



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 9, 2017 – 04:53 PM EST

PDB ID : 5I1W  
Title : Crystal structure of CrmK, a flavoenzyme involved in the shunt product recycling mechanism in caerulomycin biosynthesis  
Authors : Picard, M.-E.; Barma, J.; Shi, R.  
Deposited on : 2016-02-07  
Resolution : 2.15 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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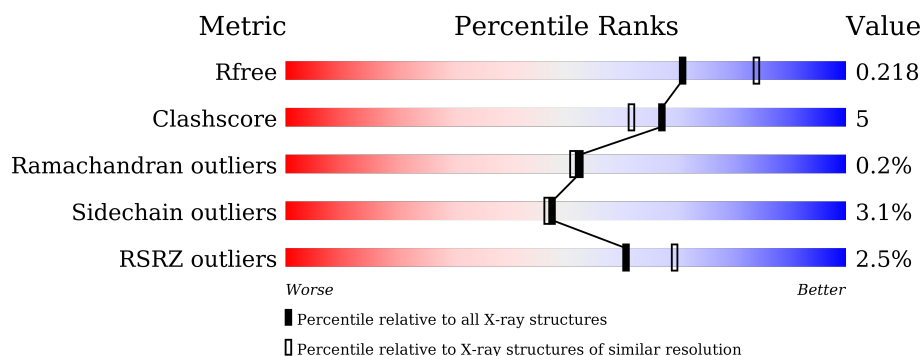
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
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)	:	rb-20028442

**i**

## X-RAY DIFFRACTION

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.



<b>Metric</b>	<b>Whole archive (#Entries)</b>	<b>Similar resolution (#Entries, resolution range(Å))</b>
$R_{free}$	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	500	<div><div></div><div></div><div></div></div> 88%	11%
1	B	500	<div><div></div><div></div><div></div></div> 86%	12%
1	C	500	<div><div></div><div></div><div></div></div> 88%	10%
1	D	500	<div><div></div><div></div><div></div></div> 89%	9%

## 2 Entry composition [i](#)

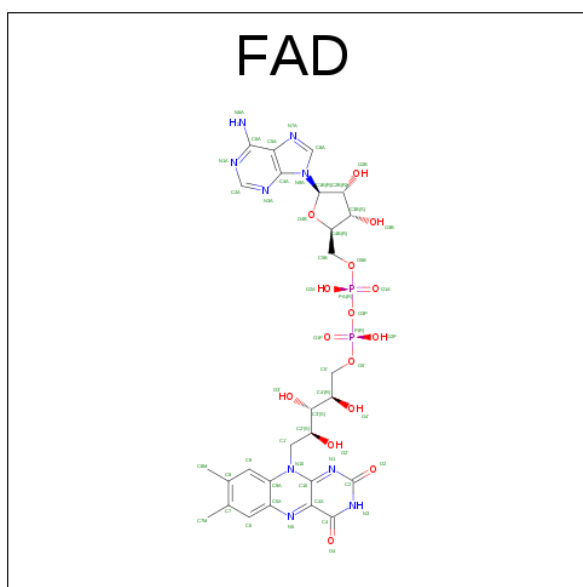
There are 5 unique types of molecules in this entry. The entry contains 16449 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CrmK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	2	0
			3896	2464	693	728	11			
1	B	498	Total	C	N	O	S	0	1	0
			3891	2461	693	726	11			
1	C	498	Total	C	N	O	S	0	2	0
			3899	2466	696	726	11			
1	D	498	Total	C	N	O	S	0	1	0
			3891	2461	693	726	11			

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



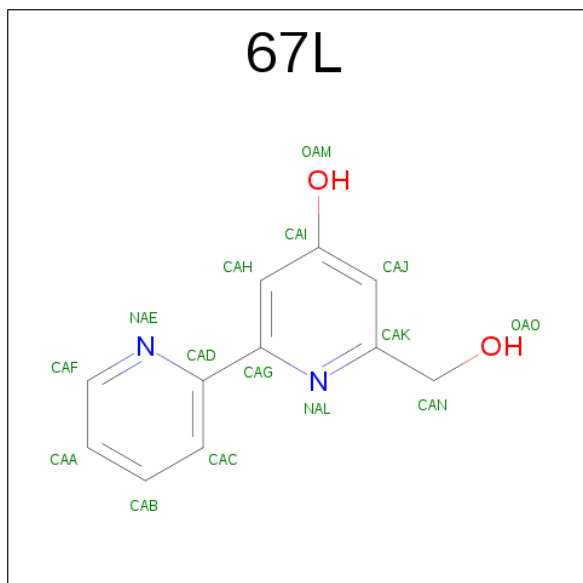
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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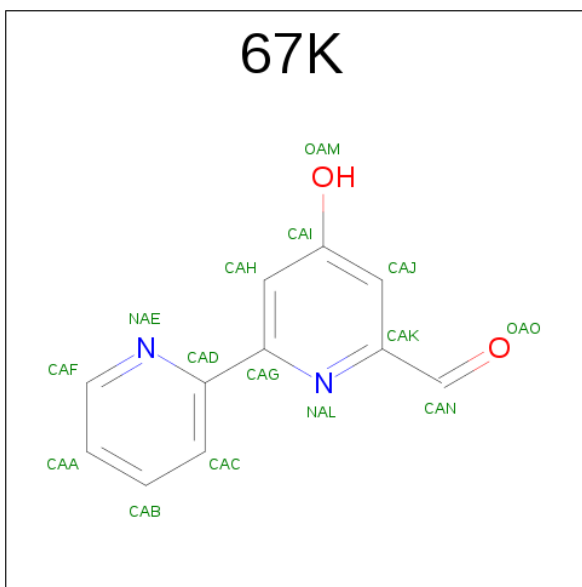
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 6-(hydroxymethyl)[2,2'-bipyridin]-4-ol (three-letter code: 67L) (formula:  $C_{11}H_{10}N_2O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	11	2	2		
3	B	1	Total	C	N	O	0	0
			15	11	2	2		
3	C	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 4 is 4-hydroxy[2,2'-bipyridine]-6-carbaldehyde (three-letter code: 67K) (formula:  $C_{11}H_8N_2O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			15	11	2	2		

