



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:28 PM GMT

PDB ID : 3BI5  
Title : Crystal structures of fms1 in complex with its inhibitors  
Authors : Huang, Q.; Hao, Q.  
Deposited on : 2007-11-29  
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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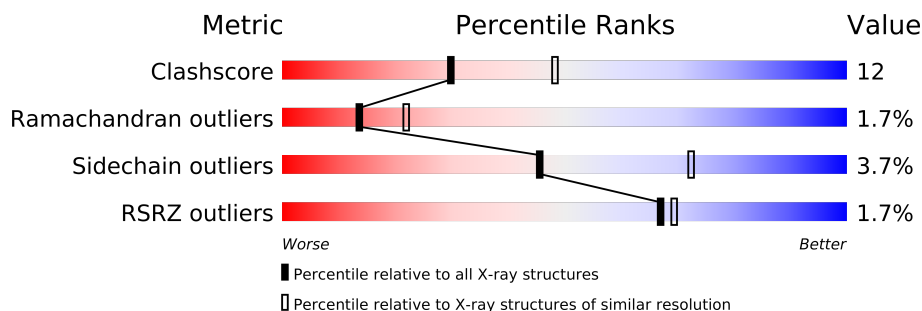
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.50 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	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	516	
1	B	516	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	DIA	A	2841	-	X
3	DIA	B	2842	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7975 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

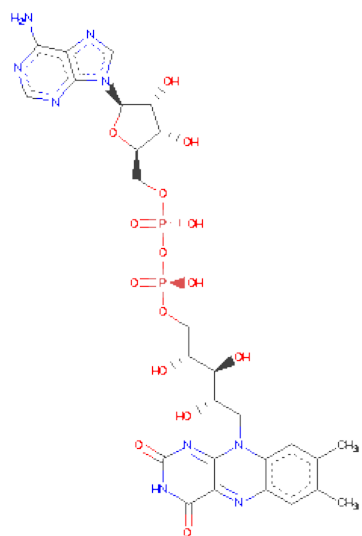
- Molecule 1 is a protein called Polyamine oxidase FMS1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	0	0
			3890	2462	681	725	22			
1	B	499	Total	C	N	O	S	0	0	0
			3842	2422	668	730	22			

There are 16 discrepancies between the modelled and reference sequences:

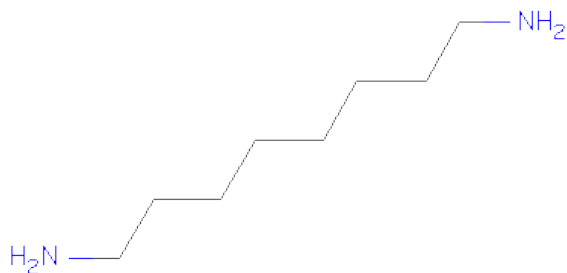
Chain	Residue	Modelled	Actual	Comment	Reference
A	509	LEU	-	EXPRESSION TAG	UNP P50264
A	510	GLU	-	EXPRESSION TAG	UNP P50264
A	511	HIS	-	EXPRESSION TAG	UNP P50264
A	512	HIS	-	EXPRESSION TAG	UNP P50264
A	513	HIS	-	EXPRESSION TAG	UNP P50264
A	514	HIS	-	EXPRESSION TAG	UNP P50264
A	515	HIS	-	EXPRESSION TAG	UNP P50264
A	516	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
B	514	HIS	-	EXPRESSION TAG	UNP P50264
B	515	HIS	-	EXPRESSION TAG	UNP P50264
B	516	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 OCTANE 1,8-DIAMINE (three-letter code: DIA) (formula:  $C_8H_{20}N_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			10	8	2		
3	B	1	Total	C	N	0	0
			10	8	2		

- Molecule 4 is water.

