



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:53 PM GMT

PDB ID : 1YY5  
Title : Crystal structure of Fms1, a polyamine oxidase from Yeast  
Authors : Huang, Q.; Liu, Q.; Hao, Q.  
Deposited on : 2005-02-23  
Resolution : 2.30 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

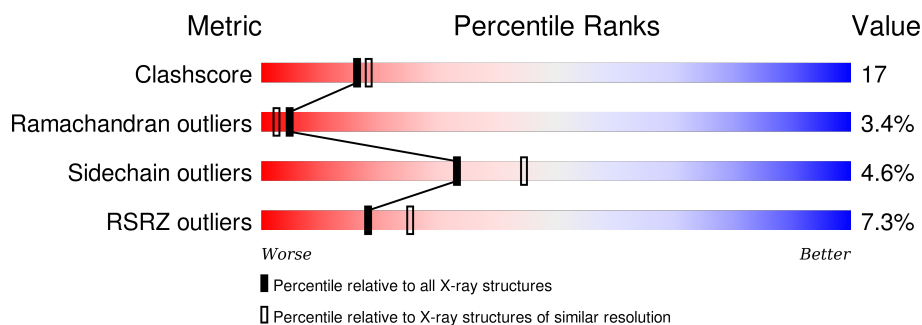
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	513	<div> <div>6%</div> <div>67%27%••</div> </div>
1	B	513	<div> <div>8%</div> <div>63%28%•5%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8083 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 FMS1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	86	0	0
			3997	2526	699	750	22			
1	B	487	Total	C	N	O	S	126	0	0
			3908	2472	679	735	22			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	509	LEU	-	EXPRESSION TAG	UNP P50264
A	510	GLU	-	EXPRESSION TAG	UNP P50264
A	511	HIS	-	EXPRESSION TAG	UNP P50264
A	512	HIS	-	EXPRESSION TAG	UNP P50264
A	513	HIS	-	EXPRESSION TAG	UNP P50264
B	509	LEU	-	EXPRESSION TAG	UNP P50264
B	510	GLU	-	EXPRESSION TAG	UNP P50264
B	511	HIS	-	EXPRESSION TAG	UNP P50264
B	512	HIS	-	EXPRESSION TAG	UNP P50264
B	513	HIS	-	EXPRESSION TAG	UNP P50264

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

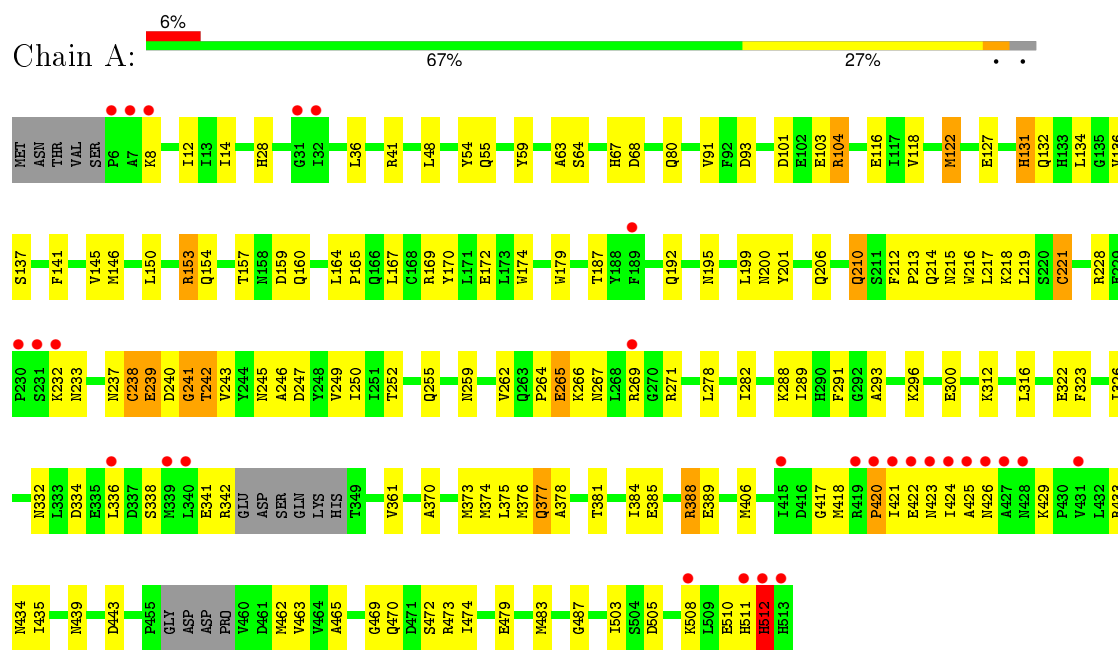
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total	O	0	0
			38	38		
3	B	34	Total	O	0	0
			34	34		