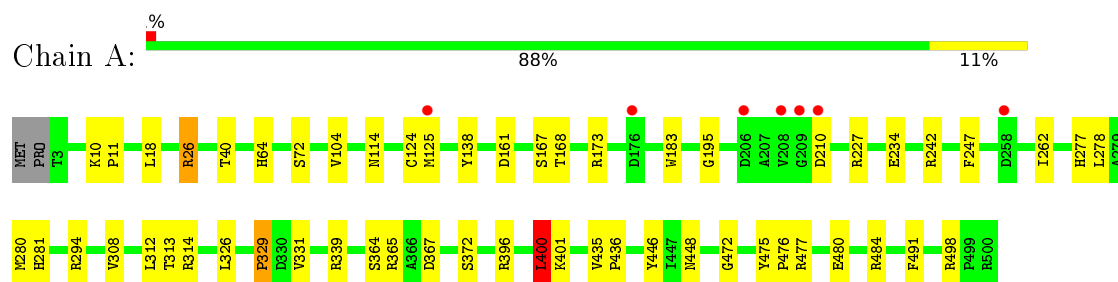
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	161	Total	O	0	0
			161	161		
5	B	124	Total	O	0	0
			124	124		
5	C	173	Total	O	0	0
			173	173		
5	D	142	Total	O	0	0
			142	142		

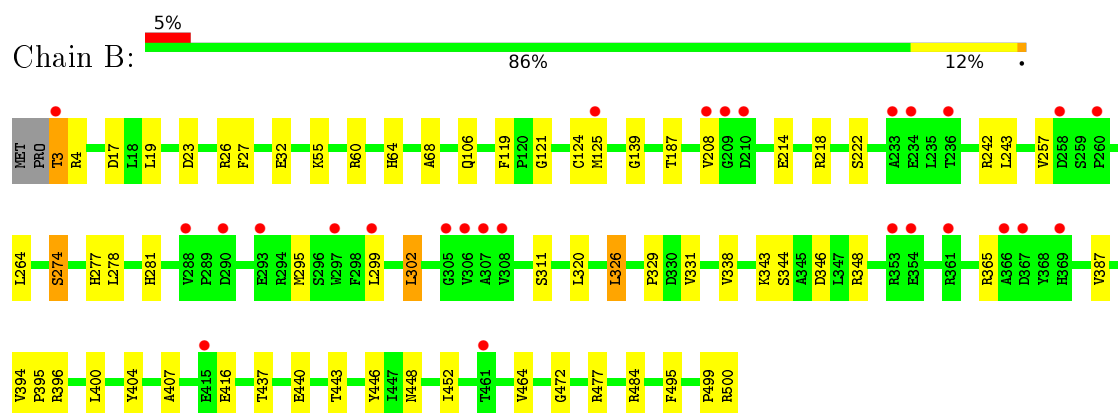
### 3 Residue-property plots [i](#)

