



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2016 – 05:29 AM EDT

PDB ID : 5HXW
Title : L-amino acid deaminase from *Proteus vulgaris*
Authors : Zhou, H.; Ju, Y.; Niu, L.; Teng, M.
Deposited on : 2016-01-31
Resolution : 2.63 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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-20027939
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-20027939

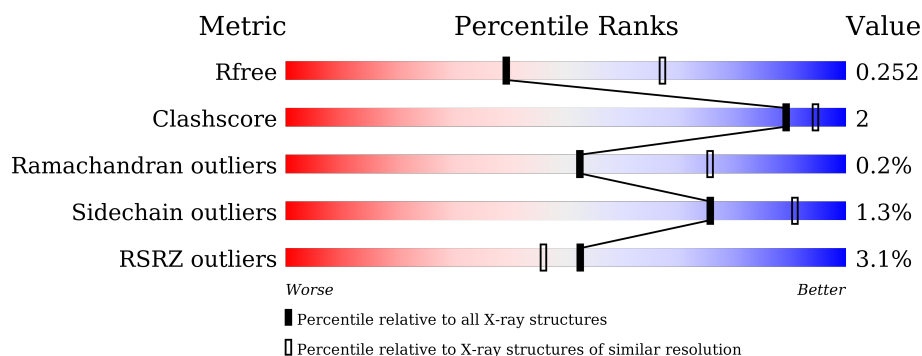
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.63 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	3377 (2.68-2.60)
Clashscore	102246	3781 (2.68-2.60)
Ramachandran outliers	100387	3722 (2.68-2.60)
Sidechain outliers	100360	3722 (2.68-2.60)
RSRZ outliers	91569	3388 (2.68-2.60)

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 ≥ 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	454	<div> <div>88%</div> <div>8% 5%</div> </div>
1	B	454	<div> <div>%</div> <div>89%</div> <div>6% 5%</div> </div>
1	C	454	<div> <div>3%</div> <div>89%</div> <div>5% 5%</div> </div>
1	D	454	<div> <div>4%</div> <div>89%</div> <div>5% 5%</div> </div>
1	E	454	<div> <div>4%</div> <div>86%</div> <div>9% 5%</div> </div>
1	F	454	<div> <div>6%</div> <div>90%</div> <div>• 5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	16A	A	503	-	-	-	X
3	16A	B	502	-	-	-	X
3	16A	B	503	-	-	-	X
3	16A	B	504	-	-	-	X
3	16A	C	502	-	-	-	X
3	16A	D	503	-	-	-	X
3	16A	E	502	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20385 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 L-amino acid deaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	0	0
			3342	2134	561	636	11			
1	B	432	Total	C	N	O	S	0	1	0
			3324	2120	560	633	11			
1	C	430	Total	C	N	O	S	0	2	0
			3252	2080	540	620	12			
1	D	430	Total	C	N	O	S	0	0	0
			3254	2072	542	629	11			
1	E	430	Total	C	N	O	S	0	2	0
			3284	2097	546	630	11			
1	F	430	Total	C	N	O	S	0	1	0
			3205	2038	535	622	10			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	expression tag	UNP Q9LCB2
A	19	ARG	-	expression tag	UNP Q9LCB2
A	20	GLY	-	expression tag	UNP Q9LCB2
A	21	SER	-	expression tag	UNP Q9LCB2
A	22	HIS	-	expression tag	UNP Q9LCB2
A	23	HIS	-	expression tag	UNP Q9LCB2
A	24	HIS	-	expression tag	UNP Q9LCB2
A	25	HIS	-	expression tag	UNP Q9LCB2
A	26	HIS	-	expression tag	UNP Q9LCB2
A	27	HIS	-	expression tag	UNP Q9LCB2
A	28	GLY	-	expression tag	UNP Q9LCB2
A	29	SER	-	expression tag	UNP Q9LCB2
B	18	MET	-	expression tag	UNP Q9LCB2
B	19	ARG	-	expression tag	UNP Q9LCB2
B	20	GLY	-	expression tag	UNP Q9LCB2
B	21	SER	-	expression tag	UNP Q9LCB2
B	22	HIS	-	expression tag	UNP Q9LCB2

