



wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 09:05 PM GMT

PDB ID : 2Q4W
Title : Ensemble refinement of the protein crystal structure of cytokinin oxidase/dehydrogenase(CKX) from Arabidopsis thaliana At5g21482
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on : 2007-05-31
Resolution : 1.70 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

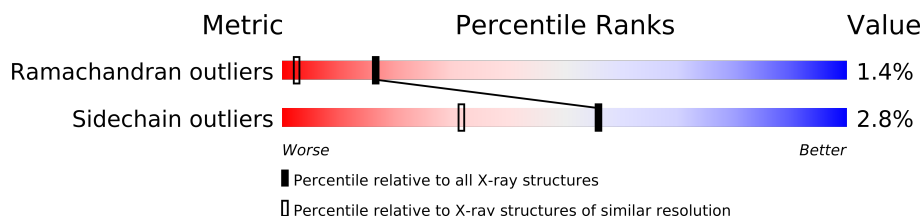
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : **FAILED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.70 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))
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1-A	524	
1	10-A	524	
1	11-A	524	
1	12-A	524	
1	13-A	524	
1	14-A	524	
1	15-A	524	
1	16-A	524	
1	2-A	524	
1	3-A	524	
1	4-A	524	
1	5-A	524	
1	6-A	524	
1	7-A	524	
1	8-A	524	
1	9-A	524	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 72624 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

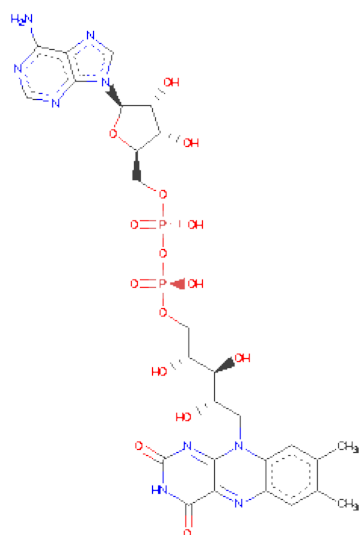
- Molecule 1 is a protein called Cytokinin dehydrogenase 7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	491	Total	C	N	O	S	Se	0	0	0
			3853	2450	667	720	8	8			
1	2-A	491	Total	C	N	O	S	Se	0	0	0
			3853	2450	667	720	8	8			
1	3-A	491	Total	C	N	O	S	Se	0	0	0
			3853	2450	667	720	8	8			
1	4-A	491	Total	C	N	O	S	Se	0	0	0
			3853	2450	667	720	8	8			
1	5-A	491	Total	C	N	O	S	Se	0	0	0
			3853	2450	667	720	8	8			
1	6-A	491	Total	C	N	O	S	Se	0	0	0
			3853	2450	667	720	8	8			
1	7-A	491	Total	C	N	O	S	Se	0	0	0
			3853	2450	667	720	8	8			
1	8-A	491	Total	C	N	O	S	Se	0	0	0
			3853	2450	667	720	8	8			
1	9-A	491	Total	C	N	O	S	Se	0	0	0
			3853	2450	667	720	8	8			
1	10-A	491	Total	C	N	O	S	Se	0	0	0
			3853	2450	667	720	8	8			
1	11-A	491	Total	C	N	O	S	Se	0	0	0
			3853	2450	667	720	8	8			
1	12-A	491	Total	C	N	O	S	Se	0	0	0
			3853	2450	667	720	8	8			
1	13-A	491	Total	C	N	O	S	Se	0	0	0
			3853	2450	667	720	8	8			
1	14-A	491	Total	C	N	O	S	Se	0	0	0
			3853	2450	667	720	8	8			
1	15-A	491	Total	C	N	O	S	Se	0	0	0
			3853	2450	667	720	8	8			
1	16-A	491	Total	C	N	O	S	Se	0	0	0
			3853	2450	667	720	8	8			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	EXPRESSION TAG	UNP Q9FUJ1
A	57	MSE	MET	MODIFIED RESIDUE	UNP Q9FUJ1
A	103	MSE	MET	MODIFIED RESIDUE	UNP Q9FUJ1
A	112	MSE	MET	MODIFIED RESIDUE	UNP Q9FUJ1
A	241	MSE	MET	MODIFIED RESIDUE	UNP Q9FUJ1
A	412	MSE	MET	MODIFIED RESIDUE	UNP Q9FUJ1
A	458	MSE	MET	MODIFIED RESIDUE	UNP Q9FUJ1
A	506	MSE	MET	MODIFIED RESIDUE	UNP Q9FUJ1
A	510	MSE	MET	MODIFIED RESIDUE	UNP Q9FUJ1