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

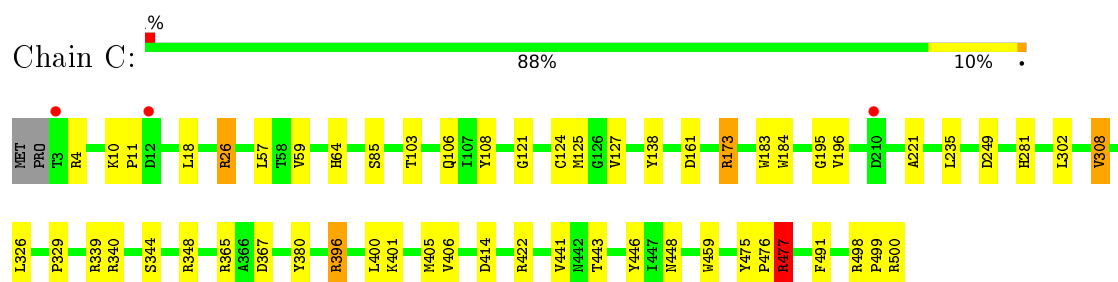
#### • Molecule 1: CrmK



#### • Molecule 1: CrmK

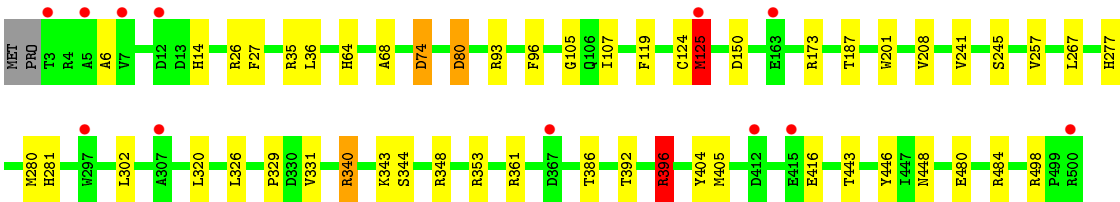


#### • Molecule 1: CrmK



#### • Molecule 1: CrmK





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.11Å 95.20Å 98.04Å 94.73° 96.56° 105.20°	Depositor
Resolution (Å)	45.60 – 2.15 45.62 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.0 (45.60-2.15) 93.1 (45.62-2.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 2.16Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.168 , 0.213 0.176 , 0.218	Depositor DCC
$R_{free}$ test set	5754 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.5	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 41.5	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	0.96	EDS
Total number of atoms	16449	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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: 67L, FAD, 67K

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	0.82	0/4015	0.91	8/5488 (0.1%)
1	B	0.68	1/4007 (0.0%)	0.84	7/5477 (0.1%)
1	C	0.84	0/4018	0.92	8/5491 (0.1%)
1	D	0.71	0/4007	0.85	7/5477 (0.1%)
All	All	0.77	1/16047 (0.0%)	0.88	30/21933 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	17	ASP	CB-CG	5.58	1.63	1.51

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	396	ARG	NE-CZ-NH2	-9.54	115.53	120.30
1	B	484	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	C	477	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	C	498	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	C	26	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	D	125	MET	CG-SD-CE	6.83	111.12	100.20
1	D	26	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	C	26	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	A	396	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	D	396	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	A	227	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	D	396	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	400	LEU	CA-CB-CG	5.97	129.04	115.30
1	B	396	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	B	484	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	D	26	ARG	NE-CZ-NH2	-5.90	117.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	396	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	D	498	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	B	26	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	B	60	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	C	308	VAL	CB-CA-C	-5.59	100.79	111.40
1	C	396	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	B	26	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	498	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	396	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	242	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	C	414	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	294	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	26	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	D	80	ASP	CB-CG-OD1	5.06	122.86	118.30