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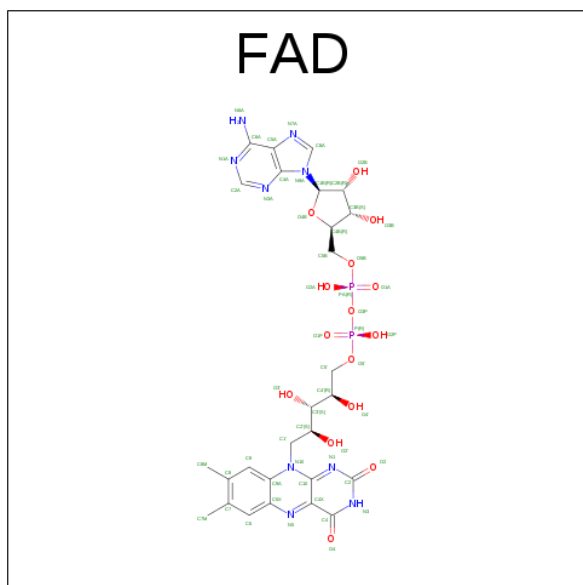
Chain	Residue	Modelled	Actual	Comment	Reference
B	23	HIS	-	expression tag	UNP Q9LCB2
B	24	HIS	-	expression tag	UNP Q9LCB2
B	25	HIS	-	expression tag	UNP Q9LCB2
B	26	HIS	-	expression tag	UNP Q9LCB2
B	27	HIS	-	expression tag	UNP Q9LCB2
B	28	GLY	-	expression tag	UNP Q9LCB2
B	29	SER	-	expression tag	UNP Q9LCB2
C	18	MET	-	expression tag	UNP Q9LCB2
C	19	ARG	-	expression tag	UNP Q9LCB2
C	20	GLY	-	expression tag	UNP Q9LCB2
C	21	SER	-	expression tag	UNP Q9LCB2
C	22	HIS	-	expression tag	UNP Q9LCB2
C	23	HIS	-	expression tag	UNP Q9LCB2
C	24	HIS	-	expression tag	UNP Q9LCB2
C	25	HIS	-	expression tag	UNP Q9LCB2
C	26	HIS	-	expression tag	UNP Q9LCB2
C	27	HIS	-	expression tag	UNP Q9LCB2
C	28	GLY	-	expression tag	UNP Q9LCB2
C	29	SER	-	expression tag	UNP Q9LCB2
D	18	MET	-	expression tag	UNP Q9LCB2
D	19	ARG	-	expression tag	UNP Q9LCB2
D	20	GLY	-	expression tag	UNP Q9LCB2
D	21	SER	-	expression tag	UNP Q9LCB2
D	22	HIS	-	expression tag	UNP Q9LCB2
D	23	HIS	-	expression tag	UNP Q9LCB2
D	24	HIS	-	expression tag	UNP Q9LCB2
D	25	HIS	-	expression tag	UNP Q9LCB2
D	26	HIS	-	expression tag	UNP Q9LCB2
D	27	HIS	-	expression tag	UNP Q9LCB2
D	28	GLY	-	expression tag	UNP Q9LCB2
D	29	SER	-	expression tag	UNP Q9LCB2
E	18	MET	-	expression tag	UNP Q9LCB2
E	19	ARG	-	expression tag	UNP Q9LCB2
E	20	GLY	-	expression tag	UNP Q9LCB2
E	21	SER	-	expression tag	UNP Q9LCB2
E	22	HIS	-	expression tag	UNP Q9LCB2
E	23	HIS	-	expression tag	UNP Q9LCB2
E	24	HIS	-	expression tag	UNP Q9LCB2
E	25	HIS	-	expression tag	UNP Q9LCB2
E	26	HIS	-	expression tag	UNP Q9LCB2
E	27	HIS	-	expression tag	UNP Q9LCB2
E	28	GLY	-	expression tag	UNP Q9LCB2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	29	SER	-	expression tag	UNP Q9LCB2
F	18	MET	-	expression tag	UNP Q9LCB2
F	19	ARG	-	expression tag	UNP Q9LCB2
F	20	GLY	-	expression tag	UNP Q9LCB2
F	21	SER	-	expression tag	UNP Q9LCB2
F	22	HIS	-	expression tag	UNP Q9LCB2
F	23	HIS	-	expression tag	UNP Q9LCB2
F	24	HIS	-	expression tag	UNP Q9LCB2
F	25	HIS	-	expression tag	UNP Q9LCB2
F	26	HIS	-	expression tag	UNP Q9LCB2
F	27	HIS	-	expression tag	UNP Q9LCB2
F	28	GLY	-	expression tag	UNP Q9LCB2
F	29	SER	-	expression tag	UNP Q9LCB2

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



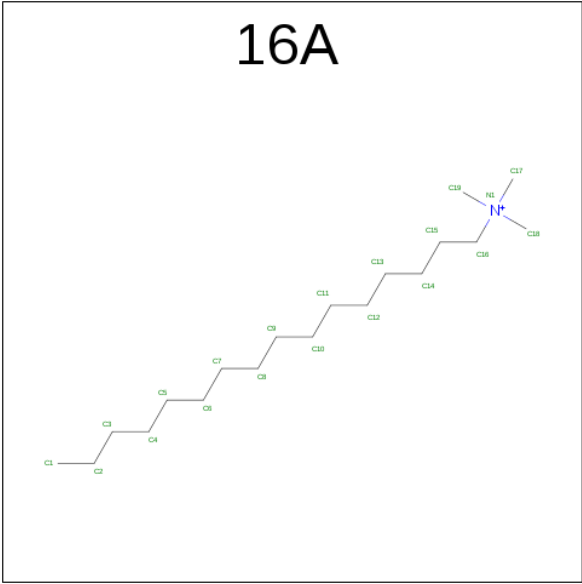
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	D	1	Total 53	C 27	N 9	O 15	P 2	0	0

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

- Molecule 3 is CETYL-TRIMETHYL-AMMONIUM (three-letter code: 16A) (formula: C₁₉H₄₂N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			20	19	1		
3	A	1	Total	C	N	0	0
			20	19	1		
3	A	1	Total	C	N	0	0
			20	19	1		
3	B	1	Total	C	N	0	0
			20	19	1		
3	B	1	Total	C	N	0	0
			20	19	1		
3	B	1	Total	C	N	0	0
			20	19	1		
3	B	1	Total	C	N	0	0
			20	19	1		
3	C	1	Total	C	N	0	0
			20	19	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	N	0	0
			20	19	1		
3	D	1	Total	C	N	0	0
			20	19	1		
3	D	1	Total	C	N	0	0
			20	19	1		
3	E	1	Total	C	N	0	0
			20	19	1		
3	F	1	Total	C	N	0	0
			20	19	1		
3	F	1	Total	C	N	0	0
			20	19	1		

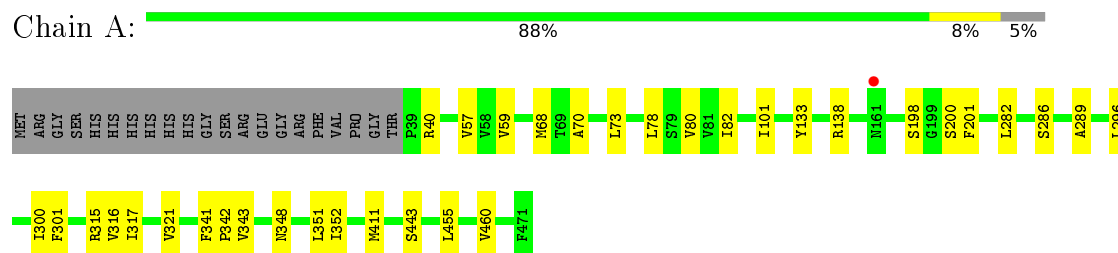
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	28	Total	O	0	0
			28	28		
4	B	18	Total	O	0	0
			18	18		
4	C	19	Total	O	0	0
			19	19		
4	D	16	Total	O	0	0
			16	16		
4	E	15	Total	O	0	0
			15	15		
4	F	10	Total	O	0	0
			10	10		