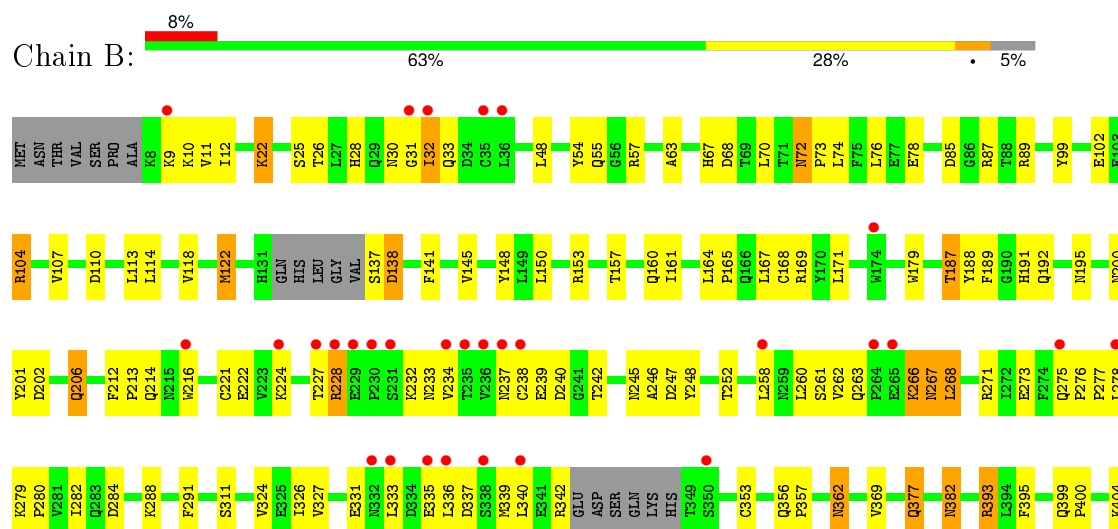
### 3 Residue-property plots

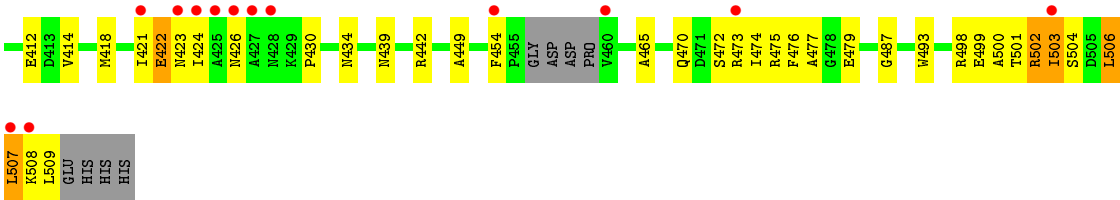
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: FMS1 protein



#### • Molecule 1: FMS1 protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.71Å 215.37Å 118.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 49.82 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.7 (50.00-2.30) 90.3 (49.82-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.20 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.249 , 0.290 0.249 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	44.3	Xtriage
Anisotropy	0.651	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 55704 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8083	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.38	0/4080	0.65	1/5515 (0.0%)
1	B	0.38	0/3985	0.61	0/5385
All	All	0.38	0/8065	0.63	1/10900 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	CYS	CA-CB-SG	5.60	124.08	114.00

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	3997	0	3916	115	2
1	B	3908	0	3842	142	0
2	A	53	0	31	3	0
2	B	53	0	31	2	0
3	A	38	0	0	1	0
3	B	34	0	0	1	0
All	All	8083	0	7820	257	2



