



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:31 PM GMT

PDB ID : 3ATZ  
Title : Crystal structure of TcOYE with pHBA  
Authors : Okamoto, N.; Yamaguchi, K.; Mizohata, E.; Tokuoka, K.; Uchiyama, N.;  
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Deposited on : 2011-01-26  
Resolution : 2.04 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (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

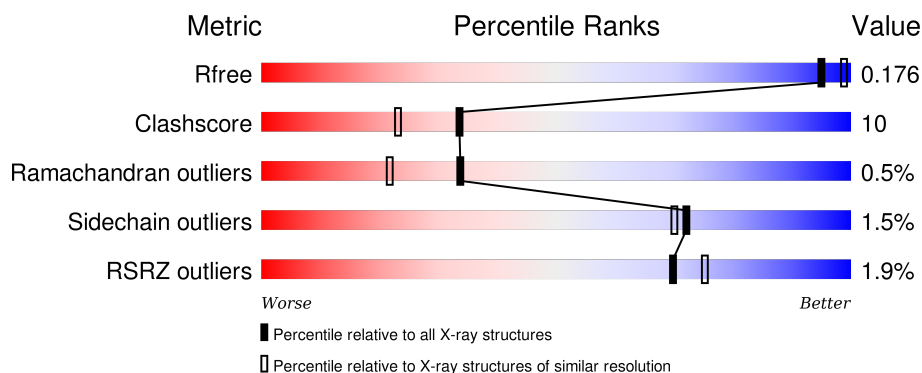
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.04 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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	379	<div> <div>2%</div> <div>75%</div> <div>22%</div> <div>..</div> </div>
1	B	379	<div> <div>2%</div> <div>76%</div> <div>21%</div> <div>..</div> </div>
1	C	379	<div> <div>%</div> <div>75%</div> <div>21%</div> <div>..</div> </div>
1	D	379	<div> <div>2%</div> <div>80%</div> <div>17%</div> <div>..</div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HBA	A	600	-	-	-	X
3	HBA	B	601	-	-	-	X
3	HBA	C	602	-	-	-	X
3	HBA	D	603	-	-	-	X

## 2 Entry composition [i](#)

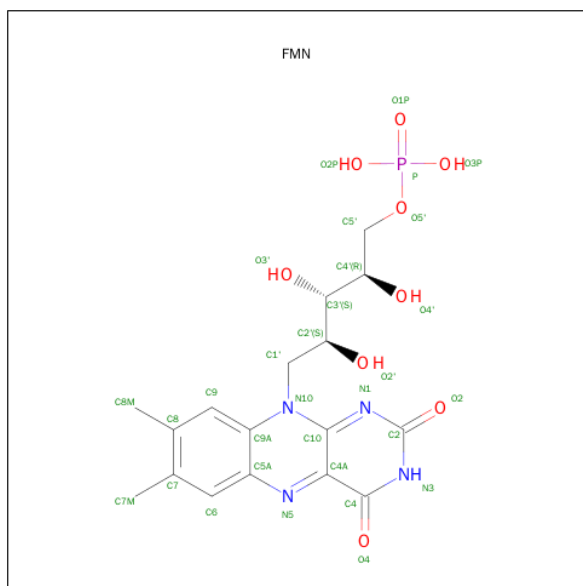
There are 4 unique types of molecules in this entry. The entry contains 12454 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Prostaglandin F2a synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	0	0
			2888	1832	504	543	9			
1	B	374	Total	C	N	O	S	0	0	0
			2931	1856	512	554	9			
1	C	374	Total	C	N	O	S	0	0	0
			2942	1864	512	557	9			
1	D	376	Total	C	N	O	S	0	0	0
			2954	1871	514	560	9			

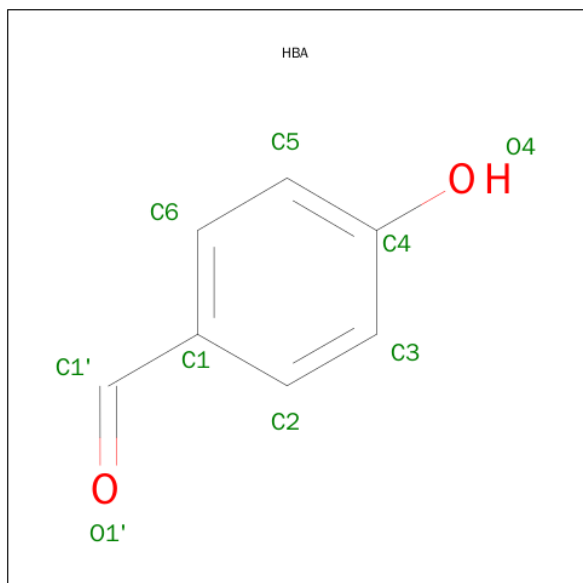
- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

- Molecule 3 is P-HYDROXYBENZALDEHYDE (three-letter code: HBA) (formula:  $C_7H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	7	2		
3	B	1	Total	C	O	0	0
			9	7	2		
3	C	1	Total	C	O	0	0
			9	7	2		
3	D	1	Total	C	O	0	0
			9	7	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	145	Total	O	0	0
			145	145		
4	B	129	Total	O	0	0
			129	129		
4	C	135	Total	O	0	0
			135	135		

