



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:31 AM UTC

PDB ID : 2X0K / pdb_00002x0k
Title : Crystal structure of modular FAD synthetase from *Corynebacterium ammoniagenes*
Authors : Herguedas, B.; Hermoso, J.A.; Martinez-Julvez, M.; Medina, M.; Frago, S.
Deposited on : 2009-12-15
Resolution : 1.95 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

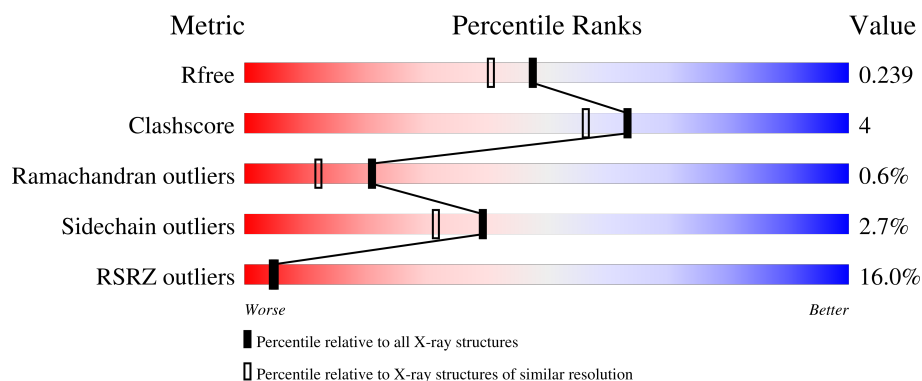
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	7% 93% 7%
1	B	338	25% 86% 12%

2 Entry composition [i](#)

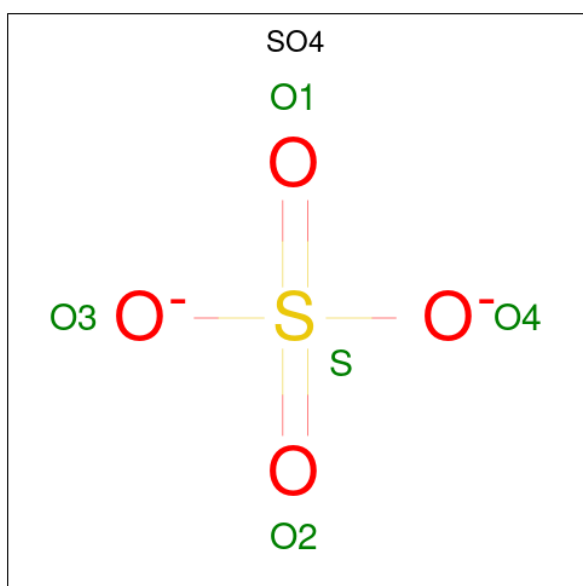
There are 4 unique types of molecules in this entry. The entry contains 5908 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

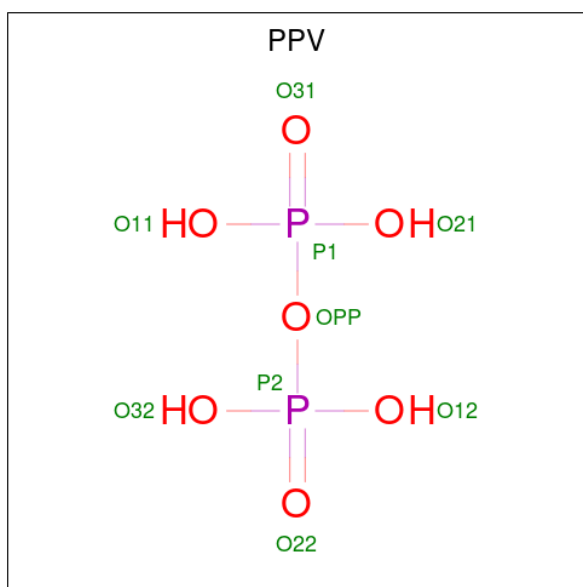
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	10	0
			2675	1690	460	517	8			
1	B	338	Total	C	N	O	S	0	11	0
			2682	1695	461	518	8			

- 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		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is PYROPHOSPHATE (CCD ID: PPV) (formula: H₄O₇P₂).



