



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:35 AM GMT

PDB ID : 2XLS  
Title : JOINT-FUNCTIONS OF PROTEIN RESIDUES AND NADP(H) IN  
OXYGEN-ACTIVATION BY FLAVIN-CONTAINING MONOOXYGE-  
NASE: ASN78LYS MUTANT  
Authors : Orru, R.; Fraaije, M.W.; Mattevi, A.  
Deposited on : 2010-07-21  
Resolution : 3.00 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

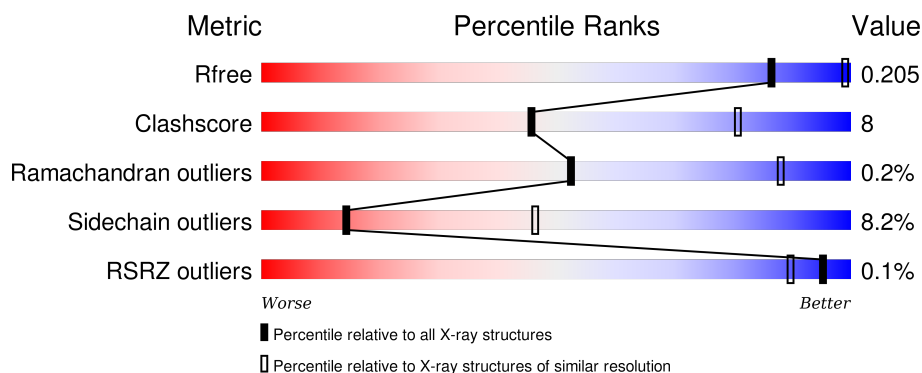
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	461	 79% 15% . .
1	B	461	 77% 16% . .
1	C	461	 78% 16% . .
1	D	461	 78% 15% . . .

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15113 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 FLAVIN-CONTAINING MONOOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3658	2348	606	683	21			
1	B	447	Total	C	N	O	S	0	0	0
			3669	2355	608	685	21			
1	C	447	Total	C	N	O	S	0	0	0
			3669	2355	608	685	21			
1	D	447	Total	C	N	O	S	0	0	0
			3669	2355	608	685	21			

There are 32 discrepancies between the modelled and reference sequences:

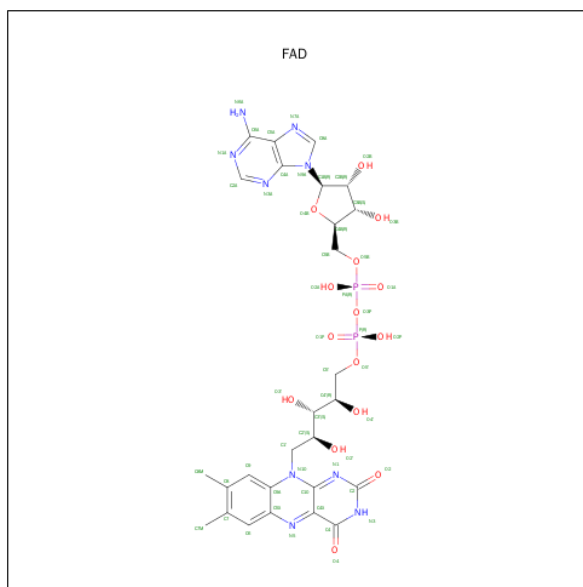
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP Q83XK4
A	2	ALA	-	EXPRESSION TAG	UNP Q83XK4
A	3	MET	-	EXPRESSION TAG	UNP Q83XK4
A	4	GLY	-	EXPRESSION TAG	UNP Q83XK4
A	5	SER	-	EXPRESSION TAG	UNP Q83XK4
A	78	LYS	ASN	ENGINEERED MUTATION	UNP Q83XK4
A	158	ALA	GLU	CONFLICT	UNP Q83XK4
A	159	ALA	GLU	CONFLICT	UNP Q83XK4
B	1	GLY	-	EXPRESSION TAG	UNP Q83XK4
B	2	ALA	-	EXPRESSION TAG	UNP Q83XK4
B	3	MET	-	EXPRESSION TAG	UNP Q83XK4
B	4	GLY	-	EXPRESSION TAG	UNP Q83XK4
B	5	SER	-	EXPRESSION TAG	UNP Q83XK4
B	78	LYS	ASN	ENGINEERED MUTATION	UNP Q83XK4
B	158	ALA	GLU	CONFLICT	UNP Q83XK4
B	159	ALA	GLU	CONFLICT	UNP Q83XK4
C	1	GLY	-	EXPRESSION TAG	UNP Q83XK4
C	2	ALA	-	EXPRESSION TAG	UNP Q83XK4
C	3	MET	-	EXPRESSION TAG	UNP Q83XK4
C	4	GLY	-	EXPRESSION TAG	UNP Q83XK4
C	5	SER	-	EXPRESSION TAG	UNP Q83XK4

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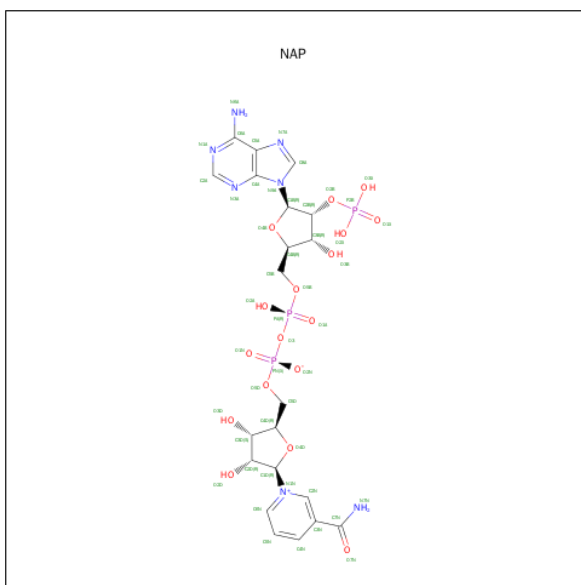
Chain	Residue	Modelled	Actual	Comment	Reference
C	78	LYS	ASN	ENGINEERED MUTATION	UNP Q83XK4
C	158	ALA	GLU	CONFLICT	UNP Q83XK4
C	159	ALA	GLU	CONFLICT	UNP Q83XK4
D	1	GLY	-	EXPRESSION TAG	UNP Q83XK4
D	2	ALA	-	EXPRESSION TAG	UNP Q83XK4
D	3	MET	-	EXPRESSION TAG	UNP Q83XK4
D	4	GLY	-	EXPRESSION TAG	UNP Q83XK4
D	5	SER	-	EXPRESSION TAG	UNP Q83XK4
D	78	LYS	ASN	ENGINEERED MUTATION	UNP Q83XK4
D	158	ALA	GLU	CONFLICT	UNP Q83XK4
D	159	ALA	GLU	CONFLICT	UNP Q83XK4