The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (257) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:LEU:HA	1:B:470:GLN:HE22	1.30	0.96
1:B:282:ILE:HD13	1:B:465:ALA:HB1	1.49	0.92
1:B:104:ARG:HG3	1:B:104:ARG:HH11	1.37	0.89
1:A:426:ASN:HB3	1:A:429:LYS:HB2	1.56	0.85
1:B:326:ILE:HG22	1:B:336:LEU:HD12	1.58	0.85
1:A:377:GLN:NE2	1:A:377:GLN:H	1.79	0.80
1:A:376:MET:HE1	1:A:384:ILE:HG21	1.65	0.79
1:B:85:ASP:OD1	1:B:87:ARG:HG3	1.85	0.77
1:A:388:ARG:HH11	1:A:388:ARG:HB2	1.50	0.76
1:B:278:LEU:HA	1:B:470:GLN:NE2	2.00	0.76
1:B:382:ASN:ND2	1:B:382:ASN:H	1.82	0.75
1:A:146:MET:HE2	1:A:336:LEU:HD21	1.68	0.75
1:A:240:ASP:OD2	1:A:242:THR:HG23	1.87	0.74
1:B:470:GLN:HB3	1:B:474:ILE:HB	1.71	0.72
1:A:388:ARG:NH2	1:A:439:ASN:HB2	2.05	0.72
1:B:227:THR:HG23	1:B:275:GLN:HB3	1.72	0.71
1:A:293:ALA:HB3	1:A:378:ALA:HB2	1.70	0.71
1:B:475:ARG:NH1	1:B:502:ARG:CZ	2.53	0.71
1:B:377:GLN:NE2	1:B:377:GLN:H	1.89	0.70
1:A:389:GLU:OE1	1:A:389:GLU:HA	1.92	0.69
1:B:72:ASN:C	1:B:72:ASN:HD22	1.96	0.69
1:A:423:ASN:HD21	1:A:426:ASN:ND2	1.94	0.66
1:A:417:GLY:O	1:A:433:ARG:HD3	1.96	0.66
1:A:423:ASN:HD21	1:A:426:ASN:HD22	1.42	0.66
1:A:41:ARG:HD2	3:A:816:HOH:O	1.95	0.66
1:B:475:ARG:HH12	1:B:502:ARG:NE	1.93	0.66
1:B:85:ASP:CG	1:B:87:ARG:HG3	2.16	0.66
1:B:439:ASN:HD21	1:B:442:ARG:HH11	1.44	0.65
1:A:41:ARG:HG2	1:A:41:ARG:HH11	1.61	0.65
1:A:247:ASP:O	1:A:473:ARG:HD2	1.97	0.65
1:A:122:MET:HE2	1:A:145:VAL:HG13	1.77	0.65
1:A:289:ILE:HD11	1:A:462:MET:HG2	1.78	0.65
1:A:326:ILE:HD11	1:A:342:ARG:HH21	1.62	0.65
1:B:157:THR:O	1:B:161:ILE:HG13	1.97	0.65
1:B:104:ARG:HG3	1:B:104:ARG:NH1	2.07	0.65
1:B:122:MET:HE1	1:B:145:VAL:HG22	1.79	0.65
1:A:48:LEU:CD2	1:A:63:ALA:HB3	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:PRO:O	1:A:216:TRP:HB2	1.98	0.64
1:B:475:ARG:HH12	1:B:502:ARG:CZ	2.11	0.62
1:B:122:MET:CE	1:B:145:VAL:HG22	2.29	0.62
1:B:393:ARG:HG2	1:B:393:ARG:NH1	2.14	0.62
1:A:288:LYS:O	1:A:289:ILE:HG23	1.98	0.62
1:B:475:ARG:NH1	1:B:502:ARG:NE	2.48	0.61
1:A:322:GLU:CG	1:A:342:ARG:HH22	2.12	0.61
1:B:9:LYS:O	1:B:246:ALA:HA	2.01	0.61
1:B:213:PRO:HG2	1:B:216:TRP:CD2	2.35	0.61
1:A:377:GLN:HE21	1:A:377:GLN:H	1.46	0.61
1:B:476:PHE:O	1:B:499:GLU:HG3	1.99	0.61
1:B:11:VAL:HG21	1:B:503:ILE:HG21	1.83	0.61
1:B:189:PHE:HE1	1:B:191:HIS:NE2	1.99	0.61
1:A:146:MET:CE	1:A:336:LEU:HD21	2.31	0.60
1:B:141:PHE:O	1:B:145:VAL:HG23	2.00	0.60
1:B:454:PHE:HD2	1:B:454:PHE:H	1.44	0.60
1:B:63:ALA:HA	2:B:804:FAD:N5	2.14	0.60
1:B:233:ASN:HB3	1:B:245:ASN:HD21	1.65	0.60
1:B:48:LEU:CD2	1:B:63:ALA:HB3	2.32	0.60
1:A:63:ALA:HA	2:A:803:FAD:N5	2.16	0.59
1:B:67:HIS:ND1	1:B:195:ASN:ND2	2.51	0.59
1:A:104:ARG:NH2	1:A:159:ASP:OD2	2.34	0.59
1:A:67:HIS:ND1	1:A:195:ASN:ND2	2.51	0.58
1:B:141:PHE:CD1	1:B:187:THR:HG21	2.38	0.58
1:B:393:ARG:HG2	1:B:393:ARG:HH11	1.68	0.58
1:B:122:MET:HE2	1:B:145:VAL:HG13	1.86	0.58
1:A:150:LEU:O	1:A:153:ARG:HD2	2.04	0.58
1:A:54:TYR:CD2	1:A:55:GLN:HG3	2.39	0.58
1:A:423:ASN:ND2	1:A:426:ASN:HD22	2.02	0.57
1:B:10:LYS:O	1:B:247:ASP:HB2	2.04	0.57
1:A:41:ARG:NH1	1:A:443:ASP:OD2	2.35	0.57
1:B:110:ASP:HB3	1:B:113:LEU:HB2	1.85	0.57
1:B:233:ASN:HB3	1:B:245:ASN:ND2	2.20	0.56
1:B:267:ASN:O	1:B:268:LEU:O	2.23	0.56
1:B:122:MET:HG2	1:B:148:TYR:CD2	2.40	0.56
1:B:382:ASN:H	1:B:382:ASN:HD22	1.53	0.56
1:B:333:LEU:O	1:B:337:ASP:HB2	2.06	0.56
1:A:54:TYR:CZ	1:A:433:ARG:HG3	2.41	0.56
1:B:150:LEU:O	1:B:153:ARG:HG2	2.06	0.56
1:B:228:ARG:HH12	1:B:232:LYS:HA	1.71	0.55
1:A:213:PRO:HB2	1:A:216:TRP:CD1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:MET:HE3	1:B:434:ASN:HA	1.89	0.55
1:A:479:GLU:OE1	1:A:487:GLY:HA2	2.06	0.55
1:A:167:LEU:HA	1:A:316:LEU:HD22	1.90	0.54
1:A:217:LEU:HD21	1:A:219:LEU:HD21	1.89	0.54
1:B:212:PHE:HB2	1:B:213:PRO:HD2	1.89	0.54
1:B:248:TYR:CE2	1:B:473:ARG:HG2	2.42	0.54