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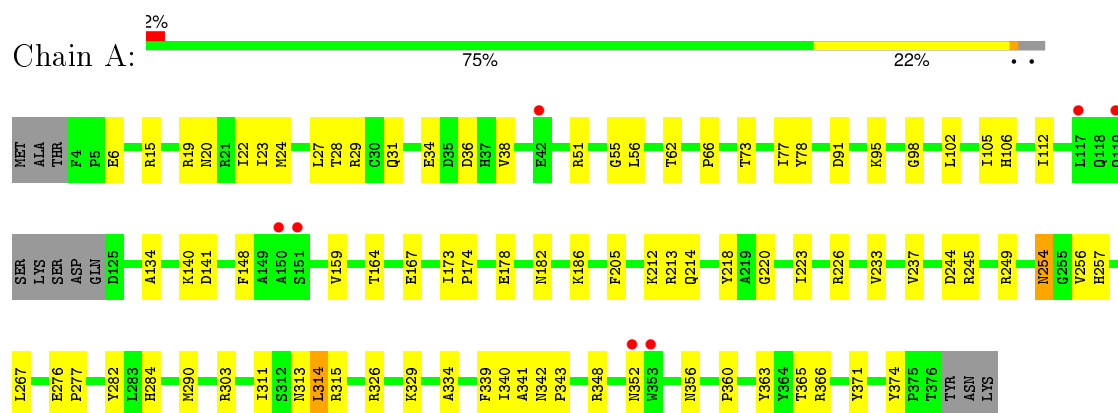
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	170	Total	O	0	0
			170	170		

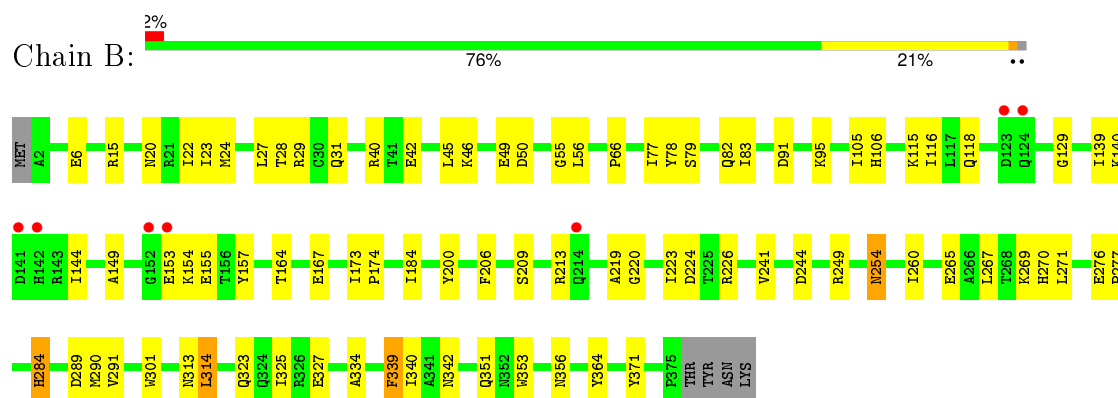
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

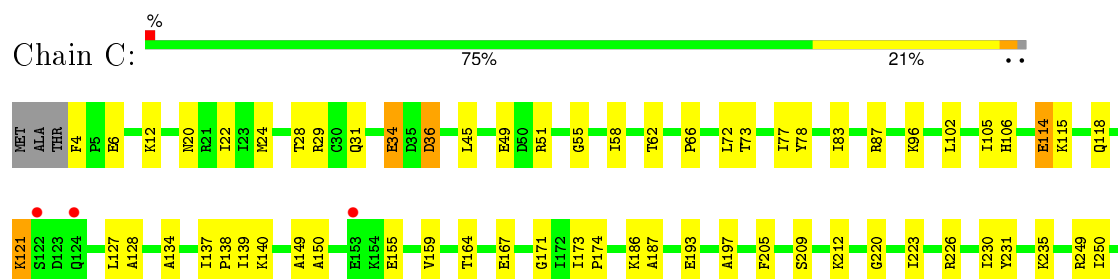
#### • Molecule 1: Prostaglandin F2a synthase



#### • Molecule 1: Prostaglandin F2a synthase

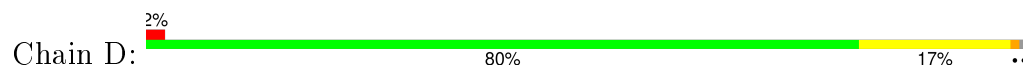


#### • Molecule 1: Prostaglandin F2a synthase





● Molecule 1: Prostaglandin F2a synthase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.33Å 119.59Å 111.53Å 90.00° 90.35° 90.00°	Depositor
Resolution (Å)	37.18 – 2.04 37.17 – 2.04	Depositor EDS
% Data completeness (in resolution range)	96.6 (37.18-2.04) 99.8 (37.17-2.04)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.54 (at 2.05Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.172 , 0.219 0.177 , 0.176	Depositor DCC
$R_{free}$ test set	3943 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.9	Xtriage
Anisotropy	0.448	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 53.4	EDS
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 78332 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12454	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.32 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.9234e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, HBA

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	0.30	0/2951	0.60	0/4002
1	B	0.30	0/2995	0.61	0/4062
1	C	0.30	0/3007	0.59	0/4078
1	D	0.30	0/3019	0.61	0/4095
All	All	0.30	0/11972	0.60	0/16237

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	2888	0	2857	57	0
1	B	2931	0	2898	61	0
1	C	2942	0	2906	74	0
1	D	2954	0	2918	52	0
2	A	31	0	19	0	0
2	B	31	0	19	3	0
2	C	31	0	19	1	0
2	D	31	0	19	0	0
3	A	9	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	9	0	6	1	0
3	C	9	0	5	0	0
3	D	9	0	5	0	0
4	A	145	0	0	1	0
4	B	129	0	0	0	0
4	C	135	0	0	3	0
4	D	170	0	0	1	0
All	All	12454	0	11676	240	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 10.

