



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:40 am GMT

PDB ID : 2GV8  
Title : Crystal structure of flavin-containing monooxygenase (FMO) from *S.pombe* and NADPH cofactor complex  
Authors : Eswaramoorthy, S.; Swaminathan, S.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2006-05-02  
Resolution : 2.10 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

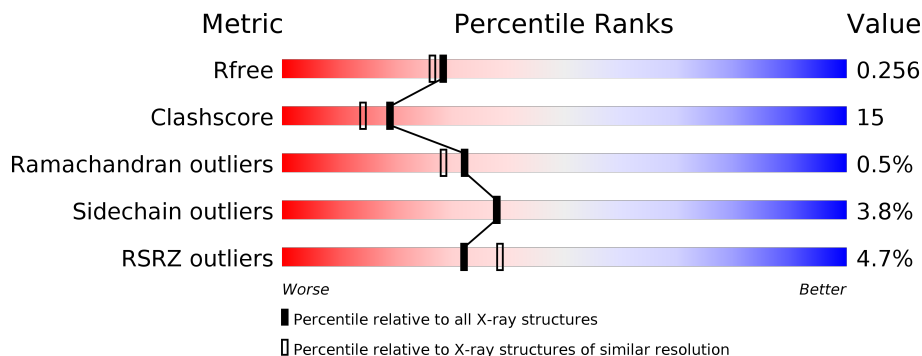
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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	447	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>23%</div> <div>••</div> </div> </div>
1	B	447	<div> <div>8%</div> <div> <div></div> <div>72%</div> <div>25%</div> <div>••</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7618 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 monooxygenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	Se	0	0	0
			3486	2259	578	641	4	4			
1	B	442	Total	C	N	O	S	Se	0	0	0
			3486	2259	578	641	4	4			

There are 10 discrepancies between the modelled and reference sequences:

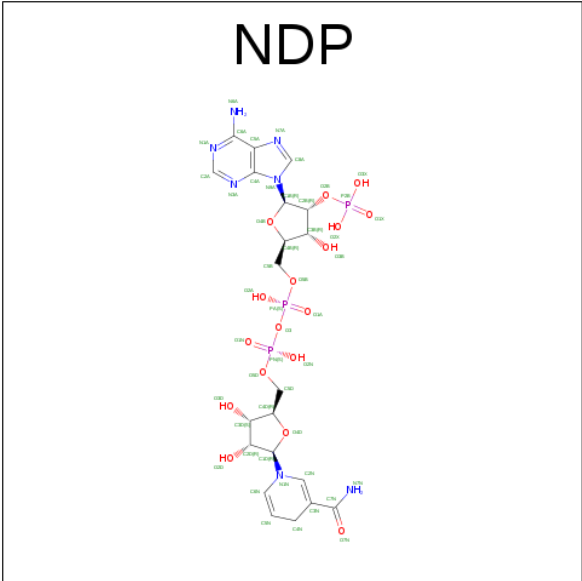
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9HFE4
A	97	MSE	MET	MODIFIED RESIDUE	UNP Q9HFE4
A	377	MSE	MET	MODIFIED RESIDUE	UNP Q9HFE4
A	386	MSE	MET	MODIFIED RESIDUE	UNP Q9HFE4
A	433	MSE	MET	MODIFIED RESIDUE	UNP Q9HFE4
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q9HFE4
B	97	MSE	MET	MODIFIED RESIDUE	UNP Q9HFE4
B	377	MSE	MET	MODIFIED RESIDUE	UNP Q9HFE4
B	386	MSE	MET	MODIFIED RESIDUE	UNP Q9HFE4
B	433	MSE	MET	MODIFIED RESIDUE	UNP Q9HFE4

- 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 NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