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		

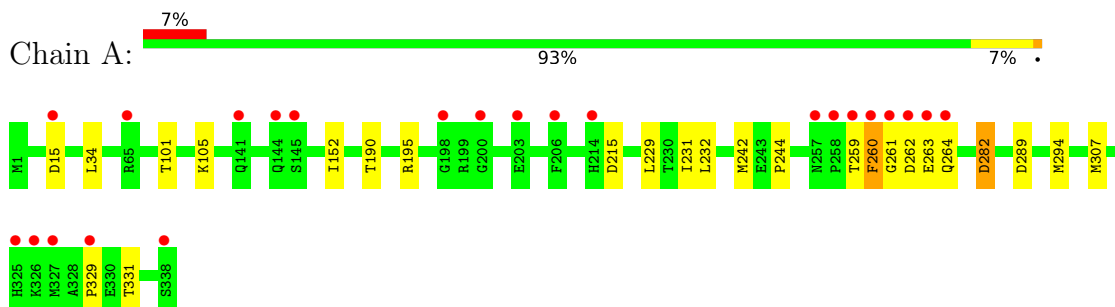
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	320	Total	O	0	0
			320	320		
4	B	203	Total	O	0	0
			203	203		

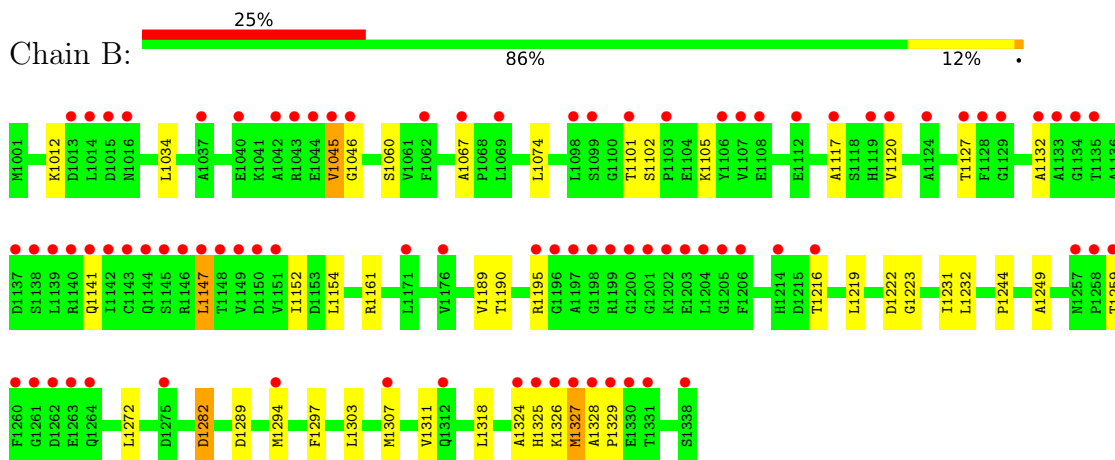
3 Residue-property plots

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	133.47 Å 133.47 Å 133.47 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.49 – 1.95 94.38 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (94.49-1.95) 99.9 (94.38-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 1.95 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.204 , 0.237 0.207 , 0.239	Depositor DCC
R_{free} test set	4189 reflections (7.25%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5908	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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, 0.333 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	0.46	0/2737	0.67	0/3721
1	B	0.42	0/2744	0.66	0/3731
All	All	0.44	0/5481	0.67	0/7452

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

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	2675	0	2613	14	0
1	B	2682	0	2619	29	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	1	0
4	A	320	0	0	0	0
4	B	203	0	0	1	0
All	All	5908	0	5232	42	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 4.