- 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	1-A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	2-A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	3-A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	4-A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	5-A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	6-A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	7-A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	8-A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	9-A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	10-A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	11-A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	12-A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	13-A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	14-A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	15-A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	16-A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-A	633	Total	O	0	0
			633	633		
3	2-A	633	Total	O	0	0
			633	633		
3	3-A	633	Total	O	0	0
			633	633		
3	4-A	633	Total	O	0	0
			633	633		
3	5-A	633	Total	O	0	0
			633	633		
3	6-A	633	Total	O	0	0
			633	633		
3	7-A	633	Total	O	0	0
			633	633		
3	8-A	633	Total	O	0	0
			633	633		
3	9-A	633	Total	O	0	0
			633	633		

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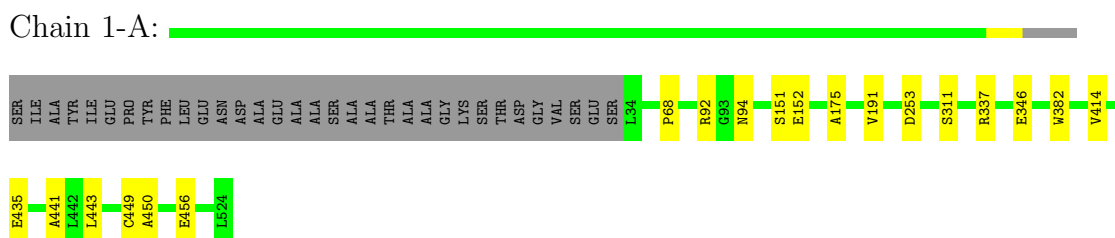
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	10-A	633	Total 633	O 633	0	0
3	11-A	633	Total 633	O 633	0	0
3	12-A	633	Total 633	O 633	0	0
3	13-A	633	Total 633	O 633	0	0
3	14-A	633	Total 633	O 633	0	0
3	15-A	633	Total 633	O 633	0	0
3	16-A	633	Total 633	O 633	0	0

3 Residue-property plots

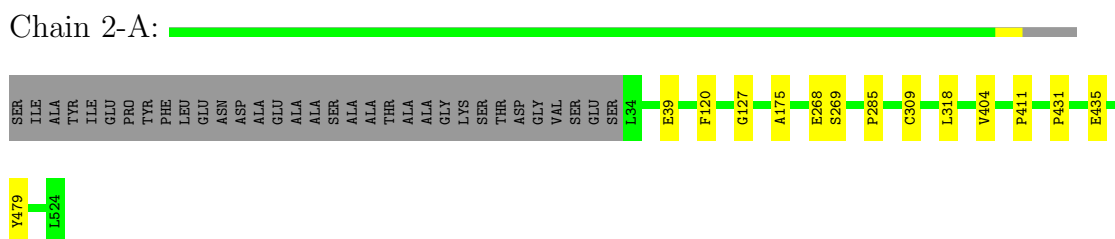
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS failed to run properly.