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	3896	0	3719	37	0
1	B	3891	0	3715	33	0
1	C	3899	0	3728	44	0
1	D	3891	0	3715	38	0
2	A	53	0	29	5	0
2	B	53	0	30	5	0
2	C	53	0	30	5	0
2	D	53	0	30	4	0
3	A	15	0	0	0	0
3	B	15	0	0	1	0
3	C	15	0	0	0	0
4	D	15	0	0	0	0
5	A	161	0	0	1	0
5	B	124	0	0	2	0
5	C	173	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	142	0	0	2	0
All	All	16449	0	14996	143	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 (143) 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:D:64:HIS:ND1	2:D:601:FAD:HM83	1.07	1.40
1:B:64:HIS:ND1	2:B:601:FAD:HM83	1.05	1.35
1:C:64:HIS:CE1	2:C:601:FAD:HM83	1.69	1.28
1:B:64:HIS:CE1	2:B:601:FAD:HM83	1.72	1.24
1:C:64:HIS:ND1	2:C:601:FAD:HM83	0.88	1.21
1:D:64:HIS:CE1	2:D:601:FAD:HM83	1.87	1.09
1:C:281[A]:HIS:NE2	1:C:326:LEU:HD11	1.80	0.95
1:B:281[A]:HIS:CD2	1:B:326:LEU:HD12	2.15	0.81
1:C:281[A]:HIS:CE1	1:C:326:LEU:HD11	2.15	0.81
1:A:64:HIS:ND1	2:A:601:FAD:HM81	1.94	0.77
1:A:64:HIS:CE1	2:A:601:FAD:C8M	2.67	0.75
1:C:64:HIS:ND1	2:C:601:FAD:HM81	1.96	0.73
1:A:281[A]:HIS:NE2	1:A:326:LEU:HD13	2.05	0.72
1:A:64:HIS:CG	2:A:601:FAD:C8M	2.73	0.70
1:A:477:ARG:NH1	1:A:480:GLU:OE2	2.24	0.70
1:B:64:HIS:ND1	2:B:601:FAD:HM81	2.00	0.69
1:C:499:PRO:O	1:C:500:ARG:CB	2.41	0.68
1:C:281[A]:HIS:NE2	1:C:326:LEU:CD1	2.57	0.67
1:C:281[A]:HIS:CE1	1:C:326:LEU:CD1	2.79	0.66
1:C:340:ARG:HD3	1:C:405:MET:HE1	1.78	0.66
1:C:365:ARG:HG2	1:C:367:ASP:OD1	1.97	0.64
1:D:281[A]:HIS:CE1	1:D:326:LEU:CD1	2.82	0.63
1:A:281[A]:HIS:CE1	1:A:326:LEU:CD1	2.84	0.61
1:D:280:MET:CE	1:D:302:LEU:HD11	2.31	0.60
1:A:281[A]:HIS:NE2	1:A:326:LEU:CD1	2.65	0.60
1:C:184:TRP:CZ3	1:C:477:ARG:HG2	2.36	0.59
1:D:281[A]:HIS:CE1	1:D:326:LEU:HD11	2.37	0.58
1:B:124:CYS:HB3	2:B:601:FAD:HM73	1.85	0.58
1:A:281[A]:HIS:CE1	1:A:326:LEU:HD13	2.38	0.58
1:C:18:LEU:HD21	1:D:320:LEU:HD23	1.86	0.58
1:D:340:ARG:HD3	1:D:405:MET:CE	2.34	0.57
1:D:150:ASP:OD2	1:D:396:ARG:NH2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:LEU:HD12	1:C:308:VAL:HG21	1.86	0.56
1:A:104:VAL:HG21	1:A:124:CYS:O	2.05	0.56
1:C:348:ARG:HD2	1:C:443:THR:HG22	1.88	0.56
1:C:64:HIS:CG	2:C:601:FAD:C8M	2.77	0.55
1:D:124:CYS:HB3	2:D:601:FAD:HM73	1.89	0.55
1:C:195:GLY:HA2	1:C:491:PHE:CE2	2.42	0.55
1:D:280:MET:HE1	1:D:302:LEU:HD11	1.89	0.54
1:D:281[A]:HIS:CE1	1:D:326:LEU:HD13	2.43	0.54
1:C:340:ARG:HD3	1:C:405:MET:CE	2.37	0.54
1:A:104:VAL:CG2	1:A:124:CYS:O	2.57	0.53
1:D:446:TYR:CZ	1:D:448:ASN:HB2	2.44	0.53
1:A:173:ARG:HB3	1:A:183:TRP:CE2	2.44	0.53
1:A:247:PHE:CD1	1:A:280:MET:HE1	2.43	0.53
1:B:499:PRO:O	1:B:500:ARG:CB	2.57	0.53
1:D:257:VAL:HG21	1:D:386:THR:CG2	2.39	0.53
1:B:281[A]:HIS:NE2	1:B:326:LEU:HD12	2.24	0.52
1:C:441:VAL:HG11	5:C:748:HOH:O	2.08	0.52
1:C:59:VAL:HG21	1:C:196:VAL:HG22	1.92	0.52
1:C:281[A]:HIS:CD2	1:C:326:LEU:CD1	2.92	0.52
1:A:475:TYR:HB3	1:A:476:PRO:HD3	1.91	0.52
1:C:124:CYS:HB3	2:C:601:FAD:HM73	1.91	0.52
1:D:150:ASP:CG	1:D:396:ARG:HH22	2.12	0.51
1:A:364:SER:O	1:A:365:ARG:C	2.47	0.51
1:A:18:LEU:HD21	1:B:320:LEU:HD23	1.92	0.51
1:D:105:GLY:HA3	1:D:125:MET:HG3	1.93	0.50
1:A:125:MET:HG3	1:B:331:VAL:HG21	1.93	0.50
1:D:36:LEU:HD23	1:D:80:ASP:HB3	1.94	0.50
1:C:138:TYR:CZ	1:C:401:LYS:HD2	2.47	0.50
1:C:326:LEU:HD21	5:C:728:HOH:O	2.11	0.50
1:D:348:ARG:HG3	1:D:443:THR:CG2	2.42	0.50
1:A:329:PRO:HB3	1:B:329:PRO:HB3	1.94	0.50
1:D:480:GLU:OE1	1:D:484:ARG:NH2	2.45	0.49
1:A:331:VAL:HG21	1:B:125:MET:HG3	1.94	0.48
1:B:27:PHE:CD1	1:B:68:ALA:HB2	2.49	0.48
1:A:64:HIS:HB3	2:A:601:FAD:HM81	1.96	0.48
1:A:195:GLY:HA2	1:A:491:PHE:CE2	2.49	0.47
