



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:17 am GMT

PDB ID : 5FN0  
Title : Crystal structure of *Pseudomonas fluorescens* kynurenine-3- monooxygenase (KMO) in complex with GSK180  
Authors : Mole, D.J.; Webster, S.P.; Uings, I.; Zheng, X.; Binnie, M.; Wilson, K.; Hutchinson, J.P.; Mirguet, O.; Walker, A.; Beaufils, B.; Ancellin, N.; Trottet, L.; Beneton, V.; Mowat, C.G.; Wilkinson, M.; Rowland, P.; Haslam, C.; McBride, A.; Homer, N.Z.M.; Baily, J.E.; Sharp, M.G.F.; Garden, O.J.; Hughes, J.; Howie, S.E.M.; Holmes, D.; Liddle, J.; Iredale, J.P.  
Deposited on : 2015-11-10  
Resolution : 3.19 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

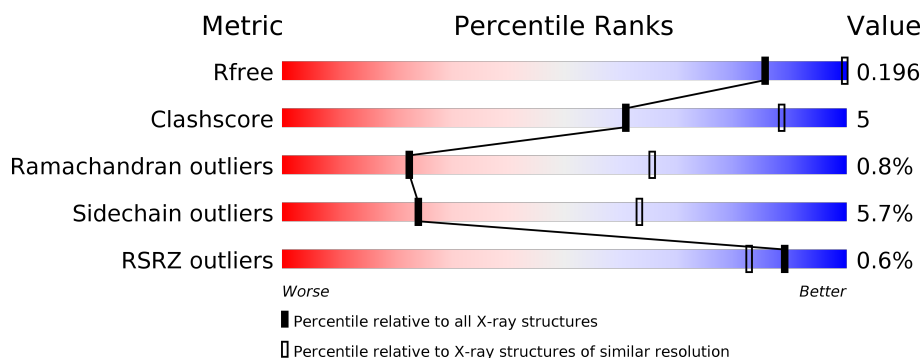
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.19 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	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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	<div> <div>81%</div> <div>17%</div> <div>..</div> </div>
1	B	461	<div> <div>79%</div> <div>19%</div> <div>..</div> </div>
1	C	461	<div> <div>%</div> <div>82%</div> <div>16%</div> <div>..</div> </div>
1	D	461	<div> <div>%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14670 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 KYNURENINE 3-MONOOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3523	2206	654	646	17			
1	B	455	Total	C	N	O	S	0	0	0
			3523	2206	654	646	17			
1	C	455	Total	C	N	O	S	0	0	0
			3523	2206	654	646	17			
1	D	455	Total	C	N	O	S	0	0	0
			3523	2206	654	646	17			

There are 8 discrepancies between the modelled and reference sequences:

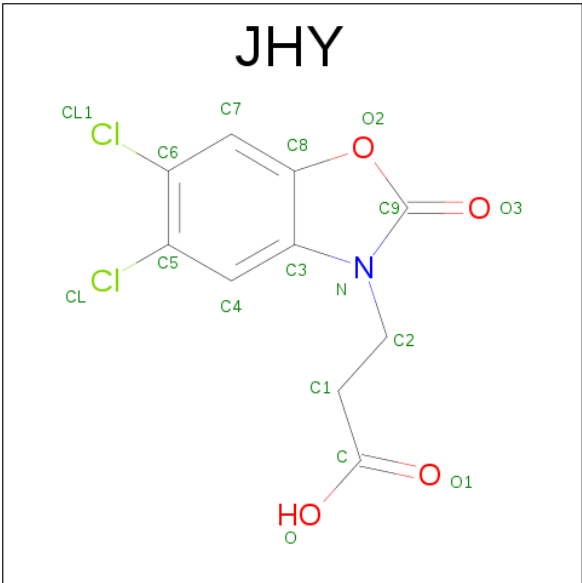
Chain	Residue	Modelled	Actual	Comment	Reference
A	461	SER	CYS	ENGINEERED MUTATION	UNP Q84HF5
A	252	SER	CYS	ENGINEERED MUTATION	UNP Q84HF5
B	461	SER	CYS	ENGINEERED MUTATION	UNP Q84HF5
B	252	SER	CYS	ENGINEERED MUTATION	UNP Q84HF5
C	461	SER	CYS	ENGINEERED MUTATION	UNP Q84HF5
C	252	SER	CYS	ENGINEERED MUTATION	UNP Q84HF5
D	461	SER	CYS	ENGINEERED MUTATION	UNP Q84HF5
D	252	SER	CYS	ENGINEERED MUTATION	UNP Q84HF5