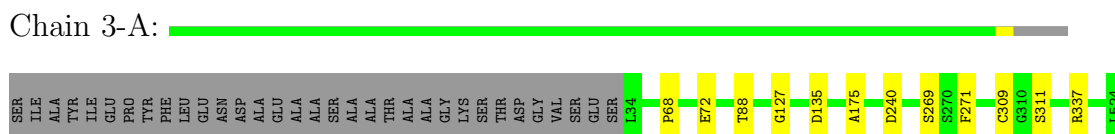
- Molecule 1: Cytokinin dehydrogenase 7



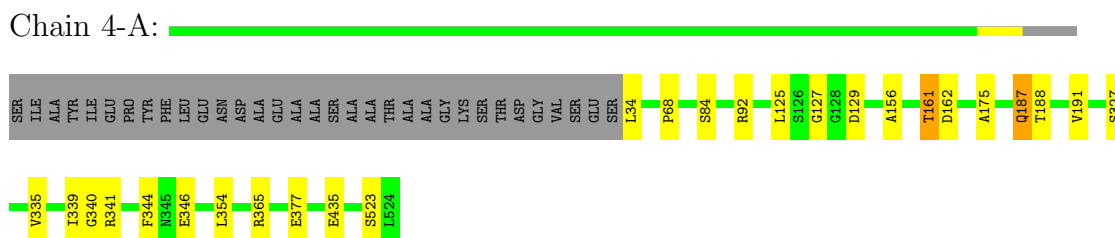
- Molecule 1: Cytokinin dehydrogenase 7



- Molecule 1: Cytokinin dehydrogenase 7

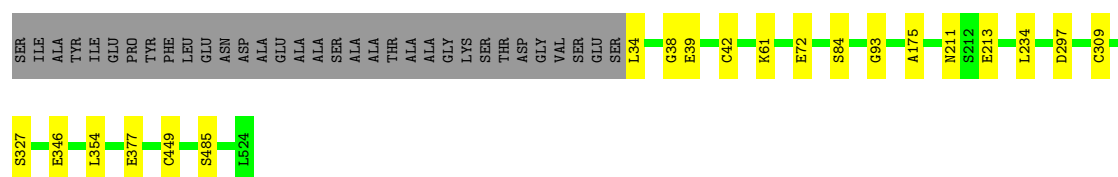


- Molecule 1: Cytokinin dehydrogenase 7



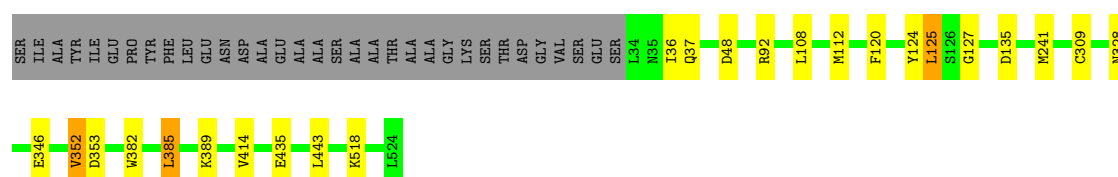
- Molecule 1: Cytokinin dehydrogenase 7





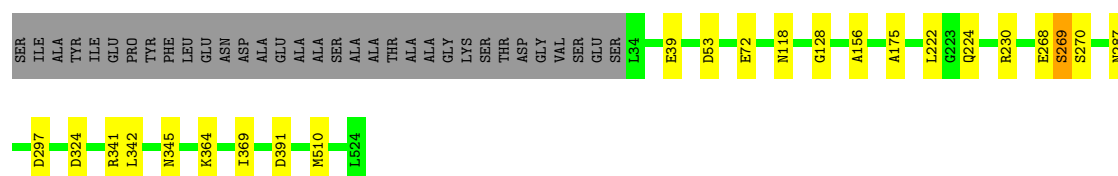
- Molecule 1: Cytokinin dehydrogenase 7

Chain 6-A:



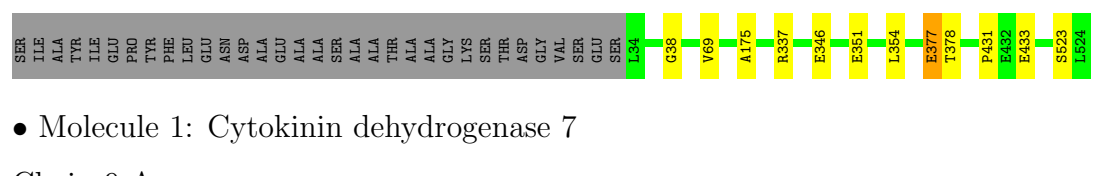
- Molecule 1: Cytokinin dehydrogenase 7

Chain 7-A:



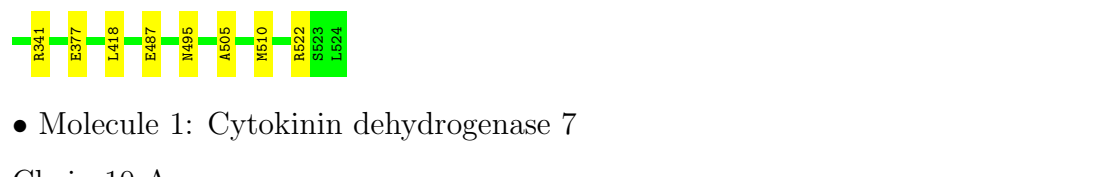
- Molecule 1: Cytokinin dehydrogenase 7

Chain 8-A:



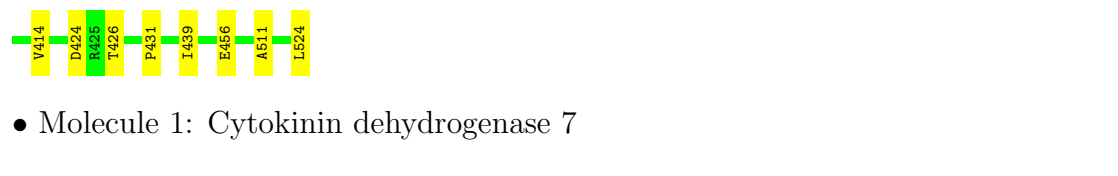
- Molecule 1: Cytokinin dehydrogenase 7

Chain 9-A:



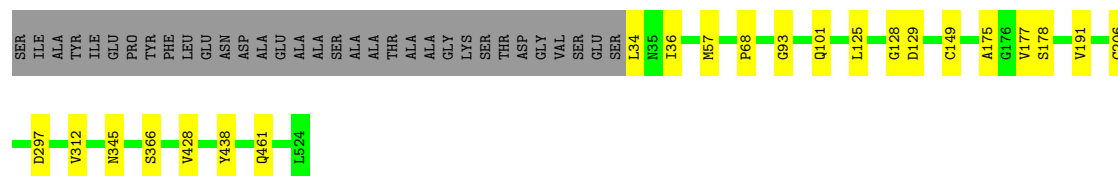
- Molecule 1: Cytokinin dehydrogenase 7

Chain 10-A:



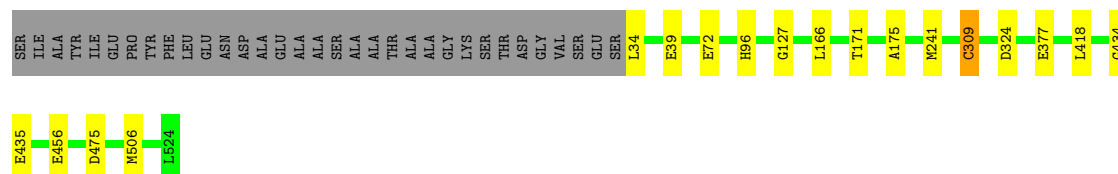
- Molecule 1: Cytokinin dehydrogenase 7

Chain 11-A:



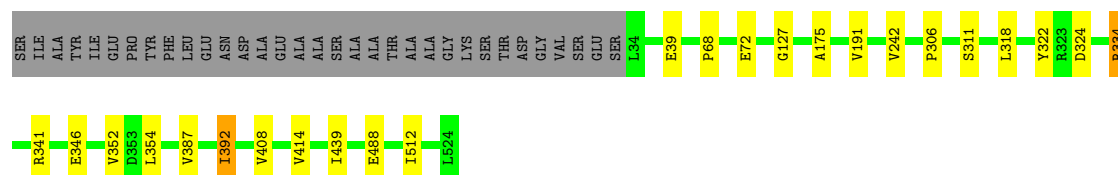
- Molecule 1: Cytokinin dehydrogenase 7

Chain 12-A:



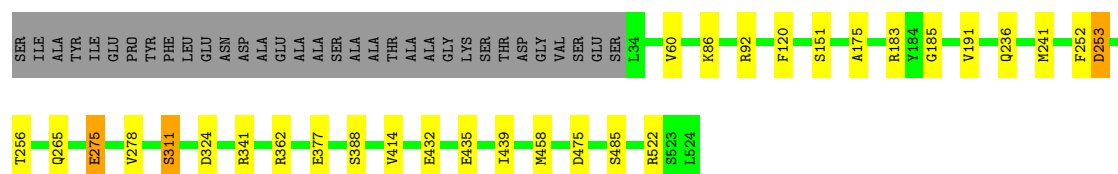
- Molecule 1: Cytokinin dehydrogenase 7

Chain 13-A:



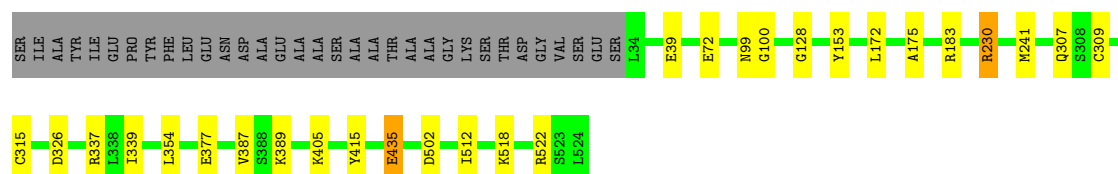
- Molecule 1: Cytokinin dehydrogenase 7

Chain 14-A:



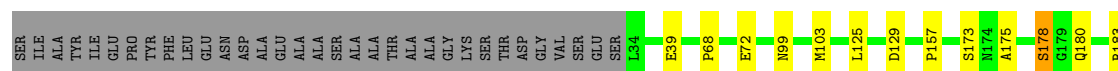
- Molecule 1: Cytokinin dehydrogenase 7

Chain 15-A:



- Molecule 1: Cytokinin dehydrogenase 7

Chain 16-A:



C206	L222	R230	M241	V242	Y273	C309	G310	S311	Y322	D326	T339	G340	R341	N345	E346	V352	D353	L354	E377	Y387	G388	K389	Y415	E435	P447	E456	S498	S514	R522	S523	L524
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	45.86Å 114.50Å 190.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.57 – 1.70	Depositor
% Data completeness (in resolution range)	94.9 (42.57-1.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.92 (at 1.70Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.143 , 0.201	Depositor
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.123	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 52917 reflections	Xtriage
Total number of atoms	72624	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1-A	0.84	3/3938 (0.1%)	0.86	1/5335 (0.0%)
1	2-A	0.83	3/3938 (0.1%)	0.88	0/5335
1	3-A	0.81	1/3938 (0.0%)	0.86	0/5335
1	4-A	0.82	2/3938 (0.1%)	0.87	3/5335 (0.1%)
1	5-A	0.82	3/3938 (0.1%)	0.85	1/5335 (0.0%)
1	6-A	0.83	2/3938 (0.1%)	0.90	4/5335 (0.1%)
1	7-A	0.82	0/3938	0.86	2/5335 (0.0%)
1	8-A	0.81	0/3938	0.84	0/5335
1	9-A	0.84	3/3938 (0.1%)	0.89	2/5335 (0.0%)
1	10-A	0.83	2/3938 (0.1%)	0.90	5/5335 (0.1%)
1	11-A	0.83	2/3938 (0.1%)	0.90	4/5335 (0.1%)
1	12-A	0.82	2/3938 (0.1%)	0.88	1/5335 (0.0%)
1	13-A	0.97	3/3938 (0.1%)	0.99	2/5335 (0.0%)
1	14-A	0.99	4/3938 (0.1%)	1.04	8/5335 (0.1%)
1	15-A	0.97	4/3938 (0.1%)	1.02	2/5335 (0.0%)
1	16-A	0.99	6/3938 (0.2%)	1.01	3/5335 (0.1%)
All	All	0.87	40/63008 (0.1%)	0.91	38/85360 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	6-A	0	1
1	13-A	0	1
1	15-A	0	2
1	16-A	0	3
All	All	0	7