1:B:437:THR:HG22	1:B:464:VAL:HG21	1.95	0.47
1:A:435:VAL:HB	1:A:436:PRO:HD2	1.96	0.47
1:B:214:GLU:OE2	1:B:218:ARG:NH2	2.47	0.47
1:D:241:VAL:O	1:D:245:SER:OG	2.20	0.47
1:D:257:VAL:HG21	1:D:386:THR:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:VAL:CG1	1:B:407:ALA:HB1	2.45	0.47
1:A:234:GLU:O	1:A:308:VAL:HG22	2.14	0.47
1:C:475:TYR:HB3	1:C:476:PRO:HD3	1.97	0.47
1:C:85:SER:HB2	1:C:106:GLN:HE22	1.80	0.46
1:C:329:PRO:HB3	1:D:329:PRO:HB3	1.97	0.46
1:A:484:ARG:HD2	5:A:860:HOH:O	2.14	0.46
1:C:326:LEU:HD23	5:C:788:HOH:O	2.14	0.46
1:C:365:ARG:NH1	5:C:710:HOH:O	2.48	0.46
1:A:124:CYS:HB3	2:A:601:FAD:HM73	1.97	0.46
1:A:281[A]:HIS:CD2	1:A:326:LEU:HD13	2.50	0.46
1:D:326:LEU:O	1:D:326:LEU:HD12	2.16	0.46
1:B:23:ASP:OD2	5:B:701:HOH:O	2.21	0.45
1:B:187:THR:O	1:B:394:VAL:HG23	2.16	0.45
1:B:452:ILE:HA	1:B:495:PHE:CZ	2.52	0.45
1:D:64:HIS:ND1	2:D:601:FAD:HM81	2.14	0.45
1:D:74:ASP:OD1	1:D:74:ASP:N	2.49	0.44
1:C:103:THR:HA	1:C:127:VAL:O	2.18	0.44
1:C:446:TYR:CZ	1:C:448:ASN:HB2	2.52	0.44
2:B:601:FAD:HM82	3:B:602:67L:CAC	2.47	0.44
1:A:331:VAL:HG21	1:B:125:MET:CG	2.48	0.44
1:C:235:LEU:CD1	1:C:308:VAL:HG21	2.47	0.44
1:C:380:TYR:CZ	1:C:401:LYS:HE2	2.53	0.44
1:B:295:MET:O	1:B:299:LEU:HG	2.18	0.44
1:C:422:ARG:HD3	1:C:459:TRP:CE2	2.53	0.43
1:C:348:ARG:HD2	1:C:443:THR:CG2	2.48	0.43
1:D:340:ARG:HD3	1:D:405:MET:HE1	2.00	0.43
1:A:114:ASN:O	1:B:4:ARG:NH1	2.51	0.43
1:C:302:LEU:HA	1:C:302:LEU:HD23	1.87	0.43
1:C:125:MET:HG3	1:D:331:VAL:HG21	2.01	0.43
1:D:96:PHE:O	1:D:201:TRP:HA	2.19	0.43
1:A:400:LEU:HD13	1:A:401:LYS:N	2.34	0.43
1:B:243:LEU:HD12	1:B:302:LEU:HD22	2.01	0.42
1:D:36:LEU:CD2	1:D:80:ASP:HB3	2.49	0.42
1:D:446:TYR:CE2	1:D:448:ASN:HB2	2.54	0.42
1:A:161:ASP:OD1	1:A:161:ASP:C	2.56	0.42
1:B:446:TYR:CE2	1:B:448:ASN:HB2	2.54	0.42
1:A:262:ILE:HA	1:A:262:ILE:HD12	1.91	0.42
1:C:173:ARG:HB2	1:C:183:TRP:CE2	2.55	0.42
1:C:173:ARG:HB2	1:C:183:TRP:CZ2	2.55	0.42
1:D:107:ILE:HG21	1:D:119:PHE:HE1	1.85	0.42
1:D:267:LEU:HB3	1:D:281[A]:HIS:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:THR:HB	1:D:392:THR:HB	2.00	0.42
1:D:27:PHE:CD1	1:D:68:ALA:HB2	2.55	0.42
1:D:6:ALA:HB1	1:D:35:ARG:HD2	2.02	0.42
1:A:312:LEU:HD11	1:A:314:ARG:CG	2.50	0.42
1:B:32:GLU:OE2	1:B:55:LYS:HE2	2.20	0.42
1:B:121:GLY:O	1:B:139:GLY:HA3	2.20	0.41
1:B:343:LYS:HB2	1:B:404:TYR:HB2	2.01	0.41
1:A:40:THR:HG21	1:A:168:THR:HG21	2.01	0.41
1:B:3:THR:HG22	1:B:4:ARG:H	1.84	0.41
1:A:446:TYR:CZ	1:A:448:ASN:HB2	2.55	0.41
1:A:10:LYS:HB3	1:A:11:PRO:HD2	2.02	0.41
1:C:281[A]:HIS:CD2	1:C:326:LEU:HD13	2.55	0.41
1:C:340:ARG:HH11	1:C:405:MET:CE	2.33	0.41
1:C:108:TYR:OH	1:C:121:GLY:C	2.59	0.41
1:D:348:ARG:NE	5:D:708:HOH:O	2.39	0.41
1:B:208:VAL:HG22	5:B:772:HOH:O	2.20	0.41
1:B:346:ASP:HB2	1:B:443:THR:OG1	2.21	0.41
1:C:26:ARG:HG3	1:C:339:ARG:HB3	2.03	0.41
1:C:221:ALA:HB2	1:D:14:HIS:CD2	2.56	0.41
1:D:343:LYS:HB2	1:D:404:TYR:HB2	2.03	0.41
1:A:138:TYR:CZ	1:A:401:LYS:HD3	2.56	0.41
1:A:26:ARG:HG3	1:A:339:ARG:HB3	2.02	0.41
1:B:19:LEU:HA	1:B:19:LEU:HD23	1.87	0.41
1:A:312:LEU:HD11	1:A:314:ARG:HG3	2.03	0.40
1:B:394:VAL:HG12	1:B:395:PRO:O	2.21	0.40
1:B:242:ARG:HD2	1:B:242:ARG:HA	1.89	0.40
1:C:10:LYS:HB3	1:C:11:PRO:CD	2.51	0.40
1:D:93:ARG:HD2	5:D:729:HOH:O	2.21	0.40
1:B:264:LEU:HD23	1:B:264:LEU:C	2.41	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	498/500 (100%)	483 (97%)	14 (3%)	1 (0%)	52	51
1	B	497/500 (99%)	482 (97%)	12 (2%)	3 (1%)	30	21
1	C	498/500 (100%)	483 (97%)	15 (3%)	0	100	100
1	D	497/500 (99%)	483 (97%)	14 (3%)	0	100	100
All	All	1990/2000 (100%)	1931 (97%)	55 (3%)	4 (0%)	52	51