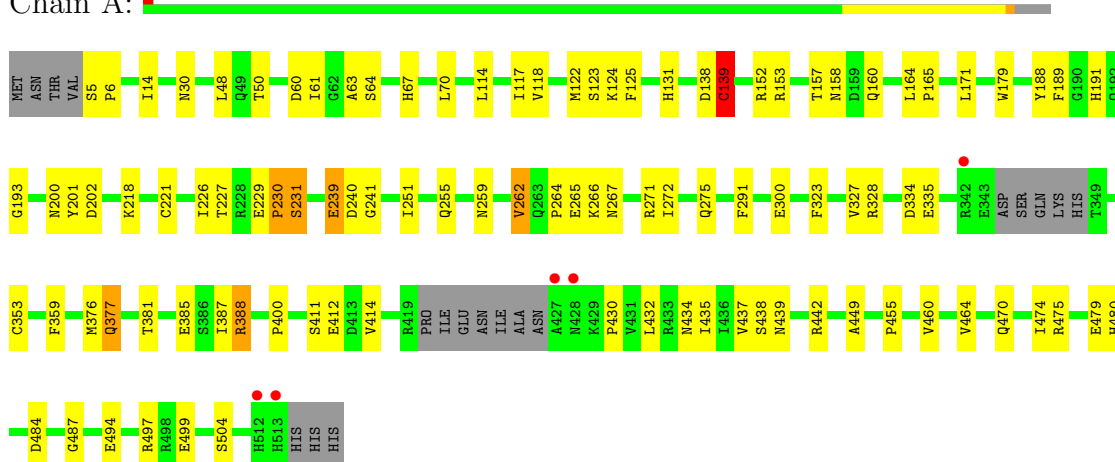
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	69	Total 69	O 69	0	0
4	B	48	Total 48	O 48	0	0

### 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.

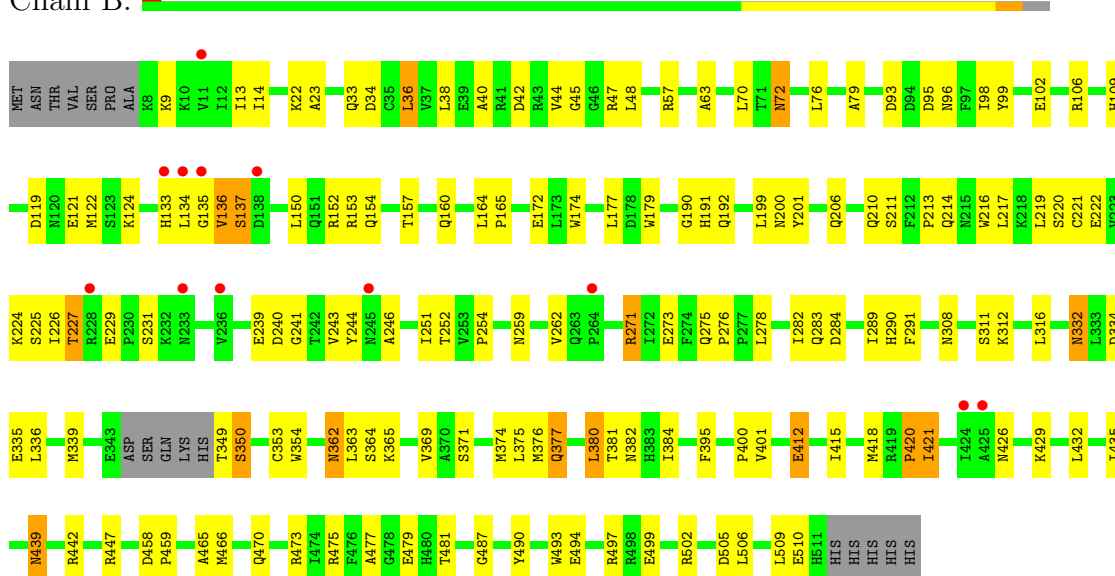
#### • Molecule 1: Polyamine oxidase FMS1

Chain A:



#### • Molecule 1: Polyamine oxidase FMS1

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	164.42Å 103.00Å 77.24Å 90.00° 94.30° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 48.28 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.4 (50.00-2.50) 72.1 (48.28-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.18 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.228 , 0.290 0.238 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	28.1	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 45.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 67830 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7975	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DIA, 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	0.40	0/3972	0.62	0/5373
1	B	0.37	0/3920	0.60	0/5306
All	All	0.39	0/7892	0.61	0/10679

