



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:33 PM GMT

PDB ID : 4P8P
Title : Crystal structure of M. tuberculosis DprE1 in complex with the non-covalent inhibitor QN127
Authors : Neres, J.; Pojer, F.; Cole, S.T.
Deposited on : 2014-03-31
Resolution : 2.20 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

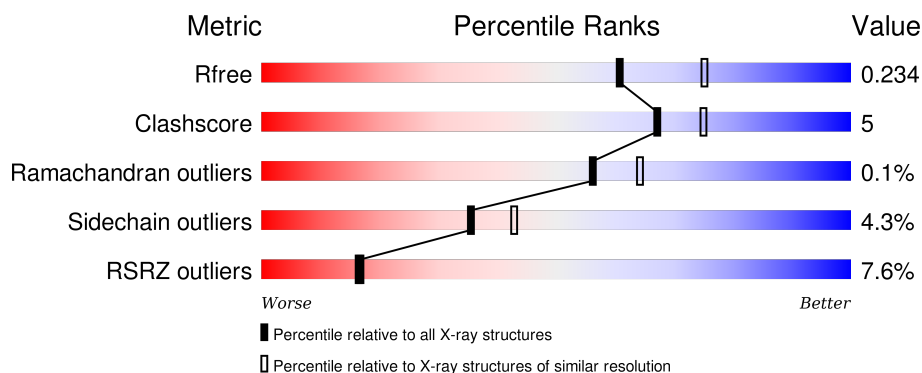
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	480	
1	B	480	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7067 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 Probable decaprenylphosphoryl-beta-D-ribose oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3461	2203	607	640	11			
1	B	420	Total	C	N	O	S	0	1	0
			3234	2052	575	597	10			

There are 38 discrepancies between the modelled and reference sequences:

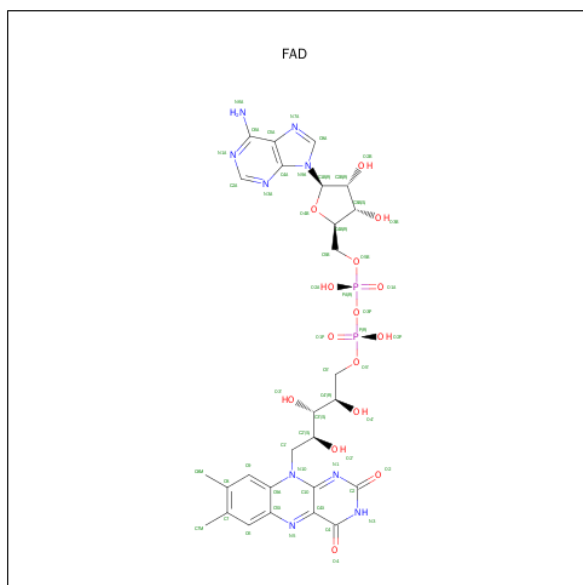
Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	expression tag	UNP P72056
A	-17	SER	-	expression tag	UNP P72056
A	-16	SER	-	expression tag	UNP P72056
A	-15	HIS	-	expression tag	UNP P72056
A	-14	HIS	-	expression tag	UNP P72056
A	-13	HIS	-	expression tag	UNP P72056
A	-12	HIS	-	expression tag	UNP P72056
A	-11	HIS	-	expression tag	UNP P72056
A	-10	HIS	-	expression tag	UNP P72056
A	-9	SER	-	expression tag	UNP P72056
A	-8	SER	-	expression tag	UNP P72056
A	-7	GLY	-	expression tag	UNP P72056
A	-6	LEU	-	expression tag	UNP P72056
A	-5	VAL	-	expression tag	UNP P72056
A	-4	PRO	-	expression tag	UNP P72056
A	-3	ARG	-	expression tag	UNP P72056
A	-2	GLY	-	expression tag	UNP P72056
A	-1	SER	-	expression tag	UNP P72056
A	0	HIS	-	expression tag	UNP P72056
B	-18	GLY	-	expression tag	UNP P72056
B	-17	SER	-	expression tag	UNP P72056
B	-16	SER	-	expression tag	UNP P72056
B	-15	HIS	-	expression tag	UNP P72056
B	-14	HIS	-	expression tag	UNP P72056
B	-13	HIS	-	expression tag	UNP P72056