- 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 3-(5,6-DICHLORO-2-OXOBENZO[D]OXAZOL-3(2H)-YL)PROPANOIC ACID (three-letter code: JHY) (formula: C<sub>10</sub>H<sub>7</sub>Cl<sub>2</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			17	10	2	1	4		
3	B	1	Total	C	Cl	N	O	0	0
			17	10	2	1	4		
3	C	1	Total	C	Cl	N	O	0	0
			17	10	2	1	4		
3	D	1	Total	C	Cl	N	O	0	0
			17	10	2	1	4		

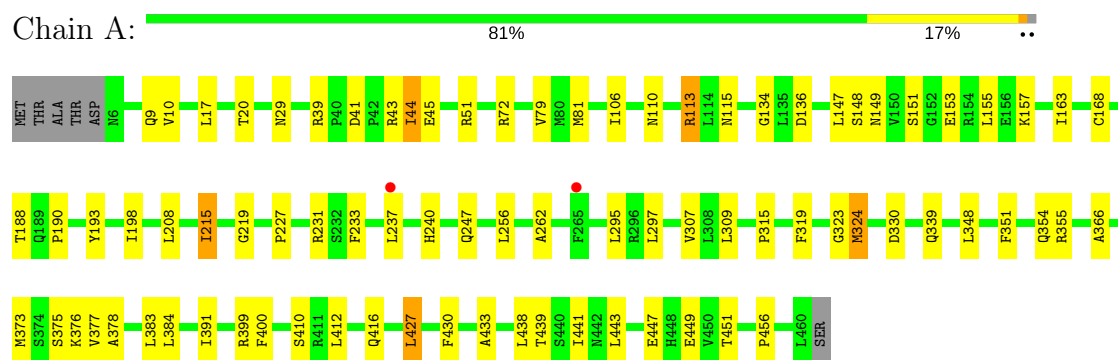
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	77	Total	O	0	0
			77	77		
4	B	73	Total	O	0	0
			73	73		
4	C	64	Total	O	0	0
			64	64		
4	D	84	Total	O	0	0
			84	84		

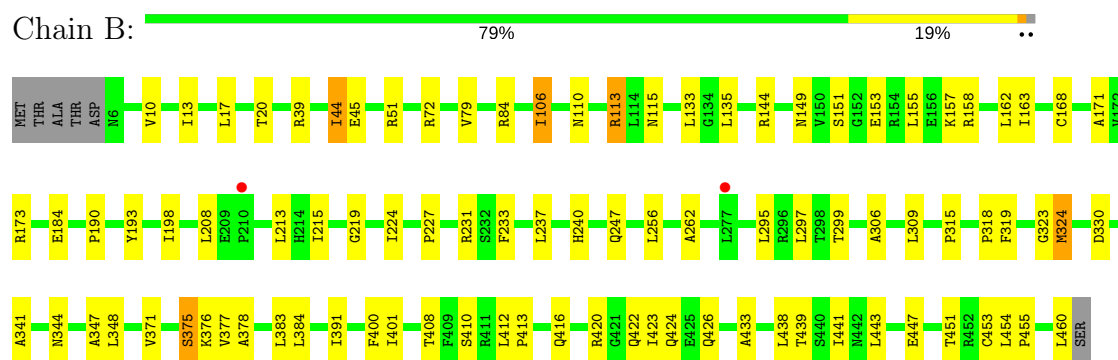
### 3 Residue-property plots [i](#)

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.

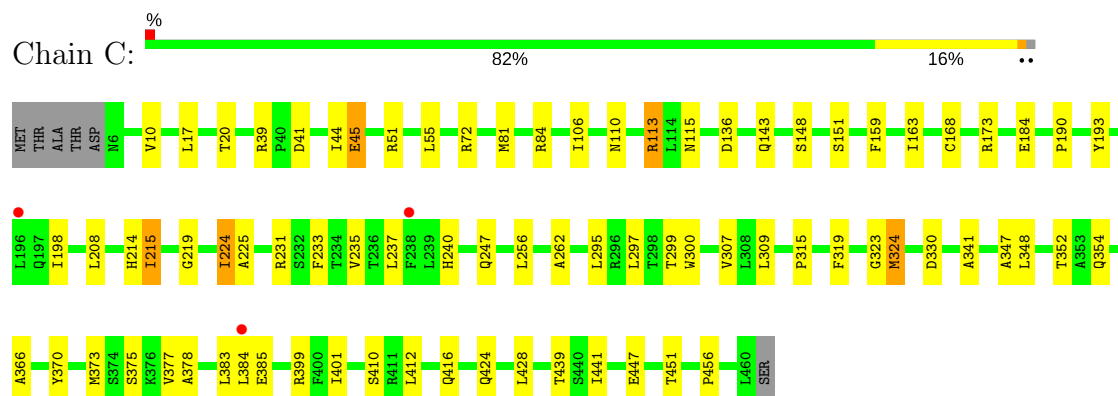
#### • Molecule 1: KYNURENINE 3-MONOOXYGENASE