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



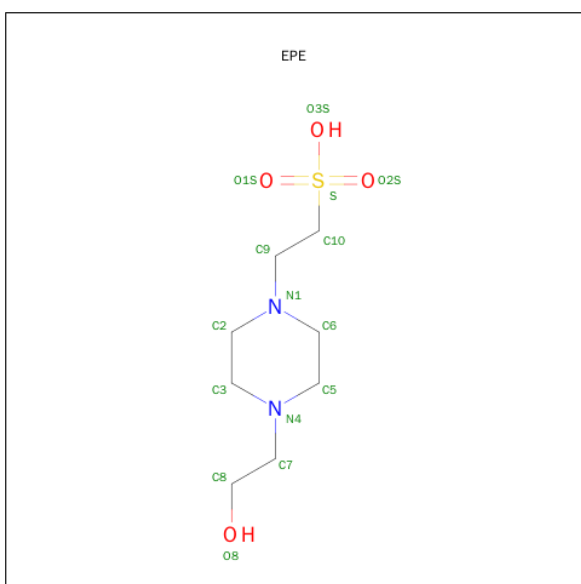
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



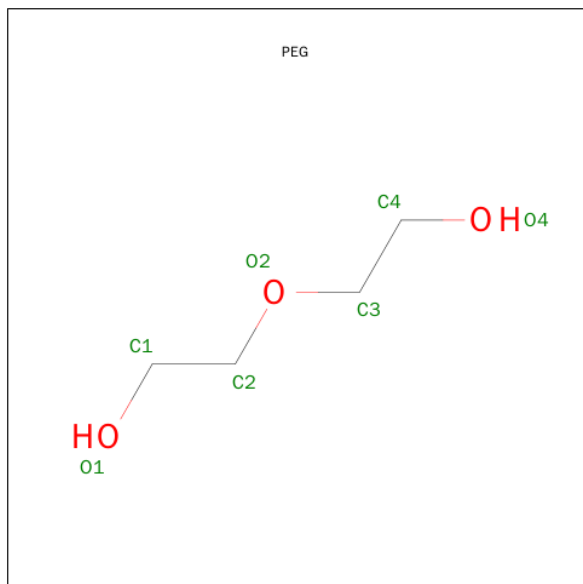
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 39	C 15	N 5	O 16	P 3	0	0
3	B	1	Total 39	C 15	N 5	O 16	P 3	0	0
3	C	1	Total 39	C 15	N 5	O 16	P 3	0	0
3	D	1	Total 39	C 15	N 5	O 16	P 3	0	0

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			7	4	3		

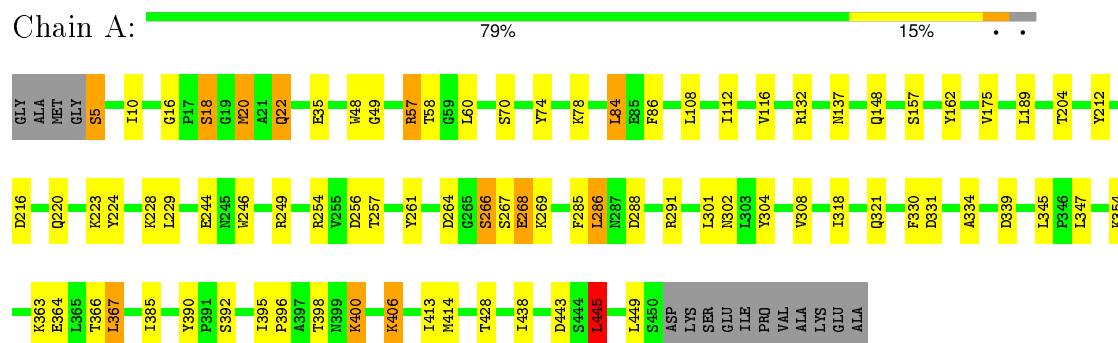
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	5	Total	O	0	0
			5	5		
6	B	7	Total	O	0	0
			7	7		
6	C	5	Total	O	0	0
			5	5		
6	D	11	Total	O	0	0
			11	11		

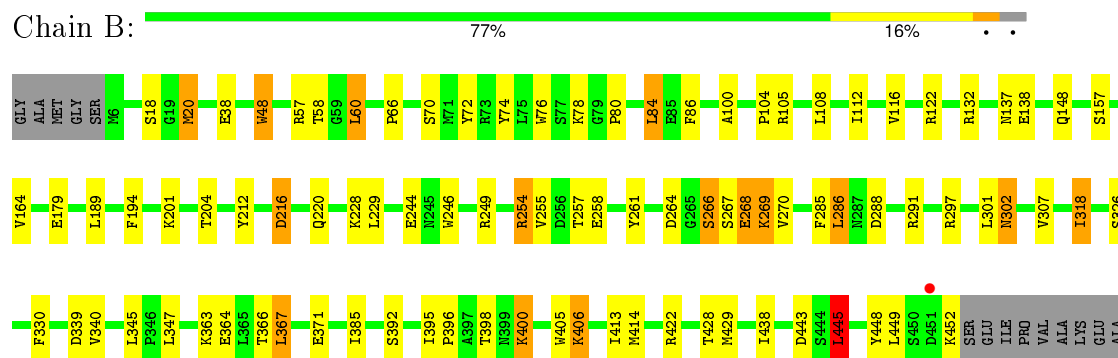
### 3 Residue-property plots

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.

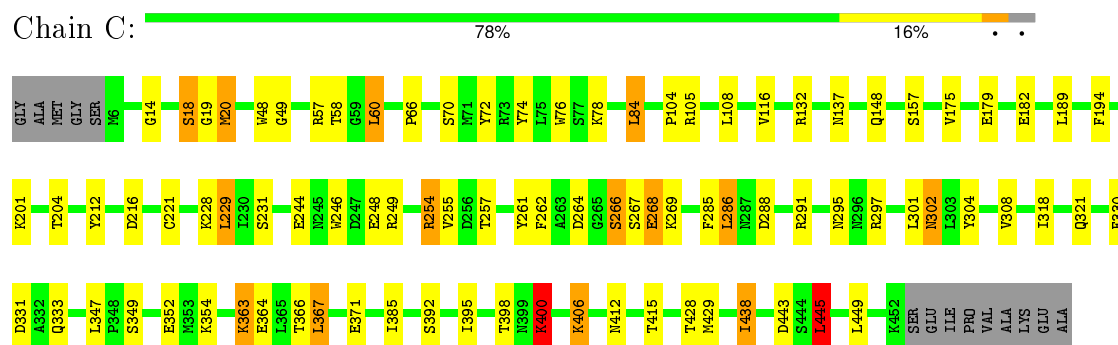
#### • Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE



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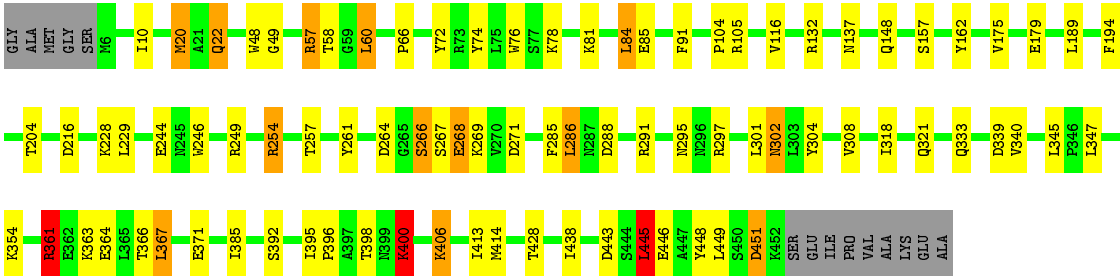
#### • Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE

Chain D: 

