



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:38 PM GMT

PDB ID : 3ULF
Title : The light state structure of the blue-light photoreceptor Aureochrome1 LOV
Authors : Mitra, D.; Yang, X.; Moffat, K.
Deposited on : 2011-11-10
Resolution : 2.90 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 ⓘ symbol.

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

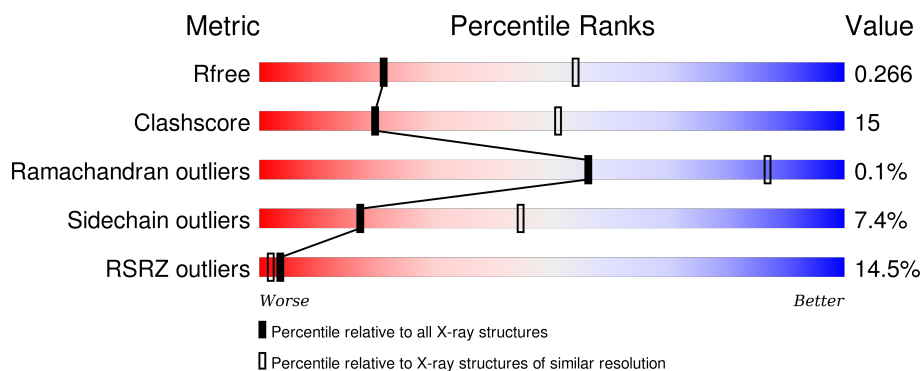
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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 $\leq 5\%$. 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	170	<div> <div>3%</div> <div>59%</div> <div>18%</div> <div>•</div> <div>21%</div> </div>
1	B	170	<div> <div>49%</div> <div>24%</div> <div>•</div> <div>25%</div> </div>
1	C	170	<div> <div>31%</div> <div>48%</div> <div>21%</div> <div>•</div> <div>29%</div> </div>
1	D	170	<div> <div>29%</div> <div>49%</div> <div>22%</div> <div>5%</div> <div>24%</div> </div>
1	E	170	<div> <div>3%</div> <div>53%</div> <div>25%</div> <div>•</div> <div>21%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	170	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FMN	C	501	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6370 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	129	Total	C	N	O	S	0	0	0
			1014	643	175	193	3			
1	E	135	Total	C	N	O	S	0	0	0
			1067	675	181	208	3			
1	F	127	Total	C	N	O	S	0	1	0
			1003	636	174	190	3			

There are 48 discrepancies between the modelled and reference sequences:

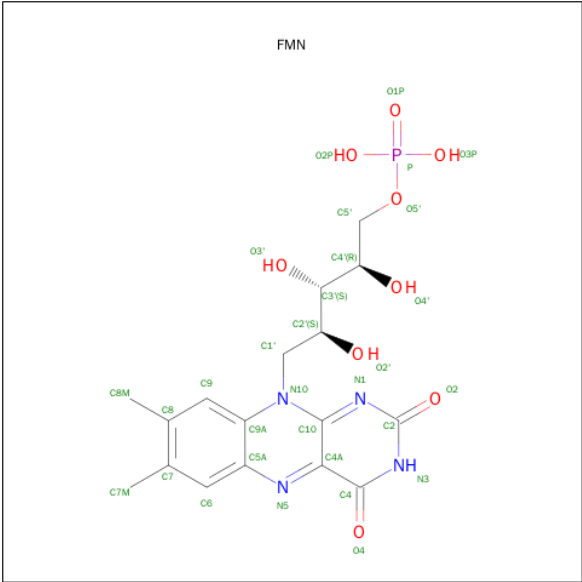
Chain	Residue	Modelled	Actual	Comment	Reference
A	168	GLY	-	EXPRESSION TAG	UNP A8QW55
A	169	SER	-	EXPRESSION TAG	UNP A8QW55
A	170	HIS	-	EXPRESSION TAG	UNP A8QW55
A	171	MET	-	EXPRESSION TAG	UNP A8QW55
A	172	GLY	-	EXPRESSION TAG	UNP A8QW55
A	173	HIS	-	EXPRESSION TAG	UNP A8QW55
A	174	SER	-	EXPRESSION TAG	UNP A8QW55
A	175	MET	-	EXPRESSION TAG	UNP A8QW55
B	168	GLY	-	EXPRESSION TAG	UNP A8QW55
B	169	SER	-	EXPRESSION TAG	UNP A8QW55
B	170	HIS	-	EXPRESSION TAG	UNP A8QW55
B	171	MET	-	EXPRESSION TAG	UNP A8QW55
B	172	GLY	-	EXPRESSION TAG	UNP A8QW55
B	173	HIS	-	EXPRESSION TAG	UNP A8QW55
B	174	SER	-	EXPRESSION TAG	UNP A8QW55
B	175	MET	-	EXPRESSION TAG	UNP A8QW55
C	168	GLY	-	EXPRESSION TAG	UNP A8QW55