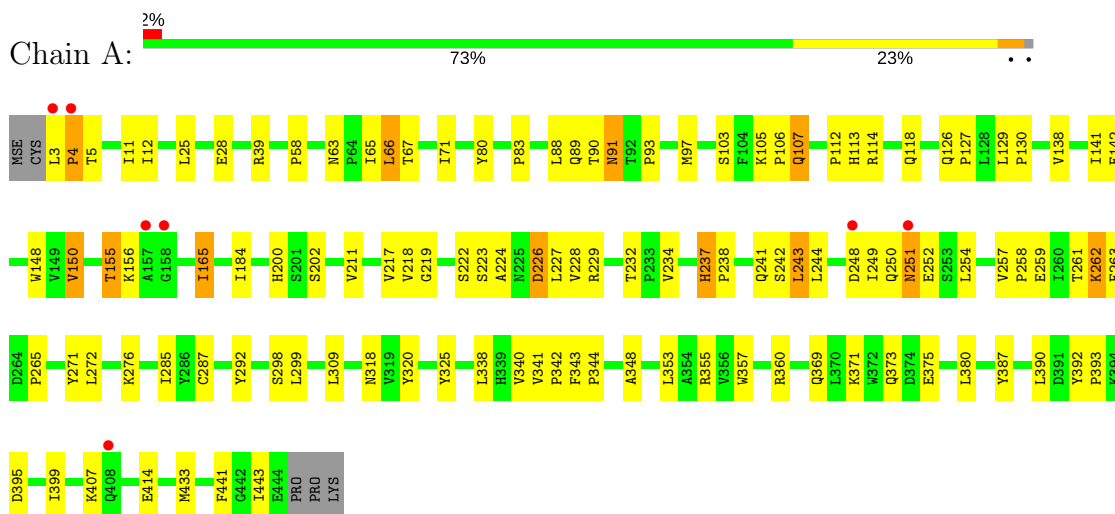
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	231	Total	O	0	0
			231	231		
5	B	201	Total	O	0	0
			201	201		

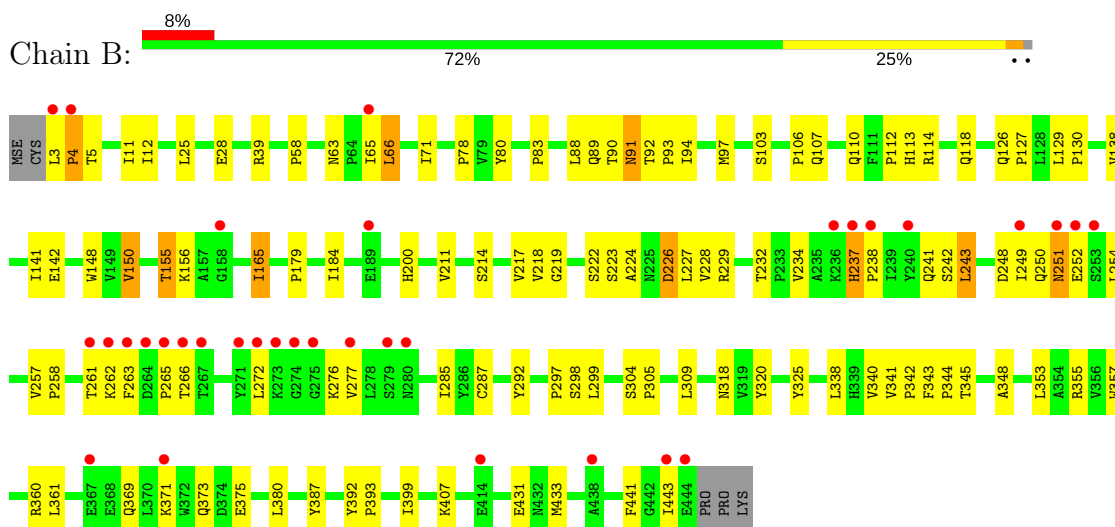
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: monooxygenase



#### • Molecule 1: monooxygenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.31Å 72.53Å 80.37Å 98.59° 107.40° 101.72°	Depositor
Resolution (Å)	50.00 – 2.10 40.54 – 2.09	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.10) 83.2 (40.54-2.09)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 2.08Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.232 , 0.259 0.231 , 0.256	Depositor DCC
$R_{free}$ test set	1940 reflections (3.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.7	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7618	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.41% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: GOL, FAD, NDP

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	0.36	0/3583	0.65	2/4880 (0.0%)
1	B	0.35	0/3583	0.64	0/4880
All	All	0.35	0/7166	0.65	2/9760 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	GLN	CA-CB-CG	-7.24	97.48	113.40
1	A	107	GLN	CB-CG-CD	5.38	125.59	111.60