78%

15%

•••





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	219.78Å 219.78Å 131.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	95.17 – 3.00 84.25 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (95.17-3.00) 99.7 (84.25-3.00)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.21 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.182 , 0.211 0.180 , 0.205	Depositor DCC
$R_{free}$ test set	3559 reflections (5.19%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.5	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 30.8	EDS
Estimated twinning fraction	0.028 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 72266 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	15113	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, NAP, EPE, 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	0.97	2/3772 (0.1%)	0.88	3/5120 (0.1%)
1	B	0.99	2/3783 (0.1%)	0.88	4/5134 (0.1%)
1	C	1.07	4/3783 (0.1%)	0.91	6/5134 (0.1%)
1	D	0.97	3/3783 (0.1%)	0.86	5/5134 (0.1%)
All	All	1.00	11/15121 (0.1%)	0.88	18/20522 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	400	LYS	CD-CE	18.61	1.97	1.51
1	C	57	ARG	CZ-NH1	-9.58	1.20	1.33
1	A	22	GLN	CD-NE2	-6.41	1.16	1.32
1	B	38	GLU	CG-CD	6.27	1.61	1.51
1	B	138	GLU	CG-CD	5.98	1.60	1.51
1	D	57	ARG	CZ-NH1	-5.68	1.25	1.33
1	A	57	ARG	CZ-NH1	-5.17	1.26	1.33
1	C	400	LYS	CE-NZ	-5.15	1.36	1.49
1	D	446	GLU	CG-CD	5.05	1.59	1.51
1	D	451	ASP	N-CA	5.02	1.56	1.46
1	C	182	GLU	CG-CD	5.00	1.59	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	57	ARG	NE-CZ-NH2	15.36	127.98	120.30
1	A	20	MET	CG-SD-CE	13.70	122.12	100.20
1	A	57	ARG	NE-CZ-NH2	7.17	123.89	120.30
1	B	105	ARG	NE-CZ-NH1	-7.04	116.78	120.30
1	B	20	MET	CG-SD-CE	6.93	111.29	100.20
1	B	445	LEU	CA-CB-CG	6.59	130.46	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	445	LEU	CA-CB-CG	6.54	130.35	115.30
1	A	445	LEU	CA-CB-CG	6.46	130.15	115.30
1	D	400	LYS	CD-CE-NZ	6.35	126.30	111.70
1	D	445	LEU	CA-CB-CG	6.34	129.87	115.30
1	C	229	LEU	CB-CG-CD1	-6.21	100.44	111.00
1	C	57	ARG	NH1-CZ-NH2	-5.92	112.88	119.40
1	D	105	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	C	331	ASP	CB-CG-OD1	5.83	123.55	118.30
1	C	20	MET	CG-SD-CE	5.75	109.40	100.20
1	B	122	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	D	20	MET	CG-SD-CE	5.35	108.77	100.20
1	D	361	ARG	CG-CD-NE	5.10	122.51	111.80

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	3658	0	3454	57	0
1	B	3669	0	3466	52	0
1	C	3669	0	3464	54	0
1	D	3669	0	3466	51	0
2	A	53	0	31	3	0
2	B	53	0	31	2	0
2	C	53	0	31	3	0
2	D	53	0	31	0	0
3	A	39	0	18	8	0
3	B	39	0	18	9	0
3	C	39	0	18	8	0
3	D	39	0	18	6	0
4	A	15	0	18	1	0
4	B	15	0	18	1	0
4	D	15	0	18	0	0
5	C	7	0	10	0	0
6	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	7	0	0	0	0
6	C	5	0	0	0	0
6	D	11	0	0	0	0
All	All	15113	0	14110	224	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 8.