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	309	CYS	CB-SG	-7.64	1.69	1.82
1	16-A	309	CYS	CB-SG	-7.54	1.69	1.82
1	10-A	309	CYS	CB-SG	-7.47	1.69	1.82
1	3-A	309	CYS	CB-SG	-7.33	1.69	1.82
1	16-A	377	GLU	CG-CD	7.32	1.62	1.51

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	14-A	475	ASP	CB-CG-OD1	9.25	126.62	118.30
1	15-A	230	ARG	NE-CZ-NH2	8.24	124.42	120.30
1	6-A	385	LEU	CA-CB-CG	6.61	130.50	115.30
1	4-A	161	THR	N-CA-C	-6.56	93.28	111.00
1	14-A	92	ARG	NE-CZ-NH1	-6.54	117.03	120.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	13-A	322	TYR	Sidechain
1	15-A	153	TYR	Sidechain
1	15-A	415	TYR	Sidechain
1	16-A	273	TYR	Sidechain
1	6-A	124	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	3853	0	3764	0	0
1	2-A	3853	0	3764	0	0
1	3-A	3853	0	3764	0	0
1	4-A	3853	0	3764	0	0
1	5-A	3853	0	3764	0	1
1	6-A	3853	0	3764	0	0
1	7-A	3853	0	3764	0	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	8-A	3853	0	3764	0	0
1	9-A	3853	0	3764	0	1
1	10-A	3853	0	3764	0	0
1	11-A	3853	0	3764	0	1
1	12-A	3853	0	3764	0	0
1	13-A	3853	0	3764	0	0
1	14-A	3853	0	3764	0	0
1	15-A	3853	0	3764	0	0
1	16-A	3853	0	3764	0	1
2	1-A	53	0	31	0	0
2	2-A	53	0	29	0	0
2	3-A	53	0	31	0	0
2	4-A	53	0	31	0	0
2	5-A	53	0	31	0	0
2	6-A	53	0	31	0	0
2	7-A	53	0	31	0	0
2	8-A	53	0	31	0	0
2	9-A	53	0	31	0	0
2	10-A	53	0	30	0	0
2	11-A	53	0	31	0	0
2	12-A	53	0	31	0	0
2	13-A	53	0	31	0	0
2	14-A	53	0	29	0	0
2	15-A	53	0	28	0	0
2	16-A	53	0	30	0	0
3	1-A	633	0	0	0	0
3	2-A	633	0	0	0	0
3	3-A	633	0	0	0	0
3	4-A	633	0	0	0	0
3	5-A	633	0	0	0	1
3	6-A	633	0	0	0	0
3	7-A	633	0	0	0	2
3	8-A	633	0	0	0	0
3	9-A	633	0	0	0	1
3	10-A	633	0	0	0	0
3	11-A	633	0	0	0	1
3	12-A	633	0	0	0	0
3	13-A	633	0	0	0	0
3	14-A	633	0	0	0	0
3	15-A	633	0	0	0	0
3	16-A	633	0	0	0	0
All	All	72624	0	60711	0	6

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

The worst 5 of 6 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:297:ASP:OD2	3:A:947:HOH:O[8_457]	1.95	0.25
1:A:297:ASP:OD2	3:A:947:HOH:O[8_457]	2.02	0.18
1:A:297:ASP:CG	3:A:947:HOH:O[8_457]	2.12	0.08
1:A:341:ARG:NH1	3:A:1280:HOH:O[8_557]	2.13	0.07
1:A:341:ARG:NH2	1:A:353:ASP:OD1[8_557]	2.13	0.07