1:B:335:GLU:O	1:B:339:MET:HG3	2.06	0.54
1:A:141:PHE:CD2	1:A:187:THR:HG21	2.42	0.54
1:B:165:PRO:O	1:B:169:ARG:HG3	2.08	0.54
1:B:278:LEU:CA	1:B:470:GLN:HE22	2.13	0.54
1:B:276:PRO:HB2	1:B:277:PRO:HD2	1.90	0.53
1:A:48:LEU:HD23	1:A:63:ALA:HB3	1.90	0.53
1:A:14:ILE:N	1:A:14:ILE:HD12	2.24	0.53
1:A:421:ILE:HG22	1:A:421:ILE:O	2.09	0.53
1:A:41:ARG:NH1	1:A:41:ARG:HG2	2.24	0.53
1:B:399:GLN:HB3	1:B:400:PRO:HD3	1.91	0.53
1:B:326:ILE:HG22	1:B:336:LEU:CD1	2.36	0.53
1:A:278:LEU:HA	1:A:470:GLN:HE22	1.72	0.53
1:A:64:SER:OG	1:A:296:LYS:NZ	2.42	0.53
1:A:322:GLU:HG3	1:A:342:ARG:HH22	1.72	0.52
1:A:322:GLU:HG2	1:A:342:ARG:HH22	1.75	0.52
1:A:12:ILE:HB	1:A:249:VAL:HG12	1.92	0.52
1:B:118:VAL:HG23	1:B:164:LEU:HD13	1.91	0.52
1:B:324:VAL:O	1:B:327:VAL:N	2.41	0.52
1:A:157:THR:OG1	1:A:160:GLN:HG3	2.10	0.52
1:A:463:VAL:HG21	1:A:483:MET:HE2	1.91	0.52
1:B:104:ARG:HD2	1:B:107:VAL:HG12	1.92	0.51
1:A:28:HIS:ND1	1:A:212:PHE:HA	2.26	0.51
1:B:137:SER:O	1:B:138:ASP:HB3	2.10	0.51
1:A:164:LEU:N	1:A:165:PRO:HD2	2.25	0.51
1:B:57:ARG:HD3	1:B:369:VAL:HG13	1.92	0.51
1:A:67:HIS:HA	1:A:195:ASN:HD22	1.76	0.50
1:B:502:ARG:HG2	1:B:502:ARG:HH11	1.77	0.50
1:B:508:LYS:O	1:B:509:LEU:C	2.49	0.50
1:B:222:GLU:O	1:B:238:CYS:HA	2.11	0.50
1:A:228:ARG:HG2	1:A:228:ARG:HH11	1.76	0.50
1:A:278:LEU:HA	1:A:470:GLN:NE2	2.27	0.50
1:B:32:ILE:HG22	1:B:33:GLN:N	2.27	0.50
1:B:393:ARG:HH11	1:B:393:ARG:CG	2.24	0.49
1:B:475:ARG:NH1	1:B:502:ARG:NH2	2.60	0.49
1:B:72:ASN:HD21	1:B:74:LEU:HB3	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ASP:HB3	1:A:192:GLN:HB2	1.95	0.49
1:A:122:MET:CE	1:A:145:VAL:HG22	2.43	0.49
1:B:157:THR:OG1	1:B:160:GLN:HG3	2.13	0.49
1:A:141:PHE:CE2	1:A:187:THR:HG21	2.48	0.48
1:B:78:GLU:OE1	1:B:89:ARG:HD3	2.13	0.48
1:B:189:PHE:HE1	1:B:191:HIS:CE1	2.31	0.48
1:A:154:GLN:O	1:A:154:GLN:HG2	2.12	0.48
1:A:8:LYS:CD	1:A:245:ASN:HD22	2.26	0.48
1:B:475:ARG:HH12	1:B:502:ARG:NH2	2.12	0.48
1:B:57:ARG:HD3	1:B:369:VAL:CG1	2.43	0.48
1:A:237:ASN:OD1	1:A:243:VAL:HG13	2.13	0.48
1:B:263:GLN:H	1:B:271:ARG:HH12	1.61	0.48
1:A:232:LYS:HB3	1:A:473:ARG:HH21	1.79	0.48
1:B:232:LYS:O	1:B:473:ARG:NH1	2.47	0.48
1:B:12:ILE:HG13	1:B:246:ALA:CB	2.44	0.48
1:A:381:THR:O	1:A:385:GLU:HG3	2.13	0.48
1:A:375:LEU:N	1:A:375:LEU:HD12	2.29	0.48
1:A:250:ILE:HD11	1:A:503:ILE:HD12	1.96	0.48
1:B:479:GLU:OE1	1:B:487:GLY:HA2	2.13	0.48
1:B:356:GLN:HB2	1:B:357:PRO:HD2	1.96	0.48
1:A:252:THR:O	2:A:803:FAD:H51A	2.14	0.47
1:A:239:GLU:C	1:A:241:GLY:H	2.17	0.47
1:B:72:ASN:HD22	1:B:73:PRO:N	2.13	0.47
1:A:418:MET:HA	1:A:433:ARG:O	2.15	0.47
1:A:508:LYS:C	1:A:510:GLU:H	2.16	0.47
1:A:206:GLN:O	1:A:210:GLN:HB2	2.15	0.47
1:B:288:LYS:HA	1:B:454:PHE:HZ	1.80	0.47
1:B:502:ARG:HG2	1:B:502:ARG:NH1	2.30	0.46
1:B:72:ASN:ND2	1:B:72:ASN:C	2.66	0.46
1:B:54:TYR:O	1:B:57:ARG:HG3	2.15	0.46
1:B:224:LYS:HE2	1:B:237:ASN:CB	2.46	0.46
1:A:259:ASN:O	1:A:262:VAL:HG22	2.14	0.46
1:B:99:TYR:CE2	1:B:167:LEU:HG	2.51	0.46
1:B:280:PRO:O	1:B:284:ASP:OD1	2.33	0.46
1:A:474:ILE:N	1:A:474:ILE:HD12	2.30	0.46
1:A:12:ILE:O	1:A:249:VAL:HA	2.15	0.46
1:A:12:ILE:HG12	1:A:246:ALA:HB2	1.98	0.46
1:B:22:LYS:HG2	1:B:493:TRP:CD1	2.51	0.46
1:B:102:GLU:O	1:B:404:LYS:HE2	2.15	0.46
1:B:70:LEU:HB2	1:B:192:GLN:O	2.16	0.46
1:A:169:ARG:O	1:A:172:GLU:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ASN:OD1	1:A:243:VAL:HG22	2.15	0.45
1:A:59:TYR:OH	1:A:300:GLU:HG2	2.17	0.45
1:A:167:LEU:O	1:A:170:TYR:HD2	1.99	0.45
1:A:264:PRO:O	1:A:265:GLU:HG3	2.15	0.45
1:B:11:VAL:HG22	1:B:248:TYR:HB2	1.98	0.45
1:A:255:GLN:OE1	1:A:289:ILE:HD12	2.16	0.45
1:B:54:TYR:CD2	1:B:55:GLN:HG3	2.52	0.45
1:B:167:LEU:HD23	1:B:167:LEU:C	2.37	0.45
1:A:266:LYS:HA	1:A:271:ARG:NH1	2.31	0.45
1:A:282:ILE:HG12	1:A:465:ALA:HB1	1.98	0.45
1:B:393:ARG:NH1	1:B:393:ARG:CG	2.80	0.45
1:B:228:ARG:NH1	1:B:232:LYS:HA	2.31	0.45