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	3486	0	3483	108	0
1	B	3486	0	3483	101	0
2	A	53	0	31	5	0
2	B	53	0	31	5	0
3	A	48	0	26	4	0
3	B	48	0	26	4	0
4	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	6	0	8	0	0
5	A	231	0	0	12	0
5	B	201	0	0	5	0
All	All	7618	0	7096	208	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 (208) 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:114:ARG:HH11	1:A:118:GLN:HE22	1.13	0.95
1:A:244:LEU:HD23	1:A:259:GLU:OE1	1.69	0.93
1:B:114:ARG:HH11	1:B:118:GLN:HE22	1.11	0.92
1:A:262:LYS:HE2	1:A:271:TYR:CG	2.06	0.91
1:A:259:GLU:HG2	5:A:646:HOH:O	1.82	0.79
1:A:407:LYS:HD3	5:A:730:HOH:O	1.85	0.76
1:B:241:GLN:HG2	1:B:243:LEU:CD2	2.17	0.75
1:B:93:PRO:HD2	1:B:433:MSE:HE2	1.68	0.75
1:A:262:LYS:HD3	1:A:271:TYR:HB2	1.67	0.74
1:A:93:PRO:HD2	1:A:433:MSE:HE2	1.69	0.73
1:A:106:PRO:HG2	1:B:106:PRO:HG2	1.68	0.73
1:A:262:LYS:CD	1:A:271:TYR:HB2	2.19	0.72
1:A:241:GLN:HG2	1:A:243:LEU:CD2	2.20	0.71
1:B:238:PRO:HB3	1:B:252:GLU:O	1.91	0.70
1:A:414:GLU:HG2	5:A:727:HOH:O	1.92	0.69
1:A:155:THR:HG21	5:A:561:HOH:O	1.92	0.68
1:B:63:ASN:OD1	1:B:65:ILE:HG22	1.93	0.68
1:B:114:ARG:NH1	1:B:118:GLN:HE22	1.89	0.67
1:A:238:PRO:HB3	1:A:252:GLU:O	1.95	0.67
1:A:63:ASN:OD1	1:A:65:ILE:HG22	1.95	0.66
1:B:249:ILE:HG21	1:B:254:LEU:HD23	1.78	0.66
1:B:249:ILE:HG23	1:B:251:ASN:OD1	1.97	0.65
1:A:67:THR:HG23	5:A:713:HOH:O	1.96	0.65
1:A:249:ILE:HG21	1:A:254:LEU:HD23	1.78	0.65
1:B:227:LEU:HD21	1:B:285:ILE:HG21	1.80	0.64
1:B:407:LYS:HD3	5:B:581:HOH:O	1.97	0.64
1:B:222:SER:OG	3:B:501:NDP:H2D	1.97	0.64
1:A:222:SER:OG	3:A:501:NDP:H2D	1.98	0.63
1:A:227:LEU:HD21	1:A:285:ILE:HG21	1.79	0.63
1:A:249:ILE:HG23	1:A:251:ASN:OD1	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:GLU:HB3	1:A:298:SER:CB	2.28	0.63
1:B:142:GLU:HB3	1:B:298:SER:CB	2.28	0.63
1:B:114:ARG:HH11	1:B:118:GLN:NE2	1.92	0.63
1:A:262:LYS:HE2	1:A:271:TYR:CD2	2.35	0.62
1:B:106:PRO:O	1:B:107:GLN:HB2	1.99	0.61
1:A:232:THR:O	1:A:237:HIS:HE1	1.83	0.61
1:B:272:LEU:HD12	1:B:276:LYS:HG3	1.83	0.61
1:B:232:THR:O	1:B:237:HIS:HE1	1.84	0.60
1:B:263:PHE:O	1:B:265:PRO:HD3	2.01	0.60
1:A:114:ARG:NH1	1:A:118:GLN:HE22	1.92	0.60
1:A:262:LYS:CE	1:A:271:TYR:CG	2.82	0.60
1:B:251:ASN:N	1:B:251:ASN:OD1	2.35	0.60
1:A:251:ASN:N	1:A:251:ASN:OD1	2.34	0.60
1:B:155:THR:HG21	5:B:527:HOH:O	2.01	0.60
1:A:39:ARG:HD2	5:A:627:HOH:O	2.02	0.59
1:B:93:PRO:CD	1:B:433:MSE:HE2	2.32	0.59