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3890	0	3743	63	0
1	B	3842	0	3633	127	0
2	A	53	0	31	3	0
2	B	53	0	31	2	0
3	A	10	0	20	2	0
3	B	10	0	20	2	0
4	A	69	0	0	2	0
4	B	48	0	0	1	0
All	All	7975	0	7478	186	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (186) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:133:HIS:HB3	1:B:136:VAL:HG13	1.36	1.08
1:B:278:LEU:HA	1:B:470:GLN:HE22	1.14	1.06
1:B:227:THR:HG23	1:B:275:GLN:HB3	1.49	0.91
1:B:282:ILE:HD13	1:B:465:ALA:HB1	1.55	0.85
1:B:278:LEU:HA	1:B:470:GLN:NE2	1.94	0.82
1:A:353:CYS:SG	1:A:400:PRO:HG2	2.21	0.80
1:A:264:PRO:O	1:A:265:GLU:HB3	1.81	0.79
1:B:353:CYS:SG	1:B:400:PRO:HG2	2.24	0.78
1:A:377:GLN:H	1:A:377:GLN:NE2	1.84	0.76
1:B:380:LEU:HD22	1:B:384:ILE:HG12	1.66	0.75
1:B:308:ASN:O	1:B:365:LYS:HD2	1.88	0.74
1:B:506:LEU:O	1:B:510:GLU:HG3	1.87	0.73
1:B:479:GLU:OE1	1:B:487:GLY:HA2	1.88	0.73
1:A:118:VAL:HG23	1:A:164:LEU:HD13	1.70	0.72
1:B:213:PRO:HG2	1:B:216:TRP:CE2	2.24	0.72
1:B:439:ASN:HD21	1:B:442:ARG:HB2	1.55	0.71
1:B:275:GLN:NE2	1:B:276:PRO:HA	2.06	0.71
1:B:213:PRO:HG2	1:B:216:TRP:CD2	2.25	0.70
1:B:252:THR:HG22	1:B:477:ALA:HB3	1.76	0.67
1:B:48:LEU:CD2	1:B:63:ALA:HB3	2.26	0.66
1:A:239:GLU:HG3	1:A:240:ASP:N	2.10	0.66
1:B:362:ASN:ND2	1:B:364:SER:H	1.93	0.66
1:A:193:GLY:HA2	1:B:121:GLU:HG3	1.78	0.65
1:B:282:ILE:CD1	1:B:465:ALA:HB1	2.26	0.65
1:A:259:ASN:O	1:A:262:VAL:HG22	1.97	0.64
1:B:72:ASN:C	1:B:72:ASN:HD22	2.01	0.64
1:B:172:GLU:HG2	1:B:177:LEU:O	1.97	0.64
1:B:251:ILE:HD12	1:B:251:ILE:N	2.13	0.62
1:A:229:GLU:O	1:A:231:SER:N	2.32	0.62
1:B:239:GLU:HA	1:B:239:GLU:OE1	1.99	0.61
1:A:414:VAL:HA	1:A:430:PRO:HG2	1.82	0.61
1:A:227:THR:HG23	1:A:275:GLN:HB2	1.82	0.61
1:A:48:LEU:CD2	1:A:63:ALA:HB3	2.32	0.60
1:A:479:GLU:OE1	1:A:487:GLY:HA2	2.02	0.60
1:B:473:ARG:HG3	1:B:473:ARG:HH11	1.65	0.60
1:B:439:ASN:ND2	1:B:442:ARG:HB2	2.15	0.60
1:B:271:ARG:HG3	1:B:271:ARG:HH11	1.65	0.60
1:A:5:SER:N	1:A:6:PRO:CD	2.65	0.60
1:B:502:ARG:HG2	1:B:502:ARG:HH11	1.68	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:362:ASN:HD21	1:B:364:SER:CB	2.17	0.58
1:B:133:HIS:O	1:B:134:LEU:HB2	2.04	0.57