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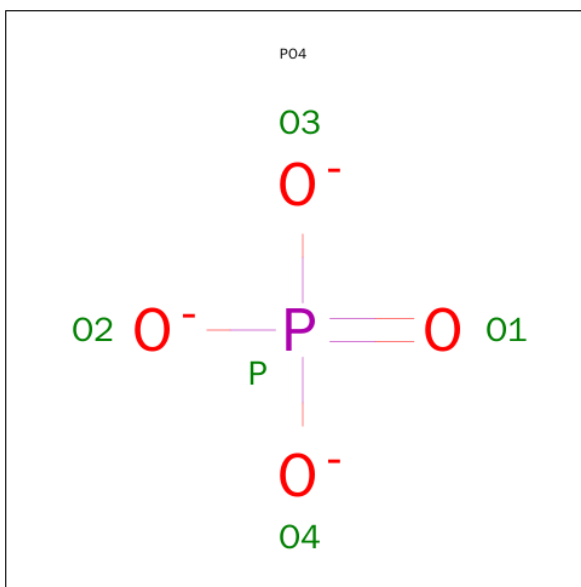
Chain	Residue	Modelled	Actual	Comment	Reference
C	169	SER	-	EXPRESSION TAG	UNP A8QW55
C	170	HIS	-	EXPRESSION TAG	UNP A8QW55
C	171	MET	-	EXPRESSION TAG	UNP A8QW55
C	172	GLY	-	EXPRESSION TAG	UNP A8QW55
C	173	HIS	-	EXPRESSION TAG	UNP A8QW55
C	174	SER	-	EXPRESSION TAG	UNP A8QW55
C	175	MET	-	EXPRESSION TAG	UNP A8QW55
D	168	GLY	-	EXPRESSION TAG	UNP A8QW55
D	169	SER	-	EXPRESSION TAG	UNP A8QW55
D	170	HIS	-	EXPRESSION TAG	UNP A8QW55
D	171	MET	-	EXPRESSION TAG	UNP A8QW55
D	172	GLY	-	EXPRESSION TAG	UNP A8QW55
D	173	HIS	-	EXPRESSION TAG	UNP A8QW55
D	174	SER	-	EXPRESSION TAG	UNP A8QW55
D	175	MET	-	EXPRESSION TAG	UNP A8QW55
E	168	GLY	-	EXPRESSION TAG	UNP A8QW55
E	169	SER	-	EXPRESSION TAG	UNP A8QW55
E	170	HIS	-	EXPRESSION TAG	UNP A8QW55
E	171	MET	-	EXPRESSION TAG	UNP A8QW55
E	172	GLY	-	EXPRESSION TAG	UNP A8QW55
E	173	HIS	-	EXPRESSION TAG	UNP A8QW55
E	174	SER	-	EXPRESSION TAG	UNP A8QW55
E	175	MET	-	EXPRESSION TAG	UNP A8QW55
F	168	GLY	-	EXPRESSION TAG	UNP A8QW55
F	169	SER	-	EXPRESSION TAG	UNP A8QW55
F	170	HIS	-	EXPRESSION TAG	UNP A8QW55
F	171	MET	-	EXPRESSION TAG	UNP A8QW55
F	172	GLY	-	EXPRESSION TAG	UNP A8QW55
F	173	HIS	-	EXPRESSION TAG	UNP A8QW55
F	174	SER	-	EXPRESSION TAG	UNP A8QW55
F	175	MET	-	EXPRESSION TAG	UNP A8QW55

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



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: O₄P).



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

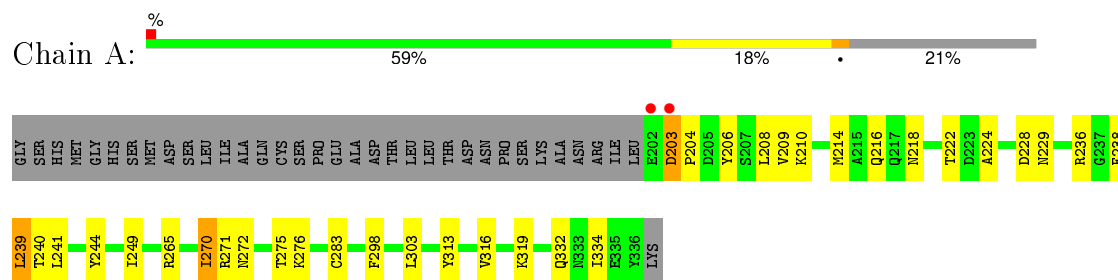
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total	O	0	0
			26	26		
4	B	19	Total	O	0	0
			19	19		
4	C	1	Total	O	0	0
			1	1		
4	E	14	Total	O	0	0
			14	14		
4	F	15	Total	O	0	0
			15	15		

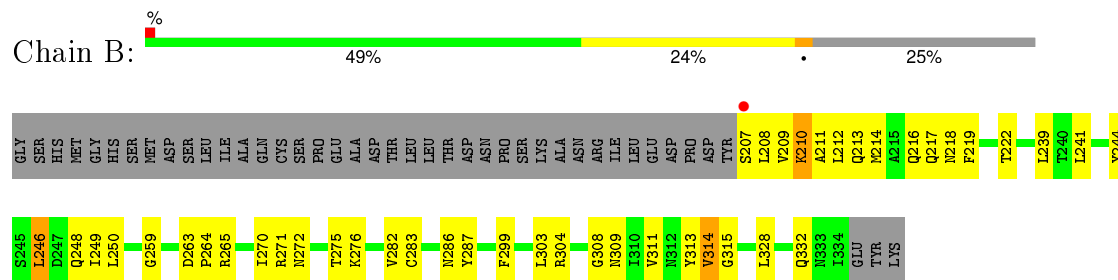
3 Residue-property plots [i](#)

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.

