



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:35 PM UTC

PDB ID : 4UZE / pdb_00004uze
Title : R66A mutant of FAD synthetase from *Corynebacterium ammoniagenes*
Authors : Martinez-Julvez, M.; Herguedas, B.; Milagros, M.
Deposited on : 2014-09-05
Resolution : 2.34 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

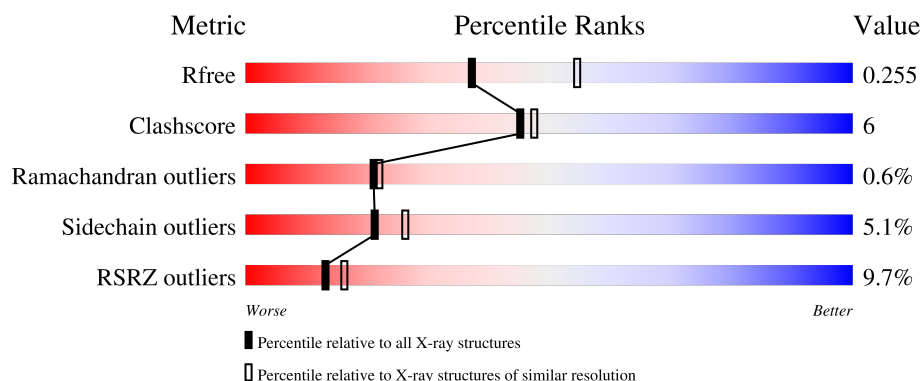
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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}	180053	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	338	6% 88% 10% ..
1	B	338	14% 85% 12% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5346 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.

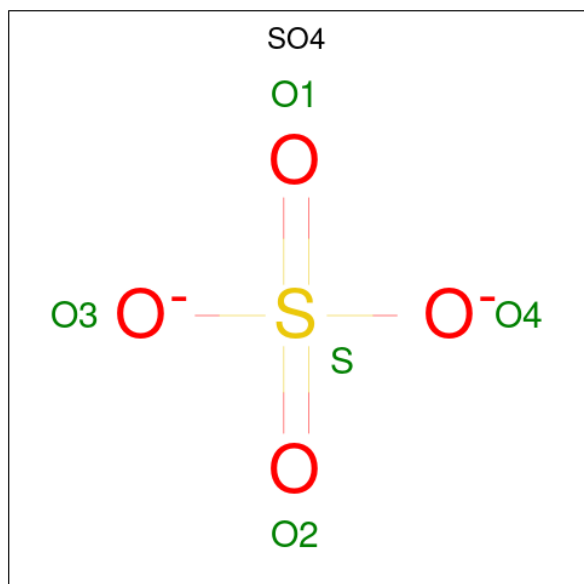
- Molecule 1 is a protein called RIBOFLAVIN BIOSYNTHESIS PROTEIN RIBF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2594	1642	441	504	7			
1	B	335	Total	C	N	O	S	0	0	0
			2571	1627	438	499	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	ALA	ARG	engineered mutation	UNP Q59263
B	66	ALA	ARG	engineered mutation	UNP Q59263

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



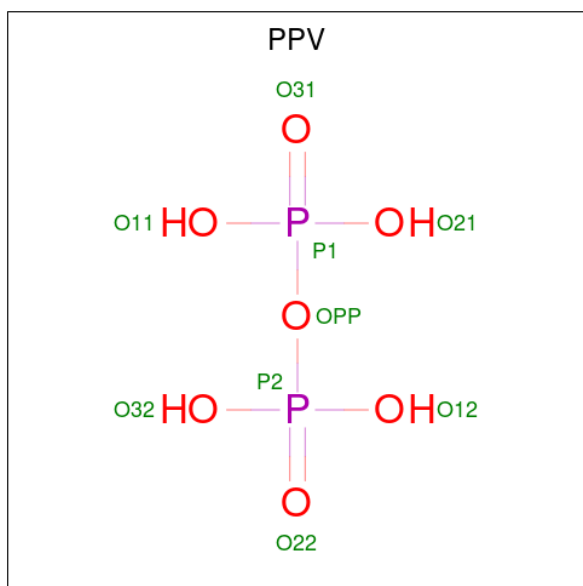
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is PYROPHOSPHATE (CCD ID: PPV) (formula: $\text{H}_4\text{O}_7\text{P}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			9	7	2		
3	B	1	Total	O	P	0	0
			9	7	2		