1:B:22:LYS:O	1:B:25:SER:HB3	2.17	0.44
1:A:116:GLU:OE2	1:A:116:GLU:N	2.34	0.44
1:A:406:MET:HE2	1:A:406:MET:HA	1.98	0.44
1:B:395:PHE:O	1:B:399:GLN:HB2	2.17	0.44
1:B:279:LYS:HB2	1:B:280:PRO:HD2	1.99	0.44
1:B:202:ASP:O	1:B:206:GLN:HB2	2.17	0.44
1:A:338:SER:O	1:A:341:GLU:HB2	2.17	0.44
1:B:171:LEU:HD13	1:B:187:THR:HG22	1.98	0.44
1:A:127:GLU:O	1:A:131:HIS:HB2	2.18	0.44
1:B:104:ARG:NH1	1:B:104:ARG:CG	2.75	0.44
1:B:507:LEU:O	1:B:508:LYS:C	2.56	0.44
1:A:101:ASP:OD2	1:A:103:GLU:HB3	2.18	0.44
1:B:247:ASP:O	1:B:473:ARG:HD3	2.18	0.44
1:B:439:ASN:HD21	1:B:442:ARG:HD3	1.82	0.44
1:B:260:LEU:O	1:B:262:VAL:N	2.50	0.44
1:B:72:ASN:ND2	1:B:74:LEU:H	2.17	0.43
1:A:63:ALA:HA	2:A:803:FAD:C4X	2.48	0.43
1:A:214:GLN:C	1:A:216:TRP:H	2.21	0.43
1:A:264:PRO:O	1:A:265:GLU:CB	2.65	0.43
1:A:91:VAL:HG13	1:A:91:VAL:O	2.17	0.43
1:B:340:LEU:O	1:B:342:ARG:N	2.50	0.43
1:B:439:ASN:ND2	1:B:442:ARG:HD3	2.34	0.43
1:A:218:LYS:HD2	1:A:221:CYS:HB3	1.99	0.43
1:B:113:LEU:O	1:B:114:LEU:C	2.57	0.43
1:A:93:ASP:O	1:A:312:LYS:HE2	2.18	0.43
1:A:289:ILE:HD11	1:A:462:MET:CG	2.47	0.43
1:A:434:ASN:ND2	1:A:435:ILE:H	2.16	0.43
1:B:273:GLU:OE1	1:B:273:GLU:HA	2.19	0.43
1:B:501:THR:O	1:B:504:SER:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:ASN:O	1:B:268:LEU:C	2.57	0.42
1:B:331:GLU:HB2	1:B:335:GLU:HG3	2.00	0.42
1:B:353:CYS:SG	1:B:400:PRO:HB2	2.59	0.42
1:B:266:LYS:HA	1:B:271:ARG:HD3	2.00	0.42
1:B:311:SER:HA	1:B:362:ASN:HB3	2.01	0.42
1:A:322:GLU:HG3	1:A:342:ARG:NH2	2.35	0.42
1:B:11:VAL:HA	1:B:248:TYR:O	2.19	0.42
1:B:228:ARG:N	1:B:275:GLN:O	2.43	0.42
1:B:240:ASP:OD2	1:B:242:THR:HG23	2.19	0.42
1:A:54:TYR:CE1	1:A:433:ARG:HB3	2.55	0.42
1:A:122:MET:HE1	1:A:145:VAL:HG22	2.00	0.42
1:B:248:TYR:CE1	1:B:507:LEU:HD21	2.55	0.42
1:B:189:PHE:CD1	1:B:189:PHE:O	2.73	0.42
1:B:266:LYS:HA	1:B:271:ARG:NE	2.34	0.42
1:B:260:LEU:C	1:B:262:VAL:H	2.22	0.42
1:B:28:HIS:O	1:B:31:GLY:N	2.52	0.42
1:A:199:LEU:HD23	1:A:199:LEU:HA	1.76	0.42
1:B:258:LEU:HD21	1:B:476:PHE:CE2	2.55	0.41
1:B:68:ASP:OD1	1:B:191:HIS:ND1	2.53	0.41
1:A:8:LYS:HD3	1:A:245:ASN:HD22	1.85	0.41
1:B:30:ASN:HD22	1:B:504:SER:HB3	1.85	0.41
1:A:288:LYS:O	1:A:289:ILE:CG2	2.66	0.41
1:A:505:ASP:O	1:A:508:LYS:HB3	2.20	0.41
1:B:161:ILE:CG2	1:B:327:VAL:HG21	2.50	0.41
1:B:63:ALA:HA	2:B:804:FAD:C4X	2.49	0.41
1:B:500:ALA:O	1:B:501:THR:C	2.58	0.41
1:A:213:PRO:HB2	1:A:216:TRP:CG	2.55	0.41
1:A:510:GLU:O	1:A:512:HIS:N	2.54	0.41
1:B:227:THR:HG23	1:B:275:GLN:CB	2.48	0.41
1:B:506:LEU:O	1:B:507:LEU:C	2.59	0.41
1:B:141:PHE:CE1	1:B:187:THR:HG21	2.55	0.41
1:A:377:GLN:N	1:A:377:GLN:NE2	2.58	0.41
1:B:26:THR:HB	1:B:500:ALA:HB1	2.03	0.41
1:A:332:ASN:OD1	1:A:334:ASP:HB2	2.20	0.41
1:B:414:VAL:HA	1:B:430:PRO:HG2	2.02	0.41
1:B:449:ALA:HB3	3:B:818:HOH:O	2.20	0.41
1:A:388:ARG:CB	1:A:388:ARG:HH11	2.24	0.41
1:A:238:CYS:HB2	1:A:240:ASP:OD2	2.21	0.41
1:A:41:ARG:CG	1:A:41:ARG:HH11	2.27	0.40
1:A:167:LEU:HA	1:A:316:LEU:CD2	2.51	0.40
1:A:470:GLN:HB3	1:A:474:ILE:HB	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:ASP:HB3	1:B:192:GLN:HB2	2.02	0.40
1:A:153:ARG:HG2	1:A:154:GLN:N	2.35	0.40
1:A:228:ARG:HD2	1:A:233:ASN:O	2.22	0.40
1:B:266:LYS:HA	1:B:271:ARG:CD	2.51	0.40
1:B:22:LYS:HG2	1:B:493:TRP:NE1	2.36	0.40
1:A:146:MET:HE1	1:A:323:PHE:HE1	1.86	0.40
1:B:234:VAL:O	1:B:245:ASN:HA	2.21	0.40
1:A:374:MET:HE1	1:A:376:MET:HE3	2.02	0.40
1:B:141:PHE:HE1	1:B:188:TYR:CE1	2.39	0.40
1:B:278:LEU:HD23	1:B:470:GLN:NE2	2.37	0.40
1:B:72:ASN:O	1:B:76:LEU:HG	2.22	0.40
1:B:164:LEU:N	1:B:165:PRO:HD2	2.36	0.40
1:B:252:THR:HG22	1:B:477:ALA:HB3	2.03	0.40
1:A:424:ILE:HG22	1:A:424:ILE:O	2.21	0.40
1:A:361:VAL:HB	1:A:373:MET:HB3	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ARG:NH2	1:A:269:ARG:NH2[4_555]	1.89	0.31
1:A:267:ASN:OD1	1:A:267:ASN:OD1[4_555]	1.90	0.30

