14%)
2	FMN	F	401	-	32,33,33	1.19	3 (9%)	34,50,50	1.67	6 (17%)
3	PO4	F	402	-	4,4,4	0.70	0	6,6,6	0.23	0

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	FMN	A	500	-	-	0/18/18/18	0/3/3/3
2	FMN	B	401	-	-	0/18/18/18	0/3/3/3
3	PO4	B	402	-	-	0/0/0/0	0/0/0/0
2	FMN	C	500	-	-	0/18/18/18	0/3/3/3
2	FMN	D	500	-	-	0/18/18/18	0/3/3/3
2	FMN	E	500	-	-	0/18/18/18	0/3/3/3
2	FMN	F	401	-	-	0/18/18/18	0/3/3/3
3	PO4	F	402	-	-	0/0/0/0	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	FMN	C1'-N10	2.00	1.50	1.48
2	F	401	FMN	C5A-N5	2.02	1.38	1.35
2	B	401	FMN	C1'-N10	2.02	1.50	1.48
2	E	500	FMN	C1'-N10	2.04	1.50	1.48
2	C	500	FMN	C5A-N5	2.09	1.38	1.35
2	E	500	FMN	C5A-N5	2.13	1.38	1.35
2	A	500	FMN	C4-N3	2.81	1.38	1.33
2	B	401	FMN	C4-N3	2.96	1.38	1.33
2	E	500	FMN	C4-N3	2.99	1.38	1.33
2	D	500	FMN	C4-N3	3.01	1.38	1.33
2	C	500	FMN	C4-N3	3.07	1.38	1.33
2	F	401	FMN	C4-N3	3.14	1.38	1.33
2	F	401	FMN	C4A-N5	3.15	1.38	1.33
2	D	500	FMN	C4A-N5	3.40	1.38	1.33
2	E	500	FMN	C4A-N5	3.50	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	FMN	C4A-N5	3.51	1.38	1.33
2	B	401	FMN	C4A-N5	3.60	1.38	1.33
2	A	500	FMN	C4A-N5	3.63	1.38	1.33

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	FMN	N3-C2-N1	-4.64	119.87	127.69
2	B	401	FMN	N3-C2-N1	-4.58	119.97	127.69
2	E	500	FMN	N3-C2-N1	-4.53	120.07	127.69
2	F	401	FMN	N3-C2-N1	-4.53	120.07	127.69
2	C	500	FMN	N3-C2-N1	-4.51	120.10	127.69
2	D	500	FMN	N3-C2-N1	-4.48	120.15	127.69
2	B	401	FMN	C4A-C4-N3	-2.97	119.64	123.52
2	A	500	FMN	C4A-C4-N3	-2.85	119.80	123.52
2	F	401	FMN	C4A-C4-N3	-2.79	119.88	123.52
2	E	500	FMN	C4A-C4-N3	-2.72	119.97	123.52
2	D	500	FMN	C4A-C4-N3	-2.71	119.98	123.52
2	C	500	FMN	C4A-C4-N3	-2.52	120.22	123.52
2	B	401	FMN	C1'-N10-C9A	2.13	121.29	118.83
2	F	401	FMN	C1'-N10-C9A	2.24	121.43	118.83
2	A	500	FMN	C1'-N10-C9A	2.42	121.63	118.83
2	F	401	FMN	C5A-C9A-N10	2.51	119.46	117.58
2	A	500	FMN	C5A-C9A-N10	2.53	119.47	117.58
2	E	500	FMN	C5A-C9A-N10	2.62	119.54	117.58
2	B	401	FMN	C4A-N5-C5A	2.63	119.82	116.72
2	C	500	FMN	C5A-C9A-N10	2.72	119.62	117.58
2	F	401	FMN	C4A-N5-C5A	2.74	119.95	116.72
2	B	401	FMN	C5A-C9A-N10	2.83	119.70	117.58
2	E	500	FMN	C4A-N5-C5A	2.91	120.15	116.72
2	A	500	FMN	C4A-N5-C5A	3.02	120.28	116.72
2	D	500	FMN	C4A-N5-C5A	3.18	120.47	116.72
2	C	500	FMN	C4A-N5-C5A	3.21	120.51	116.72
2	D	500	FMN	C5A-C9A-N10	3.33	120.07	117.58
2	C	500	FMN	C4-N3-C2	5.75	119.95	115.16
2	D	500	FMN	C4-N3-C2	5.86	120.05	115.16
2	E	500	FMN	C4-N3-C2	5.99	120.15	115.16
2	F	401	FMN	C4-N3-C2	6.08	120.23	115.16
2	B	401	FMN	C4-N3-C2	6.16	120.30	115.16
2	A	500	FMN	C4-N3-C2	6.32	120.43	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	500	FMN	2	0
2	E	500	FMN	1	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^{th} 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^2)	Q<0.9
1	A	135/166 (81%)	0.17	2 (1%)	76	72	60, 76, 112, 166	0
1	B	128/166 (77%)	0.29	3 (2%)	64	57	60, 81, 145, 191	0
1	C	120/166 (72%)	0.29	3 (2%)	61	54	81, 109, 141, 169	0
1	D	130/166 (78%)	0.28	5 (3%)	44	37	88, 112, 142, 163	0
1	E	138/166 (83%)	0.29	8 (5%)	26	20	57, 76, 126, 195	0
1	F	127/166 (76%)	0.16	3 (2%)	62	56	62, 81, 122, 183	0
All	All	778/996 (78%)	0.25	24 (3%)	52	46	57, 89, 142, 195	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	209	VAL	6.7
1	B	212	LEU	5.7
1	E	249	ILE	5.0
1	D	320	VAL	4.2
1	A	249	ILE	3.5
1	D	294	PHE	3.5
1	B	208	LEU	3.3
1	C	249	ILE	3.2
1	E	199	ARG	3.2
1	E	203	ASP	3.0
1	E	201	LEU	3.0
1	F	212	LEU	2.7
1	F	249	ILE	2.4
1	E	204	PRO	2.4
1	A	205	ASP	2.3
1	D	238	PHE	2.2
1	E	200	ILE	2.2
1	D	319	LYS	2.2
1	E	206	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	241	LEU	2.1
1	E	270	ILE	2.1
1	F	209	VAL	2.0
1	C	294	PHE	2.0
1	D	270	ILE	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^{th} 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	PO4	F	402	5/5	0.90	0.24	1.53	132,139,142,144	0
2	FMN	B	401	31/31	0.97	0.18	-0.20	59,75,84,87	0
3	PO4	B	402	5/5	0.82	0.19	-0.22	152,153,158,164	0
2	FMN	A	500	31/31	0.97	0.18	-0.23	61,74,82,86	0
2	FMN	D	500	31/31	0.91	0.18	-0.39	81,107,136,137	0
2	FMN	E	500	31/31	0.97	0.18	-0.39	57,74,87,90	0
2	FMN	F	401	31/31	0.97	0.18	-0.41	63,76,82,86	0
2	FMN	C	500	31/31	0.91	0.17	-0.56	83,106,131,133	0

6.5 Other polymers (i)

There are no such residues in this entry.