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	1-A	489/524 (93%)	439 (90%)	44 (9%)	6 (1%)	19	3
1	2-A	489/524 (93%)	458 (94%)	24 (5%)	7 (1%)	16	2
1	3-A	489/524 (93%)	451 (92%)	35 (7%)	3 (1%)	33	13
1	4-A	489/524 (93%)	442 (90%)	37 (8%)	10 (2%)	11	1
1	5-A	489/524 (93%)	454 (93%)	30 (6%)	5 (1%)	22	5
1	6-A	489/524 (93%)	441 (90%)	39 (8%)	9 (2%)	13	1
1	7-A	489/524 (93%)	434 (89%)	42 (9%)	13 (3%)	8	1
1	8-A	489/524 (93%)	447 (91%)	37 (8%)	5 (1%)	22	5
1	9-A	489/524 (93%)	441 (90%)	42 (9%)	6 (1%)	19	3
1	10-A	489/524 (93%)	442 (90%)	35 (7%)	12 (2%)	9	1
1	11-A	489/524 (93%)	444 (91%)	37 (8%)	8 (2%)	14	2
1	12-A	489/524 (93%)	454 (93%)	32 (6%)	3 (1%)	33	13
1	13-A	489/524 (93%)	444 (91%)	39 (8%)	6 (1%)	19	3
1	14-A	489/524 (93%)	433 (88%)	49 (10%)	7 (1%)	16	2
1	15-A	489/524 (93%)	439 (90%)	45 (9%)	5 (1%)	22	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	16-A	489/524 (93%)	450 (92%)	35 (7%)	4 (1%)	27	8
All	All	7824/8384 (93%)	7113 (91%)	602 (8%)	109 (1%)	16	2

5 of 109 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	382	TRP
1	1-A	414	VAL
1	2-A	269	SER
1	4-A	188	THR
1	4-A	341	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	1-A	415/430 (96%)	406 (98%)	9 (2%)	64	43
1	2-A	415/430 (96%)	411 (99%)	4 (1%)	85	76
1	3-A	415/430 (96%)	407 (98%)	8 (2%)	69	50
1	4-A	415/430 (96%)	402 (97%)	13 (3%)	52	27
1	5-A	415/430 (96%)	405 (98%)	10 (2%)	61	39
1	6-A	415/430 (96%)	403 (97%)	12 (3%)	55	30
1	7-A	415/430 (96%)	407 (98%)	8 (2%)	69	50
1	8-A	415/430 (96%)	407 (98%)	8 (2%)	69	50
1	9-A	415/430 (96%)	403 (97%)	12 (3%)	55	30
1	10-A	415/430 (96%)	408 (98%)	7 (2%)	73	55
1	11-A	415/430 (96%)	407 (98%)	8 (2%)	69	50
1	12-A	415/430 (96%)	402 (97%)	13 (3%)	52	27
1	13-A	415/430 (96%)	401 (97%)	14 (3%)	49	23
1	14-A	415/430 (96%)	398 (96%)	17 (4%)	41	17
1	15-A	415/430 (96%)	398 (96%)	17 (4%)	41	17
1	16-A	415/430 (96%)	390 (94%)	25 (6%)	27	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	6640/6880 (96%)	6455 (97%)	185 (3%)	56 32

5 of 185 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	9-A	522	ARG
1	12-A	166	LEU
1	16-A	206	CYS
1	10-A	322	TYR
1	11-A	68	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
1	8-A	119	HIS
1	9-A	211	ASN
1	15-A	467	HIS
1	8-A	211	ASN
1	8-A	345	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