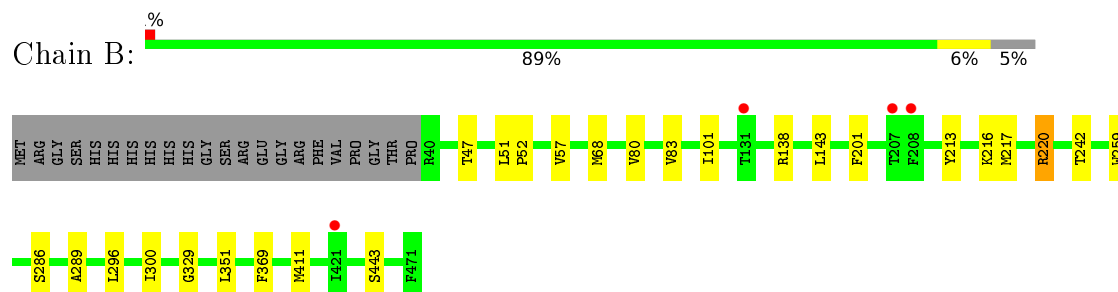
3 Residue-property plots

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.

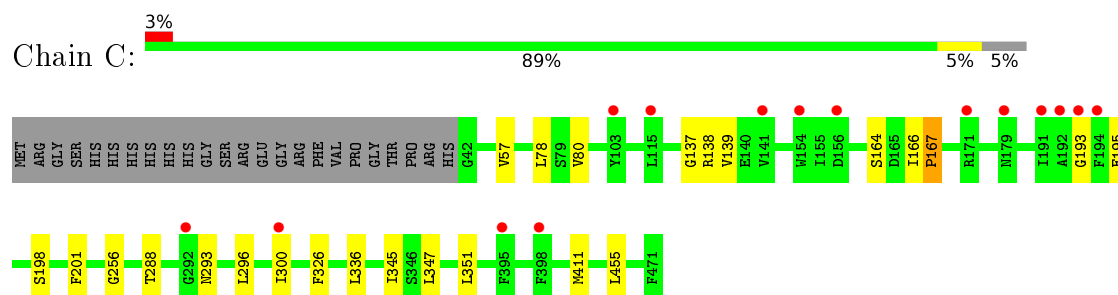
- Molecule 1: L-amino acid deaminase



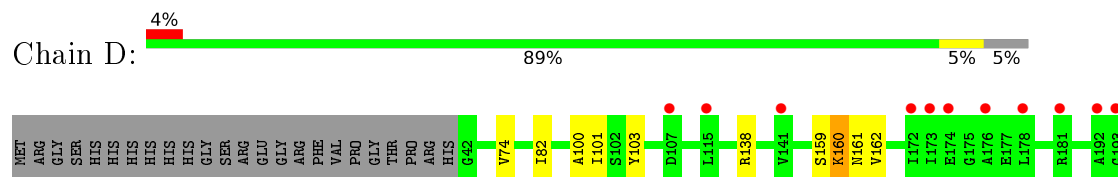
- Molecule 1: L-amino acid deaminase

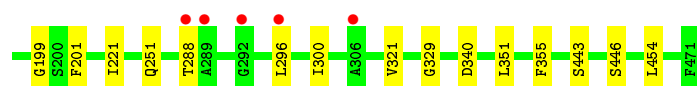


- Molecule 1: L-amino acid deaminase

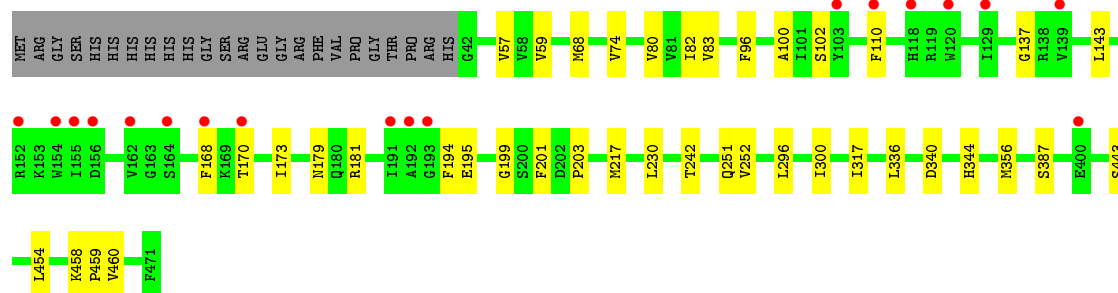
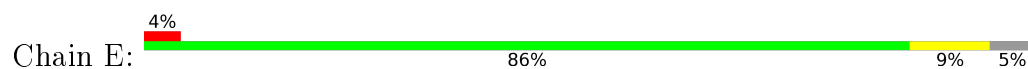