1:B:165:ILE:O	1:B:165:ILE:HG12	2.01	0.59
1:A:262:LYS:HE2	1:A:271:TYR:CD1	2.38	0.59
1:A:318:ASN:H	1:A:373:GLN:HE22	1.51	0.58
1:B:91:ASN:C	1:B:91:ASN:HD22	2.06	0.58
1:A:272:LEU:HD12	1:A:276:LYS:HG3	1.84	0.58
1:B:318:ASN:H	1:B:373:GLN:HE22	1.51	0.58
1:B:88:LEU:HD11	2:B:500:FAD:H6	1.86	0.58
1:B:58:PRO:HG3	1:B:66:LEU:CD2	2.34	0.58
1:A:414:GLU:CG	5:A:727:HOH:O	2.52	0.57
1:A:441:PHE:O	1:A:443:ILE:HG23	2.05	0.57
1:B:241:GLN:HG2	1:B:243:LEU:HD21	1.84	0.57
1:A:165:ILE:O	1:A:165:ILE:HG12	2.03	0.57
1:A:371:LYS:HE3	1:A:375:GLU:OE1	2.05	0.57
1:A:93:PRO:CD	1:A:433:MSE:HE2	2.33	0.57
1:A:88:LEU:HD11	2:A:500:FAD:H6	1.86	0.57
1:A:241:GLN:HG2	1:A:243:LEU:HD21	1.85	0.57
1:B:441:PHE:O	1:B:443:ILE:HG23	2.05	0.57
1:B:371:LYS:HE3	1:B:375:GLU:OE1	2.05	0.56
1:A:91:ASN:HD22	1:A:91:ASN:C	2.09	0.56
1:A:58:PRO:HG3	1:A:66:LEU:CD2	2.35	0.55
1:B:58:PRO:HG3	1:B:66:LEU:HD21	1.88	0.55
1:B:343:PHE:HB2	1:B:344:PRO:HD3	1.88	0.55
1:A:222:SER:HB2	5:A:562:HOH:O	2.07	0.55
1:A:299:LEU:HB3	1:A:309:LEU:HD12	1.90	0.54
1:A:263:PHE:O	1:A:265:PRO:HD3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:GLN:HG2	1:B:243:LEU:HD23	1.89	0.54
1:A:114:ARG:HH11	1:A:118:GLN:NE2	1.95	0.54
1:B:71:ILE:HD12	1:B:71:ILE:N	2.23	0.54
1:A:5:THR:HG23	5:A:699:HOH:O	2.07	0.53
1:A:58:PRO:HG3	1:A:66:LEU:HD21	1.90	0.53
1:A:343:PHE:HB2	1:A:344:PRO:HD3	1.90	0.53
1:B:179:PRO:HB3	1:B:200:HIS:CE1	2.43	0.53
1:A:71:ILE:HD12	1:A:71:ILE:N	2.24	0.53
1:A:200:HIS:CD2	1:A:202:SER:H	2.26	0.53
1:A:392:TYR:CD1	1:A:393:PRO:HA	2.44	0.53
1:B:299:LEU:HB3	1:B:309:LEU:HD12	1.90	0.53
1:B:340:VAL:O	1:B:342:PRO:HD3	2.10	0.52
1:B:341:VAL:O	1:B:344:PRO:HD2	2.09	0.52
1:A:224:ALA:O	1:A:228:VAL:HG23	2.10	0.52
1:A:341:VAL:O	1:A:344:PRO:HD2	2.10	0.52
1:B:224:ALA:O	1:B:228:VAL:HG23	2.10	0.51
1:B:392:TYR:CD1	1:B:393:PRO:HA	2.45	0.51
1:A:39:ARG:HD3	1:A:80:TYR:CE1	2.46	0.51
1:B:218:VAL:HG22	1:B:242:SER:HB3	1.93	0.51
1:A:218:VAL:HG22	1:A:242:SER:HB3	1.91	0.51
1:B:217:VAL:O	1:B:241:GLN:HA	2.11	0.51
1:B:223:SER:HA	3:B:501:NDP:H5N	1.92	0.50
1:A:83:PRO:HG2	2:A:500:FAD:HM82	1.93	0.50
1:B:83:PRO:HG2	2:B:500:FAD:HM82	1.93	0.50
1:A:243:LEU:N	1:A:243:LEU:HD23	2.27	0.50
1:A:241:GLN:HG2	1:A:243:LEU:HD23	1.93	0.50
1:A:249:ILE:CG2	1:A:251:ASN:OD1	2.59	0.50
1:B:249:ILE:CG2	1:B:251:ASN:OD1	2.60	0.50
1:A:223:SER:HA	3:A:501:NDP:H5N	1.93	0.50
1:A:67:THR:HA	5:A:713:HOH:O	2.11	0.50