All (224) 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:400:LYS:CD	1:C:400:LYS:CE	1.97	1.42
1:A:396:PRO:O	1:A:400:LYS:NZ	1.86	1.07
1:B:400:LYS:HD3	1:B:400:LYS:N	1.73	0.98
1:A:400:LYS:N	1:A:400:LYS:HD3	1.85	0.91
1:A:78:LYS:HZ2	3:A:501:NAP:H2D	1.38	0.89
1:C:78:LYS:HZ2	3:C:501:NAP:H2D	1.38	0.88
1:A:264:ASP:OD1	1:A:266:SER:OG	1.93	0.86
1:A:78:LYS:NZ	3:A:501:NAP:H2D	1.91	0.85
1:D:288:ASP:OD1	1:D:291:ARG:NH1	2.10	0.84
1:B:396:PRO:O	1:B:400:LYS:NZ	2.11	0.84
1:C:285:PHE:CD1	1:C:286:LEU:HD13	2.14	0.83
1:B:57:ARG:NH2	1:C:175:VAL:O	2.12	0.83
1:A:16:GLY:O	1:A:20:MET:HG3	1.77	0.83
1:C:78:LYS:NZ	3:C:501:NAP:H2D	1.94	0.82
1:B:285:PHE:CD1	1:B:286:LEU:HD13	2.15	0.81
1:D:228:LYS:HE3	1:D:268:GLU:OE1	1.81	0.81
1:C:228:LYS:HE3	1:C:268:GLU:OE1	1.79	0.81
1:A:288:ASP:OD1	1:A:291:ARG:NH1	2.16	0.79
1:A:285:PHE:CD1	1:A:286:LEU:HD13	2.17	0.79
1:B:78:LYS:NZ	3:B:501:NAP:H2D	1.99	0.78
1:A:228:LYS:HE3	1:A:268:GLU:OE1	1.82	0.78
1:C:288:ASP:OD1	1:C:291:ARG:NH1	2.16	0.78
1:A:175:VAL:O	1:D:57:ARG:NH2	2.17	0.78
1:A:57:ARG:NH2	1:D:175:VAL:O	2.16	0.77
1:D:285:PHE:CD1	1:D:286:LEU:HD13	2.19	0.77
1:A:5:SER:HB3	1:A:35:GLU:HG2	1.69	0.74
1:B:78:LYS:HZ2	3:B:501:NAP:H2D	1.53	0.73
1:D:396:PRO:O	1:D:400:LYS:NZ	2.18	0.73
3:B:501:NAP:H52N	3:B:501:NAP:O1A	1.88	0.73
1:D:396:PRO:C	1:D:400:LYS:HZ2	1.92	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:501:NAP:H52N	3:C:501:NAP:O1A	1.90	0.71
1:D:264:ASP:OD1	1:D:266:SER:OG	2.08	0.71
1:D:132:ARG:NH2	1:D:148:GLN:OE1	2.24	0.70
1:C:400:LYS:HD3	1:C:400:LYS:N	2.06	0.70
1:D:78:LYS:NZ	3:D:501:NAP:H2D	2.06	0.69
1:B:396:PRO:C	1:B:400:LYS:HZ2	1.95	0.69
1:B:288:ASP:OD1	1:B:291:ARG:NH1	2.24	0.69
1:B:363:LYS:O	1:B:366:THR:HB	1.92	0.68
3:D:501:NAP:O1A	3:D:501:NAP:H52N	1.92	0.68
1:B:285:PHE:HD1	1:B:286:LEU:HD13	1.55	0.68
1:C:363:LYS:O	1:C:366:THR:HB	1.95	0.67
1:A:132:ARG:NH2	1:A:148:GLN:OE1	2.26	0.67
1:B:264:ASP:OD1	1:B:266:SER:OG	2.12	0.67
1:C:301:LEU:O	1:C:302:ASN:HB2	1.95	0.66
1:B:179:GLU:HB3	1:B:254:ARG:HB2	1.77	0.66
1:D:285:PHE:HD1	1:D:286:LEU:HD13	1.60	0.65
1:A:396:PRO:C	1:A:400:LYS:NZ	2.50	0.64
3:C:501:NAP:O1A	3:C:501:NAP:C5D	2.45	0.64
3:A:501:NAP:O1A	3:A:501:NAP:H52N	1.98	0.64
1:C:285:PHE:HD1	1:C:286:LEU:HD13	1.60	0.64
1:A:445:LEU:HD13	1:A:449:LEU:HD12	1.80	0.64
1:A:363:LYS:O	1:A:366:THR:HB	1.98	0.63
3:B:501:NAP:C5D	3:B:501:NAP:O1A	2.46	0.62
1:A:18:SER:OG	2:A:500:FAD:O2P	2.16	0.62
1:A:84:LEU:HD23	1:A:84:LEU:C	2.20	0.61
1:B:301:LEU:O	1:B:302:ASN:HB2	1.99	0.61
1:B:132:ARG:NH2	1:B:148:GLN:OE1	2.33	0.61
1:C:264:ASP:OD1	1:C:266:SER:OG	2.16	0.61
1:A:321:GLN:OE1	1:A:321:GLN:N	2.34	0.61
3:A:501:NAP:C5D	3:A:501:NAP:O1A	2.49	0.60
1:A:301:LEU:O	1:A:302:ASN:CB	2.48	0.60
1:D:363:LYS:O	1:D:366:THR:HB	2.01	0.60
1:B:396:PRO:C	1:B:400:LYS:NZ	2.55	0.60
1:D:445:LEU:HD13	1:D:449:LEU:HD12	1.83	0.60
1:A:301:LEU:O	1:A:302:ASN:HB2	1.99	0.60
1:A:204:THR:HG23	1:A:228:LYS:HB3	1.83	0.60
1:D:84:LEU:C	1:D:84:LEU:HD23	2.22	0.59
1:B:228:LYS:HE3	1:B:268:GLU:OE1	2.02	0.59
1:C:78:LYS:NZ	3:C:501:NAP:C2D	2.64	0.59
3:D:501:NAP:O1A	3:D:501:NAP:C5D	2.50	0.59
1:B:84:LEU:HD23	1:B:84:LEU:C	2.23	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:LEU:O	1:B:302:ASN:CB	2.50	0.58
1:D:204:THR:HG23	1:D:228:LYS:HB3	1.85	0.58
1:A:20:MET:CE	1:A:49:GLY:HA2	2.35	0.57
1:A:20:MET:HB3	1:A:116:VAL:HG11	1.86	0.56
1:A:285:PHE:HD1	1:A:286:LEU:HD13	1.65	0.56
1:C:321:GLN:NE2	1:C:333:GLN:HE22	2.04	0.56
1:C:132:ARG:NH2	1:C:148:GLN:OE1	2.34	0.56
1:C:438:ILE:O	1:C:438:ILE:HG13	2.07	0.55
1:C:301:LEU:O	1:C:302:ASN:CB	2.55	0.54
1:D:78:LYS:HZ3	3:D:501:NAP:H2D	1.70	0.54
1:B:78:LYS:HZ3	3:B:501:NAP:C2D	2.20	0.54
1:D:321:GLN:HE22	1:D:333:GLN:HE22	1.56	0.53
1:B:413:ILE:HG23	1:B:414:MET:HG2	1.90	0.53
1:A:78:LYS:NZ	3:A:501:NAP:C2D	2.70	0.53
1:D:179:GLU:HB3	1:D:254:ARG:HB2	1.89	0.53
1:C:78:LYS:HZ3	3:C:501:NAP:C2D	2.22	0.53
1:B:78:LYS:NZ	3:B:501:NAP:C2D	2.72	0.52
1:D:445:LEU:CD1	1:D:449:LEU:HD12	2.39	0.52
1:B:385:ILE:HD12	1:B:392:SER:HA	1.92	0.52
1:D:385:ILE:HD12	1:D:392:SER:HA	1.92	0.52
1:D:72:TYR:HB3	1:D:194:PHE:O	2.10	0.51
1:D:78:LYS:HZ2	3:D:501:NAP:H2D	1.75	0.51
1:B:229:LEU:O	1:B:246:TRP:HA	2.10	0.51
1:B:100:ALA:HB3	1:B:448:TYR:OH	2.09	0.51
1:D:78:LYS:HZ3	3:D:501:NAP:C2D	2.23	0.51
1:C:20:MET:HB3	1:C:116:VAL:HG11	1.93	0.51
1:B:261:TYR:N	1:B:261:TYR:CD1	2.78	0.51
1:C:74:TYR:HA	1:C:443:ASP:HB3	1.92	0.51
1:C:400:LYS:CD	1:C:400:LYS:NZ	2.67	0.51
1:B:204:THR:HG23	1:B:228:LYS:HB3	1.93	0.50
1:B:72:TYR:HB3	1:B:194:PHE:O	2.11	0.50
1:D:321:GLN:NE2	1:D:333:GLN:HE22	2.10	0.50
1:C:445:LEU:HD13	1:C:449:LEU:HD12	1.94	0.50
1:C:385:ILE:HD12	1:C:392:SER:HA	1.94	0.50
1:A:86:PHE:HZ	1:A:112:ILE:HG22	1.78	0.49
1:A:304:TYR:HB3	1:A:308:VAL:HB	1.94	0.49
1:D:301:LEU:O	1:D:302:ASN:HB2	2.11	0.49
1:A:22:GLN:HE22	1:A:334:ALA:HA	1.78	0.49
1:D:364:GLU:HA	1:D:367:LEU:HD22	1.95	0.49
1:B:438:ILE:HG13	1:B:438:ILE:O	2.13	0.48
1:A:22:GLN:HA	1:A:334:ALA:HB1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:MET:HB3	1:B:116:VAL:HG11	1.95	0.48
1:C:70:SER:HB2	2:C:500:FAD:HM82	1.95	0.48