- Molecule 1: L-amino acid deaminase

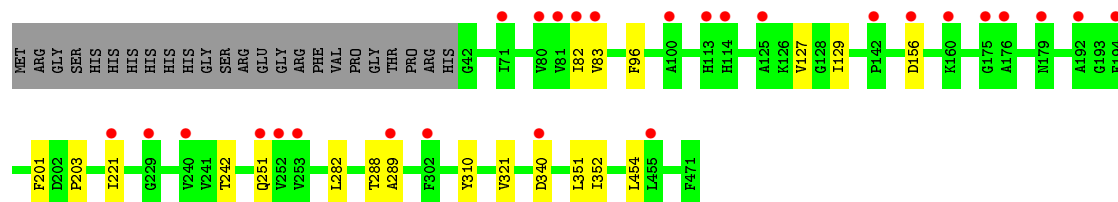
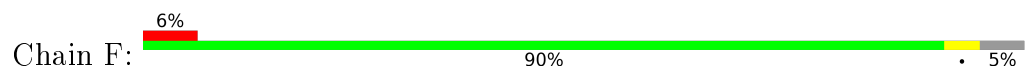




- Molecule 1: L-amino acid deaminase



- Molecule 1: L-amino acid deaminase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	100.31Å 104.58Å 105.42Å 64.52° 73.06° 61.17°	Depositor
Resolution (Å)	94.63 – 2.63 49.26 – 2.63	Depositor EDS
% Data completeness (in resolution range)	97.1 (94.63-2.63) 85.6 (49.26-2.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.221 , 0.252 0.221 , 0.252	Depositor DCC
R_{free} test set	4861 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	68.3	Xtriage
Anisotropy	0.451	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20385	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 16A, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.40	0/3419	0.60	0/4648
1	B	0.40	0/3403	0.60	0/4626
1	C	0.40	0/3329	0.59	0/4534
1	D	0.40	0/3327	0.59	0/4531
1	E	0.40	0/3362	0.59	0/4576
1	F	0.40	0/3277	0.58	0/4469
All	All	0.40	0/20117	0.59	0/27384

There are no bond length outliers.

There are no bond angle outliers.

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	3342	0	3304	18	0
1	B	3324	0	3268	17	0
1	C	3252	0	3155	15	0
1	D	3254	0	3153	11	0
1	E	3284	0	3194	21	0
1	F	3205	0	3033	7	0
2	A	53	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	53	0	31	2	0
2	C	53	0	31	2	0
2	D	53	0	31	0	0
2	E	53	0	31	0	0
2	F	53	0	31	0	0
3	A	60	0	126	5	0
3	B	100	0	210	7	0
3	C	20	0	42	1	0
3	D	60	0	126	4	0
3	E	20	0	42	2	0
3	F	40	0	84	0	0
4	A	28	0	0	0	0
4	B	18	0	0	0	0
4	C	19	0	0	0	0
4	D	16	0	0	0	0
4	E	15	0	0	0	0
4	F	10	0	0	0	0
All	All	20385	0	19923	96	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 2.