All (240) 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:C:121:LYS:H	1:C:121:LYS:HD3	1.31	0.96
1:B:342:ASN:HD21	1:B:356:ASN:H	1.05	0.94
1:C:20:ASN:HD22	1:C:22:ILE:H	1.16	0.94
1:C:342:ASN:HD21	1:C:356:ASN:H	0.99	0.92
1:D:20:ASN:HD22	1:D:22:ILE:H	1.15	0.92
1:A:254:ASN:HD21	1:A:256:VAL:HG13	1.35	0.92
1:D:342:ASN:HD21	1:D:356:ASN:H	1.11	0.91
1:A:342:ASN:HD21	1:A:356:ASN:H	1.24	0.82
1:B:20:ASN:HD22	1:B:22:ILE:H	1.26	0.81
1:B:200:TYR:HE1	3:B:601:HBA:HO4	1.28	0.81
1:A:303:ARG:HD2	1:A:329:LYS:HA	1.64	0.78
1:A:20:ASN:HD22	1:A:22:ILE:H	1.32	0.76
1:A:254:ASN:ND2	1:A:256:VAL:HG13	2.01	0.76
1:C:149:ALA:HB1	1:C:155:GLU:HG3	1.68	0.74
1:C:87:ARG:HH21	1:C:186:LYS:HB3	1.51	0.74
1:A:23:ILE:HD12	1:A:56:LEU:HB3	1.70	0.73
1:A:140:LYS:NZ	1:B:353:TRP:NE1	2.35	0.73
1:C:342:ASN:ND2	1:C:356:ASN:H	1.82	0.72
1:A:174:PRO:O	1:A:178:GLU:HG2	1.90	0.71
1:C:293:GLN:O	1:C:294:GLN:HB2	1.88	0.71
1:B:342:ASN:ND2	1:B:356:ASN:H	1.86	0.71
1:A:105:ILE:HG12	1:A:106:HIS:N	2.06	0.70
1:C:289:ASP:OD1	1:C:291:VAL:HG22	1.91	0.70
1:C:87:ARG:HG2	1:C:187:ALA:HA	1.73	0.69
1:B:115:LYS:O	1:B:118:GLN:HG2	1.92	0.69
1:D:122:SER:O	1:D:123:ASP:HB3	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:ASN:ND2	1:D:356:ASN:H	1.90	0.68
1:C:49:GLU:CG	1:C:96:LYS:HD2	2.25	0.66
1:C:34:GLU:HA	1:C:73:THR:HG22	1.78	0.66
1:C:49:GLU:HG2	1:C:96:LYS:HD2	1.77	0.66
1:A:223:ILE:HG23	1:A:267:LEU:HD12	1.78	0.66
1:A:51:ARG:HG2	1:A:343:PRO:HA	1.77	0.65
1:A:249:ARG:HA	1:A:284:HIS:O	1.97	0.64
1:A:66:PRO:HA	1:A:78:TYR:CZ	2.33	0.63
1:D:342:ASN:HD21	1:D:356:ASN:N	1.91	0.63
1:C:249:ARG:HA	1:C:284:HIS:O	1.99	0.63
1:B:149:ALA:HB1	1:B:155:GLU:HG3	1.80	0.63
1:C:223:ILE:HG23	1:C:267:LEU:HD12	1.81	0.62
1:B:342:ASN:HD21	1:B:356:ASN:N	1.86	0.62
1:B:91:ASP:O	1:B:95:LYS:HG3	2.00	0.62
1:C:72:LEU:HD11	1:C:115:LYS:HZ1	1.65	0.62
1:D:254:ASN:HD21	1:D:290:MET:HB2	1.65	0.61
1:B:23:ILE:HD12	1:B:56:LEU:HB3	1.82	0.61
1:C:361:GLU:H	1:C:361:GLU:CD	2.03	0.61
1:B:42:GLU:CD	1:B:42:GLU:H	2.04	0.61
1:D:254:ASN:ND2	1:D:290:MET:HB2	2.16	0.61
1:B:249:ARG:HA	1:B:284:HIS:O	2.00	0.61
1:A:276:GLU:HB3	1:A:277:PRO:HD3	1.83	0.61
1:C:83:ILE:O	1:C:87:ARG:HG3	2.00	0.61
1:D:164:THR:OG1	1:D:167:GLU:HG3	2.00	0.61
1:A:31:GLN:HG3	1:A:371:TYR:CZ	2.36	0.60
1:A:365:THR:O	1:A:366:ARG:HB2	2.02	0.59
1:C:342:ASN:HD21	1:C:356:ASN:N	1.84	0.59
1:D:122:SER:O	1:D:123:ASP:CB	2.51	0.59
1:C:31:GLN:HG3	1:C:371:TYR:CZ	2.37	0.59
1:B:105:ILE:HG12	1:B:106:HIS:N	2.18	0.59
1:B:223:ILE:HG23	1:B:267:LEU:HD12	1.84	0.59
1:C:276:GLU:HB3	1:C:277:PRO:HD3	1.84	0.58
1:D:149:ALA:HB1	1:D:155:GLU:HG3	1.85	0.58
1:C:173:ILE:HB	1:C:174:PRO:HD3	1.84	0.58
1:C:20:ASN:ND2	1:C:22:ILE:H	1.96	0.58