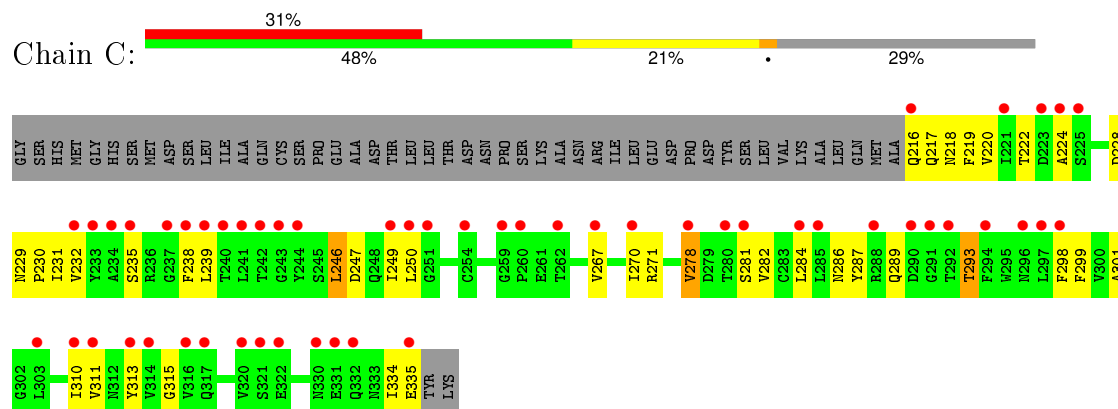
• Molecule 1: Aureochrome1



• Molecule 1: Aureochrome1

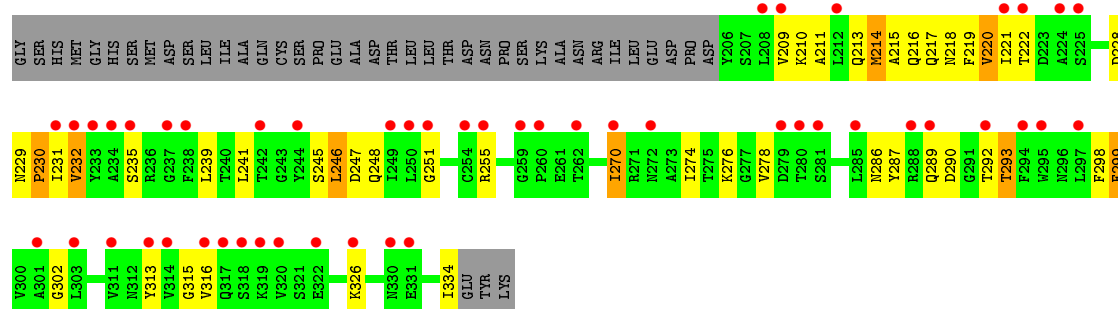


• Molecule 1: Aureochrome1

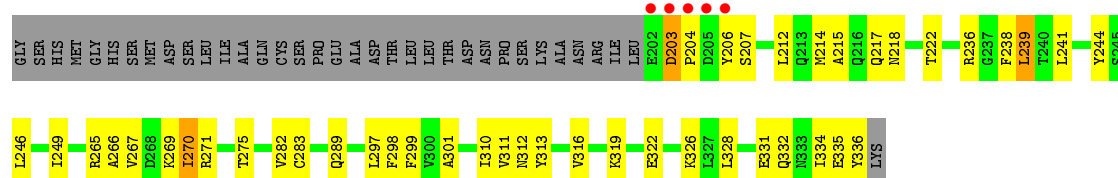


• Molecule 1: Aureochrome1

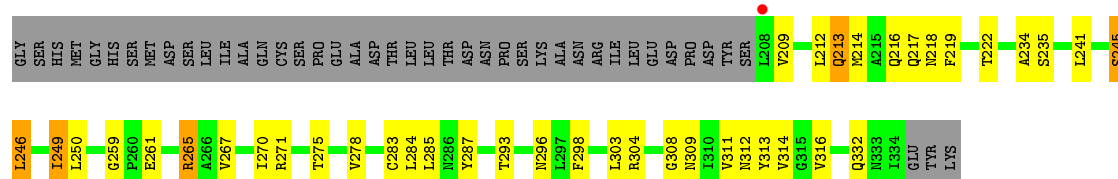




• Molecule 1: Aureochrome1



• Molecule 1: Aureochrome1



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	73.98Å 73.98Å 176.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.10 – 2.90 34.11 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.4 (34.10-2.90) 99.4 (34.11-2.89)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.201 , 0.264 0.199 , 0.266	Depositor DCC
R_{free} test set	1074 reflections (5.43%)	DCC
Wilson B-factor (Å ²)	74.4	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 71.3	EDS
Estimated twinning fraction	0.479 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	2 of 20965 reflections (0.010%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6370	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, 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	0.24	0/1086	0.42	0/1475
1	B	0.24	0/1018	0.45	0/1381
1	C	0.22	0/962	0.40	0/1306
1	D	0.22	0/1031	0.40	0/1399
1	E	0.24	0/1086	0.42	0/1475
1	F	0.24	0/1019	0.43	0/1383
All	All	0.23	0/6202	0.42	0/8419

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 [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	1067	0	1048	31	0
1	B	1002	0	1003	41	0
1	C	946	0	933	30	0
1	D	1014	0	1012	37	0
1	E	1067	0	1048	38	0
1	F	1003	0	1006	36	0
2	A	31	0	19	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	31	0	19	2	0
2	C	31	0	19	2	0
2	D	31	0	19	3	0
2	E	31	0	19	1	0
2	F	31	0	19	6	0
3	B	5	0	0	0	0
3	F	5	0	0	0	0
4	A	26	0	0	0	0
4	B	19	0	0	0	0
4	C	1	0	0	0	0
4	E	14	0	0	0	0
4	F	15	0	0	0	0
All	All	6370	0	6164	185	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 15.