1:A:158:ASN:HD22	1:A:328:ARG:HH21	1.51	0.57
1:B:376:MET:HG3	1:B:381:THR:OG1	2.04	0.57
1:B:213:PRO:O	1:B:216:TRP:HB2	2.05	0.57
1:A:385:GLU:OE2	1:A:438:SER:HB2	2.04	0.57
1:A:152:ARG:CZ	1:B:70:LEU:HD23	2.35	0.56
1:A:226:ILE:HD12	1:A:272:ILE:HG21	1.88	0.56
1:B:415:ILE:HD13	1:B:426:ASN:OD1	2.06	0.56
1:B:14:ILE:CD1	1:B:226:ILE:HD11	2.35	0.56
1:A:262:VAL:O	1:A:262:VAL:HG23	2.06	0.55
1:A:376:MET:HG3	1:A:381:THR:OG1	2.06	0.55
1:B:63:ALA:HA	2:B:802:FAD:N5	2.21	0.55
1:A:60:ASP:HB3	4:A:2850:HOH:O	2.05	0.55
1:B:311:SER:C	1:B:312:LYS:HD3	2.28	0.54
1:B:95:ASP:OD1	1:B:96:ASN:N	2.39	0.54
1:A:475:ARG:HB3	1:A:499:GLU:OE1	2.08	0.54
1:A:359:PHE:CE2	3:A:2841:DIA:HC71	2.43	0.54
1:B:225:SER:HB3	1:B:273:GLU:HB3	1.89	0.54
1:B:412:GLU:CD	1:B:429:LYS:HD2	2.28	0.53
1:B:45:GLY:O	1:B:48:LEU:HB2	2.08	0.53
1:A:157:THR:HG23	1:A:160:GLN:OE1	2.09	0.53
1:A:164:LEU:N	1:A:165:PRO:HD2	2.24	0.53
1:B:76:LEU:O	1:B:79:ALA:HB3	2.08	0.53
4:A:2862:HOH:O	1:B:109:HIS:HE1	1.92	0.53
1:B:362:ASN:C	1:B:362:ASN:ND2	2.61	0.52
1:B:382:ASN:H	1:B:382:ASN:ND2	2.06	0.52
1:B:332:ASN:ND2	1:B:334:ASP:H	2.06	0.52
1:B:48:LEU:HD23	1:B:63:ALA:HB3	1.91	0.52
1:B:502:ARG:NH1	1:B:502:ARG:HG2	2.25	0.52
1:B:251:ILE:HD12	1:B:251:ILE:H	1.74	0.52
1:B:439:ASN:ND2	1:B:442:ARG:HD3	2.25	0.52
1:B:174:TRP:CE3	3:B:2842:DIA:HC51	2.44	0.51
1:A:124:LYS:HE3	1:B:191:HIS:O	2.11	0.51
1:B:9:LYS:O	1:B:246:ALA:HA	2.11	0.51
1:B:157:THR:OG1	1:B:160:GLN:HG3	2.10	0.51
1:B:225:SER:CB	1:B:273:GLU:HB3	2.40	0.51
1:B:48:LEU:HD21	1:B:63:ALA:HB3	1.92	0.51
1:B:262:VAL:HG12	1:B:283:GLN:HG2	1.91	0.51
1:B:335:GLU:HG2	1:B:339:MET:HE3	1.92	0.50
1:A:63:ALA:HA	2:A:801:FAD:N5	2.26	0.50
1:B:271:ARG:HD3	1:B:271:ARG:C	2.32	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:219:LEU:O	1:B:220:SER:HB2	2.11	0.50
1:B:164:LEU:N	1:B:165:PRO:HD2	2.27	0.50
1:A:437:VAL:HG12	1:A:438:SER:N	2.27	0.50
1:B:135:GLY:O	1:B:137:SER:N	2.44	0.49
1:A:470:GLN:HB3	1:A:474:ILE:HB	1.95	0.49
1:B:432:LEU:HD21	1:B:435:ILE:HD11	1.94	0.49
1:B:475:ARG:HB3	1:B:499:GLU:OE1	2.13	0.49
1:B:36:LEU:HD22	1:B:38:LEU:CD2	2.43	0.49
1:A:48:LEU:HD22	1:A:63:ALA:HB3	1.95	0.49
1:A:5:SER:N	1:A:6:PRO:HD2	2.28	0.48