All (96) 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:213:TYR:CE1	1:B:217:MET:HG2	2.08	0.87
1:E:181:ARG:HD2	1:E:194:PHE:CE1	2.16	0.80
1:E:181:ARG:HD2	1:E:194:PHE:HE1	1.51	0.74
1:B:47:THR:HG21	1:B:220:ARG:HG3	1.71	0.73
1:B:213:TYR:O	1:B:216:LYS:N	2.24	0.70
1:A:348:ASN:HA	3:A:503:16A:H182	1.76	0.66
1:E:181:ARG:CD	1:E:194:PHE:HE1	2.09	0.66
1:B:213:TYR:CE1	1:B:217:MET:CG	2.82	0.62
1:C:195:GLU:HG2	1:C:198:SER:HB3	1.81	0.61
1:C:137:GLY:HA2	1:C:195:GLU:O	2.00	0.61
1:E:296:LEU:HB2	1:E:300:ILE:HB	1.84	0.59
1:C:57:VAL:HB	1:C:80:VAL:HG12	1.83	0.59
1:E:173:ILE:HG12	1:E:194:PHE:HB2	1.84	0.59
3:B:504:16A:H101	3:B:506:16A:H91	1.83	0.58
1:E:57:VAL:HG13	1:E:80:VAL:HG12	1.84	0.58
1:D:296:LEU:HB2	1:D:300:ILE:HB	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ALA:HB1	1:A:80:VAL:HG21	1.87	0.57
1:B:296:LEU:HB2	1:B:300:ILE:HB	1.87	0.56
3:B:502:16A:H151	3:B:503:16A:H161	1.89	0.55
1:B:57:VAL:HB	1:B:80:VAL:HG12	1.90	0.54
1:C:336:LEU:HD11	1:C:345:ILE:HD11	1.90	0.53
1:A:101:ILE:HG22	1:A:198:SER:HB2	1.91	0.53
1:C:296:LEU:HB2	1:C:300:ILE:HB	1.89	0.53
1:F:289:ALA:HB1	1:F:310:TYR:OH	2.10	0.52
1:A:133:TYR:HA	1:A:200:SER:O	2.10	0.52
1:A:316:VAL:HA	1:A:342:PRO:HB2	1.92	0.51
1:C:139:VAL:HA	1:C:193:GLY:O	2.09	0.51
1:E:168:PHE:CZ	1:E:170:THR:HB	2.45	0.51
1:E:74:VAL:HG23	1:E:80:VAL:HG22	1.93	0.51
1:A:296:LEU:HB2	1:A:300:ILE:HB	1.92	0.50
1:C:166:ILE:O	1:C:167:PRO:O	2.30	0.50
1:E:100:ALA:HB3	1:E:199:GLY:HA3	1.94	0.50
1:E:317:ILE:HG21	3:E:502:16A:H82	1.93	0.50
1:A:101:ILE:HG21	1:A:138:ARG:HD2	1.93	0.49
3:A:503:16A:H173	3:D:502:16A:H141	1.94	0.49
1:F:321:VAL:HG12	1:F:351:LEU:HD13	1.95	0.49
1:A:286:SER:HB3	1:A:289:ALA:HB2	1.95	0.48
1:C:347:LEU:HD11	1:C:351:LEU:HD22	1.95	0.47
1:E:102:SER:HB2	1:E:110:PHE:CE1	2.49	0.47
1:E:96:PHE:CZ	1:E:203:PRO:HA	2.49	0.47
1:B:213:TYR:HE1	1:B:217:MET:CG	2.25	0.47
1:F:251:GLN:HB3	1:F:454:LEU:HD11	1.96	0.47
1:D:355:PHE:O	3:D:502:16A:H152	2.15	0.47
3:B:502:16A:H142	3:B:503:16A:H141	1.96	0.47
3:B:502:16A:H172	3:B:506:16A:H41	1.97	0.47
1:C:78:LEU:HD11	1:C:455:LEU:HD21	1.97	0.47
1:B:83:VAL:HG11	1:B:242:THR:HG21	1.97	0.46
1:E:336:LEU:HD11	3:E:502:16A:H193	1.98	0.46
1:C:256:GLY:O	2:C:501:FAD:H8A	2.16	0.46
1:A:68:MET:HG3	1:A:443:SER:HB2	1.98	0.46
1:B:351:LEU:HD23	3:B:502:16A:H131	1.97	0.46
1:D:101:ILE:HG21	1:D:138:ARG:HD2	1.98	0.46
1:D:329:GLY:O	3:D:504:16A:H162	2.16	0.45
1:D:82:ILE:HD12	1:D:221:ILE:HG12	1.98	0.45
1:B:286:SER:HB3	1:B:289:ALA:HB2	1.97	0.45
1:D:251:GLN:HB3	1:D:454:LEU:HD11	1.99	0.45
1:E:74:VAL:HG11	1:E:217:MET:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:VAL:HB	1:A:82:ILE:HG12	2.00	0.44
1:E:59:VAL:HB	1:E:82:ILE:HG12	1.99	0.44
1:B:101:ILE:HG21	1:B:138:ARG:HD2	1.99	0.44
1:D:101:ILE:HD12	1:D:103:TYR:HB3	2.00	0.44
1:D:160:LYS:O	1:D:162:VAL:N	2.50	0.44
3:B:504:16A:H72	3:B:506:16A:H141	1.99	0.44
1:C:164:SER:C	1:C:166:ILE:H	2.20	0.44
1:B:68:MET:HG3	1:B:443:SER:HB2	1.98	0.43
1:C:411:MET:HG3	2:C:501:FAD:C8M	2.48	0.43
1:F:127:VAL:HG12	1:F:129:ILE:H	1.83	0.43
1:B:411:MET:HG3	2:B:501:FAD:C8M	2.49	0.43
3:A:503:16A:C17	3:D:502:16A:H141	2.47	0.43
1:E:83:VAL:HG11	1:E:242:THR:HG21	2.00	0.43
1:A:341:PHE:HA	1:A:342:PRO:HD3	1.85	0.43
1:B:259:TRP:HB3	1:B:369:PHE:HE1	1.83	0.43
1:D:321:VAL:HG12	1:D:351:LEU:HD13	2.00	0.42
1:E:230:LEU:HD22	1:E:252:VAL:HG21	2.00	0.42
1:A:321:VAL:HG12	1:A:351:LEU:HD13	2.00	0.42
1:E:68:MET:HG3	1:E:443:SER:HB2	2.00	0.42
1:A:301:PHE:HE2	1:A:315:ARG:HB3	1.84	0.42
1:F:96:PHE:CZ	1:F:203:PRO:HA	2.54	0.42
1:A:411:MET:SD	3:A:504:16A:H182	2.60	0.42
1:E:137:GLY:HA2	1:E:195:GLU:O	2.20	0.42
1:E:251:GLN:HB3	1:E:454:LEU:HD11	2.02	0.41
1:B:51:LEU:HA	1:B:52:PRO:HD3	1.93	0.41
1:B:411:MET:HG3	2:B:501:FAD:HM81	2.02	0.41
1:E:458:LYS:HA	1:E:459:PRO:HD3	1.85	0.41
1:A:57:VAL:HG11	1:A:73:LEU:HD13	2.01	0.41
1:C:326:PHE:HA	3:C:502:16A:H111	2.01	0.41
1:D:443:SER:HA	1:D:446:SER:HB2	2.03	0.41
1:A:352:ILE:HD11	3:A:503:16A:H142	2.01	0.41
1:B:329:GLY:HA3	3:B:505:16A:H192	2.03	0.41
1:C:138:ARG:HA	1:C:293:ASN:O	2.20	0.41
1:F:83:VAL:HG11	1:F:242:THR:HG21	2.03	0.41
1:C:138:ARG:HB2	1:C:293:ASN:HB3	2.03	0.41
1:A:317:ILE:O	1:A:343:VAL:HA	2.21	0.40
1:D:100:ALA:HB3	1:D:199:GLY:HA3	2.03	0.40
1:F:82:ILE:HD12	1:F:221:ILE:HG12	2.04	0.40
1:A:78:LEU:HD11	1:A:455:LEU:HD21	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	431/454 (95%)	418 (97%)	12 (3%)	1 (0%)	52	76
1	B	431/454 (95%)	416 (96%)	15 (4%)	0	100	100
1	C	430/454 (95%)	413 (96%)	16 (4%)	1 (0%)	52	76
1	D	428/454 (94%)	412 (96%)	14 (3%)	2 (0%)	34	57
1	E	430/454 (95%)	418 (97%)	12 (3%)	0	100	100
1	F	429/454 (94%)	412 (96%)	17 (4%)	0	100	100
All	All	2579/2724 (95%)	2489 (96%)	86 (3%)	4 (0%)	52	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	167	PRO
1	D	160	LYS
1	D	161	ASN
1	A	40	ARG