1:C:138:PRO:HB3	1:C:159:VAL:HA	1.85	0.57
1:C:295:ILE:HD12	1:C:296:GLY:H	1.69	0.57
1:D:105:ILE:HG12	1:D:106:HIS:N	2.18	0.57
1:B:276:GLU:HB2	1:B:277:PRO:HD3	1.85	0.57
1:C:105:ILE:HG12	1:C:106:HIS:N	2.20	0.57
1:D:20:ASN:ND2	1:D:22:ILE:H	1.95	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ASN:ND2	1:A:356:ASN:H	1.99	0.56
1:B:15:ARG:HB3	1:B:244:ASP:OD2	2.05	0.56
1:C:121:LYS:HB3	1:C:128:ALA:O	2.05	0.56
1:C:28:THR:O	1:C:29:ARG:HD2	2.06	0.56
1:D:276:GLU:HB3	1:D:277:PRO:HD3	1.87	0.56
1:D:261:ASP:O	1:D:264:PRO:HD3	2.06	0.55
1:A:342:ASN:HD22	1:A:348:ARG:NE	2.04	0.55
1:D:224:ASP:OD1	1:D:270:HIS:HE1	1.90	0.55
1:A:173:ILE:HB	1:A:174:PRO:HD3	1.89	0.55
1:B:45:LEU:O	1:B:49:GLU:HG2	2.06	0.55
1:A:212:LYS:HG3	1:B:351:GLN:NE2	2.22	0.55
1:B:265:GLU:HG3	1:B:301:TRP:CE2	2.42	0.55
1:B:164:THR:OG1	1:B:167:GLU:HG3	2.07	0.55
1:D:31:GLN:HG3	1:D:371:TYR:CZ	2.42	0.55
1:C:319:GLU:HG3	4:C:493:HOH:O	2.06	0.54
1:B:40:ARG:HB3	1:B:42:GLU:OE2	2.07	0.54
1:B:173:ILE:HB	1:B:174:PRO:HD3	1.89	0.54
1:C:114:GLU:HG2	1:C:150:ALA:HB3	1.89	0.54
1:B:116:ILE:O	1:B:129:GLY:HA2	2.08	0.54
1:C:114:GLU:O	1:C:118:GLN:HG3	2.08	0.54
1:B:220:GLY:HA2	1:B:226:ARG:HG2	1.88	0.54
1:D:6:GLU:HG3	1:D:326:ARG:HB2	1.91	0.53
1:C:87:ARG:CG	1:C:187:ALA:HA	2.37	0.53
1:B:31:GLN:HG3	1:B:371:TYR:CZ	2.44	0.53
1:D:237:VAL:O	1:D:241:VAL:HG22	2.07	0.53
1:C:230:ILE:HG13	4:C:408:HOH:O	2.08	0.53
1:C:4:PHE:HE2	1:C:319:GLU:HG2	1.74	0.53
1:C:164:THR:OG1	1:C:167:GLU:HG3	2.09	0.53
1:C:293:GLN:O	1:C:294:GLN:CB	2.56	0.52
1:C:231:TYR:CE1	1:C:235:LYS:HD2	2.44	0.52
1:C:149:ALA:CB	1:C:155:GLU:HG3	2.39	0.52
1:B:313:ASN:O	1:B:314:LEU:CB	2.57	0.52
1:A:342:ASN:HD21	1:A:356:ASN:N	1.98	0.51
1:C:138:PRO:HG2	1:C:140:LYS:HE3	1.92	0.51
1:C:66:PRO:HA	1:C:78:TYR:CZ	2.45	0.51
1:A:77:ILE:O	1:A:77:ILE:HG13	2.10	0.51
1:D:13:LEU:HB3	1:D:18:LEU:CD1	2.40	0.51
1:C:121:LYS:N	1:C:121:LYS:HD3	2.13	0.51
1:A:34:GLU:HA	1:A:73:THR:HG22	1.92	0.51
1:C:220:GLY:HA2	1:C:226:ARG:HG2	1.93	0.50
1:C:77:ILE:HG13	1:C:77:ILE:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:VAL:HG23	1:C:293:GLN:HG3	1.93	0.50
1:C:139:ILE:HG22	4:C:455:HOH:O	2.12	0.50
1:C:121:LYS:H	1:C:121:LYS:CD	2.08	0.50
1:C:49:GLU:HG3	1:C:96:LYS:HD2	1.94	0.50
1:A:15:ARG:NE	1:A:245:ARG:NH2	2.60	0.49
1:C:62:THR:OG1	1:C:102:LEU:HD11	2.13	0.49
1:B:77:ILE:HG13	1:B:77:ILE:O	2.12	0.49
1:D:77:ILE:HG13	1:D:77:ILE:O	2.12	0.49
1:A:91:ASP:O	1:A:95:LYS:HG2	2.12	0.49
1:B:265:GLU:HG2	1:B:269:LYS:HE2	1.94	0.49
1:D:62:THR:OG1	1:D:102:LEU:HD11	2.13	0.49
1:A:313:ASN:O	1:A:314:LEU:CB	2.60	0.49
1:A:27:LEU:HD13	1:A:340:ILE:HG13	1.94	0.48
1:B:289:ASP:OD1	1:B:291:VAL:HG22	2.13	0.48
1:C:313:ASN:O	1:C:314:LEU:HB3	2.13	0.48