1:A:30:ASN:HD22	1:A:504:SER:CB	2.26	0.48
1:B:311:SER:O	1:B:312:LYS:HD3	2.13	0.48
1:B:13:ILE:HD13	1:B:23:ALA:HB3	1.96	0.48
1:B:439:ASN:HD21	1:B:442:ARG:HD3	1.79	0.48
1:A:377:GLN:HE21	1:A:377:GLN:H	1.59	0.48
1:B:494:GLU:OE2	1:B:497:ARG:NH2	2.47	0.48
1:B:284:ASP:HA	4:B:2855:HOH:O	2.14	0.48
1:A:122:MET:O	1:A:125:PHE:HB3	2.13	0.48
1:B:353:CYS:SG	1:B:401:VAL:HG13	2.54	0.47
1:B:72:ASN:ND2	1:B:72:ASN:C	2.68	0.47
1:B:57:ARG:HD3	1:B:369:VAL:CG1	2.44	0.47
1:A:153:ARG:NH2	1:A:327:VAL:O	2.47	0.47
1:A:189:PHE:CZ	1:A:191:HIS:NE2	2.83	0.47
1:B:44:VAL:CG1	1:B:217:LEU:HD21	2.45	0.47
1:B:22:LYS:HG3	1:B:493:TRP:CD1	2.49	0.47
1:A:158:ASN:ND2	1:A:328:ARG:HH21	2.13	0.47
1:B:395:PHE:HB2	1:B:418:MET:CE	2.46	0.47
1:B:473:ARG:NH1	1:B:473:ARG:HG3	2.29	0.46
1:B:206:GLN:O	1:B:210:GLN:HG3	2.15	0.46
1:A:385:GLU:O	1:A:388:ARG:HG2	2.15	0.46
1:B:420:PRO:O	1:B:421:ILE:HG12	2.15	0.46
1:B:243:VAL:HG12	1:B:244:TYR:N	2.31	0.46
1:B:190:GLY:C	1:B:192:GLN:HE21	2.19	0.46
1:B:36:LEU:HD22	1:B:38:LEU:HD23	1.97	0.46
1:B:362:ASN:HD22	1:B:362:ASN:C	2.17	0.46
1:B:259:ASN:O	1:B:262:VAL:HG22	2.16	0.46
1:A:255:GLN:HB2	1:A:480:HIS:CD2	2.51	0.46
1:B:199:LEU:HA	1:B:199:LEU:HD23	1.82	0.45
1:B:99:TYR:HB3	1:B:316:LEU:HD11	1.99	0.45
1:B:240:ASP:OD1	1:B:241:GLY:N	2.50	0.45
1:B:214:GLN:C	1:B:216:TRP:H	2.20	0.45
1:B:213:PRO:CG	1:B:216:TRP:CE2	3.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:102:GLU:HB2	1:B:354:TRP:CZ2	2.52	0.44
1:A:114:LEU:HD22	1:A:117:ILE:HD12	1.98	0.44
1:B:98:ILE:HG23	1:B:106:ARG:NE	2.32	0.44
1:B:362:ASN:HD21	1:B:364:SER:HB3	1.82	0.44
1:B:119:ASP:O	1:B:122:MET:HB3	2.17	0.44
1:B:150:LEU:CD1	1:B:153:ARG:HH21	2.30	0.44
1:B:93:ASP:O	1:B:312:LYS:HE3	2.17	0.44
1:A:226:ILE:HD13	1:A:251:ILE:HD11	1.99	0.44
1:B:377:GLN:NE2	1:B:377:GLN:H	2.16	0.44
1:A:50:THR:OG1	1:A:202:ASP:HB3	2.16	0.44
1:A:61:ILE:HA	1:A:61:ILE:HD12	1.85	0.44
1:A:494:GLU:OE1	1:A:497:ARG:NH2	2.50	0.43
1:B:133:HIS:HB3	1:B:136:VAL:CG1	2.27	0.43
1:A:70:LEU:HD23	1:B:152:ARG:CZ	2.49	0.43
1:B:505:ASP:O	1:B:509:LEU:HG	2.18	0.43
1:A:449:ALA:HB1	2:A:801:FAD:HM83	2.01	0.43
1:B:136:VAL:HG23	1:B:136:VAL:O	2.19	0.43
1:B:362:ASN:HD21	1:B:364:SER:HB2	1.84	0.43