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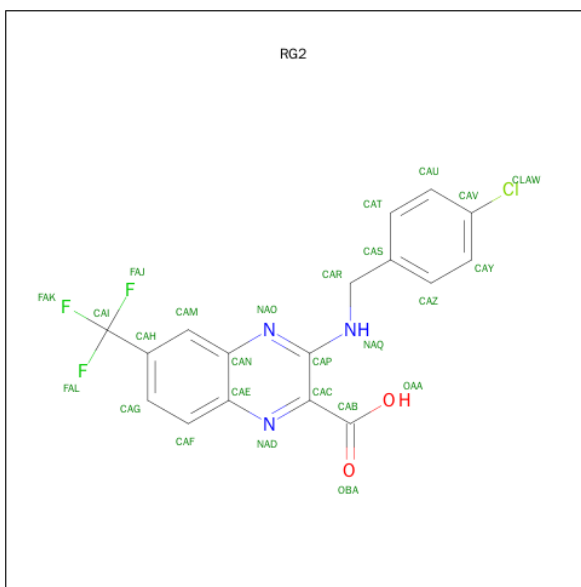
Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	expression tag	UNP P72056
B	-11	HIS	-	expression tag	UNP P72056
B	-10	HIS	-	expression tag	UNP P72056
B	-9	SER	-	expression tag	UNP P72056
B	-8	SER	-	expression tag	UNP P72056
B	-7	GLY	-	expression tag	UNP P72056
B	-6	LEU	-	expression tag	UNP P72056
B	-5	VAL	-	expression tag	UNP P72056
B	-4	PRO	-	expression tag	UNP P72056
B	-3	ARG	-	expression tag	UNP P72056
B	-2	GLY	-	expression tag	UNP P72056
B	-1	SER	-	expression tag	UNP P72056
B	0	HIS	-	expression tag	UNP P72056

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



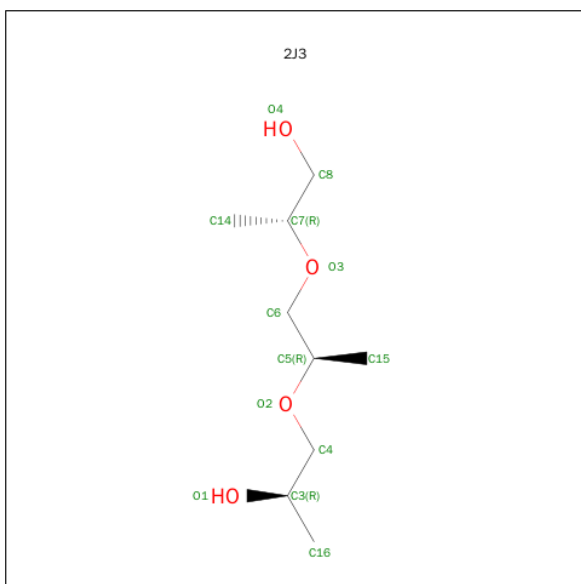
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 3-[(4-chlorobenzyl)amino]-6-(trifluoromethyl)quinoxaline-2-carboxylic acid (three-letter code: RG2) (formula: $C_{17}H_{11}ClF_3N_3O_2$).



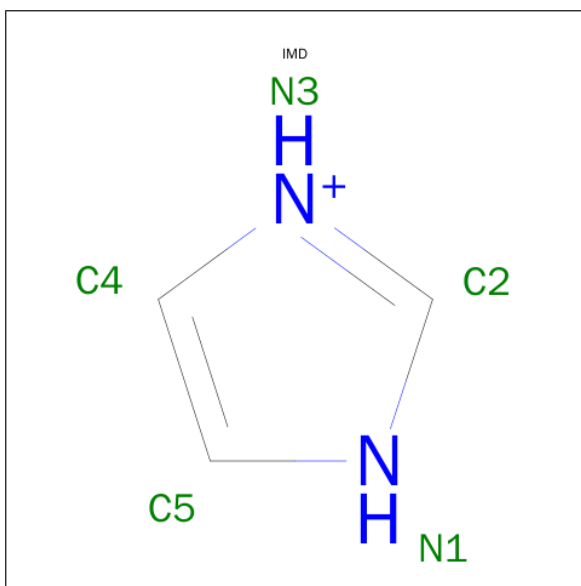
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 26	C 17	Cl 1	F 3	N 3	O 2	0	0
3	B	1	Total 26	C 17	Cl 1	F 3	N 3	O 2	0	0