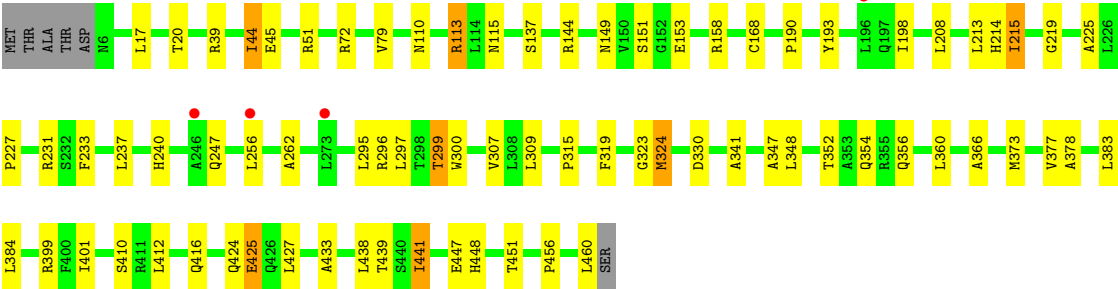
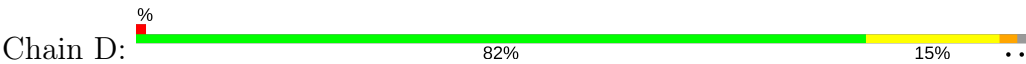
#### • Molecule 1: KYNURENINE 3-MONOOXYGENASE



#### • Molecule 1: KYNURENINE 3-MONOOXYGENASE



● Molecule 1: KYNURENINE 3-MONOOXYGENASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	186.85Å 105.29Å 133.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.43 – 3.19 93.42 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.6 (93.43-3.19) 100.0 (93.42-3.19)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.12 (at 3.19Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, $R_{free}$	0.157 , 0.196 0.160 , 0.196	Depositor DCC
$R_{free}$ test set	2244 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	89.0	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 85.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14670	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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: JHY, 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	0.51	0/3600	0.70	0/4891
1	B	0.52	0/3600	0.70	0/4891
1	C	0.50	0/3600	0.69	0/4891
1	D	0.50	0/3600	0.69	1/4891 (0.0%)
All	All	0.51	0/14400	0.70	1/19564 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	425	GLU	CA-CB-CG	5.44	125.36	113.40

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	3523	0	3482	37	0
1	B	3523	0	3482	42	0
1	C	3523	0	3482	36	0
1	D	3523	0	3482	35	0
2	A	53	0	31	1	0
2	B	53	0	31	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	53	0	31	1	0
2	D	53	0	31	1	0
3	A	17	0	6	0	0
3	B	17	0	6	1	0
3	C	17	0	6	1	0
3	D	17	0	6	0	0
4	A	77	0	0	0	0
4	B	73	0	0	2	0
4	C	64	0	0	0	0
4	D	84	0	0	4	0
All	All	14670	0	14076	149	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 5.