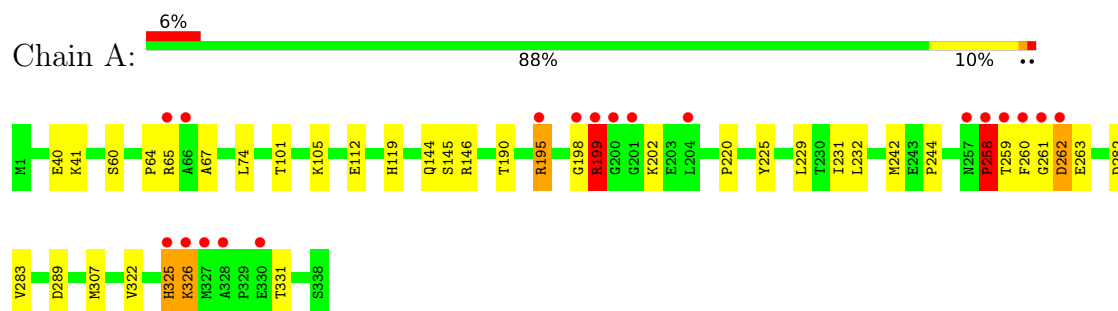
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	103	Total	O	0	0
			103	103		
4	B	50	Total	O	0	0
			50	50		

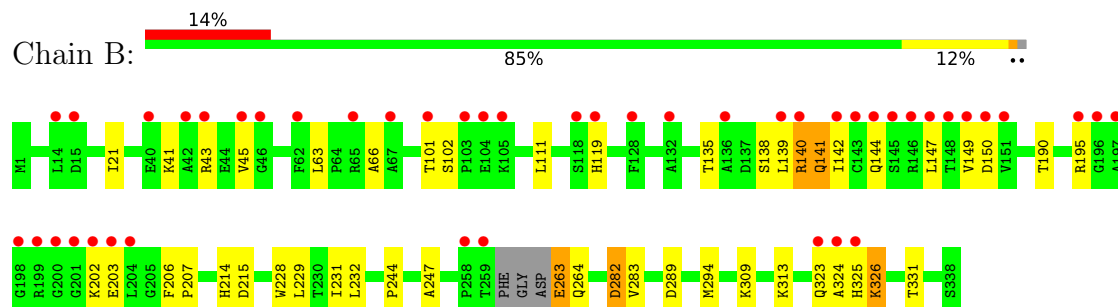
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: RIBOFLAVIN BIOSYNTHESIS PROTEIN RIBF



• Molecule 1: RIBOFLAVIN BIOSYNTHESIS PROTEIN RIBF



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	133.61Å 133.61Å 133.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.34 40.00 – 2.34	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.00-2.34) 99.7 (40.00-2.34)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.218 , 0.256 0.220 , 0.255	Depositor DCC
R_{free} test set	1711 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 25.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.034 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5346	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PPV

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	0.55	0/2649	0.86	2/3604 (0.1%)
1	B	0.53	0/2624	0.82	0/3569
All	All	0.54	0/5273	0.84	2/7173 (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	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	258	PRO	CA-N-CD	-7.92	100.91	112.00
1	A	258	PRO	N-CA-C	5.45	123.69	112.47

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	258	PRO	Peptide

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	2594	0	2530	31	0
1	B	2571	0	2513	30	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	9	0	0	0	0
3	B	9	0	0	0	0
4	A	103	0	0	0	0
4	B	50	0	0	0	0
All	All	5346	0	5043	60	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 6.