1:B:153:ARG:HG3	1:B:154:GLN:N	2.33	0.43
1:A:266:LYS:HA	1:A:271:ARG:HD3	2.00	0.43
1:B:222:GLU:O	1:B:239:GLU:N	2.52	0.42
1:A:434:ASN:ND2	1:A:435:ILE:H	2.17	0.42
1:B:33:GLN:O	1:B:34:ASP:HB2	2.19	0.42
1:A:449:ALA:CB	2:A:801:FAD:HM83	2.49	0.42
1:A:460:VAL:O	1:A:464:VAL:HG23	2.18	0.42
1:B:479:GLU:HG2	2:B:802:FAD:O3'	2.19	0.42
1:B:40:ALA:O	1:B:220:SER:HA	2.20	0.42
1:A:434:ASN:ND2	1:A:435:ILE:N	2.68	0.42
1:A:439:ASN:ND2	1:A:442:ARG:HB2	2.33	0.42
1:B:271:ARG:HG3	1:B:271:ARG:NH1	2.33	0.42
1:A:255:GLN:HB2	1:A:480:HIS:CG	2.54	0.42
1:A:138:ASP:O	1:A:139:CYS:SG	2.77	0.42
1:A:123:SER:HB3	1:A:188:TYR:CE2	2.54	0.42
1:A:411:SER:OG	1:A:412:GLU:N	2.52	0.42
1:A:229:GLU:HA	1:A:230:PRO:HD2	1.92	0.42
1:B:174:TRP:CE2	3:B:2842:DIA:HC71	2.55	0.42
1:B:99:TYR:O	1:B:106:ARG:HA	2.20	0.42
1:A:239:GLU:C	1:A:241:GLY:H	2.21	0.41
1:A:171:LEU:HD23	1:A:171:LEU:HA	1.86	0.41
1:A:14:ILE:N	1:A:14:ILE:HD12	2.35	0.41
1:A:323:PHE:O	1:A:327:VAL:HG23	2.19	0.41
1:B:36:LEU:HD23	1:B:216:TRP:O	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:109:HIS:CG	1:B:109:HIS:O	2.74	0.41
1:B:395:PHE:HB2	1:B:418:MET:HE2	2.03	0.41
1:B:229:GLU:C	1:B:231:SER:H	2.23	0.41
1:B:229:GLU:C	1:B:231:SER:N	2.74	0.41
1:B:466:MET:HG3	1:B:481:THR:HG22	2.03	0.41
1:B:42:ASP:OD1	1:B:42:ASP:C	2.59	0.41
1:A:300:GLU:O	1:A:432:LEU:HD12	2.21	0.40
1:B:363:LEU:HB2	1:B:371:SER:O	2.21	0.40
1:B:47:ARG:NH2	1:B:254:PRO:HB3	2.36	0.40
1:B:275:GLN:HE21	1:B:276:PRO:HA	1.80	0.40
1:B:72:ASN:HD21	1:B:490:TYR:HB2	1.87	0.40
1:B:376:MET:SD	1:B:381:THR:HA	2.61	0.40
1:B:466:MET:CG	1:B:481:THR:HG22	2.51	0.40
1:B:458:ASP:HA	1:B:459:PRO:HD2	1.91	0.40
1:B:251:ILE:H	1:B:251:ILE:CD1	2.35	0.40
1:B:224:LYS:HB3	1:B:239:GLU:OE1	2.22	0.40
1:A:67:HIS:NE2	3:A:2841:DIA:HC12	2.36	0.40
1:B:374:MET:HG2	1:B:375:LEU:N	2.36	0.40
1:B:133:HIS:C	1:B:135:GLY:H	2.25	0.40
1:A:138:ASP:OD2	1:A:455:PRO:HA	2.21	0.40
1:B:349:THR:O	1:B:350:SER:CB	2.70	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	491/516 (95%)	450 (92%)	34 (7%)	7 (1%)	16	27
1	B	495/516 (96%)	430 (87%)	55 (11%)	10 (2%)	11	17
All	All	986/1032 (96%)	880 (89%)	89 (9%)	17 (2%)	14	22