All (149) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:ILE:HD11	1:B:408:THR:HG21	1.64	0.78
1:C:295:LEU:HB3	1:C:315:PRO:HD2	1.73	0.70
1:A:39:ARG:HH22	1:A:115:ASN:HD21	1.44	0.66
1:A:136:ASP:OD2	1:A:148:SER:HB3	1.96	0.66
1:D:17:LEU:HD13	1:D:324:MET:HG3	1.79	0.65
1:C:41:ASP:HB3	1:C:44:ILE:HG12	1.79	0.65
1:D:39:ARG:HH22	1:D:115:ASN:HD21	1.45	0.64
1:B:17:LEU:HD13	1:B:324:MET:HG3	1.79	0.64
1:B:295:LEU:HB3	1:B:315:PRO:HD2	1.80	0.64
1:C:17:LEU:HD13	1:C:324:MET:HG3	1.79	0.63
1:D:295:LEU:HB3	1:D:315:PRO:HD2	1.81	0.62
1:A:17:LEU:HD13	1:A:324:MET:HG3	1.81	0.62
1:C:39:ARG:HH22	1:C:115:ASN:HD21	1.47	0.62
1:B:39:ARG:HH22	1:B:115:ASN:HD21	1.47	0.61
1:D:460:LEU:C	4:D:2082:HOH:O	2.38	0.61
1:A:430:PHE:HD2	1:B:426:GLN:HG2	1.66	0.61
1:B:173:ARG:HD2	1:B:297:LEU:HD11	1.81	0.61
1:C:385:GLU:HG2	1:C:428:LEU:HB3	1.82	0.61
1:D:299:THR:HA	4:D:2047:HOH:O	2.01	0.61
1:C:215:ILE:HD12	1:C:373:MET:HB2	1.83	0.61
1:B:149:ASN:HD21	1:B:153:GLU:HB2	1.66	0.60
1:B:378:ALA:HB1	1:B:383:LEU:HD21	1.83	0.60
1:A:29:ASN:ND2	1:A:339:GLN:HE22	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ALA:HB1	1:A:383:LEU:HD21	1.86	0.58
1:D:401:ILE:H	1:D:424:GLN:HE22	1.52	0.58
1:A:430:PHE:HE1	1:B:453:CYS:HG	1.50	0.58
1:A:295:LEU:HB3	1:A:315:PRO:HD2	1.85	0.57
1:A:215:ILE:HD12	1:A:373:MET:HB2	1.84	0.57
1:A:427:LEU:HD11	1:A:449:GLU:HB3	1.86	0.57
1:D:215:ILE:HD12	1:D:373:MET:HB2	1.86	0.56
1:C:378:ALA:HB1	1:C:383:LEU:HD21	1.87	0.56
1:D:378:ALA:HB1	1:D:383:LEU:HD21	1.86	0.56
1:B:110:ASN:HB3	1:B:113:ARG:HB2	1.86	0.56
1:C:224:ILE:O	1:C:235:VAL:HA	2.06	0.56
1:B:309:LEU:HD12	1:B:330:ASP:HB3	1.87	0.56
1:D:110:ASN:HB3	1:D:113:ARG:HB2	1.87	0.56
1:D:307:VAL:HB	1:D:348:LEU:HD13	1.86	0.56
1:C:309:LEU:HD12	1:C:330:ASP:HB3	1.88	0.55
1:A:110:ASN:HB3	1:A:113:ARG:HB2	1.88	0.55
1:A:51:ARG:NH2	1:A:168:CYS:HB2	2.21	0.55
1:B:44:ILE:HG13	1:B:45:GLU:H	1.72	0.55
1:D:51:ARG:NH2	1:D:168:CYS:HB2	2.22	0.55
1:C:110:ASN:HB3	1:C:113:ARG:HB2	1.88	0.54
1:A:309:LEU:HD12	1:A:330:ASP:HB3	1.87	0.54
1:B:51:ARG:NH2	1:B:168:CYS:HB2	2.24	0.53
1:C:143:GLN:HG2	1:C:159:PHE:O	2.09	0.52
1:C:173:ARG:HD2	1:C:297:LEU:HD11	1.91	0.52
1:A:44:ILE:HG13	1:A:45:GLU:H	1.74	0.52
1:D:44:ILE:HG13	1:D:45:GLU:H	1.74	0.52
1:C:307:VAL:HB	1:C:348:LEU:HD13	1.91	0.52
1:C:51:ARG:NH2	1:C:168:CYS:HB2	2.25	0.52