1:C:127:LEU:HD11	1:C:171:GLY:HA3	1.95	0.48
1:D:24:MET:HA	1:D:339:PHE:CD2	2.48	0.48
1:A:159:VAL:HG23	1:A:159:VAL:O	2.14	0.48
1:C:354:PRO:HD2	1:C:377:TYR:CE2	2.48	0.48
1:A:164:THR:OG1	1:A:167:GLU:HG3	2.14	0.48
1:D:346:VAL:O	1:D:350:GLN:HG3	2.14	0.48
1:C:359:ARG:HB3	1:C:361:GLU:OE2	2.14	0.48
1:A:290:MET:O	1:A:315:ARG:NH1	2.47	0.48
1:D:224:ASP:OD1	1:D:270:HIS:CE1	2.66	0.47
1:B:206:PHE:CZ	1:B:271:LEU:HD22	2.49	0.47
1:B:213:ARG:HB2	1:B:219:ALA:HA	1.96	0.47
1:A:6:GLU:HG3	1:A:326:ARG:HB2	1.96	0.47
1:A:19:ARG:NH1	1:A:98:GLY:HA2	2.29	0.47
1:D:249:ARG:HA	1:D:284:HIS:O	2.14	0.47
1:D:289:ASP:OD1	1:D:291:VAL:HG22	2.15	0.47
1:A:303:ARG:CD	1:A:329:LYS:HA	2.39	0.47
1:B:46:LYS:HA	1:B:49:GLU:HG2	1.97	0.47
1:A:15:ARG:HB3	1:A:244:ASP:OD2	2.14	0.47
1:C:289:ASP:CG	1:C:291:VAL:HG22	2.35	0.47
1:C:134:ALA:HA	1:C:205:PHE:CZ	2.50	0.47
1:B:66:PRO:HA	1:B:78:TYR:CZ	2.49	0.46
1:A:233:VAL:O	1:A:237:VAL:HG23	2.15	0.46
1:C:313:ASN:O	1:C:314:LEU:CB	2.63	0.46
1:A:213:ARG:HD3	1:A:218:TYR:O	2.15	0.46
1:C:342:ASN:HD22	1:C:348:ARG:CZ	2.28	0.46
1:C:51:ARG:HG2	1:C:343:PRO:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LYS:NZ	1:B:353:TRP:CD1	2.81	0.46
1:B:184:ILE:HD12	1:B:241:VAL:HG11	1.96	0.46
1:B:364:TYR:CZ	2:B:501:FMN:HM72	2.51	0.46
1:D:66:PRO:HA	1:D:78:TYR:CZ	2.51	0.46
1:D:23:ILE:HB	1:D:334:ALA:HA	1.99	0.45
1:D:233:VAL:O	1:D:237:VAL:HG13	2.16	0.45
1:D:58:ILE:HD13	1:D:193:GLU:OE2	2.16	0.45
1:B:144:ILE:O	1:B:154:LYS:HA	2.16	0.45
1:A:276:GLU:N	1:A:277:PRO:CD	2.80	0.45
1:A:212:LYS:HG3	1:B:351:GLN:HE22	1.81	0.45
1:D:294:GLN:C	1:D:295:ILE:HD12	2.37	0.45
1:C:282:TYR:CE2	1:C:284:HIS:HB2	2.52	0.45
1:B:49:GLU:HG3	1:B:50:ASP:N	2.32	0.45
1:C:58:ILE:HD13	1:C:193:GLU:OE2	2.17	0.45
1:C:289:ASP:OD2	1:C:293:GLN:O	2.35	0.45
1:C:20:ASN:HD21	1:C:55:GLY:H	1.65	0.44
1:A:62:THR:OG1	1:A:102:LEU:HD11	2.16	0.44
1:D:287:ARG:HG2	1:D:313:ASN:O	2.18	0.44
1:A:256:VAL:HG11	4:A:425:HOH:O	2.18	0.44
1:D:149:ALA:HB1	1:D:155:GLU:CG	2.47	0.44
1:D:313:ASN:O	1:D:314:LEU:CB	2.65	0.44
1:B:27:LEU:HD13	1:B:340:ILE:HG13	1.98	0.44
1:C:197:ALA:HB2	1:C:250:ILE:HA	1.98	0.44
1:B:224:ASP:OD1	1:B:270:HIS:HE1	1.99	0.44
1:B:323:GLN:HE21	1:B:327:GLU:HG3	1.83	0.44
1:B:153:GLU:O	1:B:155:GLU:HG3	2.18	0.44
1:D:173:ILE:HB	1:D:174:PRO:HD3	1.99	0.44
1:B:313:ASN:ND2	2:B:501:FMN:O3'	2.51	0.44
1:C:36:ASP:OD1	1:C:36:ASP:N	2.50	0.44
1:D:20:ASN:HD21	1:D:55:GLY:H	1.66	0.44
1:A:112:ILE:HD13	1:A:148:PHE:O	2.18	0.44
1:A:341:ALA:HA	1:A:374:TYR:CD2	2.53	0.44
1:C:134:ALA:HB2	1:C:205:PHE:CD1	2.53	0.43
1:C:364:TYR:CZ	2:C:501:FMN:HM72	2.53	0.43
1:A:20:ASN:HD21	1:A:55:GLY:H	1.66	0.43
1:A:105:ILE:HG12	1:A:106:HIS:H	1.83	0.43