1:B:242:SER:O	3:B:501:NDP:H2A	2.11	0.50
1:A:340:VAL:O	1:A:342:PRO:HD3	2.12	0.50
1:B:211:VAL:HG12	1:B:234:VAL:HB	1.94	0.49
1:A:97:MSE:HE1	1:A:112:PRO:HD2	1.94	0.49
1:A:211:VAL:HG12	1:A:234:VAL:HB	1.94	0.49
1:A:217:VAL:O	1:A:241:GLN:HA	2.13	0.49
1:B:11:ILE:HD11	1:B:25:LEU:HD12	1.94	0.49
1:B:237:HIS:HD2	1:B:252:GLU:OE2	1.96	0.49
1:B:39:ARG:HD3	1:B:80:TYR:CE1	2.47	0.49
1:B:97:MSE:O	1:B:343:PHE:HB2	2.12	0.49
1:B:292:TYR:OH	1:B:338:LEU:HD13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ILE:O	1:B:298:SER:HB2	2.13	0.49
1:A:141:ILE:O	1:A:298:SER:HB2	2.13	0.48
1:A:248:ASP:O	1:A:250:GLN:HG2	2.13	0.48
1:A:226:ASP:OD1	1:A:229:ARG:NH2	2.46	0.48
1:B:257:VAL:HB	1:B:258:PRO:HD2	1.96	0.48
1:A:106:PRO:O	1:A:107:GLN:HB2	2.13	0.48
1:B:226:ASP:OD1	1:B:229:ARG:NH2	2.46	0.48
1:B:248:ASP:O	1:B:250:GLN:HG2	2.12	0.48
1:B:380:LEU:HD11	1:B:387:TYR:HA	1.95	0.48
1:A:242:SER:O	3:A:501:NDP:H2A	2.13	0.48
1:B:97:MSE:HE1	1:B:112:PRO:HD2	1.96	0.48
1:B:39:ARG:HG2	2:B:500:FAD:N3A	2.28	0.48
1:B:243:LEU:HD23	1:B:243:LEU:N	2.29	0.47
1:A:237:HIS:HD2	1:A:252:GLU:OE2	1.97	0.47
1:A:3:LEU:O	1:A:5:THR:N	2.47	0.47
1:B:3:LEU:O	1:B:5:THR:N	2.47	0.47
1:A:39:ARG:HG2	2:A:500:FAD:N3A	2.29	0.47
1:B:39:ARG:HD2	5:B:570:HOH:O	2.14	0.47
1:B:106:PRO:O	1:B:107:GLN:CB	2.63	0.47
1:A:257:VAL:HB	1:A:258:PRO:HD2	1.97	0.46
1:A:355:ARG:HH11	1:A:355:ARG:HG3	1.79	0.46
1:A:97:MSE:O	1:A:343:PHE:HB2	2.15	0.46
1:B:214:SER:HA	5:B:649:HOH:O	2.15	0.46
1:A:11:ILE:HD11	1:A:25:LEU:HD12	1.96	0.46
1:A:292:TYR:OH	1:A:338:LEU:HD13	2.15	0.46
1:A:219:GLY:HA2	3:A:501:NDP:N3A	2.31	0.46
1:A:5:THR:HA	5:A:699:HOH:O	2.15	0.46
1:B:39:ARG:HD3	1:B:80:TYR:CD1	2.51	0.46
1:B:320:TYR:CG	1:B:369:GLN:HG2	2.50	0.46
1:A:309:LEU:HD21	1:A:325:TYR:CD1	2.51	0.46
1:B:348:ALA:HB2	1:B:399:ILE:HG23	1.98	0.45
1:A:320:TYR:CG	1:A:369:GLN:HG2	2.51	0.45
1:A:380:LEU:HD11	1:A:387:TYR:HA	1.98	0.45
1:B:222:SER:O	1:B:226:ASP:HB2	2.17	0.45
1:B:355:ARG:HG3	1:B:355:ARG:HH11	1.80	0.45
1:B:148:TRP:O	1:B:165:ILE:HA	2.17	0.45
1:A:39:ARG:HD3	1:A:80:TYR:CD1	2.52	0.45
1:B:71:ILE:CD1	1:B:71:ILE:N	2.80	0.45
1:A:89:GLN:HG2	1:A:113:HIS:HA	1.99	0.45
1:B:237:HIS:CD2	1:B:252:GLU:OE2	2.69	0.45
1:A:237:HIS:CD2	1:A:252:GLU:OE2	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:PHE:N	1:A:343:PHE:CD1	2.85	0.44
1:A:348:ALA:HB2	1:A:399:ILE:HG23	1.99	0.44
1:B:353:LEU:HD11	1:B:357:TRP:CE2	2.52	0.44
1:A:227:LEU:CD2	1:A:285:ILE:HG21	2.47	0.44
