



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:05 AM UTC

PDB ID : 5JVJ / pdb_00005jvj
Title : C4-type pyruvate phosphate dikinase: different conformational states of the nucleotide binding domain in the dimer
Authors : Minges, A.; Hoepfner, A.; Groth, G.
Deposited on : 2016-05-11
Resolution : 2.90 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

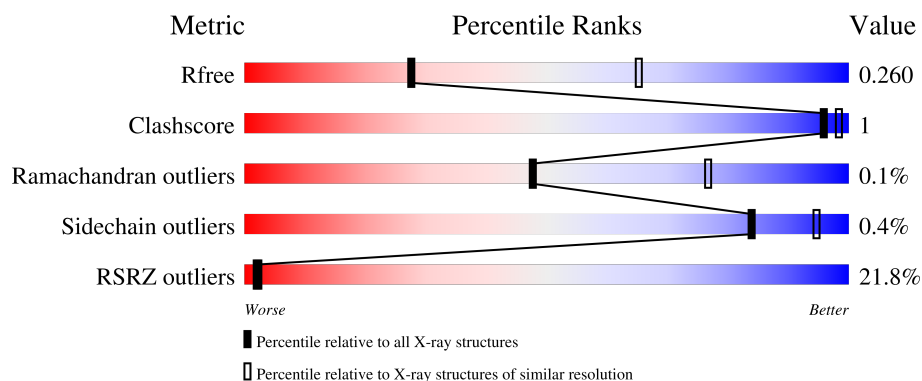
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	874	9% 96% ..
1	B	874	32% 88% • 9%

2 Entry composition [i](#)

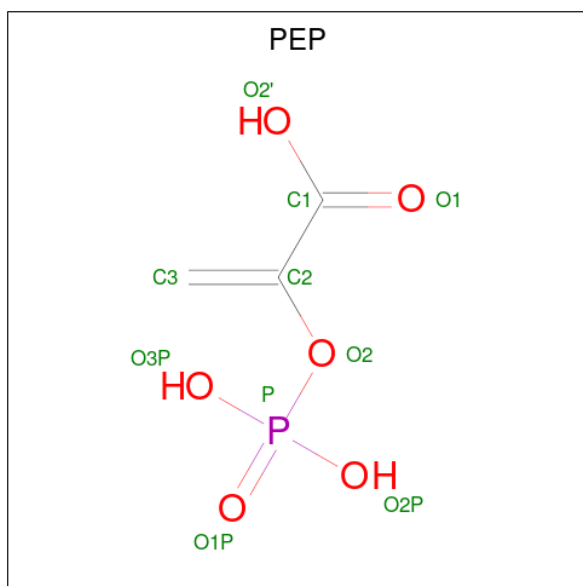
There are 3 unique types of molecules in this entry. The entry contains 11950 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pyruvate, phosphate dikinase, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	865	Total	C	N	O	S	0	2	0
			6504	4084	1127	1249	44			
1	B	797	Total	C	N	O	S	0	0	0
			5424	3386	942	1057	39			

- Molecule 2 is PHOSPHOENOLPYRUVATE (CCD ID: PEP) (formula: $C_3H_5O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			10	3	6	1		
2	B	1	Total	C	O	P	0	0
			10	3	6	1		

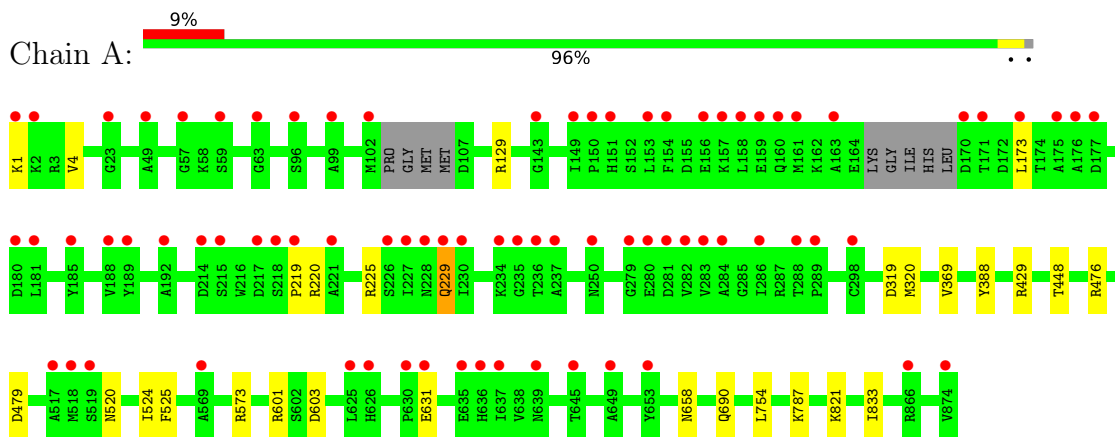
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Mg 1	0	0
3	B	1	Total 1	Mg 1	0	0