All (185) 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:A:283:CYS:H	1:A:332:GLN:HE22	1.07	0.98
1:C:222:THR:HG22	1:C:231:ILE:HG22	1.58	0.83
1:E:212:LEU:HD13	1:F:314:VAL:HG21	1.61	0.82
1:E:283:CYS:H	1:E:332:GLN:HE22	1.24	0.82
1:D:215:ALA:HB2	1:D:316:VAL:HG13	1.62	0.80
1:A:283:CYS:N	1:A:332:GLN:HE22	1.81	0.78
1:E:206:TYR:HB3	1:F:216:GLN:OE1	1.85	0.77
1:B:283:CYS:H	1:B:332:GLN:HE22	1.32	0.76
1:B:272:ASN:HD21	1:B:276:LYS:NZ	1.83	0.76
1:F:283:CYS:H	1:F:332:GLN:HE22	1.31	0.74
1:A:208:LEU:H	1:B:216:GLN:HE22	1.36	0.73
1:B:210:LYS:HD2	1:B:211:ALA:N	2.08	0.69
1:D:222:THR:HG22	1:D:231:ILE:HG22	1.75	0.69
1:F:218:ASN:HD22	1:F:241:LEU:HD22	1.59	0.68
1:D:270:ILE:HD13	1:D:298:PHE:HZ	1.60	0.67
1:C:219:PHE:CE2	1:C:235:SER:HB3	2.30	0.67
1:D:222:THR:OG1	1:D:313:TYR:HB2	1.95	0.66
1:B:207:SER:HA	1:B:210:LYS:HE3	1.78	0.66
1:B:212:LEU:HD13	1:E:331:GLU:HG3	1.78	0.66
1:C:239:LEU:HD13	1:C:246:LEU:HD12	1.79	0.65
1:A:204:PRO:HA	1:B:210:LYS:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:LEU:CD1	1:F:314:VAL:HG21	2.27	0.65
1:D:211:ALA:O	1:D:316:VAL:HG21	1.98	0.64
1:E:207:SER:HB3	1:F:216:GLN:HE22	1.61	0.64
1:B:272:ASN:HD21	1:B:276:LYS:HZ3	1.43	0.64
1:E:265:ARG:HD3	1:E:336:TYR:CZ	2.32	0.64
1:C:222:THR:OG1	1:C:313:TYR:HB2	1.98	0.64
1:C:267:VAL:HG13	2:C:501:FMN:H5'2	1.80	0.63
1:F:245:SER:O	1:F:249:ILE:HG23	1.99	0.63
1:B:218:ASN:HD22	1:B:241:LEU:HD22	1.63	0.63
1:F:267:VAL:HG13	2:F:501:FMN:H5'2	1.78	0.63
1:B:246:LEU:HD22	1:B:250:LEU:HG	1.81	0.63
1:A:271:ARG:O	1:A:275:THR:HG23	1.99	0.63
1:D:219:PHE:CE2	1:D:235:SER:HB3	2.34	0.62
1:E:271:ARG:O	1:E:275:THR:HG23	2.00	0.62
1:E:217:GLN:HE22	1:F:312:ASN:HB2	1.64	0.61
1:D:217:GLN:O	1:D:217:GLN:HG3	2.01	0.60
1:D:276:LYS:HB3	1:F:304:ARG:HH12	1.67	0.60
1:D:248:GLN:HE22	1:D:289:GLN:NE2	1.99	0.60
1:E:222:THR:OG1	1:E:313:TYR:HB2	2.02	0.60
1:B:308:GLY:HA3	1:C:278:VAL:HG11	1.85	0.59
1:C:287:TYR:CE2	1:C:293:THR:HG22	2.37	0.59
1:A:204:PRO:HA	1:B:210:LYS:CB	2.32	0.59
1:E:270:ILE:HD13	1:E:298:PHE:HZ	1.68	0.58
1:D:229:ASN:N	1:D:230:PRO:HD3	2.18	0.58
1:C:301:ALA:HB3	1:D:209:VAL:HG21	1.86	0.58
1:A:206:TYR:OH	1:B:213:GLN:HG2	2.03	0.57
1:E:266:ALA:O	1:E:269:LYS:HB3	2.05	0.57
1:C:222:THR:HA	1:C:231:ILE:HA	1.87	0.57
1:D:278:VAL:HG11	1:F:308:GLY:HA3	1.86	0.57
1:A:283:CYS:H	1:A:332:GLN:NE2	1.89	0.57
1:C:267:VAL:HG12	1:C:271:ARG:HH12	1.70	0.57
1:C:270:ILE:HD13	1:C:298:PHE:HZ	1.68	0.57
1:F:271:ARG:HD3	2:F:501:FMN:O3P	2.05	0.56
1:A:222:THR:OG1	1:A:313:TYR:HB2	2.04	0.56
1:F:313:TYR:HB3	2:F:501:FMN:HM71	1.89	0.55
1:D:218:ASN:HD22	1:D:241:LEU:HD22	1.72	0.55
1:F:259:GLY:HA3	1:F:287:TYR:CE1	2.42	0.54
1:E:322:GLU:O	1:E:326:LYS:HG3	2.07	0.54
1:F:304:ARG:HA	1:F:309:ASN:O	2.07	0.54
1:E:218:ASN:HD21	1:E:241:LEU:HD22	1.73	0.53
1:E:265:ARG:HD3	1:E:336:TYR:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:222:THR:OG1	1:F:313:TYR:HB2	2.09	0.53
1:A:270:ILE:HD13	1:A:298:PHE:HZ	1.74	0.53
1:F:246:LEU:HD22	1:F:250:LEU:HG	1.91	0.52
1:F:213:GLN:HE21	1:F:214:MET:N	2.08	0.52
1:A:272:ASN:HD21	1:A:276:LYS:HE3	1.73	0.52
1:D:215:ALA:HB2	1:D:316:VAL:CG1	2.38	0.52
1:D:245:SER:H	1:D:248:GLN:HB2	1.74	0.52
1:B:213:GLN:HE22	1:B:299:PHE:HB2	1.76	0.51
1:C:270:ILE:HG23	1:C:282:VAL:HG21	1.93	0.51
1:E:283:CYS:N	1:E:332:GLN:HE22	2.02	0.50
1:F:271:ARG:O	1:F:275:THR:HG23	2.11	0.50
1:F:285:LEU:HD11	1:F:293:THR:HB	1.92	0.50
1:D:228:ASP:HB3	1:D:230:PRO:HD3	1.94	0.50
1:A:238:PHE:HE2	1:A:249:ILE:HD13	1.75	0.50
1:C:249:ILE:O	1:C:249:ILE:HG22	2.12	0.49
1:D:287:TYR:CE2	1:D:293:THR:HG22	2.48	0.49
1:B:271:ARG:O	1:B:275:THR:HG23	2.12	0.49
1:A:208:LEU:HD13	1:A:303:LEU:HD11	1.94	0.49
1:E:270:ILE:HD12	2:E:501:FMN:H4'	1.95	0.49
1:D:274:ILE:HD11	2:D:501:FMN:O3'	2.13	0.49
1:B:270:ILE:HG21	1:B:282:VAL:HG11	1.95	0.49
1:D:230:PRO:HB3	1:D:251:GLY:O	2.12	0.49
1:D:302:GLY:HA2	1:D:313:TYR:HA	1.96	0.48
1:B:217:GLN:HG2	1:B:218:ASN:OD1	2.14	0.48
1:E:238:PHE:HE2	1:E:249:ILE:HD13	1.79	0.48
1:D:315:GLY:HA3	2:D:501:FMN:HM73	1.96	0.47
1:D:290:ASP:OD2	1:D:292:THR:HG22	2.15	0.47
1:D:334:ILE:HD12	1:E:319:LYS:HD2	1.97	0.47
1:C:219:PHE:CD2	1:C:235:SER:HB3	2.50	0.47
1:A:319:LYS:NZ	1:C:334:ILE:HG23	2.29	0.47
1:E:269:LYS:NZ	1:E:335:GLU:OE1	2.46	0.47
1:D:239:LEU:CD1	1:D:246:LEU:HD12	2.45	0.47
1:A:218:ASN:HD21	1:A:241:LEU:HD22	1.79	0.46