1:B:227:LEU:HD22	1:B:287:CYS:SG	2.58	0.44
1:A:371:LYS:O	1:A:375:GLU:HG3	2.17	0.44
1:B:343:PHE:N	1:B:343:PHE:CD1	2.84	0.44
1:B:28:GLU:OE1	1:B:360:ARG:HD3	2.17	0.44
1:A:251:ASN:HB2	1:A:252:GLU:H	1.56	0.44
1:B:219:GLY:HA2	3:B:501:NDP:N3A	2.31	0.44
1:A:83:PRO:CG	2:A:500:FAD:HM82	2.48	0.44
1:B:91:ASN:C	1:B:91:ASN:ND2	2.69	0.44
1:A:222:SER:O	1:A:226:ASP:HB2	2.17	0.44
1:B:257:VAL:CG2	1:B:272:LEU:HD13	2.47	0.44
1:B:345:THR:HB	5:B:536:HOH:O	2.17	0.44
1:B:90:THR:HA	2:B:500:FAD:O4	2.18	0.44
1:A:360:ARG:NH1	5:A:656:HOH:O	2.26	0.44
1:A:90:THR:HA	2:A:500:FAD:O4	2.17	0.44
1:A:148:TRP:O	1:A:165:ILE:HA	2.18	0.43
1:A:257:VAL:CG2	1:A:272:LEU:HD13	2.48	0.43
1:B:309:LEU:HD21	1:B:325:TYR:CD1	2.53	0.43
1:B:407:LYS:HA	1:B:407:LYS:HD2	1.79	0.43
1:A:355:ARG:NH1	1:A:355:ARG:HG3	2.33	0.43
1:B:83:PRO:CG	2:B:500:FAD:HM82	2.48	0.43
1:A:227:LEU:HD22	1:A:287:CYS:SG	2.59	0.43
1:A:91:ASN:ND2	1:A:91:ASN:C	2.72	0.43
1:B:371:LYS:O	1:B:375:GLU:HG3	2.18	0.43
1:A:126:GLN:HB3	1:A:127:PRO:CD	2.49	0.43
1:B:355:ARG:NH1	1:B:355:ARG:HG3	2.34	0.43
1:B:126:GLN:HB3	1:B:127:PRO:CD	2.49	0.43
1:A:184:ILE:HG22	1:A:262:LYS:HA	2.01	0.43
1:A:97:MSE:HA	1:A:341:VAL:CG1	2.49	0.43
1:B:89:GLN:HG2	1:B:113:HIS:HA	2.00	0.43
1:A:28:GLU:OE1	1:A:360:ARG:HD3	2.19	0.42
1:A:71:ILE:CD1	1:A:71:ILE:N	2.82	0.42
1:B:179:PRO:HB3	1:B:200:HIS:ND1	2.34	0.42
1:B:392:TYR:CE2	1:B:431:GLU:HG3	2.54	0.42
1:B:12:ILE:HD12	1:B:138:VAL:HG21	2.01	0.42
1:B:251:ASN:HB2	1:B:252:GLU:H	1.56	0.42
1:B:94:ILE:HG12	1:B:110:GLN:HA	2.01	0.42
1:A:353:LEU:HD11	1:A:357:TRP:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:THR:O	1:B:97:MSE:HE2	2.20	0.42
1:A:138:VAL:HG13	1:A:150:VAL:HG23	2.02	0.41
1:A:390:LEU:O	1:A:395:ASP:HB3	2.20	0.41
1:B:107:GLN:HA	1:B:107:GLN:OE1	2.19	0.41
1:B:304:SER:HA	1:B:305:PRO:HD3	1.96	0.41
1:B:138:VAL:HG13	1:B:150:VAL:HG23	2.03	0.41
1:A:200:HIS:HD2	1:A:202:SER:OG	2.03	0.41
1:B:184:ILE:CG2	1:B:262:LYS:HA	2.51	0.41
1:A:129:LEU:N	1:A:130:PRO:HD2	2.36	0.41
1:B:129:LEU:N	1:B:130:PRO:HD2	2.36	0.41
1:B:91:ASN:ND2	1:B:92:THR:HG23	2.36	0.41
1:A:12:ILE:HD12	1:A:138:VAL:HG21	2.02	0.40
1:B:361:LEU:HD23	1:B:361:LEU:HA	1.96	0.40
1:B:78:PRO:HD2	1:B:155:THR:CG2	2.51	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	440/447 (98%)	414 (94%)	24 (6%)	2 (0%)	32	28
1	B	440/447 (98%)	415 (94%)	23 (5%)	2 (0%)	32	28
All	All	880/894 (98%)	829 (94%)	47 (5%)	4 (0%)	32	28