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	357/379 (94%)	354 (99%)	3 (1%)	86	95
1	B	352/379 (93%)	349 (99%)	3 (1%)	84	94
1	C	335/379 (88%)	333 (99%)	2 (1%)	90	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	339/379 (89%)	334 (98%)	5 (2%)	72	89
1	E	344/379 (91%)	336 (98%)	8 (2%)	58	81
1	F	322/379 (85%)	316 (98%)	6 (2%)	65	85
All	All	2049/2274 (90%)	2022 (99%)	27 (1%)	76	91

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	201	PHE
1	A	282	LEU
1	A	460	VAL
1	B	143	LEU
1	B	201	PHE
1	B	220	ARG
1	C	201	PHE
1	C	288	THR
1	D	74	VAL
1	D	159	SER
1	D	201	PHE
1	D	288	THR
1	D	340	ASP
1	E	143	LEU
1	E	179	ASN
1	E	201	PHE
1	E	340	ASP
1	E	344	HIS
1	E	356	MET
1	E	387	SER
1	E	460	VAL
1	F	156	ASP
1	F	201	PHE
1	F	282	LEU
1	F	288	THR
1	F	340	ASP
1	F	352	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

21 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	501	-	52,58,58	1.47	7 (13%)	52,89,89	2.25	8 (15%)
3	16A	A	502	-	19,19,19	0.40	0	21,21,21	0.62	0
3	16A	A	503	-	19,19,19	0.49	0	21,21,21	0.56	0
3	16A	A	504	-	19,19,19	0.45	0	21,21,21	0.62	0
2	FAD	B	501	-	52,58,58	1.50	7 (13%)	52,89,89	2.13	8 (15%)
3	16A	B	502	-	19,19,19	0.38	0	21,21,21	0.63	0
3	16A	B	503	-	19,19,19	0.45	0	21,21,21	0.70	0
3	16A	B	504	-	19,19,19	0.46	0	21,21,21	0.66	0
3	16A	B	505	-	19,19,19	0.45	0	21,21,21	0.61	0
3	16A	B	506	-	19,19,19	0.42	0	21,21,21	0.57	0
2	FAD	C	501	-	52,58,58	1.50	7 (13%)	52,89,89	2.18	8 (15%)
3	16A	C	502	-	19,19,19	0.44	0	21,21,21	0.59	0
2	FAD	D	501	-	52,58,58	1.48	7 (13%)	52,89,89	2.24	9 (17%)
3	16A	D	502	-	19,19,19	0.44	0	21,21,21	0.58	0
3	16A	D	503	-	19,19,19	0.43	0	21,21,21	0.59	0
3	16A	D	504	-	19,19,19	0.45	0	21,21,21	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	E	501	-	52,58,58	1.52	7 (13%)	52,89,89	2.06	8 (15%)
3	16A	E	502	-	19,19,19	0.44	0	21,21,21	0.62	0
2	FAD	F	501	-	52,58,58	1.51	8 (15%)	52,89,89	2.15	9 (17%)
3	16A	F	502	-	19,19,19	0.41	0	21,21,21	0.54	0
3	16A	F	503	-	19,19,19	0.46	0	21,21,21	0.62	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	501	-	-	0/30/50/50	0/6/6/6
3	16A	A	502	-	-	0/17/17/17	0/0/0/0
3	16A	A	503	-	-	0/17/17/17	0/0/0/0
3	16A	A	504	-	-	0/17/17/17	0/0/0/0
2	FAD	B	501	-	-	0/30/50/50	0/6/6/6
3	16A	B	502	-	-	0/17/17/17	0/0/0/0
3	16A	B	503	-	-	0/17/17/17	0/0/0/0
3	16A	B	504	-	-	0/17/17/17	0/0/0/0
3	16A	B	505	-	-	0/17/17/17	0/0/0/0
3	16A	B	506	-	-	0/17/17/17	0/0/0/0
2	FAD	C	501	-	-	0/30/50/50	0/6/6/6
3	16A	C	502	-	-	0/17/17/17	0/0/0/0
2	FAD	D	501	-	-	0/30/50/50	0/6/6/6
3	16A	D	502	-	-	0/17/17/17	0/0/0/0
3	16A	D	503	-	-	0/17/17/17	0/0/0/0
3	16A	D	504	-	-	0/17/17/17	0/0/0/0
2	FAD	E	501	-	-	0/30/50/50	0/6/6/6
3	16A	E	502	-	-	0/17/17/17	0/0/0/0
2	FAD	F	501	-	-	0/30/50/50	0/6/6/6
3	16A	F	502	-	-	0/17/17/17	0/0/0/0
3	16A	F	503	-	-	0/17/17/17	0/0/0/0