16 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	1-A	701	-	58,58,58	1.99	13 (22%)	85,89,89	1.96	17 (20%)
2	FAD	10-A	701	-	58,58,58	2.39	20 (34%)	85,89,89	2.16	15 (17%)
2	FAD	11-A	701	-	58,58,58	2.52	20 (34%)	85,89,89	1.89	15 (17%)
2	FAD	12-A	701	-	58,58,58	1.97	16 (27%)	85,89,89	1.65	14 (16%)
2	FAD	13-A	701	-	58,58,58	2.34	14 (24%)	85,89,89	2.12	18 (21%)
2	FAD	14-A	701	-	58,58,58	3.12	23 (39%)	85,89,89	2.16	25 (29%)
2	FAD	15-A	701	-	58,58,58	2.90	21 (36%)	85,89,89	1.69	11 (12%)
2	FAD	16-A	701	-	58,58,58	2.56	19 (32%)	85,89,89	2.13	26 (30%)
2	FAD	2-A	701	-	58,58,58	2.48	15 (25%)	85,89,89	1.94	21 (24%)
2	FAD	3-A	701	-	58,58,58	2.30	15 (25%)	85,89,89	1.69	21 (24%)
2	FAD	4-A	701	-	58,58,58	2.43	13 (22%)	85,89,89	1.85	20 (23%)
2	FAD	5-A	701	-	58,58,58	2.02	19 (32%)	85,89,89	1.89	17 (20%)
2	FAD	6-A	701	-	58,58,58	2.58	14 (24%)	85,89,89	1.68	15 (17%)
2	FAD	7-A	701	-	58,58,58	2.42	14 (24%)	85,89,89	1.96	19 (22%)
2	FAD	8-A	701	-	58,58,58	2.14	12 (20%)	85,89,89	1.92	20 (23%)
2	FAD	9-A	701	-	58,58,58	2.23	17 (29%)	85,89,89	1.69	17 (20%)

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	1-A	701	-	-	0/34/50/50	0/1/6/6
2	FAD	10-A	701	-	-	0/34/50/50	0/1/6/6
2	FAD	11-A	701	-	-	0/34/50/50	0/1/6/6
2	FAD	12-A	701	-	-	0/34/50/50	0/1/6/6
2	FAD	13-A	701	-	-	0/34/50/50	0/1/6/6
2	FAD	14-A	701	-	-	0/34/50/50	0/1/6/6
2	FAD	15-A	701	-	-	0/34/50/50	0/1/6/6
2	FAD	16-A	701	-	-	0/34/50/50	0/1/6/6
2	FAD	2-A	701	-	-	0/34/50/50	0/1/6/6
2	FAD	3-A	701	-	-	0/34/50/50	0/1/6/6
2	FAD	4-A	701	-	-	1/34/50/50	0/1/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	5-A	701	-	-	0/34/50/50	0/1/6/6
2	FAD	6-A	701	-	-	0/34/50/50	0/1/6/6
2	FAD	7-A	701	-	-	0/34/50/50	0/1/6/6
2	FAD	8-A	701	-	-	0/34/50/50	0/1/6/6
2	FAD	9-A	701	-	-	0/34/50/50	0/1/6/6

The worst 5 of 265 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	15-A	701	FAD	C5'-C4'	-14.55	1.28	1.51
2	14-A	701	FAD	C5'-C4'	-13.74	1.29	1.51
2	2-A	701	FAD	C5'-C4'	-10.54	1.34	1.51
2	14-A	701	FAD	C9A-N10	10.32	1.54	1.38
2	8-A	701	FAD	C5'-C4'	-10.13	1.35	1.51

The worst 5 of 291 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	10-A	701	FAD	O4B-C1B-N9A	-9.89	99.24	108.44
2	13-A	701	FAD	C4'-C3'-C2'	-9.00	92.91	113.25
2	14-A	701	FAD	O4B-C1B-N9A	-8.65	100.39	108.44
2	10-A	701	FAD	C5'-C4'-C3'	8.35	127.82	112.06
2	7-A	701	FAD	O4B-C1B-N9A	-8.30	100.72	108.44

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	4-A	701	FAD	PA-O5B-C5B-C4B

There are no ring outliers.

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 ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.