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	274	SER
1	A	472	GLY
1	B	365	ARG
1	B	472	GLY

### 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	401/402 (100%)	391 (98%)	10 (2%)	55	58
1	B	400/402 (100%)	382 (96%)	18 (4%)	34	30
1	C	401/402 (100%)	391 (98%)	10 (2%)	55	58
1	D	400/402 (100%)	389 (97%)	11 (3%)	51	52
All	All	1602/1608 (100%)	1553 (97%)	49 (3%)	47	47

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	SER
1	A	167	SER
1	A	210	ASP
1	A	277	HIS
1	A	278	LEU
1	A	313	THR
1	A	329	PRO

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Mol	Chain	Res	Type
1	A	367	ASP
1	A	372	SER
1	A	400	LEU
1	B	3	THR
1	B	106	GLN
1	B	119	PHE
1	B	222	SER
1	B	257	VAL
1	B	274	SER
1	B	277	HIS
1	B	278	LEU
1	B	302	LEU
1	B	311	SER
1	B	326	LEU
1	B	344	SER
1	B	348	ARG
1	B	387	VAL
1	B	400	LEU
1	B	416	GLU
1	B	440	GLU
1	B	477	ARG
1	C	4	ARG
1	C	57	LEU
1	C	161	ASP
1	C	173	ARG
1	C	249	ASP
1	C	344	SER
1	C	396	ARG
1	C	400	LEU
1	C	406	VAL
1	C	477	ARG
1	D	74	ASP
1	D	125	MET
1	D	173	ARG
1	D	208	VAL
1	D	277	HIS
1	D	340	ARG
1	D	344	SER
1	D	353	ARG
1	D	361	ARG
1	D	396	ARG
1	D	416	GLU



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	GLN
1	B	14	HIS
1	C	106	GLN
1	D	14	HIS

### 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
2	FAD	A	601	1	52,58,58	1.28	7 (13%)	52,89,89	2.33	12 (23%)
3	67L	A	602	-	16,16,16	2.32	3 (18%)	21,21,21	1.79	4 (19%)
2	FAD	B	601	1	52,58,58	1.31	8 (15%)	52,89,89	1.82	12 (23%)
3	67L	B	602	-	16,16,16	2.31	3 (18%)	21,21,21	1.93	7 (33%)
2	FAD	C	601	1	52,58,58	1.27	7 (13%)	52,89,89	2.30	11 (21%)
3	67L	C	602	-	16,16,16	2.35	4 (25%)	21,21,21	2.12	8 (38%)
2	FAD	D	601	1	52,58,58	1.32	6 (11%)	52,89,89	2.37	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	67K	D	602	-	16,16,16	2.16	3 (18%)	18,21,21	2.43	9 (50%)

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	601	1	-	0/30/50/50	0/6/6/6
3	67L	A	602	-	-	0/6/6/6	0/2/2/2
2	FAD	B	601	1	-	0/30/50/50	0/6/6/6
3	67L	B	602	-	-	0/6/6/6	0/2/2/2
2	FAD	C	601	1	-	0/30/50/50	0/6/6/6
3	67L	C	602	-	-	0/6/6/6	0/2/2/2
2	FAD	D	601	1	-	0/30/50/50	0/6/6/6
4	67K	D	602	-	-	0/6/6/6	0/2/2/2

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	67L	CAN-CAK	-7.02	1.40	1.51
3	C	602	67L	CAN-CAK	-6.72	1.40	1.51
4	D	602	67K	CAK-CAN	-6.10	1.40	1.48
3	A	602	67L	CAN-CAK	-6.00	1.41	1.51
3	B	602	67L	CAD-CAG	-4.45	1.39	1.49
3	C	602	67L	CAD-CAG	-4.35	1.39	1.49
3	A	602	67L	CAD-CAG	-4.29	1.39	1.49
2	B	601	FAD	C1'-N10	-3.77	1.44	1.48
2	C	601	FAD	C1'-N10	-3.01	1.45	1.48
2	D	601	FAD	C1'-N10	-2.93	1.45	1.48
2	A	601	FAD	C1'-N10	-2.87	1.45	1.48
2	B	601	FAD	C6-C5X	-2.85	1.37	1.41
4	D	602	67K	CAD-CAG	-2.84	1.42	1.49
2	D	601	FAD	C4A-N3A	-2.57	1.31	1.35
2	C	601	FAD	C4A-N3A	-2.44	1.32	1.35
2	B	601	FAD	C2'-C3'	-2.12	1.49	1.53
2	C	601	FAD	C9A-C5X	2.00	1.46	1.42
2	B	601	FAD	C8-C7	2.13	1.46	1.41
2	B	601	FAD	C4-C4X	2.19	1.45	1.41
3	C	602	67L	CAG-NAL	2.21	1.38	1.34
2	B	601	FAD	C5A-C4A	2.22	1.45	1.40
2	C	601	FAD	C4-N3	2.29	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C4X-N5	2.35	1.37	1.33
2	A	601	FAD	C4-C4X	2.43	1.46	1.41
2	D	601	FAD	C8-C7	2.50	1.47	1.41
2	A	601	FAD	C7M-C7	2.53	1.56	1.51
2	B	601	FAD	C9A-C5X	2.55	1.47	1.42
2	D	601	FAD	C9A-C5X	2.88	1.48	1.42
2	C	601	FAD	C4X-C10	2.89	1.46	1.40
2	A	601	FAD	C9A-C5X	2.92	1.48	1.42
2	C	601	FAD	C4-C4X	2.99	1.47	1.41
2	C	601	FAD	C8-C7	3.02	1.49	1.41
2	D	601	FAD	C4X-C10	3.06	1.46	1.40
2	A	601	FAD	C4X-C10	3.07	1.46	1.40
2	B	601	FAD	C4X-C10	3.11	1.46	1.40
2	A	601	FAD	C8-C7	3.19	1.49	1.41
3	B	602	67L	CAF-NAE	3.36	1.41	1.34
3	C	602	67L	CAF-NAE	3.40	1.42	1.34
2	D	601	FAD	C4-C4X	3.46	1.48	1.41
4	D	602	67K	CAF-NAE	4.38	1.44	1.34
3	A	602	67L	CAF-NAE	4.53	1.44	1.34