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	B	4	PRO
1	A	66	LEU
1	B	66	LEU

### 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	384/385 (100%)	370 (96%)	14 (4%)	40	41
1	B	384/385 (100%)	369 (96%)	15 (4%)	37	37
All	All	768/770 (100%)	739 (96%)	29 (4%)	38	38

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	A	91	ASN
1	A	103	SER
1	A	105	LYS
1	A	150	VAL
1	A	155	THR
1	A	156	LYS
1	A	165	ILE
1	A	226	ASP
1	A	237	HIS
1	A	243	LEU
1	A	251	ASN
1	A	261	THR
1	A	262	LYS
1	B	4	PRO
1	B	91	ASN
1	B	103	SER
1	B	150	VAL
1	B	155	THR
1	B	156	LYS
1	B	165	ILE
1	B	226	ASP
1	B	237	HIS
1	B	243	LEU
1	B	251	ASN
1	B	261	THR
1	B	266	THR

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Mol	Chain	Res	Type
1	B	277	VAL
1	B	297	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	91	ASN
1	A	118	GLN
1	A	121	GLN
1	A	200	HIS
1	A	237	HIS
1	A	373	GLN
1	B	48	ASN
1	B	91	ASN
1	B	118	GLN
1	B	121	GLN
1	B	237	HIS
1	B	373	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 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	500	-	51,58,58	2.68	13 (25%)	54,89,89	2.25	8 (14%)
3	NDP	A	501	-	43,52,52	1.47	4 (9%)	49,80,80	1.56	6 (12%)
4	GOL	A	502	-	5,5,5	0.40	0	5,5,5	0.59	0
2	FAD	B	500	-	51,58,58	2.72	16 (31%)	54,89,89	2.27	8 (14%)
3	NDP	B	501	-	43,52,52	1.53	5 (11%)	49,80,80	1.61	7 (14%)
4	GOL	B	502	-	5,5,5	0.40	0	5,5,5	0.56	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	FAD	A	500	-	-	0/28/50/50	0/6/6/6
3	NDP	A	501	-	-	0/30/77/77	0/5/5/5
4	GOL	A	502	-	-	0/4/4/4	0/0/0/0
2	FAD	B	500	-	-	0/28/50/50	0/6/6/6
3	NDP	B	501	-	-	0/30/77/77	0/5/5/5
4	GOL	B	502	-	-	0/4/4/4	0/0/0/0

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	FAD	C1'-N10	-5.42	1.42	1.48
2	A	500	FAD	C1'-N10	-5.21	1.43	1.48
3	B	501	NDP	C4N-C5N	-5.04	1.38	1.49
3	A	501	NDP	C4N-C5N	-4.72	1.38	1.49
2	B	500	FAD	C5A-C4A	-3.68	1.32	1.40
2	A	500	FAD	C5A-C4A	-3.64	1.32	1.40
3	B	501	NDP	P2B-O2B	-2.88	1.54	1.59
3	A	501	NDP	P2B-O2B	-2.75	1.54	1.59
2	B	500	FAD	C2B-C3B	-2.61	1.46	1.53
2	B	500	FAD	C5'-C4'	-2.53	1.48	1.51
2	A	500	FAD	C2B-C3B	-2.48	1.46	1.53
2	B	500	FAD	C8A-N7A	-2.19	1.30	1.34
2	A	500	FAD	C6-C7	2.07	1.43	1.37
2	B	500	FAD	O4B-C1B	2.14	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	FAD	C6-C7	2.17	1.43	1.37
3	B	501	NDP	C4A-N3A	2.37	1.39	1.35
2	A	500	FAD	C9A-C5X	2.47	1.47	1.42
2	B	500	FAD	C9A-C5X	2.49	1.47	1.42
3	A	501	NDP	C2N-C3N	2.57	1.42	1.34
3	B	501	NDP	C2N-C3N	2.61	1.42	1.34
3	B	501	NDP	C6N-C5N	3.69	1.40	1.33
3	A	501	NDP	C6N-C5N	3.75	1.40	1.33
2	B	500	FAD	C10-N1	4.06	1.39	1.33
2	A	500	FAD	C10-N1	4.22	1.39	1.33
2	B	500	FAD	C4-N3	4.72	1.41	1.33
2	B	500	FAD	P-O5'	4.89	1.80	1.59
2	A	500	FAD	P-O5'	5.11	1.81	1.59
2	A	500	FAD	C5X-N5	5.15	1.43	1.35
2	B	500	FAD	C5X-N5	5.17	1.43	1.35
2	A	500	FAD	C4-N3	5.18	1.42	1.33
2	A	500	FAD	C2A-N3A	5.44	1.41	1.32
2	A	500	FAD	C4A-N3A	5.60	1.43	1.35
2	B	500	FAD	C4A-N3A	5.64	1.43	1.35
2	B	500	FAD	C2A-N3A	5.73	1.41	1.32
2	A	500	FAD	C4X-N5	7.26	1.43	1.33
2	A	500	FAD	C9A-N10	7.62	1.48	1.38
2	B	500	FAD	C4X-N5	7.64	1.44	1.33
2	B	500	FAD	C9A-N10	7.70	1.48	1.38