1:C:193:TYR:HA	1:C:237:LEU:O	2.10	0.51
1:B:384:LEU:HD12	1:B:438:LEU:HD12	1.92	0.51
1:B:193:TYR:HA	1:B:237:LEU:O	2.11	0.50
1:C:214:HIS:HB2	1:C:225:ALA:HB3	1.93	0.50
1:A:29:ASN:HD22	1:A:339:GLN:HE22	1.58	0.49
1:D:256:LEU:HD22	1:D:262:ALA:HA	1.93	0.49
1:A:193:TYR:HA	1:A:237:LEU:O	2.12	0.49
1:B:135:LEU:HD23	1:B:171:ALA:HB3	1.93	0.49
1:C:256:LEU:HD22	1:C:262:ALA:HA	1.95	0.49
1:D:214:HIS:HB2	1:D:225:ALA:HB3	1.94	0.49
1:B:401:ILE:H	1:B:424:GLN:HE22	1.60	0.49
1:D:149:ASN:HD21	1:D:153:GLU:HB2	1.77	0.49
1:C:136:ASP:OD2	1:C:148:SER:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:PHE:HA	3:C:4000:JHY:CL	2.50	0.49
1:D:193:TYR:HA	1:D:237:LEU:O	2.12	0.49
1:A:256:LEU:HD22	1:A:262:ALA:HA	1.94	0.49
1:B:256:LEU:HD22	1:B:262:ALA:HA	1.95	0.48
1:B:13:ILE:HG13	1:B:135:LEU:HD22	1.96	0.48
1:D:341:ALA:HB3	1:D:347:ALA:HB2	1.95	0.48
1:B:144:ARG:NH1	1:B:158:ARG:HE	2.12	0.48
1:A:307:VAL:HB	1:A:348:LEU:HD13	1.95	0.47
1:D:384:LEU:HG	1:D:438:LEU:HD12	1.96	0.47
1:D:412:LEU:HD11	1:D:416:GLN:OE1	2.14	0.47
1:D:299:THR:HG23	4:D:2047:HOH:O	2.14	0.47
1:C:341:ALA:HB3	1:C:347:ALA:HB2	1.96	0.47
1:C:224:ILE:HD11	1:C:373:MET:HE2	1.97	0.47
1:D:309:LEU:HD12	1:D:330:ASP:HB3	1.96	0.47
1:B:318:PRO:HA	4:B:2045:HOH:O	2.14	0.47
1:A:412:LEU:HD11	1:A:416:GLN:OE1	2.15	0.47
1:B:460:LEU:C	4:B:2073:HOH:O	2.52	0.47
1:C:184:GLU:HG2	1:C:297:LEU:HD22	1.96	0.46
1:A:384:LEU:HD12	1:A:438:LEU:HD12	1.97	0.46
1:A:198:ILE:HB	1:A:233:PHE:HB2	1.98	0.46
1:D:447:GLU:O	1:D:451:THR:HG23	2.15	0.46
1:A:134:GLY:O	1:A:147:LEU:HA	2.16	0.45
1:A:190:PRO:HB2	1:A:240:HIS:CD2	2.52	0.45
1:A:29:ASN:HD22	1:A:339:GLN:NE2	2.14	0.45
1:C:319:PHE:CD2	1:C:370:TYR:HB2	2.51	0.45
1:C:447:GLU:O	1:C:451:THR:HG23	2.16	0.45
1:D:198:ILE:HB	1:D:233:PHE:HB2	1.99	0.45
1:C:198:ILE:HB	1:C:233:PHE:HB2	1.99	0.45
1:D:190:PRO:HB2	1:D:240:HIS:CD2	2.52	0.45
1:B:106:ILE:HD11	1:B:408:THR:CG2	2.41	0.44
1:B:190:PRO:HB2	1:B:240:HIS:CD2	2.52	0.44
1:B:198:ILE:HB	1:B:233:PHE:HB2	2.00	0.44
1:B:184:GLU:HG2	1:B:297:LEU:HD22	1.99	0.44
1:B:412:LEU:HD11	1:B:416:GLN:OE1	2.17	0.44
1:C:190:PRO:HB2	1:C:240:HIS:CD2	2.52	0.44
1:C:401:ILE:H	1:C:424:GLN:HE22	1.64	0.44
1:B:149:ASN:ND2	1:B:153:GLU:HB2	2.29	0.44
1:C:323:GLY:HA3	2:C:462:FAD:H1'2	2.00	0.44
1:A:81:MET:HB2	1:A:106:ILE:HG13	1.99	0.43
1:B:344:ASN:O	1:B:348:LEU:HG	2.18	0.43