- Molecule 4 is (2R)-2-{\[(2R)-2-{\[(2R)-2-hydroxypropyl]oxy}propyl]oxy}propan-1-ol (three-letter code: 2J3) (formula: C₉H₂₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	9	4		

- Molecule 5 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			5	3	2		

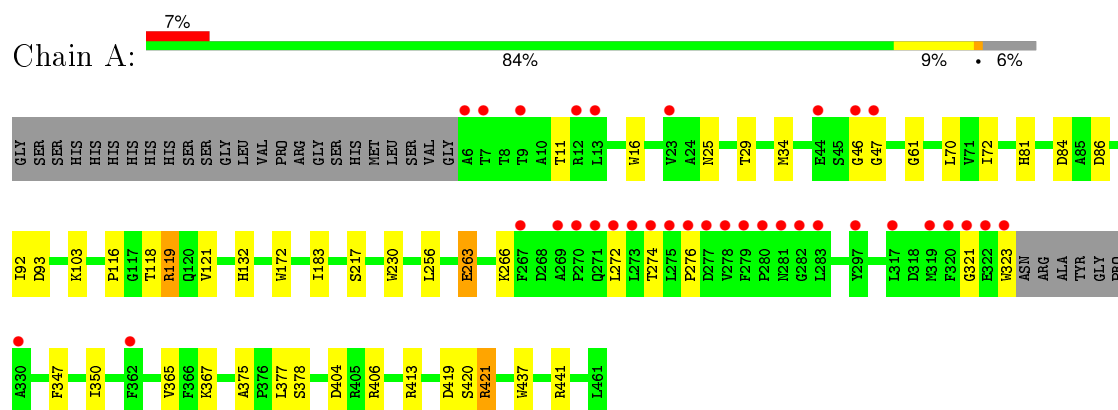
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	112	Total	O	0	0
			112	112		
6	B	84	Total	O	0	0
			84	84		

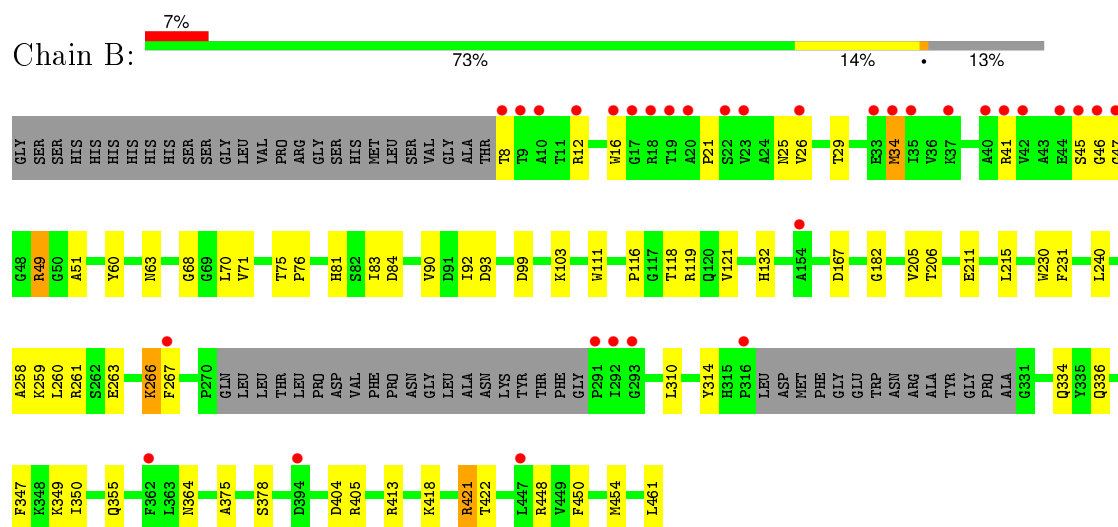
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Probable decaprenylphosphoryl-beta-D-ribose oxidase