All (60) 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:A:261:GLY:HA2	1:A:262:ASP:C	1.86	0.98
1:B:141:GLN:O	1:B:144:GLN:HG2	1.66	0.94
1:B:263:GLU:HB3	1:B:264:GLN:HA	1.59	0.85
1:A:258:PRO:HG3	1:A:263:GLU:HA	1.63	0.80
1:A:198:GLY:HA2	1:A:199:ARG:HB2	1.68	0.75
1:A:258:PRO:HG3	1:A:260:PHE:O	1.87	0.75
1:A:258:PRO:CG	1:A:263:GLU:HA	2.22	0.69
1:B:263:GLU:CB	1:B:264:GLN:HA	2.22	0.68
1:B:263:GLU:HB2	1:B:264:GLN:HB2	1.74	0.67
1:A:74:LEU:HD23	1:B:195:ARG:HH21	1.59	0.67
1:B:215:ASP:H	1:B:263:GLU:HG2	1.61	0.66
1:A:60:SER:HB3	1:A:67:ALA:HB2	1.77	0.65
1:A:258:PRO:HB3	1:A:260:PHE:O	2.00	0.62
1:B:41:LYS:HG2	1:B:119:HIS:CD2	2.36	0.61
1:B:63:LEU:HB3	1:B:66:ALA:HB3	1.82	0.61
1:B:323:GLN:C	1:B:325:HIS:H	2.10	0.60
1:B:263:GLU:CB	1:B:264:GLN:CA	2.80	0.59
1:A:41:LYS:HG2	1:A:119:HIS:CD2	2.38	0.58
1:A:198:GLY:CA	1:A:199:ARG:HB2	2.35	0.57
1:B:231:ILE:HB	1:B:244:PRO:HA	1.87	0.56
1:B:323:GLN:C	1:B:325:HIS:N	2.64	0.55
1:A:202:LYS:HA	1:A:202:LYS:HE2	1.89	0.54
1:A:258:PRO:CG	1:A:260:PHE:O	2.55	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:PRO:CB	1:A:260:PHE:O	2.56	0.54
1:A:322:VAL:O	1:A:325:HIS:HD2	1.91	0.54
1:A:261:GLY:HA2	1:A:262:ASP:O	2.08	0.54
1:B:232:LEU:HD12	1:B:282:ASP:HB3	1.90	0.53
1:B:215:ASP:CG	1:B:263:GLU:HG3	2.34	0.53
1:A:64:PRO:O	1:A:65:ARG:HB2	2.09	0.52
1:B:215:ASP:H	1:B:263:GLU:CG	2.23	0.52
1:B:263:GLU:HB3	1:B:264:GLN:CA	2.35	0.51
1:B:215:ASP:N	1:B:263:GLU:HG2	2.25	0.51
1:B:294:MET:HE3	1:B:294:MET:HA	1.92	0.51
1:B:323:GLN:O	1:B:324:ALA:HB3	2.12	0.50
1:A:258:PRO:C	1:A:260:PHE:H	2.20	0.49
1:B:135:THR:H	1:B:138:SER:HB2	1.78	0.48
1:B:101:THR:HG22	1:B:102:SER:O	2.13	0.47
1:B:228:TRP:HB3	1:B:247:ALA:HB1	1.97	0.46
1:A:261:GLY:CA	1:A:262:ASP:C	2.74	0.45
1:A:60:SER:HB3	1:A:67:ALA:CB	2.45	0.45
1:A:190:THR:HG21	1:A:232:LEU:HD11	1.97	0.45
1:B:140:ARG:HA	1:B:149:VAL:HG21	1.98	0.44
1:B:149:VAL:HG12	1:B:150:ASP:N	2.33	0.44
1:B:141:GLN:HG2	1:B:142:ILE:N	2.33	0.43
1:A:144:GLN:O	1:A:145:SER:HB3	2.18	0.43
1:A:229:LEU:HD22	1:A:242:MET:HE1	2.01	0.42
1:A:258:PRO:CA	1:A:260:PHE:H	2.32	0.42
1:A:229:LEU:HD23	1:A:229:LEU:C	2.43	0.42
1:A:220:PRO:HB2	1:A:225:TYR:CZ	2.54	0.42
1:A:112:GLU:CD	1:A:146:ARG:HH21	2.26	0.42
1:B:214:HIS:HA	1:B:263:GLU:HG2	2.00	0.42
1:A:326:LYS:HE2	1:A:326:LYS:H	1.84	0.42
1:B:324:ALA:O	1:B:326:LYS:N	2.42	0.42
1:A:258:PRO:HA	1:A:260:PHE:H	1.85	0.41
1:A:101:THR:CG2	1:A:105:LYS:HB2	2.50	0.41
1:A:231:ILE:HB	1:A:244:PRO:HA	2.02	0.41
1:B:206:PHE:HA	1:B:207:PRO:HD3	1.94	0.40
1:B:21:ILE:HD11	1:B:111:LEU:HD21	2.03	0.40
1:A:195:ARG:HA	1:A:195:ARG:HD2	1.92	0.40
1:B:229:LEU:HD23	1:B:229:LEU:C	2.46	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	336/338 (99%)	324 (96%)	9 (3%)	3 (1%)	14	13
1	B	331/338 (98%)	308 (93%)	22 (7%)	1 (0%)	36	41
All	All	667/676 (99%)	632 (95%)	31 (5%)	4 (1%)	21	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	258	PRO
1	A	199	ARG
1	A	262	ASP
1	B	45	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	274/274 (100%)	262 (96%)	12 (4%)	25	33
1	B	272/274 (99%)	256 (94%)	16 (6%)	18	21
All	All	546/548 (100%)	518 (95%)	28 (5%)	21	26