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	ASN
1	A	230	PRO
1	A	231	SER
1	B	136	VAL
1	B	200	ASN
1	B	289	ILE
1	B	290	HIS
1	B	137	SER
1	B	421	ILE
1	A	131	HIS
1	B	211	SER
1	B	420	PRO
1	A	262	VAL
1	B	291	PHE
1	A	139	CYS
1	A	387	ILE
1	B	350	SER

### 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	414/457 (91%)	400 (97%)	14 (3%)	49	75
1	B	403/457 (88%)	387 (96%)	16 (4%)	42	68
All	All	817/914 (89%)	787 (96%)	30 (4%)	45	72

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	SER
1	A	139	CYS
1	A	179	TRP
1	A	201	TYR
1	A	218	LYS
1	A	221	CYS
1	A	239	GLU
1	A	267	ASN
1	A	291	PHE

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Mol	Chain	Res	Type
1	A	334	ASP
1	A	335	GLU
1	A	377	GLN
1	A	388	ARG
1	A	484	ASP
1	B	36	LEU
1	B	72	ASN
1	B	124	LYS
1	B	179	TRP
1	B	201	TYR
1	B	221	CYS
1	B	227	THR
1	B	271	ARG
1	B	332	ASN
1	B	336	LEU
1	B	362	ASN
1	B	377	GLN
1	B	380	LEU
1	B	412	GLU
1	B	439	ASN
1	B	447	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	30	ASN
1	A	80	GLN
1	A	84	ASN
1	A	109	HIS
1	A	158	ASN
1	A	192	GLN
1	A	267	ASN
1	A	362	ASN
1	A	377	GLN
1	A	434	ASN
1	A	439	ASN
1	B	29	GLN
1	B	72	ASN
1	B	109	HIS
1	B	191	HIS
1	B	192	GLN

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Mol	Chain	Res	Type
1	B	275	GLN
1	B	329	ASN
1	B	362	ASN
1	B	377	GLN
1	B	382	ASN
1	B	434	ASN
1	B	439	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

4 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	$\# Z  > 2$
3	DIA	A	2841	-	9,9,9	0.25	0	8,8,8	0.98	0
2	FAD	A	801	-	58,58,58	1.35	9 (15%)	85,89,89	1.98	16 (18%)
3	DIA	B	2842	-	9,9,9	0.26	0	8,8,8	0.87	0
2	FAD	B	802	-	58,58,58	1.35	6 (10%)	85,89,89	1.96	15 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DIA	A	2841	-	-	0/7/7/7	0/0/0/0
2	FAD	A	801	-	-	0/34/50/50	0/1/6/6
3	DIA	B	2842	-	-	0/7/7/7	0/0/0/0
2	FAD	B	802	-	-	0/34/50/50	0/1/6/6

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	802	FAD	C9A-N10	3.80	1.44	1.38
2	A	801	FAD	C9A-N10	3.69	1.44	1.38
2	A	801	FAD	C2A-N3A	2.75	1.37	1.32
2	B	802	FAD	C1'-C2'	2.75	1.54	1.51
2	B	802	FAD	C1'-N10	2.68	1.51	1.48
2	A	801	FAD	PA-O3P	2.64	1.64	1.59
2	A	801	FAD	C5B-C4B	2.61	1.60	1.51
2	A	801	FAD	C5X-N5	2.54	1.39	1.35
2	A	801	FAD	C2A-N1A	2.47	1.38	1.33
2	B	802	FAD	C2A-N1A	2.40	1.38	1.33
2	A	801	FAD	C1'-N10	2.30	1.50	1.48
2	B	802	FAD	C2A-N3A	2.16	1.36	1.32
2	A	801	FAD	C5'-C4'	2.14	1.55	1.51
2	B	802	FAD	PA-O3P	2.03	1.63	1.59
2	A	801	FAD	O2'-C2'	-2.01	1.38	1.43