## 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	492/513 (96%)	444 (90%)	34 (7%)	14 (3%)	6	4
1	B	479/513 (93%)	406 (85%)	54 (11%)	19 (4%)	4	2
All	All	971/1026 (95%)	850 (88%)	88 (9%)	33 (3%)	5	2

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	VAL
1	A	265	GLU
1	A	422	GLU
1	A	511	HIS
1	B	200	ASN
1	B	267	ASN
1	B	268	LEU
1	B	422	GLU
1	B	426	ASN
1	B	506	LEU
1	A	420	PRO
1	A	512	HIS
1	B	421	ILE
1	B	423	ASN
1	B	424	ILE
1	B	502	ARG
1	A	200	ASN
1	A	370	ALA
1	A	472	SER
1	B	261	SER
1	B	266	LYS
1	B	472	SER
1	B	507	LEU
1	A	137	SER
1	B	138	ASP
1	B	498	ARG
1	A	215	ASN
1	A	425	ALA
1	B	187	THR
1	B	503	ILE
1	A	241	GLY
1	B	32	ILE
1	A	469	GLY

### 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	439/454 (97%)	418 (95%)	21 (5%)	31	42
1	B	431/454 (95%)	412 (96%)	19 (4%)	35	46
All	All	870/908 (96%)	830 (95%)	40 (5%)	33	44