- Molecule 1: Probable decaprenylphosphoryl-beta-D-ribose oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.62Å 83.96Å 80.87Å 90.00° 103.25° 90.00°	Depositor
Resolution (Å)	49.20 – 2.20 49.17 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.20-2.20) 98.4 (49.17-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.195 , 0.234 0.194 , 0.234	Depositor DCC
R_{free} test set	2553 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.1	EDS
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 50451 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7067	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: RG2, 2J3, IMD, FAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	5/3544 (0.1%)	0.60	0/4815
1	B	0.50	3/3311 (0.1%)	0.57	0/4492
All	All	0.51	8/6855 (0.1%)	0.58	0/9307

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	323	TRP	CD2-CE2	5.19	1.47	1.41
1	A	172	TRP	CD2-CE2	5.12	1.47	1.41
1	A	230	TRP	CD2-CE2	5.12	1.47	1.41
1	B	16	TRP	CD2-CE2	5.12	1.47	1.41
1	A	437	TRP	CD2-CE2	5.10	1.47	1.41
1	B	230	TRP	CD2-CE2	5.07	1.47	1.41
1	A	16	TRP	CD2-CE2	5.02	1.47	1.41
1	B	111	TRP	CD2-CE2	5.01	1.47	1.41

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	3461	0	3430	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3234	0	3218	41	0
2	A	53	0	31	2	0
2	B	53	0	31	0	0
3	A	26	0	10	0	0
3	B	26	0	10	1	0
4	A	13	0	20	1	0
5	A	5	0	5	2	0
6	A	112	0	0	1	0
6	B	84	0	0	3	0
All	All	7067	0	6755	66	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 (66) 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:103:LYS:HE3	1:B:267:PHE:CE2	1.73	1.22
1:B:103:LYS:HE3	1:B:267:PHE:CZ	2.03	0.94
1:A:406:ARG:HH11	1:A:406:ARG:HG2	1.41	0.85
1:A:119:ARG:HB2	1:A:119:ARG:HH11	1.41	0.84
1:B:103:LYS:CE	1:B:267:PHE:CZ	2.72	0.72
1:A:406:ARG:NH1	1:A:406:ARG:HG2	2.05	0.71
1:B:49:ARG:HG3	1:B:68:GLY:O	1.91	0.71
1:B:99:ASP:OD2	1:B:103:LYS:NZ	2.25	0.69
1:B:119:ARG:HG3	1:B:119:ARG:HH11	1.57	0.68
1:B:81:HIS:HE1	1:B:93:ASP:OD1	1.75	0.68
1:A:81:HIS:HE1	1:A:93:ASP:OD1	1.76	0.68
1:A:119:ARG:CB	1:A:119:ARG:HH11	2.08	0.66
1:A:118:THR:HG23	2:A:501:FAD:HM73	1.80	0.65
1:B:258:ALA:HA	1:B:261:ARG:HD2	1.80	0.64
1:A:347:PHE:O	1:A:350:ILE:HG22	1.98	0.64
1:B:334:GLN:HG3	1:B:418:LYS:HD3	1.83	0.60
1:A:263:GLU:HB3	1:A:266:LYS:HG3	1.84	0.59
1:B:347:PHE:O	1:B:350:ILE:HG22	2.03	0.59
1:A:132:HIS:HD2	6:A:623:HOH:O	1.86	0.58
1:B:60:TYR:HB2	1:B:418:LYS:HA	1.86	0.57
1:B:132:HIS:HD2	6:B:626:HOH:O	1.87	0.56