1:A:24:MET:HA	1:A:339:PHE:CD2	2.53	0.43
1:A:23:ILE:HB	1:A:334:ALA:HA	2.01	0.43
1:D:276:GLU:N	1:D:277:PRO:CD	2.81	0.43
1:A:28:THR:O	1:A:29:ARG:HD2	2.18	0.43
1:C:276:GLU:N	1:C:277:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:MET:HA	1:B:339:PHE:CD2	2.54	0.43
1:D:265:GLU:HG3	1:D:301:TRP:CE2	2.53	0.43
1:D:313:ASN:O	1:D:314:LEU:HB3	2.19	0.43
1:A:348:ARG:NH2	1:A:356:ASN:HD21	2.17	0.43
1:A:360:PRO:HA	1:A:363:TYR:CD2	2.54	0.43
1:B:364:TYR:CE1	2:B:501:FMN:HM72	2.54	0.42
1:B:323:GLN:HE21	1:B:327:GLU:CG	2.32	0.42
1:D:182:ASN:O	1:D:186:LYS:HB2	2.18	0.42
1:C:149:ALA:HB1	1:C:155:GLU:CG	2.45	0.42
1:A:220:GLY:HA2	1:A:226:ARG:HG2	2.01	0.42
1:D:149:ALA:HB1	1:D:155:GLU:CD	2.40	0.42
1:D:105:ILE:CG1	1:D:106:HIS:N	2.82	0.42
1:D:27:LEU:HD13	1:D:340:ILE:HG13	2.01	0.42
1:C:137:ILE:HD11	1:C:212:LYS:CG	2.50	0.42
1:D:116:ILE:O	1:D:129:GLY:HA2	2.19	0.42
1:D:118:GLN:HA	4:D:543:HOH:O	2.18	0.42
1:B:276:GLU:N	1:B:277:PRO:CD	2.83	0.42
1:A:282:TYR:CD2	1:A:311:ILE:HD12	2.55	0.42
1:C:24:MET:HA	1:C:339:PHE:CD2	2.55	0.42
1:A:141:ASP:OD1	1:A:257:HIS:HA	2.19	0.41
1:C:209:SER:HB3	1:C:260:ILE:O	2.20	0.41
1:C:249:ARG:HH11	1:C:284:HIS:CE1	2.37	0.41
1:D:13:LEU:HB3	1:D:18:LEU:HD11	2.02	0.41
1:C:45:LEU:C	1:C:45:LEU:HD23	2.41	0.41
1:B:209:SER:HB3	1:B:260:ILE:O	2.21	0.41
1:B:6:GLU:HB3	1:B:325:ILE:CG2	2.49	0.41
1:B:254:ASN:ND2	1:B:290:MET:H	2.17	0.41
1:D:282:TYR:CE2	1:D:284:HIS:HB2	2.55	0.41
1:D:33:THR:O	1:D:37:HIS:HA	2.20	0.41
1:D:51:ARG:HG2	1:D:343:PRO:HA	2.03	0.41
1:A:182:ASN:O	1:A:186:LYS:HB2	2.21	0.41
1:B:265:GLU:HG3	1:B:301:TRP:NE1	2.36	0.41
1:B:289:ASP:CG	1:B:291:VAL:HG22	2.40	0.41
1:D:115:LYS:O	1:D:118:GLN:HG2	2.20	0.41
1:B:79:SER:OG	1:B:82:GLN:HG3	2.21	0.41
1:C:342:ASN:HA	1:C:343:PRO:HD2	1.93	0.41
1:B:79:SER:O	1:B:83:ILE:HG13	2.21	0.41
1:B:28:THR:O	1:B:29:ARG:HD2	2.21	0.41
1:A:36:ASP:HB3	1:A:38:VAL:HG23	2.02	0.41
1:D:41:THR:OG1	1:D:85:GLU:HB3	2.21	0.41
1:B:23:ILE:HB	1:B:334:ALA:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ILE:CG1	1:B:106:HIS:N	2.84	0.40
1:D:313:ASN:CG	1:D:314:LEU:N	2.73	0.40
1:C:72:LEU:HD11	1:C:115:LYS:NZ	2.33	0.40
1:B:313:ASN:O	1:B:314:LEU:HB3	2.20	0.40
1:C:313:ASN:CG	1:C:314:LEU:N	2.75	0.40
1:B:20:ASN:HD21	1:B:55:GLY:H	1.68	0.40
1:B:139:ILE:HD12	1:B:157:TYR:CD2	2.56	0.40
1:A:105:ILE:CG1	1:A:106:HIS:N	2.79	0.40
1:A:134:ALA:HB2	1:A:205:PHE:CD1	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	364/379 (96%)	345 (95%)	18 (5%)	1 (0%)	46	36
1	B	372/379 (98%)	351 (94%)	19 (5%)	2 (0%)	34	22
1	C	372/379 (98%)	354 (95%)	15 (4%)	3 (1%)	24	12
1	D	374/379 (99%)	354 (95%)	18 (5%)	2 (0%)	34	22
All	All	1482/1516 (98%)	1404 (95%)	70 (5%)	8 (0%)	34	22