1:C:310:ILE:HG21	1:C:313:TYR:CZ	2.50	0.46
1:C:334:ILE:O	1:C:335:GLU:HB3	2.15	0.46
1:A:270:ILE:HD12	2:A:501:FMN:H4'	1.97	0.46
1:E:244:TYR:HB2	1:E:249:ILE:HD11	1.98	0.46
1:F:267:VAL:CG1	2:F:501:FMN:H5'2	2.44	0.46
1:C:219:PHE:HA	1:C:315:GLY:O	2.15	0.46
1:F:270:ILE:HD12	2:F:501:FMN:H1'2	1.97	0.46
1:D:316:VAL:HG12	1:D:316:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:LEU:H	1:B:216:GLN:NE2	2.10	0.45
1:A:238:PHE:CE2	1:A:249:ILE:HD13	2.51	0.45
1:D:315:GLY:CA	2:D:501:FMN:HM73	2.47	0.45
1:B:244:TYR:HB3	1:B:248:GLN:HG3	1.98	0.45
1:C:228:ASP:HB3	1:C:230:PRO:HD3	1.97	0.45
1:B:304:ARG:HA	1:B:309:ASN:O	2.16	0.45
1:C:247:ASP:O	1:C:250:LEU:HG	2.16	0.45
1:A:203:ASP:HA	1:A:204:PRO:HD3	1.69	0.45
1:F:209:VAL:HA	1:F:212:LEU:HD13	1.99	0.45
1:E:270:ILE:HG23	1:E:282:VAL:CG2	2.47	0.44
1:B:272:ASN:HD21	1:B:276:LYS:HZ2	1.62	0.44
1:A:206:TYR:HE1	1:B:214:MET:HA	1.82	0.44
1:F:219:PHE:CE2	1:F:235:SER:HB3	2.52	0.44
1:A:209:VAL:HG11	1:B:299:PHE:HE1	1.81	0.44
1:D:219:PHE:O	1:D:220:VAL:HG13	2.17	0.44
1:B:286:ASN:HD22	1:B:286:ASN:HA	1.61	0.44
1:E:206:TYR:HE1	1:F:214:MET:HB2	1.83	0.44
1:A:298:PHE:HA	1:A:316:VAL:O	2.18	0.44
1:E:297:LEU:HD22	1:E:328:LEU:HD11	2.00	0.44
1:B:209:VAL:O	1:B:213:GLN:HB2	2.18	0.44
1:C:281:SER:O	1:C:282:VAL:HG23	2.18	0.43
1:B:328:LEU:O	1:B:332:GLN:HG3	2.18	0.43
1:F:213:GLN:HE21	1:F:213:GLN:C	2.20	0.43
1:E:267:VAL:O	1:E:270:ILE:HG13	2.18	0.43
1:B:222:THR:OG1	1:B:313:TYR:HB2	2.19	0.43
1:F:265:ARG:HH11	1:F:265:ARG:HB2	1.83	0.43
1:D:210:LYS:O	1:D:214:MET:HG2	2.19	0.43
1:A:236:ARG:O	1:A:240:THR:HG23	2.18	0.43
1:B:239:LEU:HD22	1:B:249:ILE:HD12	1.99	0.43
1:C:270:ILE:HD13	1:C:298:PHE:CZ	2.51	0.43
1:D:209:VAL:HG13	1:D:210:LYS:N	2.33	0.43
1:C:281:SER:OG	1:C:299:PHE:HD2	2.01	0.43
1:E:206:TYR:CE1	1:F:214:MET:HB2	2.54	0.43
1:F:217:GLN:HG2	1:F:218:ASN:OD1	2.17	0.43
1:E:282:VAL:HA	1:E:332:GLN:NE2	2.33	0.42
1:A:206:TYR:HB3	1:B:216:GLN:NE2	2.34	0.42
1:E:212:LEU:O	1:E:215:ALA:HB3	2.19	0.42
1:D:211:ALA:HA	1:D:214:MET:CE	2.49	0.42
1:D:299:PHE:HB3	1:D:316:VAL:HB	2.00	0.42
1:D:221:ILE:HG13	1:D:232:VAL:HG23	2.01	0.42
1:D:278:VAL:HB	1:F:304:ARG:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:303:LEU:HD11	1:F:314:VAL:HG23	2.00	0.42
1:C:315:GLY:N	2:C:501:FMN:HM73	2.34	0.42
1:F:271:ARG:HB2	2:F:501:FMN:C5'	2.50	0.42
1:A:271:ARG:HD3	2:A:501:FMN:O3P	2.19	0.42
1:C:301:ALA:CB	1:D:209:VAL:HG21	2.49	0.42
1:F:298:PHE:HA	1:F:316:VAL:O	2.20	0.42
1:E:270:ILE:HG23	1:E:282:VAL:HG21	2.02	0.42
1:C:219:PHE:CD1	1:C:219:PHE:C	2.93	0.42
1:E:217:GLN:NE2	1:F:312:ASN:HB2	2.33	0.42
1:D:216:GLN:O	1:D:217:GLN:HB3	2.20	0.42
1:E:311:VAL:HG13	1:E:312:ASN:OD1	2.20	0.42
1:C:224:ALA:HA	1:C:229:ASN:HD22	1.85	0.42
1:E:283:CYS:H	1:E:332:GLN:NE2	2.05	0.41
1:B:283:CYS:H	1:B:332:GLN:NE2	2.08	0.41
1:F:283:CYS:HA	1:F:296:ASN:O	2.20	0.41
1:D:222:THR:HA	1:D:231:ILE:HA	2.02	0.41
1:F:234:ALA:CB	1:F:249:ILE:HD11	2.50	0.41
1:B:313:TYR:HB3	2:B:501:FMN:HM71	2.03	0.41
1:E:334:ILE:HD13	1:E:334:ILE:HA	1.83	0.41
1:E:310:ILE:HG21	1:E:313:TYR:CZ	2.55	0.41
1:B:271:ARG:HD3	2:B:501:FMN:O3P	2.20	0.41
1:E:299:PHE:CE2	1:E:301:ALA:HB2	2.55	0.41
1:B:259:GLY:HA3	1:B:287:TYR:CE1	2.55	0.41
1:B:208:LEU:HD11	1:B:212:LEU:HD11	2.02	0.41
1:C:218:ASN:O	1:C:238:PHE:HD1	2.03	0.41
1:A:239:LEU:HD13	1:A:244:TYR:O	2.20	0.41
1:A:224:ALA:HA	1:A:229:ASN:HD22	1.86	0.41
1:B:303:LEU:HD11	1:B:314:VAL:HG22	2.02	0.41
1:A:206:TYR:CE1	1:B:214:MET:HA	2.56	0.41
1:C:219:PHE:CZ	1:C:235:SER:HB3	2.56	0.41
1:A:228:ASP:O	1:A:229:ASN:C	2.60	0.41
1:E:203:ASP:HA	1:E:204:PRO:HD3	1.71	0.41
1:A:206:TYR:OH	1:B:213:GLN:CG	2.69	0.40
1:A:206:TYR:HB2	1:A:209:VAL:HB	2.02	0.40
1:B:210:LYS:HD2	1:B:210:LYS:C	2.41	0.40
1:B:304:ARG:HD3	1:C:278:VAL:HB	2.03	0.40
1:B:219:PHE:HA	1:B:315:GLY:O	2.21	0.40
1:E:236:ARG:O	1:E:239:LEU:HB2	2.21	0.40
1:D:209:VAL:HG22	1:D:213:GLN:CD	2.41	0.40
1:E:298:PHE:HA	1:E:316:VAL:O	2.21	0.40
1:B:263:ASP:HA	1:B:264:PRO:HD2	1.92	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	133/170 (78%)	131 (98%)	2 (2%)	0	100	100
1	B	126/170 (74%)	117 (93%)	9 (7%)	0	100	100
1	C	118/170 (69%)	110 (93%)	8 (7%)	0	100	100
1	D	127/170 (75%)	116 (91%)	10 (8%)	1 (1%)	24	60
1	E	133/170 (78%)	129 (97%)	4 (3%)	0	100	100
1	F	126/170 (74%)	121 (96%)	5 (4%)	0	100	100
All	All	763/1020 (75%)	724 (95%)	38 (5%)	1 (0%)	56	87