1:B:240:LEU:HD13	1:B:355:GLN:HG3	1.88	0.56
1:A:84:ASP:OD2	5:A:504:IMD:H5	2.07	0.54
1:B:375:ALA:HB3	1:B:378:SER:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:504:IMD:H2	1:B:84:ASP:OD2	2.09	0.53
1:B:83:ILE:HG12	1:B:90:VAL:HG12	1.92	0.52
1:B:405:ARG:NH1	6:B:601:HOH:O	2.39	0.52
1:A:119:ARG:HB2	1:A:119:ARG:NH1	2.19	0.51
1:A:263:GLU:CB	1:A:266:LYS:HG3	2.41	0.51
1:A:365:VAL:HG22	4:A:503:2J3:H16	1.93	0.51
1:B:132:HIS:HE1	3:B:502:RG2:H10	1.76	0.50
1:B:116:PRO:HG2	1:B:118:THR:O	2.12	0.50
1:A:375:ALA:HB3	1:A:378:SER:HB2	1.94	0.50
1:B:51:ALA:HA	1:B:70:LEU:O	2.12	0.49
1:B:29:THR:HG21	1:B:34:MET:HB3	1.94	0.49
1:B:45:SER:N	1:B:46:GLY:HA3	2.28	0.48
1:B:448:ARG:HD3	1:B:461:LEU:HG	1.95	0.48
1:B:46:GLY:HA2	1:B:47:GLY:HA2	1.60	0.47
1:B:12:ARG:HH21	1:B:21:PRO:HG3	1.78	0.47
1:A:72:ILE:HD12	1:A:183:ILE:HD11	1.95	0.47
1:A:116:PRO:HG2	1:A:118:THR:O	2.14	0.46
1:A:118:THR:CG2	2:A:501:FAD:HM73	2.45	0.46
1:B:119:ARG:HB2	6:B:664:HOH:O	2.15	0.46
1:B:99:ASP:OD1	1:B:119:ARG:NE	2.49	0.46
1:A:119:ARG:HH11	1:A:119:ARG:CG	2.28	0.46
1:A:274:THR:HG23	1:A:276:PRO:HD2	1.98	0.45
1:B:206:THR:HB	1:B:211:GLU:HB3	1.98	0.45
1:B:75:THR:N	1:B:76:PRO:HD2	2.31	0.45
1:A:86:ASP:OD1	1:B:81:HIS:HD2	1.99	0.45
1:B:119:ARG:HG3	1:B:119:ARG:NH1	2.30	0.45
1:B:26:VAL:HA	1:B:71:VAL:O	2.17	0.44
1:A:25:ASN:O	1:A:70:LEU:HD12	2.18	0.44
1:B:49:ARG:HA	1:B:49:ARG:HD2	1.32	0.43
1:A:61:GLY:HA3	1:A:419:ASP:O	2.18	0.43
1:B:8:THR:HG23	1:B:25:ASN:HB3	2.02	0.42
1:B:182:GLY:HA2	1:B:450:PHE:CE2	2.53	0.42
1:B:119:ARG:HD3	1:B:310:LEU:HD21	2.01	0.42
1:B:63:ASN:HB3	1:B:454:MET:SD	2.59	0.41
1:A:404:ASP:CG	1:A:421:ARG:HH22	2.23	0.41
1:A:61:GLY:HA2	1:A:420:SER:HB3	2.03	0.41
1:B:231:PHE:CE2	1:B:364:ASN:HB3	2.56	0.41
1:B:263:GLU:OE1	1:B:266:LYS:HG2	2.21	0.41
1:B:132:HIS:CE1	1:B:336:GLN:HE22	2.39	0.40
1:B:404:ASP:CG	1:B:421:ARG:HH22	2.25	0.40
1:A:29:THR:HG21	1:A:34:MET:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:GLY:HA2	1:A:47:GLY:HA2	1.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	446/480 (93%)	439 (98%)	6 (1%)	1 (0%)	52	59
1	B	415/480 (86%)	407 (98%)	8 (2%)	0	100	100
All	All	861/960 (90%)	846 (98%)	14 (2%)	1 (0%)	56	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	321	GLY

5.3.2 Protein sidechains [i](#)

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	360/384 (94%)	346 (96%)	14 (4%)	39	48
1	B	337/384 (88%)	321 (95%)	16 (5%)	32	39
All	All	697/768 (91%)	667 (96%)	30 (4%)	35	43