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	FAD	O5B-PA-O1A	7.09	137.15	109.37
2	A	801	FAD	O2A-PA-O5B	-7.04	73.04	108.51
2	B	802	FAD	O5B-PA-O1A	6.84	136.16	109.37
2	B	802	FAD	O2A-PA-O5B	-6.55	75.50	108.51
2	A	801	FAD	O3P-PA-O1A	-5.34	72.93	111.28
2	B	802	FAD	O3P-PA-O1A	-5.21	73.85	111.28
2	A	801	FAD	O2A-PA-O1A	-4.92	84.73	112.21
2	B	802	FAD	C2-N1-C10	4.75	119.76	114.98
2	B	802	FAD	O2A-PA-O1A	-4.60	86.52	112.21
2	B	802	FAD	O3P-PA-O5B	-4.39	83.77	103.41
2	A	801	FAD	C2-N1-C10	4.21	119.22	114.98
2	A	801	FAD	N3A-C2A-N1A	-4.09	125.29	128.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	802	FAD	C4X-N5-C5X	4.08	121.27	116.69
2	B	802	FAD	O2A-PA-O3P	4.02	124.19	105.14
2	A	801	FAD	O4B-C1B-C2B	-3.86	100.86	106.77
2	A	801	FAD	C4X-N5-C5X	3.83	121.00	116.69
2	B	802	FAD	O4B-C1B-C2B	-3.70	101.11	106.77
2	A	801	FAD	O3P-PA-O5B	-3.67	86.99	103.41
2	B	802	FAD	N3A-C2A-N1A	-3.65	125.66	128.71
2	A	801	FAD	C1'-N10-C9A	3.29	122.08	118.87
2	A	801	FAD	O2A-PA-O3P	3.14	120.03	105.14
2	B	802	FAD	C4X-C10-N10	-3.10	118.96	120.51
2	B	802	FAD	C1'-N10-C9A	2.74	121.53	118.87
2	A	801	FAD	C4X-C10-N10	-2.66	119.18	120.51
2	A	801	FAD	C2'-C1'-N10	2.58	115.87	112.45
2	B	802	FAD	O3'-C3'-C4'	-2.42	102.62	108.74
2	B	802	FAD	C5X-C9A-N10	2.36	119.13	116.80
2	A	801	FAD	C5X-C9A-N10	2.30	119.06	116.80
2	B	802	FAD	C4B-O4B-C1B	-2.24	107.32	109.75
2	A	801	FAD	N3A-C4A-N9A	2.08	129.19	125.43
2	A	801	FAD	O4B-C1B-N9A	-2.01	106.58	108.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	497/516 (96%)	-0.34	5 (1%) 79 81	22, 39, 65, 90	0
1	B	499/516 (96%)	-0.19	12 (2%) 56 58	27, 46, 74, 97	0
All	All	996/1032 (96%)	-0.27	17 (1%) 67 69	22, 43, 73, 97	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	425	ALA	4.0
1	A	342	ARG	3.6
1	B	134	LEU	3.5
1	A	512	HIS	3.4
1	B	236	VAL	3.3
1	B	245	ASN	2.9
1	B	11	VAL	2.8
1	A	427	ALA	2.7
1	B	135	GLY	2.6
1	B	138	ASP	2.5
1	B	228	ARG	2.3
1	B	264	PRO	2.3
1	A	428	ASN	2.2
1	B	233	ASN	2.2
1	B	424	ILE	2.2
1	B	133	HIS	2.2
1	A	513	HIS	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	DIA	B	2842	10/10	0.40	16.81	72,75,78,78	0
3	DIA	A	2841	10/10	0.33	7.93	49,59,65,66	0
2	FAD	A	801	53/53	0.16	0.43	16,25,32,40	0
2	FAD	B	802	53/53	0.12	-0.24	32,40,45,50	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.