1:D:301:LEU:O	1:D:302:ASN:CB	2.61	0.48
1:C:261:TYR:CD1	1:C:261:TYR:N	2.81	0.48
1:B:74:TYR:HA	1:B:443:ASP:HB3	1.96	0.48
1:B:78:LYS:HZ3	3:B:501:NAP:H2D	1.76	0.48
1:C:321:GLN:HE22	1:C:333:GLN:HE22	1.60	0.48
1:C:412:ASN:HB3	1:C:415:THR:OG1	2.14	0.48
1:A:331:ASP:HB3	1:A:390:TYR:CE1	2.48	0.48
4:A:1451:EPE:H71	1:C:295:ASN:HB3	1.95	0.47
1:D:445:LEU:CD1	1:D:445:LEU:C	2.82	0.47
1:C:364:GLU:HA	1:C:367:LEU:HD22	1.97	0.47
1:A:86:PHE:CZ	1:A:112:ILE:HG22	2.50	0.47
1:B:216:ASP:O	1:B:220:GLN:HG2	2.14	0.47
1:D:20:MET:HB3	1:D:116:VAL:HG11	1.97	0.47
3:B:501:NAP:H51N	3:B:501:NAP:PA	2.54	0.47
1:A:78:LYS:HZ3	3:A:501:NAP:C2D	2.28	0.47
1:A:445:LEU:CD1	1:A:449:LEU:HD12	2.45	0.47
1:D:413:ILE:HG23	1:D:414:MET:HG2	1.96	0.47
1:D:10:ILE:HD12	1:D:162:TYR:HB2	1.97	0.47
1:B:364:GLU:HA	1:B:367:LEU:HD22	1.97	0.47
1:C:18:SER:OG	2:C:500:FAD:O2P	2.33	0.46
1:D:304:TYR:HB3	1:D:308:VAL:HB	1.96	0.46
1:C:20:MET:HE3	1:C:49:GLY:N	2.31	0.46
1:A:16:GLY:O	1:A:20:MET:CG	2.59	0.46
1:A:223:LYS:HE2	1:A:224:TYR:CE1	2.50	0.46
1:A:330:PHE:CE2	2:A:500:FAD:H5'2	2.51	0.46
1:B:297:ARG:HB2	1:B:364:GLU:OE2	2.16	0.46
1:D:20:MET:HE3	1:D:49:GLY:N	2.31	0.45
1:A:78:LYS:HZ3	3:A:501:NAP:H2D	1.77	0.45
1:C:14:GLY:O	1:C:19:GLY:HA3	2.16	0.45
1:C:78:LYS:HB2	1:C:212:TYR:CE2	2.51	0.45
1:A:261:TYR:CD1	1:A:261:TYR:N	2.84	0.45
1:C:84:LEU:C	1:C:84:LEU:HD23	2.37	0.45
1:D:104:PRO:HD3	1:D:448:TYR:CE1	2.52	0.45
1:B:18:SER:HB3	1:B:318:ILE:HG22	1.98	0.45
1:B:86:PHE:CZ	1:B:112:ILE:HG22	2.51	0.45
1:D:361:ARG:HD2	1:D:361:ARG:HH11	1.66	0.45
1:C:76:TRP:HA	1:C:104:PRO:HA	1.97	0.45
1:C:330:PHE:CE2	2:C:500:FAD:H5'2	2.52	0.45
1:C:72:TYR:HB3	1:C:194:PHE:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:LEU:O	1:D:246:TRP:HA	2.16	0.45
1:A:400:LYS:N	1:A:400:LYS:CD	2.71	0.44
1:C:204:THR:HG23	1:C:228:LYS:HB3	1.99	0.44
1:A:229:LEU:O	1:A:246:TRP:HA	2.18	0.44
1:B:339:ASP:HB3	1:B:345:LEU:HD12	1.99	0.44
1:A:364:GLU:HA	1:A:367:LEU:HD22	2.00	0.44
1:C:179:GLU:HB3	1:C:254:ARG:HB2	2.00	0.44
1:A:20:MET:HE2	1:A:49:GLY:HA2	2.00	0.43
1:D:339:ASP:HB3	1:D:345:LEU:HD12	1.99	0.43
1:C:108:LEU:HA	1:C:108:LEU:HD23	1.75	0.43
1:D:400:LYS:HA	1:D:400:LYS:HD3	1.63	0.43
1:C:297:ARG:HB2	1:C:364:GLU:OE2	2.17	0.43
1:B:330:PHE:N	1:B:330:PHE:CD1	2.81	0.43
1:C:445:LEU:C	1:C:445:LEU:CD1	2.87	0.43
1:D:85:GLU:HG3	1:D:91:PHE:CD2	2.53	0.43
1:C:304:TYR:HB3	1:C:308:VAL:HB	2.00	0.43
1:B:78:LYS:HB2	1:B:212:TYR:CE2	2.53	0.43
3:B:501:NAP:C5D	3:B:501:NAP:PA	3.07	0.43
1:A:286:LEU:HB3	1:A:291:ARG:HB2	1.99	0.43
1:C:262:PHE:N	1:C:262:PHE:CD2	2.85	0.42
1:A:108:LEU:HD23	1:A:108:LEU:HA	1.81	0.42
1:B:76:TRP:HA	1:B:104:PRO:HA	2.01	0.42
1:A:445:LEU:CD1	1:A:445:LEU:C	2.88	0.42
1:D:396:PRO:C	1:D:400:LYS:NZ	2.68	0.42
1:A:256:ASP:C	1:A:256:ASP:OD1	2.58	0.42
1:D:76:TRP:HA	1:D:104:PRO:HA	2.01	0.42
1:B:406:LYS:HD3	1:B:406:LYS:HA	1.58	0.42
1:B:70:SER:HB2	2:B:500:FAD:HM82	2.00	0.42
1:D:60:LEU:HD12	1:D:66:PRO:HA	2.02	0.42
1:B:422:ARG:HB2	1:B:429:MET:HE2	2.01	0.42
3:A:501:NAP:PA	3:A:501:NAP:H51N	2.60	0.42
1:B:326:SER:OG	2:B:500:FAD:O2	2.33	0.42
1:A:10:ILE:HD12	1:A:162:TYR:HB2	2.01	0.42
1:C:229:LEU:O	1:C:246:TRP:HA	2.19	0.42
1:D:261:TYR:CD1	1:D:261:TYR:N	2.87	0.42
1:C:400:LYS:CG	1:C:400:LYS:CE	2.93	0.42
1:A:78:LYS:HB2	1:A:212:TYR:CE2	2.55	0.42
1:C:445:LEU:CD1	1:C:449:LEU:HD12	2.50	0.42
1:A:74:TYR:HA	1:A:443:ASP:HB3	2.02	0.42
1:A:385:ILE:HD12	1:A:392:SER:HA	2.02	0.42
1:A:216:ASP:O	1:A:220:GLN:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:ILE:HG23	1:A:414:MET:HG2	2.02	0.41
1:D:204:THR:O	1:D:271:ASP:HB2	2.20	0.41
1:A:70:SER:HB2	2:A:500:FAD:HM82	2.01	0.41
1:A:406:LYS:HD3	1:A:406:LYS:HA	1.66	0.41
1:D:22:GLN:HA	1:D:22:GLN:NE2	2.35	0.41
1:C:231:SER:O	1:C:248:GLU:HA	2.20	0.41
1:B:445:LEU:HD13	1:B:449:LEU:HD12	2.01	0.41
1:C:349:SER:OG	1:C:352:GLU:HG3	2.20	0.41
3:C:501:NAP:O1A	3:C:501:NAP:H51N	2.20	0.41
1:D:297:ARG:HB2	1:D:364:GLU:OE2	2.20	0.41
1:B:86:PHE:HZ	1:B:112:ILE:HG22	1.85	0.41
1:B:108:LEU:HD23	1:B:108:LEU:HA	1.94	0.41
1:A:438:ILE:O	1:A:438:ILE:HG13	2.21	0.41
1:D:74:TYR:HA	1:D:443:ASP:HB3	2.03	0.41
1:C:330:PHE:CD1	1:C:330:PHE:N	2.85	0.41
1:C:429:MET:HE2	1:C:429:MET:HB2	1.98	0.41
1:B:60:LEU:HD12	1:B:66:PRO:HA	2.02	0.41
1:B:164:VAL:CG1	1:B:318:ILE:HG13	2.51	0.41
1:B:258:GLU:OE1	1:B:269:LYS:NZ	2.54	0.41
1:C:406:LYS:HA	1:C:406:LYS:HD3	1.74	0.40
1:B:80:PRO:HD3	1:B:405:TRP:CD1	2.56	0.40
1:D:438:ILE:O	1:D:438:ILE:HG13	2.21	0.40
1:C:105:ARG:HD3	1:C:105:ARG:HH11	1.72	0.40
3:C:501:NAP:PA	3:C:501:NAP:H51N	2.61	0.40
1:D:81:LYS:O	1:D:84:LEU:HD22	2.22	0.40
1:D:406:LYS:HD3	1:D:406:LYS:HA	1.75	0.40
1:B:48:TRP:CD1	1:B:48:TRP:N	2.89	0.40
1:C:60:LEU:HD12	1:C:66:PRO:HA	2.04	0.40
4:B:1453:EPE:H81	1:D:295:ASN:HB3	2.02	0.40
1:A:339:ASP:HB3	1:A:345:LEU:HD12	2.02	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	444/461 (96%)	427 (96%)	17 (4%)	0	100	100
1	B	445/461 (96%)	426 (96%)	18 (4%)	1 (0%)	52	88
1	C	445/461 (96%)	424 (95%)	20 (4%)	1 (0%)	52	88
1	D	445/461 (96%)	426 (96%)	18 (4%)	1 (0%)	52	88
All	All	1779/1844 (96%)	1703 (96%)	73 (4%)	3 (0%)	52	88