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	THR
1	A	92	ILE
1	A	103	LYS
1	A	119	ARG
1	A	121	VAL
1	A	217	SER
1	A	256	LEU
1	A	263	GLU
1	A	272	LEU
1	A	367	LYS
1	A	377	LEU
1	A	413	ARG
1	A	421	ARG
1	A	441	ARG
1	B	34	MET
1	B	41	ARG
1	B	49	ARG
1	B	92	ILE
1	B	121	VAL
1	B	167	ASP
1	B	205	VAL
1	B	215	LEU
1	B	259	LYS
1	B	260	LEU
1	B	266	LYS
1	B	314	TYR
1	B	349	LYS
1	B	413	ARG
1	B	421	ARG
1	B	422	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	HIS
1	A	132	HIS
1	A	271	GLN
1	A	364	ASN
1	B	81	HIS
1	B	132	HIS
1	B	364	ASN

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 ⓘ

6 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	-	48,58,58	1.32	6 (12%)	54,89,89	2.23	13 (24%)
3	RG2	A	502	-	24,28,28	1.33	3 (12%)	36,41,41	1.21	2 (5%)
4	2J3	A	503	-	12,12,12	0.72	0	11,14,14	0.57	0
5	IMD	A	504	-	3,5,5	0.33	0	4,5,5	0.73	0
2	FAD	B	501	-	48,58,58	1.40	6 (12%)	54,89,89	2.27	11 (20%)
3	RG2	B	502	-	24,28,28	1.34	3 (12%)	36,41,41	1.08	2 (5%)

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	RG2	A	502	-	-	0/11/15/15	0/3/3/3
4	2J3	A	503	-	-	0/12/12/12	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	IMD	A	504	-	-	0/0/0/0	0/1/1/1
2	FAD	B	501	-	-	0/30/50/50	0/6/6/6
3	RG2	B	502	-	-	0/11/15/15	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FAD	C9A-N10	2.05	1.41	1.38
3	A	502	RG2	CAC-NAD	2.38	1.35	1.32
3	A	502	RG2	CAV-CLAW	2.46	1.80	1.74
2	A	501	FAD	C9A-N10	2.49	1.42	1.38
3	B	502	RG2	CAV-CLAW	2.54	1.80	1.74
3	B	502	RG2	CAC-NAD	2.61	1.36	1.32
2	A	501	FAD	C5A-C4A	2.97	1.47	1.40
2	B	501	FAD	C5A-C4A	3.00	1.47	1.40
2	A	501	FAD	C4-C4X	3.05	1.47	1.41
2	A	501	FAD	C8-C7	3.10	1.49	1.41
2	B	501	FAD	C8-C7	3.31	1.49	1.41
2	B	501	FAD	C9A-C5X	3.43	1.49	1.42
2	A	501	FAD	C9A-C5X	3.49	1.49	1.42
3	B	502	RG2	CAP-NAO	3.59	1.36	1.31
2	A	501	FAD	C4X-C10	3.73	1.48	1.41
2	B	501	FAD	C4X-C10	3.75	1.48	1.41
3	A	502	RG2	CAP-NAO	3.78	1.36	1.31
2	B	501	FAD	C4-C4X	3.79	1.48	1.41