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	80	GLN
1	A	104	ARG
1	A	118	VAL
1	A	122	MET
1	A	131	HIS
1	A	132	GLN
1	A	134	LEU
1	A	153	ARG
1	A	174	TRP
1	A	179	TRP
1	A	201	TYR
1	A	210	GLN
1	A	221	CYS
1	A	239	GLU
1	A	242	THR
1	A	291	PHE
1	A	377	GLN
1	A	388	ARG
1	A	420	PRO
1	A	512	HIS
1	B	22	LYS
1	B	72	ASN
1	B	104	ARG
1	B	122	MET
1	B	168	CYS
1	B	179	TRP
1	B	201	TYR
1	B	206	GLN
1	B	214	GLN
1	B	221	CYS
1	B	228	ARG
1	B	239	GLU
1	B	291	PHE
1	B	362	ASN

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Mol	Chain	Res	Type
1	B	377	GLN
1	B	382	ASN
1	B	393	ARG
1	B	412	GLU
1	B	422	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	49	GLN
1	A	80	GLN
1	A	131	HIS
1	A	195	ASN
1	A	245	ASN
1	A	362	ASN
1	A	377	GLN
1	A	426	ASN
1	A	434	ASN
1	B	30	ASN
1	B	33	GLN
1	B	72	ASN
1	B	109	HIS
1	B	120	ASN
1	B	195	ASN
1	B	259	ASN
1	B	283	GLN
1	B	318	ASN
1	B	329	ASN
1	B	362	ASN
1	B	377	GLN
1	B	382	ASN
1	B	399	GLN
1	B	434	ASN
1	B	439	ASN
1	B	468	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 ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	FAD	A	803	-	48,58,58	1.45	9 (18%)	54,89,89	2.72	13 (24%)
2	FAD	B	804	-	48,58,58	1.40	7 (14%)	54,89,89	2.70	15 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	803	-	-	0/30/50/50	0/6/6/6
2	FAD	B	804	-	-	0/30/50/50	0/6/6/6

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	803	FAD	C2A-N1A	2.06	1.37	1.33
2	B	804	FAD	C5B-C4B	2.08	1.58	1.51
2	A	803	FAD	C1'-N10	2.09	1.50	1.48
2	B	804	FAD	C2A-N3A	2.14	1.36	1.32
2	A	803	FAD	C2A-N3A	2.18	1.36	1.32
2	B	804	FAD	C2A-N1A	2.27	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	803	FAD	C5B-C4B	2.38	1.59	1.51
2	A	803	FAD	C5X-N5	2.56	1.39	1.35
2	B	804	FAD	C5X-N5	2.63	1.39	1.35
2	A	803	FAD	O4B-C1B	2.75	1.44	1.41
2	A	803	FAD	C4-N3	2.97	1.38	1.33
2	B	804	FAD	C9A-N10	3.22	1.43	1.38
2	B	804	FAD	C4-N3	3.51	1.39	1.33
2	A	803	FAD	C4X-N5	3.77	1.39	1.33
2	B	804	FAD	C4X-N5	3.85	1.39	1.33
2	A	803	FAD	C9A-N10	4.12	1.44	1.38