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	302	ASN
1	D	302	ASN
1	C	302	ASN

### 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	387/397 (98%)	359 (93%)	28 (7%)	18	53
1	B	388/397 (98%)	355 (92%)	33 (8%)	13	45
1	C	388/397 (98%)	354 (91%)	34 (9%)	12	42
1	D	388/397 (98%)	356 (92%)	32 (8%)	14	46
All	All	1551/1588 (98%)	1424 (92%)	127 (8%)	14	46

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	18	SER
1	A	48	TRP
1	A	58	THR
1	A	60	LEU

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Mol	Chain	Res	Type
1	A	84	LEU
1	A	137	ASN
1	A	157	SER
1	A	189	LEU
1	A	244	GLU
1	A	249	ARG
1	A	254	ARG
1	A	257	THR
1	A	266	SER
1	A	267	SER
1	A	268	GLU
1	A	269	LYS
1	A	286	LEU
1	A	318	ILE
1	A	347	LEU
1	A	354	LYS
1	A	367	LEU
1	A	395	ILE
1	A	398	THR
1	A	400	LYS
1	A	406	LYS
1	A	428	THR
1	A	445	LEU
1	B	48	TRP
1	B	58	THR
1	B	60	LEU
1	B	84	LEU
1	B	137	ASN
1	B	157	SER
1	B	189	LEU
1	B	201	LYS
1	B	216	ASP
1	B	244	GLU
1	B	249	ARG
1	B	254	ARG
1	B	255	VAL
1	B	257	THR
1	B	266	SER
1	B	267	SER
1	B	268	GLU
1	B	269	LYS
1	B	270	VAL

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Mol	Chain	Res	Type
1	B	286	LEU
1	B	307	VAL
1	B	318	ILE
1	B	340	VAL
1	B	347	LEU
1	B	367	LEU
1	B	371	GLU
1	B	395	ILE
1	B	398	THR
1	B	400	LYS
1	B	406	LYS
1	B	428	THR
1	B	445	LEU
1	B	452	LYS
1	C	18	SER
1	C	48	TRP
1	C	58	THR
1	C	60	LEU
1	C	84	LEU
1	C	137	ASN
1	C	157	SER
1	C	189	LEU
1	C	201	LYS
1	C	216	ASP
1	C	221	CYS
1	C	244	GLU
1	C	249	ARG
1	C	254	ARG
1	C	255	VAL
1	C	257	THR
1	C	266	SER
1	C	267	SER
1	C	268	GLU
1	C	269	LYS
1	C	286	LEU
1	C	318	ILE
1	C	347	LEU
1	C	354	LYS
1	C	363	LYS
1	C	367	LEU
1	C	371	GLU
1	C	395	ILE

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Mol	Chain	Res	Type
1	C	398	THR
1	C	400	LYS
1	C	406	LYS
1	C	428	THR
1	C	438	ILE
1	C	445	LEU
1	D	22	GLN
1	D	48	TRP
1	D	58	THR
1	D	60	LEU
1	D	84	LEU
1	D	137	ASN
1	D	157	SER
1	D	189	LEU
1	D	216	ASP
1	D	244	GLU
1	D	249	ARG
1	D	254	ARG
1	D	257	THR
1	D	266	SER
1	D	267	SER
1	D	268	GLU
1	D	269	LYS
1	D	286	LEU
1	D	318	ILE
1	D	340	VAL
1	D	347	LEU
1	D	354	LYS
1	D	361	ARG
1	D	367	LEU
1	D	371	GLU
1	D	395	ILE
1	D	398	THR
1	D	400	LYS
1	D	406	LYS
1	D	428	THR
1	D	445	LEU
1	D	451	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	45	GLN
1	A	141	GLN
1	B	63	ASN
1	B	128	ASN
1	B	141	GLN
1	C	45	GLN
1	C	63	ASN
1	C	128	ASN
1	C	141	GLN
1	C	321	GLN
1	D	45	GLN
1	D	141	GLN
1	D	321	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](#)

12 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	$\# Z  > 2$
4	EPE	A	1451	-	14,15,15	0.92	0	18,20,20	2.22	6 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FAD	A	500	-	48,58,58	1.24	4 (8%)	54,89,89	2.34	11 (20%)
3	NAP	A	501	-	35,42,52	1.53	4 (11%)	46,65,80	1.87	14 (30%)
4	EPE	B	1453	-	14,15,15	0.74	0	18,20,20	2.24	5 (27%)
2	FAD	B	500	-	48,58,58	1.36	8 (16%)	54,89,89	1.97	11 (20%)
3	NAP	B	501	-	35,42,52	1.42	5 (14%)	46,65,80	1.96	11 (23%)
5	PEG	C	1453	-	6,6,6	0.88	0	5,5,5	0.68	0
2	FAD	C	500	-	48,58,58	1.26	4 (8%)	54,89,89	2.05	9 (16%)
3	NAP	C	501	-	35,42,52	1.53	6 (17%)	46,65,80	2.01	13 (28%)
4	EPE	D	1453	-	14,15,15	0.88	0	18,20,20	2.35	6 (33%)
2	FAD	D	500	-	48,58,58	1.39	8 (16%)	54,89,89	2.13	11 (20%)
3	NAP	D	501	-	35,42,52	1.57	5 (14%)	46,65,80	1.81	13 (28%)

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
4	EPE	A	1451	-	-	0/9/19/19	0/1/1/1
2	FAD	A	500	-	-	0/30/50/50	0/6/6/6
3	NAP	A	501	-	-	0/23/56/67	0/4/4/5
4	EPE	B	1453	-	-	0/9/19/19	0/1/1/1
2	FAD	B	500	-	-	0/30/50/50	0/6/6/6
3	NAP	B	501	-	-	0/23/56/67	0/4/4/5
5	PEG	C	1453	-	-	0/4/4/4	0/0/0/0
2	FAD	C	500	-	-	0/30/50/50	0/6/6/6
3	NAP	C	501	-	-	0/23/56/67	0/4/4/5
4	EPE	D	1453	-	-	0/9/19/19	0/1/1/1
2	FAD	D	500	-	-	0/30/50/50	0/6/6/6
3	NAP	D	501	-	-	0/23/56/67	0/4/4/5