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	FAD	N3A-C2A-N1A	-9.29	121.57	128.87
2	A	601	FAD	N3A-C2A-N1A	-7.27	123.16	128.87
2	C	601	FAD	N3A-C2A-N1A	-6.76	123.56	128.87
2	A	601	FAD	C4-C4X-C10	-6.58	115.73	119.94
2	C	601	FAD	C4-C4X-C10	-6.36	115.87	119.94
2	A	601	FAD	C1B-N9A-C4A	-5.79	120.34	126.81
2	D	601	FAD	C4-C4X-C10	-5.01	116.73	119.94
2	B	601	FAD	N3A-C2A-N1A	-4.97	124.97	128.87
4	D	602	67K	CAJ-CAK-CAN	-4.52	118.88	121.49
2	B	601	FAD	C4-C4X-C10	-4.21	117.25	119.94
2	C	601	FAD	N3-C2-N1	-4.16	120.68	127.69
2	B	601	FAD	C4X-C10-N10	-4.09	117.55	120.52
2	D	601	FAD	C4X-C4-N3	-4.08	118.19	123.52
3	A	602	67L	CAJ-CAK-NAL	-3.75	118.73	122.90
2	C	601	FAD	C1B-N9A-C4A	-3.73	122.64	126.81
4	D	602	67K	CAC-CAD-NAE	-3.68	116.63	122.28
2	D	601	FAD	C1B-N9A-C4A	-3.61	122.77	126.81
4	D	602	67K	CAH-CAG-NAL	-3.53	118.05	122.40
2	A	601	FAD	N3-C2-N1	-3.53	121.75	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	FAD	C4X-C4-N3	-3.50	118.94	123.52
2	D	601	FAD	C4X-C10-N10	-3.40	118.05	120.52
3	B	602	67L	CAJ-CAK-NAL	-3.39	119.13	122.90
3	C	602	67L	CAJ-CAK-NAL	-3.38	119.14	122.90
3	B	602	67L	CAA-CAF-NAE	-3.33	117.75	123.42
2	D	601	FAD	N3-C2-N1	-3.13	122.43	127.69
2	C	601	FAD	O4'-C4'-C5'	-2.82	103.94	110.09
2	B	601	FAD	C4X-C4-N3	-2.72	119.97	123.52
2	B	601	FAD	C1B-N9A-C4A	-2.70	123.80	126.81
2	A	601	FAD	C4X-C4-N3	-2.68	120.03	123.52
4	D	602	67K	OAo-CAN-CAK	-2.62	122.28	124.47
3	A	602	67L	CAI-CAH-CAG	-2.61	117.34	119.01
3	C	602	67L	CAI-CAH-CAG	-2.59	117.35	119.01
2	D	601	FAD	O2'-C2'-C1'	-2.52	103.69	109.93
2	D	601	FAD	O4'-C4'-C5'	-2.48	104.68	110.09
2	A	601	FAD	C6-C7-C8	-2.36	115.36	119.97
2	B	601	FAD	O3B-C3B-C2B	-2.32	104.36	111.86
2	B	601	FAD	N3-C2-N1	-2.29	123.83	127.69
3	C	602	67L	CAA-CAF-NAE	-2.27	119.55	123.42
3	C	602	67L	OAo-CAN-CAK	-2.22	108.05	112.23
2	B	601	FAD	O3'-C3'-C2'	-2.17	103.10	108.73
2	A	601	FAD	C4X-C10-N10	-2.08	119.01	120.52
2	D	601	FAD	O3B-C3B-C2B	-2.06	105.19	111.86
3	B	602	67L	CAH-CAG-NAL	-2.04	119.89	122.40
3	B	602	67L	OAo-CAN-CAK	-2.01	108.45	112.23
2	B	601	FAD	O2P-P-O3P	2.01	113.86	105.27
4	D	602	67K	CAI-CAH-CAG	2.03	120.32	119.01
2	D	601	FAD	C4B-O4B-C1B	2.06	111.82	109.64
2	B	601	FAD	O2P-P-O1P	2.09	123.44	112.56
4	D	602	67K	CAA-CAB-CAC	2.13	123.16	120.20
2	D	601	FAD	C4-C4X-N5	2.14	121.31	118.70
3	C	602	67L	CAD-CAG-NAL	2.15	118.95	116.27
4	D	602	67K	CAG-CAD-NAE	2.22	120.43	116.72
2	C	601	FAD	O2B-C2B-C1B	2.26	118.70	111.61
2	A	601	FAD	C4X-N5-C5X	2.42	119.57	116.72
2	B	601	FAD	C1'-N10-C9A	2.46	121.68	118.83
2	A	601	FAD	O2A-PA-O3P	2.49	115.92	105.27
2	C	601	FAD	O2P-P-O3P	2.67	116.73	105.27
4	D	602	67K	CAD-CAG-NAL	2.92	119.92	116.27