1:B:155:LEU:HD21	1:B:157:LYS:HE3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:VAL:HG11	1:D:227:PRO:HB2	2.01	0.43
1:D:441:ILE:H	1:D:441:ILE:HG13	1.71	0.43
1:C:412:LEU:HD11	1:C:416:GLN:OE1	2.19	0.43
1:C:44:ILE:HG13	1:C:45:GLU:N	2.34	0.43
1:C:341:ALA:CB	1:C:347:ALA:HB2	2.48	0.42
1:B:323:GLY:HA3	2:B:462:FAD:H1'2	2.01	0.42
1:A:79:VAL:HG11	1:A:227:PRO:HB2	2.00	0.42
1:B:447:GLU:O	1:B:451:THR:HG23	2.19	0.42
1:D:319:PHE:HB2	1:D:366:ALA:O	2.19	0.42
1:A:447:GLU:O	1:A:451:THR:HG23	2.20	0.42
1:B:420:ARG:HA	1:B:423:ILE:HD12	2.01	0.42
1:D:399:ARG:CZ	1:D:456:PRO:HG3	2.49	0.42
1:B:79:VAL:HG11	1:B:227:PRO:HB2	2.01	0.42
1:D:323:GLY:HA3	2:D:462:FAD:H1'2	2.00	0.42
1:A:155:LEU:HD21	1:A:157:LYS:HE3	2.02	0.42
1:A:323:GLY:HA3	2:A:462:FAD:H1'2	2.01	0.42
1:D:149:ASN:ND2	1:D:153:GLU:HB2	2.34	0.42
1:C:319:PHE:HB2	1:C:366:ALA:O	2.19	0.42
1:A:149:ASN:HD21	1:A:153:GLU:HB2	1.85	0.42
1:A:319:PHE:HB2	1:A:366:ALA:O	2.20	0.42
1:D:300:TRP:HB2	1:D:352:THR:HG23	2.01	0.42
1:A:10:VAL:HG21	1:A:163:ILE:HD12	2.01	0.42
1:C:10:VAL:HG21	1:C:163:ILE:HD12	2.02	0.42
1:B:319:PHE:HA	3:B:4000:JHY:CL	2.57	0.41
1:D:352:THR:O	1:D:356:GLN:HB2	2.19	0.41
1:A:351:PHE:CE1	1:A:355:ARG:HG3	2.55	0.41
1:B:162:LEU:O	1:B:306:ALA:HA	2.21	0.41
1:B:391:ILE:HG21	1:B:443:LEU:HD13	2.02	0.41
1:C:300:TRP:HB2	1:C:352:THR:HG23	2.01	0.41
1:A:399:ARG:CZ	1:A:456:PRO:HG3	2.51	0.41
1:B:133:LEU:HD23	1:B:133:LEU:HA	1.88	0.41
1:A:41:ASP:HB3	1:A:44:ILE:HG12	2.03	0.40
1:B:341:ALA:HB3	1:B:347:ALA:HB2	2.04	0.40
1:D:296:ARG:HD3	1:D:360:LEU:HD22	2.03	0.40
1:D:448:HIS:HE1	4:D:2078:HOH:O	2.04	0.40
1:A:391:ILE:HG21	1:A:443:LEU:HD13	2.03	0.40
1:A:399:ARG:HD3	1:A:451:THR:HA	2.03	0.40
1:B:454:LEU:HA	1:B:455:PRO:HD3	1.96	0.40
1:C:81:MET:HB2	1:C:106:ILE:HG13	2.02	0.40
1:B:10:VAL:HG21	1:B:163:ILE:HD12	2.03	0.40
2:B:462:FAD:H1'1	2:B:462:FAD:H9	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:PRO:HG2	1:B:416:GLN:HB2	2.04	0.40
1:C:399:ARG:CZ	1:C:456:PRO:HG3	2.52	0.40
1:D:144:ARG:NH1	1:D:158:ARG:HE	2.19	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	453/461 (98%)	432 (95%)	17 (4%)	4 (1%)	20	64
1	B	453/461 (98%)	431 (95%)	17 (4%)	5 (1%)	17	58
1	C	453/461 (98%)	430 (95%)	21 (5%)	2 (0%)	38	77
1	D	453/461 (98%)	431 (95%)	19 (4%)	3 (1%)	25	68
All	All	1812/1844 (98%)	1724 (95%)	74 (4%)	14 (1%)	22	65