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	230	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	118/148 (80%)	110 (93%)	8 (7%)	20	49
1	B	111/148 (75%)	106 (96%)	5 (4%)	34	70
1	C	105/148 (71%)	94 (90%)	11 (10%)	8	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	112/148 (76%)	101 (90%)	11 (10%)	10	30
1	E	118/148 (80%)	112 (95%)	6 (5%)	29	65
1	F	111/148 (75%)	102 (92%)	9 (8%)	15	39
All	All	675/888 (76%)	625 (93%)	50 (7%)	17	44

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	ASP
1	A	210	LYS
1	A	214	MET
1	A	216	GLN
1	A	239	LEU
1	A	265	ARG
1	A	270	ILE
1	A	334	ILE
1	B	210	LYS
1	B	246	LEU
1	B	265	ARG
1	B	311	VAL
1	B	314	VAL
1	C	216	GLN
1	C	217	GLN
1	C	220	VAL
1	C	232	VAL
1	C	246	LEU
1	C	278	VAL
1	C	284	LEU
1	C	286	ASN
1	C	289	GLN
1	C	293	THR
1	C	311	VAL
1	D	214	MET
1	D	220	VAL
1	D	232	VAL
1	D	246	LEU
1	D	247	ASP
1	D	255	ARG
1	D	270	ILE
1	D	286	ASN
1	D	293	THR

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Mol	Chain	Res	Type
1	D	299	PHE
1	D	326	LYS
1	E	203	ASP
1	E	214	MET
1	E	239	LEU
1	E	246	LEU
1	E	270	ILE
1	E	289	GLN
1	F	213	GLN
1	F	245	SER
1	F	246	LEU
1	F	249	ILE
1	F	261	GLU
1	F	265	ARG
1	F	278	VAL
1	F	284	LEU
1	F	311	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	GLN
1	A	229	ASN
1	A	272	ASN
1	A	330	ASN
1	A	332	GLN
1	B	213	GLN
1	B	216	GLN
1	B	229	ASN
1	B	272	ASN
1	B	332	GLN
1	C	217	GLN
1	C	229	ASN
1	C	317	GLN
1	D	217	GLN
1	D	218	ASN
1	D	289	GLN
1	E	216	GLN
1	E	217	GLN
1	E	229	ASN
1	E	272	ASN
1	E	309	ASN

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Mol	Chain	Res	Type
1	E	330	ASN
1	E	332	GLN
1	F	213	GLN
1	F	229	ASN
1	F	332	GLN