2	C	601	FAD	N6A-C6A-N1A	2.95	123.46	118.52
2	A	601	FAD	C1'-N10-C9A	3.23	122.57	118.83
3	C	602	67L	CAF-NAE-CAD	3.35	121.86	117.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	67L	CAG-NAL-CAK	3.38	122.45	118.31
3	C	602	67L	CAG-NAL-CAK	3.45	122.54	118.31
3	B	602	67L	CAF-NAE-CAD	3.50	122.06	117.21
3	B	602	67L	CAN-CAK-NAL	3.55	118.47	114.98
2	A	601	FAD	C4-C4X-N5	3.61	123.09	118.70
2	C	601	FAD	C4-C4X-N5	3.62	123.10	118.70
3	B	602	67L	CAG-NAL-CAK	3.84	123.01	118.31
3	A	602	67L	CAN-CAK-NAL	3.94	118.86	114.98
4	D	602	67K	CAF-NAE-CAD	4.39	123.30	117.21
3	C	602	67L	CAN-CAK-NAL	5.00	119.90	114.98
2	B	601	FAD	C4-N3-C2	5.77	119.97	115.16
2	A	601	FAD	C4-N3-C2	7.65	121.54	115.16
2	C	601	FAD	C4-N3-C2	8.11	121.92	115.16
2	D	601	FAD	C4-N3-C2	8.21	122.01	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FAD	5	0
2	B	601	FAD	5	0
3	B	602	67L	1	0
2	C	601	FAD	5	0
2	D	601	FAD	4	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	498/500 (99%)	-0.13	7 (1%) 78 83	18, 29, 51, 65	0
1	B	498/500 (99%)	0.21	27 (5%) 29 40	19, 38, 64, 83	0
1	C	498/500 (99%)	-0.14	3 (0%) 90 92	16, 28, 49, 72	0
1	D	498/500 (99%)	0.08	12 (2%) 62 71	22, 34, 55, 75	0
All	All	1992/2000 (99%)	0.01	49 (2%) 61 69	16, 32, 56, 83	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	208	VAL	5.9
1	B	367	ASP	4.1
1	B	258	ASP	4.1
1	B	415	GLU	4.0
1	D	307	ALA	3.9
1	B	288	VAL	3.8
1	B	209	GLY	3.8
1	A	206	ASP	3.7
1	B	208	VAL	3.7
1	B	297	TRP	3.7
1	C	12	ASP	3.6
1	D	3	THR	3.5
1	D	415	GLU	3.5
1	B	353	ARG	3.2
1	D	125	MET	3.2
1	B	305	GLY	3.2
1	B	290	ASP	3.2
1	A	209	GLY	3.2
1	D	5	ALA	3.0
1	B	210	ASP	3.0
1	C	3	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	293	GLU	2.9
1	B	308	VAL	2.9
1	D	12	ASP	2.8
1	D	367	ASP	2.8
1	B	260	PRO	2.7
1	D	412	ASP	2.5
1	D	297	TRP	2.5
1	B	354	GLU	2.5
1	A	258	ASP	2.4
1	B	307	ALA	2.4
1	B	125	MET	2.4
1	B	369	HIS	2.3
1	A	125	MET	2.3
1	D	163	GLU	2.3
1	B	306	VAL	2.2
1	B	366	ALA	2.2
1	B	234	GLU	2.2
1	A	210	ASP	2.2
1	B	236	THR	2.2
1	A	176	ASP	2.1
1	B	3	THR	2.1
1	B	233	ALA	2.1
1	B	461	THR	2.1
1	D	500	ARG	2.1
1	B	299	LEU	2.1
1	B	361	ARG	2.1
1	C	210	ASP	2.0
1	D	7	VAL	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
3	67L	C	602	15/15	0.84	0.16	1.55	33,41,54,55	0
3	67L	B	602	15/15	0.89	0.15	0.80	47,51,58,60	0
3	67L	A	602	15/15	0.90	0.14	0.59	35,39,55,57	0
4	67K	D	602	15/15	0.90	0.15	0.17	37,46,59,60	0
2	FAD	C	601	53/53	0.98	0.12	0.05	16,20,27,29	0
2	FAD	A	601	53/53	0.98	0.11	-0.01	16,21,30,34	0
2	FAD	B	601	53/53	0.98	0.12	-0.07	20,25,34,36	0
2	FAD	D	601	53/53	0.98	0.13	-0.09	19,24,29,32	0

## 6.5 Other polymers

There are no such residues in this entry.