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	FAD	N3A-C2A-N1A	-8.00	122.77	128.89
2	A	501	FAD	N3A-C2A-N1A	-7.92	122.83	128.89
2	A	501	FAD	C4-C4X-C10	-6.80	115.59	119.94
2	B	501	FAD	C4-C4X-C10	-6.47	115.80	119.94
3	A	502	RG2	CAC-CAP-NAO	-3.56	119.09	122.02
2	B	501	FAD	C4X-C4-N3	-3.48	118.83	123.59
3	B	502	RG2	CAC-CAP-NAO	-2.98	119.57	122.02
2	A	501	FAD	C4X-C4-N3	-2.97	119.52	123.59
2	B	501	FAD	P-O3P-PA	-2.89	124.62	132.73
2	B	501	FAD	C4A-C5A-N7A	-2.87	106.84	109.48
2	A	501	FAD	C4X-C10-N10	-2.39	119.11	120.52
2	A	501	FAD	O3P-PA-O5B	-2.24	97.00	102.94
2	A	501	FAD	C4A-C5A-N7A	-2.23	107.42	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	FAD	C2B-C1B-N9A	-2.18	110.96	114.29
2	A	501	FAD	C1B-N9A-C4A	-2.11	123.75	126.94
3	B	502	RG2	CAP-NAO-CAN	2.01	120.82	116.84
2	A	501	FAD	C2A-N1A-C6A	2.06	122.44	118.77
2	B	501	FAD	O4B-C1B-N9A	2.11	112.51	108.10
3	A	502	RG2	NAQ-CAP-NAO	2.32	121.50	118.67
2	A	501	FAD	C5X-C9A-N10	2.78	119.73	117.62
2	A	501	FAD	C4-C4X-N5	3.06	122.43	118.72
2	B	501	FAD	C1'-N10-C9A	3.15	122.40	118.86
2	A	501	FAD	C4X-N5-C5X	3.29	120.54	116.76
2	B	501	FAD	C4X-N5-C5X	3.72	121.04	116.76
2	B	501	FAD	C4-C4X-N5	3.85	123.39	118.72
2	A	501	FAD	C1'-N10-C9A	3.86	123.19	118.86
2	A	501	FAD	C4-N3-C2	7.50	121.73	115.25
2	B	501	FAD	C4-N3-C2	8.05	122.20	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FAD	2	0
4	A	503	2J3	1	0
5	A	504	IMD	2	0
3	B	502	RG2	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	450/480 (93%)	0.23	34 (7%) 17 16	22, 36, 88, 117	0
1	B	420/480 (87%)	0.28	32 (7%) 17 16	26, 43, 77, 95	0
All	All	870/960 (90%)	0.25	66 (7%) 17 16	22, 40, 81, 117	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	273	LEU	6.6
1	A	323	TRP	6.3
1	A	321	GLY	5.7
1	B	8	THR	5.7
1	A	281	ASN	5.3
1	A	274	THR	5.3
1	B	47	GLY	5.3
1	A	279	PHE	5.2
1	A	320	PHE	5.2
1	A	278	VAL	5.1
1	A	280	PRO	5.1
1	B	20	ALA	4.8
1	A	283	LEU	4.8
1	A	330	ALA	4.7
1	A	275	LEU	4.6
1	B	46	GLY	4.5
1	A	269	ALA	4.5
1	A	276	PRO	4.5
1	A	277	ASP	4.5
1	A	7	THR	4.4
1	B	45	SER	4.1
1	A	6	ALA	4.0
1	A	322	GLU	4.0
1	B	291	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	272	LEU	3.9
1	A	317	LEU	3.8
1	B	17	GLY	3.7
1	B	37	LYS	3.6
1	B	44	GLU	3.6
1	B	447	LEU	3.6
1	A	47	GLY	3.5
1	A	319	MET	3.5
1	B	292	ILE	3.4
1	B	40	ALA	3.3
1	B	41	ARG	3.3
1	A	23	VAL	3.2
1	B	10	ALA	3.0
1	B	34	MET	3.0
1	A	282	GLY	2.9
1	B	154	ALA	2.8
1	A	9	THR	2.8
1	B	35	ILE	2.7
1	B	362	PHE	2.7
1	A	46	GLY	2.7
1	B	293	GLY	2.6
1	B	12	ARG	2.6
1	B	22	SER	2.5
1	B	42	VAL	2.5
1	A	44	GLU	2.5
1	A	362	PHE	2.4
1	B	316	PRO	2.4
1	B	394	ASP	2.3
1	B	16	TRP	2.3
1	B	33	GLU	2.3
1	B	267	PHE	2.3
1	A	270	PRO	2.2
1	A	267	PHE	2.2
1	A	271	GLN	2.2
1	B	9	THR	2.2
1	A	12	ARG	2.2
1	B	18	ARG	2.2
1	A	13	LEU	2.2
1	B	23	VAL	2.1
1	B	26	VAL	2.1
1	B	19	THR	2.1
1	A	297	TYR	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	RG2	B	502	26/26	0.91	0.17	0.49	49,52,66,70	0
2	FAD	A	501	53/53	0.97	0.15	0.46	26,29,30,32	0
4	2J3	A	503	13/13	0.82	0.20	0.33	71,74,77,77	0
2	FAD	B	501	53/53	0.98	0.13	-0.44	28,34,37,38	0
3	RG2	A	502	26/26	0.95	0.14	-0.51	35,38,63,76	0
5	IMD	A	504	5/5	0.96	0.14	-	39,39,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.