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	501	1	32,33,33	2.59	6 (18%)	34,50,50	4.00	8 (23%)
2	FMN	B	501	1	32,33,33	2.49	4 (12%)	34,50,50	4.25	7 (20%)
3	PO4	B	502	-	4,4,4	0.53	0	6,6,6	0.25	0
2	FMN	C	501	1	32,33,33	2.54	5 (15%)	34,50,50	4.38	7 (20%)
2	FMN	D	501	1	32,33,33	2.55	5 (15%)	34,50,50	4.30	7 (20%)
2	FMN	E	501	1	32,33,33	2.55	5 (15%)	34,50,50	4.17	7 (20%)
2	FMN	F	501	1	32,33,33	2.52	6 (18%)	34,50,50	3.97	7 (20%)
3	PO4	F	502	-	4,4,4	0.53	0	6,6,6	0.24	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	501	1	-	0/18/18/18	0/3/3/3
2	FMN	B	501	1	-	0/18/18/18	0/3/3/3
3	PO4	B	502	-	-	0/0/0/0	0/0/0/0
2	FMN	C	501	1	-	0/18/18/18	0/3/3/3
2	FMN	D	501	1	-	0/18/18/18	0/3/3/3
2	FMN	E	501	1	-	0/18/18/18	0/3/3/3
2	FMN	F	501	1	-	0/18/18/18	0/3/3/3
3	PO4	F	502	-	-	0/0/0/0	0/0/0/0

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	FMN	C5A-N5	2.05	1.38	1.35
2	A	501	FMN	C5A-N5	2.06	1.38	1.35
2	E	501	FMN	C1'-N10	2.10	1.50	1.48
2	F	501	FMN	C1'-N10	2.19	1.50	1.48
2	A	501	FMN	C1'-N10	2.27	1.50	1.48
2	D	501	FMN	C1'-N10	2.27	1.50	1.48
2	C	501	FMN	C1'-N10	2.65	1.51	1.48
2	B	501	FMN	C4-N3	2.80	1.38	1.33
2	F	501	FMN	C4-N3	2.92	1.38	1.33
2	A	501	FMN	C4-N3	2.94	1.38	1.33
2	C	501	FMN	C4-N3	2.96	1.38	1.33
2	E	501	FMN	C4-N3	2.97	1.38	1.33
2	D	501	FMN	C4-N3	2.99	1.38	1.33
2	B	501	FMN	C4-C4A	6.24	1.54	1.41
2	E	501	FMN	C4-C4A	6.30	1.54	1.41
2	F	501	FMN	C4-C4A	6.36	1.54	1.41
2	C	501	FMN	C4-C4A	6.42	1.54	1.41
2	D	501	FMN	C4-C4A	6.42	1.54	1.41
2	A	501	FMN	C4-C4A	6.53	1.54	1.41
2	F	501	FMN	C4A-C10	7.06	1.53	1.40
2	B	501	FMN	C4A-C10	7.06	1.53	1.40
2	E	501	FMN	C4A-C10	7.10	1.54	1.40
2	A	501	FMN	C4A-C10	7.19	1.54	1.40
2	D	501	FMN	C4A-C10	7.29	1.54	1.40
2	C	501	FMN	C4A-C10	7.32	1.54	1.40
2	C	501	FMN	C4A-N5	8.83	1.46	1.33
2	B	501	FMN	C4A-N5	8.94	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	FMN	C4A-N5	8.99	1.47	1.33
2	D	501	FMN	C4A-N5	9.00	1.47	1.33
2	E	501	FMN	C4A-N5	9.23	1.47	1.33
2	A	501	FMN	C4A-N5	9.36	1.47	1.33

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	FMN	C4-C4A-C10	-22.64	105.45	119.94
2	D	501	FMN	C4-C4A-C10	-22.27	105.69	119.94
2	B	501	FMN	C4-C4A-C10	-21.90	105.92	119.94
2	E	501	FMN	C4-C4A-C10	-20.71	106.69	119.94
2	A	501	FMN	C4-C4A-C10	-19.99	107.15	119.94
2	F	501	FMN	C4-C4A-C10	-19.76	107.30	119.94
2	E	501	FMN	C4-C4A-N5	-6.35	110.98	118.70
2	B	501	FMN	C4-C4A-N5	-6.23	111.12	118.70
2	C	501	FMN	C4-C4A-N5	-5.88	111.55	118.70
2	A	501	FMN	C4-C4A-N5	-5.18	112.39	118.70
2	F	501	FMN	C4-C4A-N5	-5.14	112.44	118.70
2	D	501	FMN	C4-C4A-N5	-5.09	112.50	118.70
2	F	501	FMN	C4A-C4-N3	-4.36	117.82	123.52
2	A	501	FMN	C4A-C4-N3	-4.31	117.89	123.52
2	C	501	FMN	N3-C2-N1	-4.20	120.62	127.69
2	D	501	FMN	N3-C2-N1	-4.18	120.66	127.69
2	E	501	FMN	N3-C2-N1	-4.04	120.88	127.69
2	E	501	FMN	C4A-C4-N3	-3.96	118.35	123.52
2	B	501	FMN	N3-C2-N1	-3.92	121.09	127.69
2	B	501	FMN	C4A-C4-N3	-3.88	118.45	123.52
2	F	501	FMN	N3-C2-N1	-3.85	121.20	127.69
2	A	501	FMN	N3-C2-N1	-3.83	121.25	127.69
2	C	501	FMN	C4A-C4-N3	-3.63	118.78	123.52
2	D	501	FMN	C4A-C4-N3	-3.55	118.88	123.52
2	E	501	FMN	C4A-C10-N10	-3.53	117.95	120.52
2	F	501	FMN	C4A-C10-N10	-2.86	118.44	120.52
2	C	501	FMN	C4A-C10-N10	-2.77	118.51	120.52
2	D	501	FMN	C4A-C10-N10	-2.63	118.61	120.52
2	B	501	FMN	C4A-C10-N10	-2.49	118.71	120.52
2	A	501	FMN	C4A-C10-N10	-2.41	118.77	120.52
2	A	501	FMN	C4A-N5-C5A	2.11	119.21	116.72
2	B	501	FMN	C5A-C9A-N10	3.30	120.05	117.58
2	C	501	FMN	C5A-C9A-N10	3.63	120.30	117.58
2	D	501	FMN	C5A-C9A-N10	3.90	120.50	117.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	501	FMN	C5A-C9A-N10	4.01	120.58	117.58
2	A	501	FMN	C5A-C9A-N10	4.06	120.62	117.58
2	E	501	FMN	C5A-C9A-N10	4.70	121.10	117.58
2	B	501	FMN	C4-N3-C2	6.08	120.23	115.16
2	C	501	FMN	C4-N3-C2	6.45	120.54	115.16
2	D	501	FMN	C4-N3-C2	6.46	120.55	115.16
2	E	501	FMN	C4-N3-C2	6.61	120.68	115.16
2	A	501	FMN	C4-N3-C2	6.92	120.93	115.16
2	F	501	FMN	C4-N3-C2	7.13	121.11	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FMN	2	0
2	B	501	FMN	2	0
2	C	501	FMN	2	0
2	D	501	FMN	3	0
2	E	501	FMN	1	0
2	F	501	FMN	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å ²)	Q<0.9
1	A	135/170 (79%)	0.12	2 (1%) 76 74	49, 67, 103, 178	0
1	B	128/170 (75%)	0.12	1 (0%) 87 86	49, 74, 153, 173	0
1	C	120/170 (70%)	2.06	53 (44%) 0 0	117, 169, 212, 222	0
1	D	129/170 (75%)	1.93	50 (38%) 0 0	108, 169, 217, 225	0
1	E	135/170 (79%)	0.17	5 (3%) 45 38	48, 65, 106, 188	0
1	F	127/170 (74%)	0.04	1 (0%) 87 86	49, 74, 125, 177	0
All	All	774/1020 (75%)	0.72	112 (14%) 3 2	48, 82, 200, 225	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	250	LEU	18.9
1	C	238	PHE	10.5
1	C	291	GLY	9.1
1	D	232	VAL	8.9
1	C	292	THR	8.8
1	D	280	THR	7.3
1	D	294	PHE	6.6
1	D	234	ALA	6.3
1	C	221	ILE	6.2
1	C	240	THR	5.9
1	D	260	PRO	5.9
1	C	280	THR	5.8
1	C	239	LEU	5.8
1	D	259	GLY	5.8
1	E	204	PRO	5.7
1	D	249	ILE	5.7
1	C	294	PHE	5.6
1	C	232	VAL	5.5
1	C	285	LEU	5.4