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	FAD	C4-C4X	-2.59	1.36	1.41
2	D	500	FAD	C9A-C5X	-2.51	1.37	1.42
2	B	500	FAD	C4X-C10	-2.43	1.36	1.41
2	D	500	FAD	C6-C5X	-2.29	1.38	1.41
2	A	500	FAD	C6-C5X	-2.26	1.38	1.41
2	B	500	FAD	C6-C5X	-2.11	1.38	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	FAD	C9A-C5X	-2.02	1.38	1.42
3	C	501	NAP	C3B-C4B	2.05	1.58	1.53
2	B	500	FAD	C1'-N10	2.07	1.50	1.48
3	B	501	NAP	P2B-O1X	2.18	1.58	1.51
3	B	501	NAP	O4B-C1B	2.23	1.44	1.41
3	C	501	NAP	O4D-C4D	2.28	1.48	1.44
3	B	501	NAP	O4D-C4D	2.28	1.48	1.44
2	C	500	FAD	C2A-N1A	2.30	1.38	1.33
3	C	501	NAP	P2B-O3X	2.33	1.63	1.54
2	D	500	FAD	C2A-N1A	2.33	1.38	1.33
2	D	500	FAD	C4X-N5	2.36	1.37	1.33
2	B	500	FAD	C2A-N1A	2.40	1.38	1.33
3	B	501	NAP	P2B-O3X	2.41	1.63	1.54
2	D	500	FAD	C10-N1	2.44	1.39	1.35
2	C	500	FAD	C1'-N10	2.52	1.51	1.48
3	D	501	NAP	C2D-C3D	2.55	1.57	1.53
3	A	501	NAP	O4B-C1B	2.58	1.44	1.41
2	A	500	FAD	C2A-N3A	2.65	1.36	1.32
3	D	501	NAP	O4D-C4D	2.66	1.49	1.44
3	A	501	NAP	P2B-O3X	2.67	1.64	1.54
2	A	500	FAD	C4-N3	2.73	1.38	1.33
3	D	501	NAP	P2B-O1X	2.79	1.60	1.51
2	C	500	FAD	C4X-N5	2.84	1.37	1.33
2	B	500	FAD	C4X-N5	2.88	1.37	1.33
2	D	500	FAD	C2A-N3A	2.98	1.37	1.32
3	C	501	NAP	O4B-C1B	3.11	1.45	1.41
2	D	500	FAD	C4-N3	3.32	1.39	1.33
3	C	501	NAP	P2B-O1X	3.41	1.62	1.51
3	A	501	NAP	P2B-O1X	3.55	1.62	1.51
2	D	500	FAD	C1'-N10	3.56	1.52	1.48
2	A	500	FAD	C4X-N5	3.59	1.39	1.33
2	C	500	FAD	C2A-N3A	3.72	1.38	1.32
3	D	501	NAP	O4B-C1B	3.81	1.46	1.41
2	B	500	FAD	C2A-N3A	3.81	1.38	1.32
3	C	501	NAP	C1D-C2D	3.86	1.58	1.51
3	B	501	NAP	C1D-C2D	3.93	1.58	1.51
3	D	501	NAP	C1D-C2D	4.43	1.59	1.51
3	A	501	NAP	C1D-C2D	4.69	1.60	1.51