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	FAD	C2A-N3A	2.02	1.35	1.32
2	D	501	FAD	C10-N10	2.21	1.41	1.39
2	A	501	FAD	C10-N10	2.33	1.41	1.39
2	E	501	FAD	C9A-N10	2.41	1.42	1.38
2	C	501	FAD	C9A-N10	2.44	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	FAD	C10-N10	2.46	1.42	1.39
2	A	501	FAD	C9A-N10	2.52	1.42	1.38
2	D	501	FAD	C9A-N10	2.56	1.42	1.38
2	B	501	FAD	C10-N10	2.60	1.42	1.39
2	B	501	FAD	C9A-N10	2.61	1.42	1.38
2	F	501	FAD	C10-N10	2.61	1.42	1.39
2	E	501	FAD	C10-N10	2.83	1.42	1.39
2	F	501	FAD	C9A-N10	2.91	1.42	1.38
2	A	501	FAD	C5A-C4A	3.22	1.47	1.40
2	F	501	FAD	C5A-C4A	3.29	1.47	1.40
2	C	501	FAD	C5A-C4A	3.32	1.48	1.40
2	B	501	FAD	C8-C7	3.32	1.49	1.41
2	B	501	FAD	C5A-C4A	3.32	1.48	1.40
2	D	501	FAD	C5A-C4A	3.35	1.48	1.40
2	A	501	FAD	C8-C7	3.38	1.50	1.41
2	D	501	FAD	C8-C7	3.46	1.50	1.41
2	C	501	FAD	C8-C7	3.48	1.50	1.41
2	E	501	FAD	C5A-C4A	3.48	1.48	1.40
2	A	501	FAD	C9A-C5X	3.54	1.50	1.42
2	E	501	FAD	C8-C7	3.54	1.50	1.41
2	F	501	FAD	C8-C7	3.56	1.50	1.41
2	B	501	FAD	C9A-C5X	3.87	1.50	1.42
2	D	501	FAD	C4-C4X	3.88	1.49	1.41
2	D	501	FAD	C9A-C5X	3.89	1.50	1.42
2	F	501	FAD	C9A-C5X	3.91	1.50	1.42
2	C	501	FAD	C9A-C5X	3.91	1.50	1.42
2	E	501	FAD	C9A-C5X	3.94	1.50	1.42
2	C	501	FAD	C4-C4X	3.97	1.49	1.41
2	F	501	FAD	C4-C4X	4.11	1.49	1.41
2	A	501	FAD	C4-C4X	4.15	1.49	1.41
2	E	501	FAD	C4-C4X	4.19	1.49	1.41
2	B	501	FAD	C4-C4X	4.23	1.49	1.41
2	A	501	FAD	C4X-C10	4.49	1.49	1.40
2	C	501	FAD	C4X-C10	4.66	1.49	1.40
2	F	501	FAD	C4X-C10	4.68	1.49	1.40
2	B	501	FAD	C4X-C10	4.68	1.49	1.40
2	D	501	FAD	C4X-C10	4.69	1.49	1.40
2	E	501	FAD	C4X-C10	4.74	1.49	1.40