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Mol	Chain	Res	Type	RSRZ
1	C	260	PRO	5.4
1	C	259	GLY	5.1
1	D	285	LEU	5.1
1	C	224	ALA	4.9
1	D	251	GLY	4.6
1	D	238	PHE	4.6
1	C	233	TYR	4.5
1	C	250	LEU	4.5
1	D	313	TYR	4.5
1	C	234	ALA	4.4
1	D	322	GLU	4.2
1	C	314	VAL	4.2
1	C	317	GLN	4.1
1	D	303	LEU	4.1
1	C	297	LEU	4.1
1	D	221	ILE	4.1
1	D	233	TYR	4.1
1	D	320	VAL	4.1
1	D	235	SER	4.0
1	D	316	VAL	3.9
1	D	270	ILE	3.9
1	D	279	ASP	3.7
1	C	249	ILE	3.7
1	C	288	ARG	3.6
1	C	237	GLY	3.6
1	D	292	THR	3.6
1	D	311	VAL	3.5
1	C	244	TYR	3.5
1	C	270	ILE	3.5
1	B	207	SER	3.4
1	C	313	TYR	3.4
1	C	281	SER	3.3
1	C	322	GLU	3.3
1	C	284	LEU	3.3
1	D	231	ILE	3.3
1	D	318	SER	3.2
1	C	311	VAL	3.2
1	C	316	VAL	3.2
1	D	208	LEU	3.2
1	D	222	THR	3.2
1	C	243	GLY	3.2
1	D	209	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	254	CYS	3.0
1	C	223	ASP	3.0
1	C	296	ASN	2.9
1	E	205	ASP	2.9
1	D	319	LYS	2.9
1	E	203	ASP	2.9
1	C	303	LEU	2.9
1	C	335	GLU	2.8
1	C	254	CYS	2.8
1	D	288	ARG	2.8
1	C	310	ILE	2.8
1	D	242	THR	2.8
1	C	330	ASN	2.7
1	D	237	GLY	2.7
1	D	314	VAL	2.7
1	C	331	GLU	2.7
1	C	320	VAL	2.7
1	D	224	ALA	2.7
1	D	297	LEU	2.7
1	E	206	TYR	2.7
1	C	216	GLN	2.7
1	C	242	THR	2.7
1	C	225	SER	2.6
1	D	289	GLN	2.6
1	D	255	ARG	2.6
1	D	225	SER	2.5
1	D	281	SER	2.4
1	D	301	ALA	2.4
1	A	202	GLU	2.4
1	C	235	SER	2.4
1	C	332	GLN	2.4
1	D	330	ASN	2.4
1	C	321	SER	2.3
1	D	244	TYR	2.3
1	D	262	THR	2.3
1	D	331	GLU	2.3
1	D	212	LEU	2.3
1	D	295	TRP	2.3
1	E	202	GLU	2.3
1	C	290	ASP	2.3
1	F	208	LEU	2.2
1	D	272	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	251	GLY	2.2
1	C	241	LEU	2.2
1	D	326	LYS	2.2
1	C	278	VAL	2.1
1	C	262	THR	2.1
1	D	317	GLN	2.1
1	A	203	ASP	2.0
1	C	298	PHE	2.0
1	C	267	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, 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	PO4	F	502	5/5	0.83	0.24	1.41	100,118,125,133	0
3	PO4	B	502	5/5	0.91	0.23	1.03	117,124,131,141	0
2	FMN	D	501	31/31	0.75	0.36	0.32	150,167,181,182	0
2	FMN	C	501	31/31	0.74	0.43	0.18	148,169,189,194	0
2	FMN	F	501	31/31	0.97	0.21	-0.04	50,64,72,74	0
2	FMN	E	501	31/31	0.96	0.20	-0.04	33,58,65,67	0
2	FMN	B	501	31/31	0.97	0.20	-0.35	48,63,69,72	0
2	FMN	A	501	31/31	0.96	0.17	-0.99	33,57,64,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.