All (42) 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:1045:VAL:HG12	1:B:1046:GLY:H	1.46	0.81
1:A:259:THR:O	1:A:260:PHE:HB3	1.96	0.64
1:B:1127:THR:HG21	1:B:1132:ALA:HB1	1.81	0.61
1:B:1272:LEU:HD13	1:B:1311:VAL:HG13	1.82	0.60
1:B:1223:GLY:HA2	1:B:1294:MET:HE3	1.83	0.60
1:A:34:LEU:HD23	1:A:152:ILE:HD12	1.83	0.60
1:B:1101:THR:HG22	1:B:1102:SER:O	2.04	0.56
1:B:1223:GLY:CA	1:B:1294:MET:HE3	2.35	0.56
1:B:1045:VAL:HG12	1:B:1046:GLY:N	2.20	0.56
1:B:1034:LEU:HD23	1:B:1152:ILE:HD12	1.89	0.55
1:B:1326[B]:LYS:O	1:B:1327[B]:MET:C	2.51	0.54
1:A:232:LEU:HD12	1:A:282:ASP:HB3	1.89	0.54
1:A:195[A]:ARG:NH2	1:B:1074:LEU:HD23	2.22	0.54
1:B:1325[A]:HIS:O	1:B:1327[A]:MET:N	2.42	0.53
1:B:1190:THR:CG2	1:B:1232:LEU:HD11	2.39	0.52
3:B:2340:PPV:P2	4:B:2200:HOH:O	2.66	0.52
1:A:190:THR:CG2	1:A:232:LEU:HD11	2.40	0.51
1:A:190:THR:HG21	1:A:232:LEU:HD11	1.91	0.51
1:B:1294:MET:HE2	1:B:1294:MET:HA	1.94	0.49
1:B:1297:PHE:CD2	1:B:1303:LEU:HD13	2.46	0.49
1:A:229:LEU:HD22	1:A:242:MET:HE1	1.95	0.49
1:B:1190:THR:HG21	1:B:1232:LEU:HD11	1.94	0.48
1:A:195[A]:ARG:HH21	1:B:1074:LEU:HD23	1.79	0.47
1:B:1325[A]:HIS:O	1:B:1326[A]:LYS:C	2.57	0.46
1:B:1259:THR:HG23	1:B:1259:THR:O	2.15	0.46
1:B:1232:LEU:HD12	1:B:1282:ASP:HB3	1.99	0.45
1:A:101:THR:HG22	1:A:105:LYS:HB2	1.98	0.45
1:A:215:ASP:CB	1:A:263:GLU:HG3	2.46	0.44
1:B:1117:ALA:HB3	1:B:1147:LEU:HD23	1.98	0.44
1:B:1249:ALA:HB1	1:B:1318:LEU:HD12	2.00	0.44
1:A:231:ILE:HB	1:A:244:PRO:HA	2.00	0.43
1:A:101:THR:CG2	1:A:105:LYS:HB2	2.49	0.43
1:B:1222:ASP:HB3	1:B:1294:MET:HG3	2.01	0.43
1:B:1060:SER:HB3	1:B:1067:ALA:HB2	2.02	0.42
1:A:261:GLY:C	1:A:263:GLU:H	2.28	0.41
1:A:329[B]:PRO:O	1:A:331[B]:THR:N	2.53	0.41
1:B:1154:LEU:HB2	1:B:1161:ARG:NH1	2.36	0.41
1:B:1189:VAL:HG11	1:B:1219:LEU:HD21	2.02	0.41
1:B:1324[A]:ALA:O	1:B:1325[A]:HIS:C	2.64	0.41
1:B:1101:THR:HG23	1:B:1105:LYS:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1231:ILE:HB	1:B:1244:PRO:HA	2.02	0.40
1:B:1328[A]:ALA:HB1	1:B:1329[A]:PRO:CD	2.50	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	346/338 (102%)	332 (96%)	12 (4%)	2 (1%)	21	12
1	B	347/338 (103%)	329 (95%)	15 (4%)	3 (1%)	14	6
All	All	693/676 (102%)	661 (95%)	27 (4%)	5 (1%)	21	10

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	260	PHE
1	B	1327[A]	MET
1	B	1327[B]	MET
1	A	262	ASP
1	B	1045	VAL

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	283/275 (103%)	277 (98%)	6 (2%)	47	41
1	B	284/275 (103%)	274 (96%)	10 (4%)	32	22
All	All	567/550 (103%)	551 (97%)	16 (3%)	39	30

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	264	GLN
1	A	282	ASP
1	A	289	ASP
1	A	294	MET
1	A	307	MET
1	B	1012	LYS
1	B	1120	VAL
1	B	1141	GLN
1	B	1147	LEU
1	B	1195[A]	ARG
1	B	1195[B]	ARG
1	B	1216	THR
1	B	1282	ASP
1	B	1289	ASP
1	B	1307	MET

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

Mol	Chain	Res	Type
1	A	312	GLN
1	B	1116	HIS
1	B	1141	GLN
1	B	1302	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

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	2339	-	4,4,4	0.24	0	6,6,6	0.34	0
3	PPV	A	1340	-	6,8,8	0.79	0	12,13,13	0.95	0
3	PPV	B	2340	-	6,8,8	0.80	0	12,13,13	0.94	0
2	SO4	A	1339	-	4,4,4	0.25	0	6,6,6	0.26	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	2340	-	-	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2340	PPV	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	338/338 (100%)	0.50	23 (6%)	23 27	9, 23, 35, 46	10 (2%)
1	B	338/338 (100%)	1.39	85 (25%)	1 1	16, 29, 46, 49	11 (3%)
All	All	676/676 (100%)	0.94	108 (15%)	5 5	9, 26, 44, 49	21 (3%)