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	433	ALA
1	B	376	LYS
1	B	433	ALA
1	D	433	ALA
1	C	377	VAL
1	D	377	VAL
1	A	219	GLY
1	A	376	LYS
1	A	377	VAL
1	B	219	GLY
1	B	375	SER
1	C	219	GLY

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Mol	Chain	Res	Type
1	D	219	GLY
1	B	377	VAL

### 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	367/372 (99%)	346 (94%)	21 (6%)	24	63
1	B	367/372 (99%)	345 (94%)	22 (6%)	22	61
1	C	367/372 (99%)	347 (95%)	20 (5%)	26	65
1	D	367/372 (99%)	347 (95%)	20 (5%)	26	65
All	All	1468/1488 (99%)	1385 (94%)	83 (6%)	24	63

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	20	THR
1	A	43	ARG
1	A	44	ILE
1	A	72	ARG
1	A	113	ARG
1	A	151	SER
1	A	188	THR
1	A	208	LEU
1	A	215	ILE
1	A	231	ARG
1	A	247	GLN
1	A	297	LEU
1	A	324	MET
1	A	354	GLN
1	A	375	SER
1	A	400	PHE
1	A	410	SER
1	A	427	LEU

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Mol	Chain	Res	Type
1	A	439	THR
1	A	441	ILE
1	B	20	THR
1	B	44	ILE
1	B	72	ARG
1	B	84	ARG
1	B	106	ILE
1	B	113	ARG
1	B	151	SER
1	B	208	LEU
1	B	213	LEU
1	B	215	ILE
1	B	224	ILE
1	B	231	ARG
1	B	247	GLN
1	B	299	THR
1	B	324	MET
1	B	371	VAL
1	B	375	SER
1	B	400	PHE
1	B	410	SER
1	B	422	GLN
1	B	439	THR
1	B	441	ILE
1	C	20	THR
1	C	45	GLU
1	C	55	LEU
1	C	72	ARG
1	C	84	ARG
1	C	113	ARG
1	C	151	SER
1	C	208	LEU
1	C	215	ILE
1	C	224	ILE
1	C	231	ARG
1	C	247	GLN
1	C	299	THR
1	C	324	MET
1	C	354	GLN
1	C	375	SER
1	C	384	LEU
1	C	410	SER

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Mol	Chain	Res	Type
1	C	439	THR
1	C	441	ILE
1	D	20	THR
1	D	44	ILE
1	D	72	ARG
1	D	113	ARG
1	D	137	SER
1	D	151	SER
1	D	208	LEU
1	D	213	LEU
1	D	215	ILE
1	D	231	ARG
1	D	247	GLN
1	D	297	LEU
1	D	299	THR
1	D	324	MET
1	D	354	GLN
1	D	410	SER
1	D	425	GLU
1	D	427	LEU
1	D	439	THR
1	D	441	ILE

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

Mol	Chain	Res	Type
1	A	34	ASN
1	A	54	ASN
1	A	96	GLN
1	A	115	ASN
1	A	197	GLN
1	A	240	HIS
1	A	339	GLN
1	A	424	GLN
1	A	459	HIS
1	B	34	ASN
1	B	54	ASN
1	B	96	GLN
1	B	115	ASN
1	B	197	GLN
1	B	240	HIS
1	B	339	GLN

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Mol	Chain	Res	Type
1	B	390	GLN
1	B	424	GLN
1	B	448	HIS
1	B	459	HIS
1	C	34	ASN
1	C	54	ASN
1	C	115	ASN
1	C	197	GLN
1	C	240	HIS
1	C	255	GLN
1	C	305	GLN
1	C	339	GLN
1	C	424	GLN
1	D	34	ASN
1	D	54	ASN
1	D	96	GLN
1	D	115	ASN
1	D	197	GLN
1	D	240	HIS
1	D	339	GLN
1	D	390	GLN
1	D	424	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](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	JHY	A	4000	-	10,18,18	0.84	0	11,26,26	1.08	1 (9%)
2	FAD	A	462	-	51,58,58	1.08	5 (9%)	54,89,89	2.22	5 (9%)
3	JHY	B	4000	-	10,18,18	0.89	0	11,26,26	1.12	1 (9%)
2	FAD	B	462	-	51,58,58	1.07	4 (7%)	54,89,89	2.22	6 (11%)
3	JHY	C	4000	-	10,18,18	0.85	0	11,26,26	1.11	1 (9%)
2	FAD	C	462	-	51,58,58	1.01	5 (9%)	54,89,89	2.23	6 (11%)
3	JHY	D	4000	-	10,18,18	0.93	0	11,26,26	1.08	1 (9%)
2	FAD	D	462	-	51,58,58	1.04	5 (9%)	54,89,89	2.24	6 (11%)

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	JHY	A	4000	-	-	0/3/5/5	0/1/2/2
2	FAD	A	462	-	-	0/28/50/50	0/6/6/6
3	JHY	B	4000	-	-	0/3/5/5	0/1/2/2
2	FAD	B	462	-	-	0/28/50/50	0/6/6/6
3	JHY	C	4000	-	-	0/3/5/5	0/1/2/2
2	FAD	C	462	-	-	0/28/50/50	0/6/6/6
3	JHY	D	4000	-	-	0/3/5/5	0/1/2/2
2	FAD	D	462	-	-	0/28/50/50	0/6/6/6

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	462	FAD	C4-C4X	2.06	1.45	1.41
2	D	462	FAD	C5X-N5	2.34	1.38	1.35
2	D	462	FAD	C4-C4X	2.35	1.45	1.41
2	B	462	FAD	C5X-N5	2.48	1.39	1.35
2	A	462	FAD	C4-C4X	2.48	1.46	1.41
2	A	462	FAD	C5X-N5	2.62	1.39	1.35
2	C	462	FAD	C4X-C10	2.74	1.45	1.41
2	C	462	FAD	C5X-N5	2.81	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	462	FAD	C9A-N10	2.83	1.42	1.38
2	C	462	FAD	C9A-N10	2.95	1.42	1.38
2	C	462	FAD	C4-N3	3.00	1.38	1.33
2	A	462	FAD	C4X-C10	3.05	1.46	1.41
2	B	462	FAD	C4-N3	3.14	1.38	1.33
2	D	462	FAD	C4-N3	3.17	1.38	1.33
2	B	462	FAD	C4X-C10	3.19	1.46	1.41
2	B	462	FAD	C9A-N10	3.20	1.42	1.38
2	D	462	FAD	C4X-C10	3.20	1.46	1.41
2	A	462	FAD	C4-N3	3.24	1.38	1.33
2	A	462	FAD	C9A-N10	3.40	1.43	1.38