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	314	LEU
1	B	140	LYS
1	B	314	LEU
1	C	314	LEU
1	D	314	LEU
1	C	294	GLN

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Mol	Chain	Res	Type
1	C	34	GLU
1	D	123	ASP

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	303/314 (96%)	300 (99%)	3 (1%)	82	81
1	B	308/314 (98%)	305 (99%)	3 (1%)	82	81
1	C	310/314 (99%)	301 (97%)	9 (3%)	50	42
1	D	311/314 (99%)	308 (99%)	3 (1%)	82	81
All	All	1232/1256 (98%)	1214 (98%)	18 (2%)	72	70

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	GLN
1	A	254	ASN
1	A	352	ASN
1	B	254	ASN
1	B	284	HIS
1	B	339	PHE
1	C	6	GLU
1	C	12	LYS
1	C	36	ASP
1	C	114	GLU
1	C	121	LYS
1	C	254	ASN
1	C	284	HIS
1	C	293	GLN
1	C	339	PHE
1	D	254	ASN
1	D	290	MET
1	D	339	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	118	GLN
1	A	182	ASN
1	A	254	ASN
1	A	270	HIS
1	A	313	ASN
1	A	323	GLN
1	A	342	ASN
1	A	352	ASN
1	A	356	ASN
1	B	20	ASN
1	B	119	GLN
1	B	182	ASN
1	B	198	ASN
1	B	257	HIS
1	B	270	HIS
1	B	313	ASN
1	B	323	GLN
1	B	342	ASN
1	B	350	GLN
1	B	351	GLN
1	C	20	ASN
1	C	182	ASN
1	C	254	ASN
1	C	270	HIS
1	C	313	ASN
1	C	323	GLN
1	C	342	ASN
1	C	351	GLN
1	D	20	ASN
1	D	118	GLN
1	D	119	GLN
1	D	182	ASN
1	D	214	GLN
1	D	254	ASN
1	D	270	HIS
1	D	313	ASN
1	D	342	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	501	-	32,33,33	2.00	10 (31%)	34,50,50	2.65	7 (20%)
3	HBA	A	600	-	9,9,9	1.29	1 (11%)	11,11,11	0.75	0
2	FMN	B	501	-	32,33,33	1.95	8 (25%)	34,50,50	2.66	7 (20%)
3	HBA	B	601	-	9,9,9	1.34	1 (11%)	11,11,11	0.75	0
2	FMN	C	501	-	32,33,33	1.95	9 (28%)	34,50,50	2.66	7 (20%)
3	HBA	C	602	-	9,9,9	1.26	1 (11%)	11,11,11	0.73	0
2	FMN	D	501	-	32,33,33	1.92	9 (28%)	34,50,50	2.64	7 (20%)
3	HBA	D	603	-	9,9,9	1.30	1 (11%)	11,11,11	0.74	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	-	-	0/18/18/18	0/3/3/3
3	HBA	A	600	-	-	0/2/2/2	0/1/1/1
2	FMN	B	501	-	-	0/18/18/18	0/3/3/3
3	HBA	B	601	-	-	0/2/2/2	0/1/1/1
2	FMN	C	501	-	-	0/18/18/18	0/3/3/3
3	HBA	C	602	-	-	0/2/2/2	0/1/1/1
2	FMN	D	501	-	-	0/18/18/18	0/3/3/3
3	HBA	D	603	-	-	0/2/2/2	0/1/1/1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	FMN	C4'-C3'	2.08	1.57	1.53
2	A	501	FMN	C4A-N5	2.08	1.36	1.33
2	A	501	FMN	C6-C5A	2.09	1.45	1.41
3	B	601	HBA	C6-C1	2.21	1.43	1.39
2	A	501	FMN	C8-C7	2.24	1.47	1.41
3	C	602	HBA	C6-C1	2.26	1.43	1.39
2	C	501	FMN	C4A-N5	2.30	1.36	1.33
3	D	603	HBA	C6-C1	2.31	1.43	1.39
2	C	501	FMN	C8-C7	2.33	1.47	1.41
2	D	501	FMN	C8-C7	2.36	1.47	1.41
3	A	600	HBA	C6-C1	2.40	1.44	1.39
2	B	501	FMN	C8-C7	2.41	1.47	1.41
2	C	501	FMN	C10-N10	2.45	1.42	1.39
2	B	501	FMN	C10-N10	2.57	1.42	1.39
2	C	501	FMN	C9-C9A	2.66	1.46	1.40
2	D	501	FMN	C9-C9A	2.73	1.46	1.40
2	D	501	FMN	C5A-N5	2.78	1.39	1.35
2	D	501	FMN	C10-N10	2.81	1.42	1.39
2	A	501	FMN	C10-N10	2.83	1.42	1.39
2	A	501	FMN	C9-C9A	2.86	1.47	1.40
2	B	501	FMN	C9-C9A	2.96	1.47	1.40
2	C	501	FMN	C5A-N5	2.96	1.40	1.35
2	B	501	FMN	C4A-C10	3.04	1.46	1.40
2	B	501	FMN	C5A-N5	3.05	1.40	1.35
2	C	501	FMN	C4A-C10	3.12	1.46	1.40
2	D	501	FMN	C4A-C10	3.14	1.46	1.40
2	A	501	FMN	P-O5'	3.18	1.69	1.59
2	A	501	FMN	C4A-C10	3.26	1.46	1.40
2	B	501	FMN	P-O5'	3.31	1.69	1.59