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	259	THR	7.4
1	B	1326[A]	LYS	7.3
1	B	1200	GLY	6.8
1	B	1258	PRO	6.8
1	B	1046	GLY	6.5
1	B	1260	PHE	6.4
1	A	262	ASP	6.1
1	A	329[A]	PRO	6.1
1	A	260	PHE	5.7
1	B	1259	THR	5.6
1	B	1204	LEU	5.6
1	B	1142	ILE	5.3
1	A	258	PRO	5.3
1	B	1261	GLY	5.2
1	A	326[A]	LYS	5.1
1	B	1328[A]	ALA	5.0
1	B	1201	GLY	5.0
1	A	263	GLU	4.9
1	B	1045	VAL	4.9
1	B	1262	ASP	4.8
1	B	1144	GLN	4.5
1	B	1145	SER	4.5
1	B	1147	LEU	4.5
1	A	261	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	1043	ARG	4.2
1	B	1327[A]	MET	4.2
1	B	1044	GLU	4.2
1	B	1143	CYS	4.1
1	B	1015	ASP	4.1
1	A	325[A]	HIS	3.9
1	B	1206	PHE	3.9
1	B	1149	VAL	3.5
1	B	1197	ALA	3.5
1	B	1133	ALA	3.4
1	B	1329[A]	PRO	3.4
1	B	1203	GLU	3.3
1	B	1138	SER	3.3
1	A	200	GLY	3.3
1	B	1128	PHE	3.2
1	B	1140	ARG	3.2
1	B	1108	GLU	3.2
1	B	1199	ARG	3.1
1	B	1331[A]	THR	3.1
1	B	1120	VAL	3.1
1	B	1042	ALA	2.9
1	B	1330[A]	GLU	2.9
1	B	1257	ASN	2.9
1	B	1099	SER	2.9
1	B	1146	ARG	2.8
1	B	1195[A]	ARG	2.8
1	B	1198	GLY	2.8
1	B	1103	PRO	2.8
1	B	1112	GLU	2.8
1	B	1294	MET	2.8
1	A	257	ASN	2.8
1	B	1119	HIS	2.8
1	B	1214	HIS	2.8
1	B	1014	LEU	2.7
1	B	1324[A]	ALA	2.7
1	B	1013	ASP	2.7
1	B	1176	VAL	2.7
1	A	198	GLY	2.6
1	A	203	GLU	2.6
1	B	1132	ALA	2.6
1	A	206	PHE	2.5
1	B	1139	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	1216	THR	2.5
1	B	1263	GLU	2.5
1	A	214	HIS	2.5
1	B	1171	LEU	2.5
1	B	1037	ALA	2.5
1	B	1135	THR	2.5
1	B	1150	ASP	2.5
1	A	65	ARG	2.4
1	B	1137	ASP	2.4
1	B	1040	GLU	2.4
1	A	327[A]	MET	2.4
1	B	1275	ASP	2.4
1	B	1127	THR	2.4
1	B	1124	ALA	2.4
1	B	1134	GLY	2.4
1	B	1151	VAL	2.4
1	B	1196	GLY	2.4
1	B	1338	SER	2.4
1	A	264	GLN	2.3
1	B	1062	PHE	2.3
1	B	1067	ALA	2.3
1	B	1264	GLN	2.3
1	B	1202	LYS	2.3
1	B	1141	GLN	2.2
1	A	15	ASP	2.2
1	B	1307	MET	2.1
1	B	1148	THR	2.1
1	A	145	SER	2.1
1	B	1016	ASN	2.1
1	A	338	SER	2.1
1	B	1107	VAL	2.1
1	A	144	GLN	2.1
1	B	1069	LEU	2.1
1	B	1098	LEU	2.1
1	B	1117	ALA	2.1
1	A	141	GLN	2.0
1	B	1325[A]	HIS	2.0
1	B	1101	THR	2.0
1	B	1129	GLY	2.0
1	B	1205	GLY	2.0
1	B	1312	GLN	2.0
1	B	1106	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 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	2339	5/5	0.81	0.14	49,49,50,50	0
3	PPV	B	2340	9/9	0.88	0.13	28,31,32,32	4
2	SO4	A	1339	5/5	0.91	0.19	38,41,41,42	0
3	PPV	A	1340	9/9	0.94	0.12	22,26,28,29	4

6.5 Other polymers [i](#)

There are no such residues in this entry.