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	FAD	C4X-C4-N3	-5.73	115.33	123.48
2	B	500	FAD	C4X-C4-N3	-5.63	115.47	123.48
2	B	500	FAD	N3A-C2A-N1A	-4.48	124.95	128.86
3	A	501	NDP	C1D-N1N-C2N	-4.34	113.72	121.09
3	B	501	NDP	C1D-N1N-C2N	-4.34	113.72	121.09
2	B	500	FAD	C5X-C9A-N10	-4.16	114.57	117.66
3	B	501	NDP	N3A-C2A-N1A	-4.15	125.24	128.86
2	A	500	FAD	C5X-C9A-N10	-4.15	114.57	117.66
2	A	500	FAD	N3A-C2A-N1A	-4.15	125.25	128.86
3	A	501	NDP	C4B-O4B-C1B	-4.06	105.44	109.77
3	B	501	NDP	C3N-C2N-N1N	-4.02	117.25	123.08
3	B	501	NDP	C4B-O4B-C1B	-3.99	105.52	109.77
3	A	501	NDP	C3N-C2N-N1N	-3.89	117.44	123.08
3	A	501	NDP	N3A-C2A-N1A	-3.74	125.60	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	FAD	O3'-C3'-C4'	-2.79	101.89	108.82
2	A	500	FAD	O3'-C3'-C4'	-2.74	102.03	108.82
2	A	500	FAD	O2'-C2'-C1'	-2.71	103.51	109.79
2	B	500	FAD	O2'-C2'-C1'	-2.70	103.55	109.79
3	B	501	NDP	O7N-C7N-N7N	-2.48	116.90	122.92
3	B	501	NDP	O5B-C5B-C4B	-2.35	100.66	109.00
3	A	501	NDP	O7N-C7N-N7N	-2.33	117.27	122.92
3	A	501	NDP	O5B-C5B-C4B	-2.27	100.95	109.00
3	B	501	NDP	O2A-PA-O1A	2.09	123.11	112.28
2	B	500	FAD	O2B-C2B-C3B	2.55	120.01	111.83
2	A	500	FAD	O2B-C2B-C3B	2.60	120.16	111.83
2	B	500	FAD	O5'-P-O1P	2.80	120.56	109.25
2	A	500	FAD	O5'-P-O1P	2.81	120.59	109.25
2	A	500	FAD	C4-N3-C2	11.53	125.24	115.16
2	B	500	FAD	C4-N3-C2	11.70	125.40	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	FAD	5	0
3	A	501	NDP	4	0
2	B	500	FAD	5	0
3	B	501	NDP	4	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	438/447 (97%)	0.10	7 (1%) 72 76	11, 28, 42, 51	0
1	B	438/447 (97%)	0.42	34 (7%) 14 18	11, 30, 44, 52	0
All	All	876/894 (97%)	0.26	41 (4%) 32 38	11, 29, 43, 52	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	LEU	6.8
1	B	271	TYR	5.7
1	B	266	THR	5.4
1	A	3	LEU	4.8
1	B	4	PRO	4.5
1	B	444	GLU	4.1
1	A	4	PRO	4.0
1	B	251	ASN	3.8
1	B	249	ILE	3.6
1	B	272	LEU	3.3
1	B	263	PHE	3.3
1	B	238	PRO	3.3
1	B	277	VAL	3.2
1	B	240	TYR	3.2
1	A	157	ALA	3.1
1	B	252	GLU	3.0
1	B	264	ASP	3.0
1	B	275	GLY	3.0
1	B	262	LYS	2.9
1	B	267	THR	2.9
1	B	274	GLY	2.9
1	B	443	ILE	2.9
1	B	261	THR	2.8
1	B	253	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	273	LYS	2.8
1	B	279	SER	2.8
1	B	189	GLU	2.7
1	B	158	GLY	2.7
1	A	251	ASN	2.5
1	B	367	GLU	2.5
1	B	237	HIS	2.4
1	B	280	ASN	2.4
1	B	265	PRO	2.4
1	B	438	ALA	2.3
1	B	65	ILE	2.2
1	A	248	ASP	2.2
1	B	236	LYS	2.2
1	B	414	GLU	2.1
1	B	371	LYS	2.1
1	A	158	GLY	2.1
1	A	408	GLN	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(Å <sup>2</sup> )	Q<0.9
2	FAD	B	500	53/53	0.94	0.20	1.70	14,20,23,25	0
2	FAD	A	500	53/53	0.95	0.18	1.24	15,18,24,24	0
4	GOL	A	502	6/6	0.94	0.18	1.19	15,18,19,20	0
3	NDP	A	501	48/48	0.89	0.16	0.86	24,27,43,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	B	502	6/6	0.95	0.17	0.82	16,18,20,21	0
3	NDP	B	501	48/48	0.89	0.14	0.15	27,32,47,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.