2	A	501	FMN	C5A-N5	3.34	1.40	1.35
2	D	501	FMN	P-O5'	3.35	1.69	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	FMN	P-O5'	3.67	1.70	1.59
2	C	501	FMN	C9A-N10	3.94	1.44	1.38
2	A	501	FMN	C9A-N10	3.98	1.44	1.38
2	B	501	FMN	C9A-N10	4.05	1.44	1.38
2	D	501	FMN	C9A-N10	4.24	1.44	1.38
2	D	501	FMN	C4-N3	4.73	1.41	1.33
2	C	501	FMN	C4-N3	4.83	1.41	1.33
2	A	501	FMN	C4-N3	4.86	1.41	1.33
2	B	501	FMN	C4-N3	4.86	1.41	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	FMN	C4-C4A-C10	-7.55	115.11	119.94
2	A	501	FMN	C4-C4A-C10	-7.49	115.15	119.94
2	D	501	FMN	C4-C4A-C10	-7.42	115.19	119.94
2	C	501	FMN	C4-C4A-C10	-7.41	115.20	119.94
2	C	501	FMN	C4A-C10-N10	-5.49	116.53	120.52
2	A	501	FMN	C4A-C10-N10	-5.39	116.60	120.52
2	B	501	FMN	C4A-C10-N10	-5.34	116.64	120.52
2	D	501	FMN	C4A-C10-N10	-5.32	116.65	120.52
2	D	501	FMN	N3-C2-N1	-4.78	119.64	127.69
2	C	501	FMN	N3-C2-N1	-4.72	119.74	127.69
2	B	501	FMN	N3-C2-N1	-4.71	119.76	127.69
2	A	501	FMN	N3-C2-N1	-4.67	119.83	127.69
2	A	501	FMN	C4A-C4-N3	-3.67	118.72	123.52
2	C	501	FMN	C4A-C4-N3	-3.65	118.75	123.52
2	B	501	FMN	C4A-C4-N3	-3.58	118.84	123.52
2	D	501	FMN	C4A-C4-N3	-3.57	118.86	123.52
2	D	501	FMN	C4-C4A-N5	2.48	121.71	118.70
2	C	501	FMN	C4-C4A-N5	2.62	121.88	118.70
2	B	501	FMN	C4-C4A-N5	2.66	121.94	118.70
2	A	501	FMN	C4-C4A-N5	2.78	122.08	118.70
2	C	501	FMN	C4A-N5-C5A	2.98	120.23	116.72
2	B	501	FMN	C4A-N5-C5A	3.04	120.30	116.72
2	D	501	FMN	C4A-N5-C5A	3.05	120.31	116.72
2	A	501	FMN	C4A-N5-C5A	3.08	120.35	116.72
2	A	501	FMN	C4-N3-C2	8.61	122.34	115.16
2	B	501	FMN	C4-N3-C2	8.73	122.44	115.16
2	D	501	FMN	C4-N3-C2	8.73	122.44	115.16
2	C	501	FMN	C4-N3-C2	8.82	122.52	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	FMN	3	0
3	B	601	HBA	1	0
2	C	501	FMN	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	368/379 (97%)	-0.17	7 (1%) 70 75	17, 27, 47, 70	0
1	B	374/379 (98%)	-0.18	7 (1%) 70 75	15, 26, 42, 76	0
1	C	374/379 (98%)	-0.17	5 (1%) 79 83	16, 26, 50, 75	0
1	D	376/379 (99%)	-0.19	9 (2%) 62 68	16, 24, 44, 81	0
All	All	1492/1516 (98%)	-0.18	28 (1%) 70 75	15, 26, 47, 81	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	124	GLN	4.3
1	B	124	GLN	4.1
1	B	141	ASP	3.9
1	B	123	ASP	3.4
1	C	124	GLN	3.4
1	A	352	ASN	3.3
1	A	42	GLU	3.1
1	D	121	LYS	3.1
1	A	353	TRP	3.0
1	C	153	GLU	3.0
1	B	142	HIS	2.8
1	C	292	ASN	2.7
1	D	141	ASP	2.6
1	D	120	SER	2.6
1	C	293	GLN	2.6
1	D	114	GLU	2.5
1	A	150	ALA	2.4
1	A	151	SER	2.4
1	B	153	GLU	2.3
1	A	119	GLN	2.3
1	C	122	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	122	SER	2.2
1	D	150	ALA	2.2
1	D	142	HIS	2.1
1	B	214	GLN	2.1
1	B	152	GLY	2.0
1	D	153	GLU	2.0
1	A	117	LEU	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( $\text{\AA}^2$ )	Q<0.9
3	HBA	B	601	9/9	0.75	0.34	29.25	20,44,66,76	0
3	HBA	C	602	9/9	0.91	0.17	7.43	21,33,41,43	0
3	HBA	D	603	9/9	0.89	0.20	4.51	22,30,42,59	0
3	HBA	A	600	9/9	0.92	0.17	3.87	19,26,33,40	0
2	FMN	B	501	31/31	0.97	0.13	0.21	10,17,26,29	0
2	FMN	C	501	31/31	0.97	0.11	-0.06	17,19,26,32	0
2	FMN	D	501	31/31	0.97	0.11	-0.25	11,17,22,22	0
2	FMN	A	501	31/31	0.97	0.11	-0.28	10,21,29,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.