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	462	FAD	C4X-C4-N3	-6.50	114.22	123.48
2	D	462	FAD	C4X-C4-N3	-6.47	114.27	123.48
2	A	462	FAD	C4X-C4-N3	-6.46	114.28	123.48
2	C	462	FAD	C4X-C4-N3	-6.41	114.35	123.48
2	A	462	FAD	C4X-C10-N10	-5.32	116.83	120.52
2	C	462	FAD	C4X-C10-N10	-5.32	116.83	120.52
2	D	462	FAD	C4X-C10-N10	-5.31	116.83	120.52
2	B	462	FAD	C4X-C10-N10	-5.19	116.92	120.52
2	C	462	FAD	C4-C4X-C10	-2.98	117.55	119.96
2	A	462	FAD	C4-C4X-C10	-2.95	117.57	119.96
2	D	462	FAD	C4-C4X-C10	-2.93	117.59	119.96
3	B	4000	JHY	C6-C7-C8	-2.69	116.95	119.64
2	B	462	FAD	C4-C4X-C10	-2.65	117.81	119.96
3	A	4000	JHY	C6-C7-C8	-2.64	117.00	119.64
3	C	4000	JHY	C6-C7-C8	-2.53	117.11	119.64
3	D	4000	JHY	C6-C7-C8	-2.47	117.17	119.64
2	B	462	FAD	O2P-P-O5'	2.03	117.74	108.14
2	C	462	FAD	O2P-P-O5'	2.07	117.94	108.14
2	D	462	FAD	O2P-P-O5'	2.16	118.32	108.14
2	B	462	FAD	C10-C4X-N5	3.08	124.14	120.59
2	C	462	FAD	C10-C4X-N5	3.16	124.22	120.59
2	A	462	FAD	C10-C4X-N5	3.19	124.26	120.59
2	D	462	FAD	C10-C4X-N5	3.20	124.28	120.59
2	A	462	FAD	C4-N3-C2	12.11	125.75	115.16
2	B	462	FAD	C4-N3-C2	12.15	125.79	115.16
2	D	462	FAD	C4-N3-C2	12.23	125.86	115.16
2	C	462	FAD	C4-N3-C2	12.26	125.88	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	462	FAD	1	0
3	B	4000	JHY	1	0
2	B	462	FAD	2	0
3	C	4000	JHY	1	0
2	C	462	FAD	1	0
2	D	462	FAD	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [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	455/461 (98%)	0.02	2 (0%) 92 89	49, 99, 181, 198	0
1	B	455/461 (98%)	-0.01	2 (0%) 92 89	47, 103, 182, 210	0
1	C	455/461 (98%)	-0.08	3 (0%) 87 80	60, 103, 180, 194	0
1	D	455/461 (98%)	-0.03	4 (0%) 84 75	56, 110, 194, 221	0
All	All	1820/1844 (98%)	-0.03	11 (0%) 89 83	47, 104, 184, 221	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	196	LEU	2.9
1	C	384	LEU	2.8
1	D	273	LEU	2.7
1	B	210	PRO	2.7
1	C	238	PHE	2.6
1	D	246	ALA	2.6
1	D	196	LEU	2.5
1	B	277	LEU	2.4
1	A	265	PHE	2.1
1	A	237	LEU	2.1
1	D	256	LEU	2.1

### 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
3	JHY	D	4000	17/17	0.94	0.32	0.52	103,107,121,131	0
3	JHY	B	4000	17/17	0.94	0.30	0.06	104,107,113,123	0
3	JHY	A	4000	17/17	0.96	0.31	0.03	99,105,113,122	0
3	JHY	C	4000	17/17	0.94	0.27	-0.04	105,111,115,122	0
2	FAD	A	462	53/53	0.97	0.21	-0.49	73,86,101,112	0
2	FAD	C	462	53/53	0.97	0.20	-0.50	70,85,104,106	0
2	FAD	B	462	53/53	0.97	0.20	-0.71	67,80,98,105	0
2	FAD	D	462	53/53	0.98	0.18	-0.83	76,87,98,102	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.