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	804	FAD	O2A-PA-O5B	-7.18	72.23	108.46
2	A	803	FAD	O2A-PA-O5B	-7.03	73.00	108.46
2	B	804	FAD	O2A-PA-O1A	-5.54	82.48	112.53
2	A	803	FAD	O3P-PA-O5B	-5.32	88.81	102.94
2	B	804	FAD	O3P-PA-O5B	-5.19	89.18	102.94
2	A	803	FAD	O2A-PA-O1A	-5.14	84.68	112.53
2	A	803	FAD	C4X-C4-N3	-4.69	117.18	123.59
2	A	803	FAD	N3A-C2A-N1A	-4.61	125.37	128.89
2	B	804	FAD	C4X-C4-N3	-4.60	117.30	123.59
2	B	804	FAD	N3A-C2A-N1A	-4.44	125.49	128.89
2	A	803	FAD	C4-C4X-C10	-2.90	118.08	119.94
2	B	804	FAD	O3'-C3'-C4'	-2.79	101.71	108.75
2	B	804	FAD	C4-C4X-C10	-2.65	118.24	119.94
2	A	803	FAD	O3'-C3'-C4'	-2.32	102.90	108.75
2	B	804	FAD	C4X-C10-N10	-2.10	119.28	120.52
2	B	804	FAD	C4B-O4B-C1B	-2.05	107.47	109.72
2	A	803	FAD	O3P-P-O5'	2.46	109.46	102.94
2	B	804	FAD	O3P-P-O5'	2.48	109.51	102.94
2	B	804	FAD	C1'-N10-C9A	2.64	121.82	118.86
2	A	803	FAD	C1'-N10-C9A	3.14	122.38	118.86
2	A	803	FAD	C4X-N5-C5X	3.53	120.82	116.76
2	A	803	FAD	O2A-PA-O3P	3.81	122.37	105.09
2	B	804	FAD	C4X-N5-C5X	3.91	121.26	116.76
2	B	804	FAD	O2A-PA-O3P	4.05	123.48	105.09
2	B	804	FAD	O5B-PA-O1A	6.53	134.94	109.62
2	A	803	FAD	O5B-PA-O1A	6.86	136.26	109.62
2	B	804	FAD	C4-N3-C2	9.89	123.80	115.25
2	A	803	FAD	C4-N3-C2	10.69	124.49	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	803	FAD	3	0
2	B	804	FAD	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	498/513 (97%)	0.51	29 (5%)	26 35	30, 47, 75, 116	22 (4%)
1	B	487/513 (94%)	0.51	43 (8%)	12 18	31, 48, 81, 98	33 (6%)
All	All	985/1026 (96%)	0.51	72 (7%)	18 25	30, 48, 80, 116	55 (5%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	424	ILE	12.0
1	A	425	ALA	11.2
1	A	512	HIS	8.7
1	A	511	HIS	8.0
1	B	423	ASN	8.0
1	A	428	ASN	6.9
1	B	424	ILE	6.7
1	A	423	ASN	6.5
1	A	422	GLU	6.3
1	A	513	HIS	6.3
1	B	231	SER	6.2
1	A	7	ALA	5.9
1	A	426	ASN	5.9
1	A	421	ILE	5.7
1	B	264	PRO	5.5
1	B	425	ALA	5.3
1	A	189	PHE	5.3
1	A	6	PRO	4.6
1	A	427	ALA	4.4
1	A	231	SER	4.3
1	B	507	LEU	4.2
1	B	265	GLU	4.0
1	B	238	CYS	3.9
1	B	460	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	9	LYS	3.6
1	A	230	PRO	3.5
1	A	31	GLY	3.4
1	B	333	LEU	3.4
1	B	224	LYS	3.4
1	A	420	PRO	3.3
1	B	235	THR	3.2
1	A	8	LYS	3.2
1	B	230	PRO	3.2
1	B	275	GLN	3.2
1	B	174	TRP	3.1
1	B	31	GLY	3.1
1	B	335	GLU	3.0
1	B	503	ILE	3.0
1	B	428	ASN	3.0
1	B	36	LEU	3.0
1	A	508	LYS	2.9
1	B	427	ALA	2.9
1	B	278	LEU	2.9
1	B	426	ASN	2.9
1	A	336	LEU	2.8
1	A	419	ARG	2.8
1	B	508	LYS	2.8
1	B	234	VAL	2.7
1	B	237	ASN	2.7
1	B	473	ARG	2.7
1	B	227	THR	2.7
1	B	229	GLU	2.7
1	A	340	LEU	2.6
1	B	258	LEU	2.6
1	B	35	CYS	2.6
1	B	340	LEU	2.6
1	A	431	VAL	2.6
1	A	339	MET	2.5
1	B	336	LEU	2.5
1	B	350	SER	2.5
1	B	236	VAL	2.5
1	B	32	ILE	2.4
1	B	338	SER	2.4
1	A	269	ARG	2.3
1	B	228	ARG	2.2
1	A	415	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	421	ILE	2.2
1	A	232	LYS	2.2
1	B	332	ASN	2.2
1	A	32	ILE	2.2
1	B	454	PHE	2.1
1	B	216	TRP	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
2	FAD	A	803	53/53	0.95	0.17	0.63	27,35,45,52	0
2	FAD	B	804	53/53	0.93	0.14	0.08	25,41,48,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.