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	GLU
1	A	195	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	199	ARG
1	A	258	PRO
1	A	259	THR
1	A	282	ASP
1	A	283	VAL
1	A	289	ASP
1	A	307	MET
1	A	325	HIS
1	A	326	LYS
1	A	331	THR
1	B	43	ARG
1	B	139	LEU
1	B	140	ARG
1	B	141	GLN
1	B	147	LEU
1	B	190	THR
1	B	202	LYS
1	B	203	GLU
1	B	263	GLU
1	B	282	ASP
1	B	283	VAL
1	B	289	ASP
1	B	309	LYS
1	B	313	LYS
1	B	326	LYS
1	B	331	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	A	312	GLN
1	A	323	GLN
1	A	325	HIS
1	A	335	GLN
1	B	119	HIS
1	B	131	ASN
1	B	141	GLN
1	B	144	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	SO4	B	1339	-	4,4,4	0.48	0	6,6,6	0.37	0
3	PPV	A	1340	-	6,8,8	0.69	0	12,13,13	0.97	0
2	SO4	A	1339	-	4,4,4	0.48	0	6,6,6	0.28	0
3	PPV	B	1340	-	6,8,8	0.70	0	12,13,13	0.87	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
3	PPV	A	1340	-	-	0/6/6/6	-
3	PPV	B	1340	-	-	0/6/6/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	338/338 (100%)	0.06	19 (5%) 30 35	19, 31, 64, 113	0
1	B	335/338 (99%)	0.55	46 (13%) 6 7	21, 39, 81, 107	0
All	All	673/676 (99%)	0.30	65 (9%) 13 16	19, 35, 78, 113	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	324	ALA	5.1
1	B	43	ARG	4.9
1	B	204	LEU	4.7
1	A	260	PHE	4.7
1	B	200	GLY	4.5
1	B	149	VAL	4.3
1	A	65	ARG	4.2
1	A	199	ARG	4.1
1	B	258	PRO	4.0
1	B	259	THR	3.8
1	B	140	ARG	3.8
1	B	145	SER	3.7
1	A	200	GLY	3.6
1	A	259	THR	3.6
1	B	197	ALA	3.6
1	B	143	CYS	3.5
1	A	258	PRO	3.4
1	B	128	PHE	3.3
1	B	136	ALA	3.3
1	B	142	ILE	3.0
1	A	257	ASN	3.0
1	B	45	VAL	3.0
1	B	65	ARG	3.0
1	B	323	GLN	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	202	LYS	2.8
1	B	46	GLY	2.8
1	A	325	HIS	2.8
1	B	144	GLN	2.8
1	A	261	GLY	2.8
1	B	148	THR	2.8
1	B	151	VAL	2.8
1	A	262	ASP	2.7
1	B	139	LEU	2.7
1	B	203	GLU	2.6
1	A	198	GLY	2.6
1	A	328	ALA	2.6
1	A	66	ALA	2.6
1	B	150	ASP	2.6
1	B	195	ARG	2.5
1	B	132	ALA	2.5
1	B	325	HIS	2.5
1	B	147	LEU	2.5
1	B	199	ARG	2.5
1	B	146	ARG	2.4
1	B	67	ALA	2.4
1	B	118	SER	2.3
1	A	204	LEU	2.3
1	A	330	GLU	2.3
1	B	62	PHE	2.3
1	A	201	GLY	2.3
1	B	42	ALA	2.3
1	B	15	ASP	2.2
1	B	119	HIS	2.2
1	B	196	GLY	2.2
1	B	40	GLU	2.2
1	B	101	THR	2.2
1	B	198	GLY	2.2
1	B	14	LEU	2.1
1	A	195	ARG	2.1
1	A	327	MET	2.1
1	B	104	GLU	2.1
1	B	201	GLY	2.1
1	A	326	LYS	2.0
1	B	105	LYS	2.0
1	B	103	PRO	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 oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	1339	5/5	0.79	0.17	69,69,74,74	0
2	SO4	A	1339	5/5	0.83	0.15	61,68,70,73	0
3	PPV	B	1340	9/9	0.84	0.12	49,55,69,74	0
3	PPV	A	1340	9/9	0.90	0.11	46,47,63,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.