All (110) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	FAD	N3A-C2A-N1A	-11.66	119.97	128.89
2	D	500	FAD	N3A-C2A-N1A	-9.22	121.84	128.89
2	B	500	FAD	N3A-C2A-N1A	-9.06	121.96	128.89
2	C	500	FAD	N3A-C2A-N1A	-8.12	122.68	128.89
3	B	501	NAP	N3A-C2A-N1A	-7.37	123.25	128.89
3	A	501	NAP	N3A-C2A-N1A	-5.43	124.73	128.89
3	D	501	NAP	N3A-C2A-N1A	-5.41	124.75	128.89
3	C	501	NAP	N3A-C2A-N1A	-5.03	125.05	128.89
3	C	501	NAP	O3X-P2B-O1X	-4.91	94.76	110.58
3	C	501	NAP	C4B-O4B-C1B	-4.57	104.70	109.72
3	D	501	NAP	P2B-O2B-C2B	-4.32	111.20	121.56
3	C	501	NAP	PN-O3-PA	-4.24	120.83	132.73
2	C	500	FAD	P-O3P-PA	-3.91	121.75	132.73
2	B	500	FAD	P-O3P-PA	-3.88	121.82	132.73
2	A	500	FAD	C4X-C4-N3	-3.76	118.44	123.59
2	A	500	FAD	P-O3P-PA	-3.69	122.36	132.73
2	D	500	FAD	C4X-C4-N3	-3.67	118.57	123.59
2	C	500	FAD	C4A-C5A-N7A	-3.65	106.12	109.48
2	D	500	FAD	P-O3P-PA	-3.63	122.53	132.73
3	A	501	NAP	PN-O3-PA	-3.50	122.90	132.73
3	A	501	NAP	O3X-P2B-O1X	-3.49	99.36	110.58
3	B	501	NAP	O3X-P2B-O1X	-3.46	99.43	110.58
2	B	500	FAD	C4B-O4B-C1B	-3.40	105.98	109.72
3	B	501	NAP	P2B-O2B-C2B	-3.34	113.56	121.56
3	C	501	NAP	P2B-O2B-C2B	-3.20	113.90	121.56
3	D	501	NAP	O3X-P2B-O1X	-3.14	100.46	110.58
3	A	501	NAP	P2B-O2B-C2B	-3.12	114.09	121.56
3	B	501	NAP	PN-O3-PA	-3.10	124.03	132.73
2	A	500	FAD	O2'-C2'-C1'	-3.08	102.37	109.94
2	D	500	FAD	O3'-C3'-C4'	-3.07	101.02	108.75
3	B	501	NAP	C4B-O4B-C1B	-3.01	106.41	109.72
3	D	501	NAP	C3B-C2B-C1B	-2.88	97.16	102.73
3	A	501	NAP	O2B-C2B-C1B	-2.75	99.29	110.02
3	A	501	NAP	C4B-O4B-C1B	-2.72	106.73	109.72
3	D	501	NAP	PN-O3-PA	-2.68	125.22	132.73
4	D	1453	EPE	O1S-S-C10	-2.65	104.64	106.91
2	D	500	FAD	C4A-C5A-N7A	-2.63	107.06	109.48
3	C	501	NAP	O5B-C5B-C4B	-2.59	99.56	109.12
3	A	501	NAP	C3B-C2B-C1B	-2.56	97.78	102.73
3	C	501	NAP	O2B-C2B-C1B	-2.54	100.11	110.02
3	D	501	NAP	O5B-C5B-C4B	-2.49	99.92	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	FAD	C4-C4X-C10	-2.49	118.34	119.94
3	A	501	NAP	O5B-C5B-C4B	-2.49	99.93	109.12
2	B	500	FAD	C4A-C5A-N7A	-2.46	107.22	109.48
2	C	500	FAD	C4X-C4-N3	-2.46	120.23	123.59
3	B	501	NAP	C3B-C2B-C1B	-2.41	98.08	102.73
2	D	500	FAD	O2'-C2'-C1'	-2.40	104.04	109.94
3	C	501	NAP	C3B-C2B-C1B	-2.38	98.13	102.73
2	C	500	FAD	O2'-C2'-C1'	-2.32	104.24	109.94
2	B	500	FAD	O2'-C2'-C1'	-2.28	104.33	109.94
3	B	501	NAP	O2B-C2B-C1B	-2.24	101.31	110.02
3	D	501	NAP	C1B-N9A-C4A	-2.21	123.60	126.94
2	A	500	FAD	C4B-O4B-C1B	-2.14	107.37	109.72
3	A	501	NAP	C5D-C4D-C3D	-2.13	106.74	115.21
3	D	501	NAP	C4B-O4B-C1B	-2.13	107.38	109.72
3	D	501	NAP	O2B-C2B-C1B	-2.11	101.79	110.02
2	B	500	FAD	O3'-C3'-C4'	-2.09	103.49	108.75
3	C	501	NAP	C4A-C5A-N7A	-2.03	107.61	109.48
2	D	500	FAD	C4X-C10-N10	-2.03	119.32	120.52
3	A	501	NAP	O2X-P2B-O1X	2.03	117.13	110.58
4	A	1451	EPE	C8-C7-N4	2.03	120.98	113.41
3	A	501	NAP	O2B-P2B-O1X	2.10	112.35	107.11
2	A	500	FAD	C6-C5X-C9A	2.11	121.75	118.98
2	A	500	FAD	C5X-C9A-N10	2.25	119.33	117.62
3	A	501	NAP	C1D-C2D-C3D	2.26	105.28	101.64
3	B	501	NAP	O3-PN-O5D	2.35	109.16	102.94
2	B	500	FAD	C4-C4X-N5	2.38	121.60	118.72
2	C	500	FAD	O3P-P-O5'	2.41	109.33	102.94
2	D	500	FAD	O2A-PA-O3P	2.43	116.12	105.09
2	A	500	FAD	O4'-C4'-C5'	2.47	115.57	110.19
4	D	1453	EPE	C5-C6-N1	2.47	115.06	110.63
3	C	501	NAP	O4D-C4D-C3D	2.49	108.82	104.43
4	B	1453	EPE	C7-N4-C3	2.59	117.91	111.27
3	D	501	NAP	O3-PN-O5D	2.63	109.92	102.94
3	B	501	NAP	C1D-C2D-C3D	2.71	106.00	101.64
4	D	1453	EPE	C7-N4-C3	2.75	118.32	111.27
3	C	501	NAP	C1D-C2D-C3D	2.76	106.09	101.64
4	B	1453	EPE	O1S-S-C10	2.82	109.31	106.91
4	A	1451	EPE	C2-C3-N4	2.82	115.67	110.63
3	C	501	NAP	O2X-P2B-O1X	2.89	119.90	110.58
4	B	1453	EPE	O2S-S-C10	2.91	109.39	106.91
3	D	501	NAP	C1D-C2D-C3D	2.93	106.35	101.64
2	B	500	FAD	C4X-N5-C5X	2.95	120.16	116.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	NAP	O4D-C4D-C3D	3.01	109.73	104.43
3	B	501	NAP	O2B-P2B-O1X	3.02	114.66	107.11
4	A	1451	EPE	C7-N4-C5	3.04	119.05	111.27
3	D	501	NAP	O2B-P2B-O1X	3.07	114.78	107.11
2	C	500	FAD	C4X-N5-C5X	3.11	120.34	116.76
3	A	501	NAP	O4D-C4D-C3D	3.18	110.04	104.43
3	B	501	NAP	O4D-C4D-C3D	3.36	110.35	104.43
4	B	1453	EPE	C6-C5-N4	3.41	116.73	110.63
2	A	500	FAD	C4X-N5-C5X	3.63	120.94	116.76
3	A	501	NAP	O3-PN-O5D	3.65	112.62	102.94
4	A	1451	EPE	C5-N4-C3	3.67	116.85	108.90
2	B	500	FAD	C4-N3-C2	3.85	118.58	115.25
4	A	1451	EPE	C7-N4-C3	3.97	121.44	111.27
2	D	500	FAD	C4X-N5-C5X	4.00	121.36	116.76
4	D	1453	EPE	C5-N4-C3	4.17	117.94	108.90
3	C	501	NAP	O3-PN-O5D	4.20	114.08	102.94
2	D	500	FAD	C1'-N10-C9A	4.46	123.87	118.86
4	A	1451	EPE	O1S-S-C10	4.66	110.88	106.91
2	A	500	FAD	C1'-N10-C9A	4.70	124.13	118.86
2	B	500	FAD	C1'-N10-C9A	4.74	124.18	118.86
4	D	1453	EPE	C7-N4-C5	4.79	123.56	111.27
4	D	1453	EPE	O2S-S-C10	4.99	111.16	106.91
2	C	500	FAD	C1'-N10-C9A	5.43	124.96	118.86
2	D	500	FAD	C4-N3-C2	5.49	120.00	115.25
4	B	1453	EPE	C5-N4-C3	6.04	121.98	108.90
2	A	500	FAD	C4-N3-C2	6.50	120.86	115.25
2	C	500	FAD	C4-N3-C2	6.72	121.06	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1451	EPE	1	0
2	A	500	FAD	3	0
3	A	501	NAP	8	0
4	B	1453	EPE	1	0
2	B	500	FAD	2	0
3	B	501	NAP	9	0
2	C	500	FAD	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	NAP	8	0
3	D	501	NAP	6	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	446/461 (96%)	-0.39	0 <span>100</span> <span>100</span>	20, 31, 46, 56	0
1	B	447/461 (96%)	-0.48	1 (0%) <span>95</span> <span>87</span>	20, 32, 47, 71	0
1	C	447/461 (96%)	-0.60	0 <span>100</span> <span>100</span>	20, 32, 47, 72	0
1	D	447/461 (96%)	-0.47	0 <span>100</span> <span>100</span>	20, 32, 46, 72	0
All	All	1787/1844 (96%)	-0.48	1 (0%) <span>95</span> <span>90</span>	20, 32, 47, 72	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	451	ASP	2.6

### 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
4	EPE	B	1453	15/15	0.94	0.26	1.65	59,63,67,67	0
4	EPE	A	1451	15/15	0.95	0.22	1.42	52,55,58,58	0
4	EPE	D	1453	15/15	0.92	0.23	1.40	51,68,78,79	0
5	PEG	C	1453	7/7	0.87	0.22	1.26	41,44,47,50	0
2	FAD	C	500	53/53	0.99	0.15	0.19	16,20,26,28	0
2	FAD	D	500	53/53	0.98	0.17	0.12	16,20,26,28	0
2	FAD	A	500	53/53	0.98	0.17	-0.21	16,20,26,28	0
2	FAD	B	500	53/53	0.98	0.15	-0.25	16,21,26,28	0
3	NAP	A	501	39/48	0.97	0.18	-0.28	31,35,48,52	0
3	NAP	D	501	39/48	0.97	0.18	-0.41	30,34,48,52	0
3	NAP	B	501	39/48	0.98	0.14	-0.70	31,35,48,52	0
3	NAP	C	501	39/48	0.97	0.14	-0.86	31,35,48,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.