All (50) 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	D	501	FAD	N3A-C2A-N1A	-7.85	122.71	128.87
2	F	501	FAD	N3A-C2A-N1A	-7.53	122.95	128.87
2	A	501	FAD	N3A-C2A-N1A	-7.41	123.05	128.87
2	B	501	FAD	N3A-C2A-N1A	-7.21	123.21	128.87
2	C	501	FAD	N3A-C2A-N1A	-7.17	123.23	128.87
2	E	501	FAD	N3A-C2A-N1A	-7.16	123.25	128.87
2	D	501	FAD	C4-C4X-C10	-5.83	116.21	119.94
2	C	501	FAD	C4-C4X-C10	-5.82	116.22	119.94
2	A	501	FAD	C4-C4X-C10	-5.78	116.25	119.94
2	B	501	FAD	C4-C4X-C10	-5.40	116.49	119.94
2	F	501	FAD	C4-C4X-C10	-5.15	116.65	119.94
2	E	501	FAD	C4-C4X-C10	-4.99	116.75	119.94
2	A	501	FAD	C4X-C4-N3	-3.83	118.51	123.52
2	D	501	FAD	C4X-C4-N3	-3.83	118.52	123.52
2	E	501	FAD	C4X-C4-N3	-3.80	118.56	123.52
2	C	501	FAD	C4X-C4-N3	-3.76	118.61	123.52
2	F	501	FAD	C4X-C4-N3	-3.68	118.71	123.52
2	B	501	FAD	C4X-C4-N3	-3.61	118.81	123.52
2	A	501	FAD	N3-C2-N1	-3.24	122.24	127.69
2	C	501	FAD	N3-C2-N1	-3.23	122.26	127.69
2	D	501	FAD	N3-C2-N1	-3.19	122.32	127.69
2	B	501	FAD	N3-C2-N1	-3.11	122.46	127.69
2	F	501	FAD	N3-C2-N1	-3.08	122.50	127.69
2	E	501	FAD	N3-C2-N1	-2.95	122.73	127.69
2	D	501	FAD	C1'-N10-C9A	2.06	121.21	118.83
2	D	501	FAD	C5X-C9A-N10	2.30	119.30	117.58
2	C	501	FAD	C5X-C9A-N10	2.33	119.32	117.58
2	B	501	FAD	C5X-C9A-N10	2.33	119.32	117.58
2	F	501	FAD	C5X-C9A-N10	2.41	119.39	117.58
2	E	501	FAD	C5X-C9A-N10	2.46	119.42	117.58
2	F	501	FAD	C1'-N10-C9A	2.47	121.69	118.83
2	A	501	FAD	C5X-C9A-N10	2.71	119.61	117.58
2	F	501	FAD	C4-C4X-N5	2.99	122.34	118.70
2	E	501	FAD	C4-C4X-N5	3.04	122.40	118.70
2	D	501	FAD	C4-C4X-N5	3.25	122.65	118.70
2	C	501	FAD	C4-C4X-N5	3.32	122.73	118.70
2	B	501	FAD	C4-C4X-N5	3.33	122.75	118.70
2	A	501	FAD	C4-C4X-N5	3.44	122.88	118.70
2	E	501	FAD	C4X-N5-C5X	3.73	121.12	116.72
2	D	501	FAD	C4X-N5-C5X	3.80	121.20	116.72
2	C	501	FAD	C4X-N5-C5X	3.80	121.20	116.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	501	FAD	C4X-N5-C5X	3.93	121.35	116.72
2	B	501	FAD	C4X-N5-C5X	4.14	121.60	116.72
2	A	501	FAD	C4X-N5-C5X	4.16	121.63	116.72
2	E	501	FAD	C4-N3-C2	8.11	121.93	115.16
2	F	501	FAD	C4-N3-C2	8.30	122.08	115.16
2	B	501	FAD	C4-N3-C2	8.39	122.16	115.16
2	A	501	FAD	C4-N3-C2	8.71	122.42	115.16
2	C	501	FAD	C4-N3-C2	8.75	122.46	115.16
2	D	501	FAD	C4-N3-C2	8.77	122.47	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	16A	4	0
3	A	504	16A	1	0
2	B	501	FAD	2	0
3	B	502	16A	4	0
3	B	503	16A	2	0
3	B	504	16A	2	0
3	B	505	16A	1	0
3	B	506	16A	3	0
2	C	501	FAD	2	0
3	C	502	16A	1	0
3	D	502	16A	3	0
3	D	504	16A	1	0
3	E	502	16A	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	433/454 (95%)	-0.14	1 (0%) 95 95	58, 74, 103, 127	0
1	B	432/454 (95%)	-0.11	4 (0%) 85 83	51, 88, 123, 138	0
1	C	430/454 (94%)	0.19	15 (3%) 48 41	55, 83, 148, 180	0
1	D	430/454 (94%)	0.19	16 (3%) 45 38	56, 93, 155, 192	0
1	E	430/454 (94%)	0.10	18 (4%) 40 33	54, 96, 139, 165	0
1	F	430/454 (94%)	0.30	27 (6%) 23 18	55, 117, 165, 190	0
All	All	2585/2724 (94%)	0.09	81 (3%) 52 46	51, 89, 149, 192	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	192	ALA	7.3
1	C	191	ILE	5.2
1	F	81	VAL	4.9
1	D	176	ALA	4.8
1	F	252	VAL	4.8
1	F	192	ALA	4.3
1	C	193	GLY	4.2
1	F	194	PHE	4.1
1	D	292	GLY	4.0
1	D	193	GLY	3.9
1	D	192	ALA	3.9
1	E	155	ILE	3.7
1	F	289	ALA	3.7
1	E	191	ILE	3.6
1	E	139	VAL	3.5
1	F	113	HIS	3.5
1	A	161	ASN	3.5
1	C	115	LEU	3.4
1	C	179	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	152	ARG	3.3
1	F	229	GLY	3.3
1	F	156	ASP	3.2
1	F	80	VAL	3.2
1	F	302	PHE	3.2
1	C	194	PHE	3.1
1	F	125	ALA	3.1
1	F	240	VAL	3.1
1	F	176	ALA	3.1
1	E	120	TRP	3.0
1	B	131	THR	3.0
1	C	292	GLY	2.9
1	E	118	HIS	2.9
1	E	156	ASP	2.9
1	F	455	LEU	2.9
1	D	288	THR	2.9
1	E	154	TRP	2.8
1	C	171	ARG	2.8
1	F	340	ASP	2.8
1	C	103	TYR	2.7
1	D	289	ALA	2.7
1	F	221	ILE	2.7
1	E	193	GLY	2.6
1	C	156	ASP	2.6
1	F	179	ASN	2.6
1	D	172	ILE	2.5
1	E	129	ILE	2.5
1	D	178	LEU	2.5
1	C	154	TRP	2.5
1	D	115	LEU	2.5
1	D	181	ARG	2.5
1	F	100	ALA	2.4
1	B	421	ILE	2.4
1	E	164	SER	2.4
1	F	83	VAL	2.4
1	E	192	ALA	2.4
1	B	208	PHE	2.4
1	C	300	ILE	2.4
1	C	395	PHE	2.3
1	E	170	THR	2.3
1	F	82	ILE	2.3
1	D	296	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	141	VAL	2.3
1	F	160	LYS	2.2
1	F	71	ILE	2.2
1	E	168	PHE	2.2
1	C	398	PHE	2.2
1	B	207	THR	2.2
1	E	110	PHE	2.1
1	F	251	GLN	2.1
1	E	162	VAL	2.1
1	D	174	GLU	2.1
1	D	306	ALA	2.1
1	E	103	TYR	2.1
1	D	107	ASP	2.1
1	F	114	HIS	2.1
1	F	175	GLY	2.0
1	D	141	VAL	2.0
1	E	400	GLU	2.0
1	F	142	PRO	2.0
1	F	253	VAL	2.0
1	D	173	ILE	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, 95th 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 ²)	Q<0.9
3	16A	B	503	20/20	0.85	0.33	3.77	82,85,88,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	16A	A	503	20/20	0.74	0.35	3.65	80,89,95,96	0
3	16A	E	502	20/20	0.85	0.34	3.36	76,80,88,89	0
3	16A	D	503	20/20	0.76	0.34	2.97	71,80,84,84	0
3	16A	B	504	20/20	0.87	0.30	2.12	68,73,86,87	0
3	16A	C	502	20/20	0.77	0.29	2.12	91,97,100,101	0
3	16A	B	502	20/20	0.84	0.27	2.00	73,79,88,88	0
3	16A	F	502	20/20	0.92	0.25	1.60	67,71,75,76	0
3	16A	A	504	20/20	0.92	0.27	1.50	70,79,89,90	0
3	16A	D	504	20/20	0.85	0.26	1.48	72,77,80,81	0
3	16A	B	505	20/20	0.89	0.22	1.18	67,68,73,74	0
3	16A	F	503	20/20	0.93	0.21	0.89	62,75,92,92	0
3	16A	A	502	20/20	0.88	0.23	0.88	64,71,88,88	0
3	16A	D	502	20/20	0.89	0.20	0.61	68,71,79,79	0
2	FAD	D	501	53/53	0.97	0.17	-0.01	62,66,77,79	0
2	FAD	F	501	53/53	0.96	0.17	-0.12	77,90,97,102	0
2	FAD	A	501	53/53	0.97	0.16	-0.13	54,57,62,62	0
2	FAD	C	501	53/53	0.97	0.17	-0.14	57,60,79,83	0
2	FAD	E	501	53/53	0.97	0.15	-0.31	67,75,85,87	0
3	16A	B	506	20/20	0.92	0.21	-0.40	67,69,72,72	0
2	FAD	B	501	53/53	0.98	0.13	-0.76	61,69,76,79	0

6.5 Other polymers ⓘ

There are no such residues in this entry.