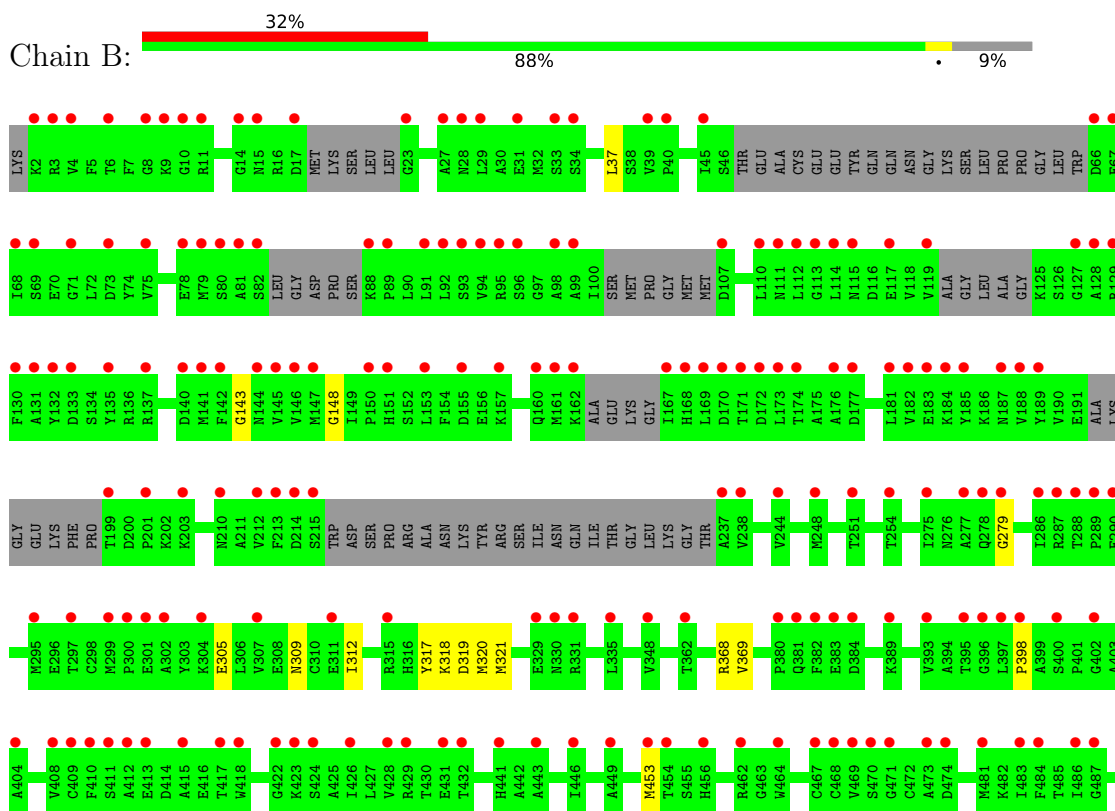
3 Residue-property plots

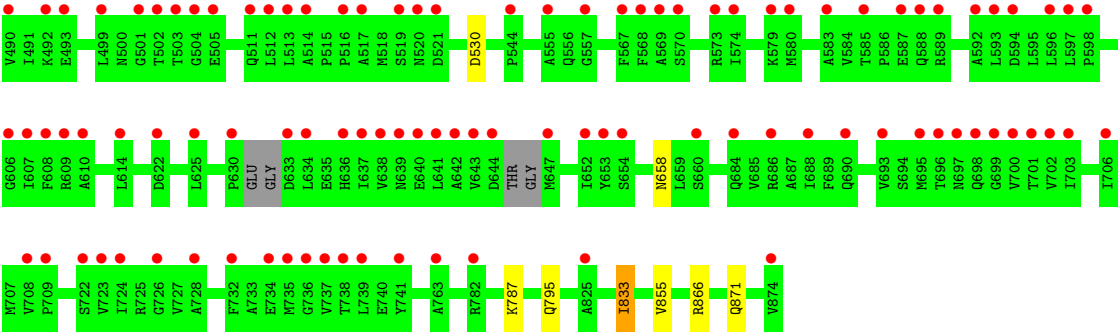
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Pyruvate, phosphate dikinase, chloroplastic



- Molecule 1: Pyruvate, phosphate dikinase, chloroplastic





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	208.74Å 69.04Å 166.76Å 90.00° 112.84° 90.00°	Depositor
Resolution (Å)	38.42 – 2.90 38.42 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.1 (38.42-2.90) 98.0 (38.42-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.90Å)	Xtriage
Refinement program	PHENIX dev_2386	Depositor
R, R_{free}	0.237 , 0.261 0.237 , 0.260	Depositor DCC
R_{free} test set	1228 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å ²)	39.7	Xtriage
Anisotropy	0.903	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	11950	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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: PEP, MG

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	0.13	0/6623	0.27	0/8961
1	B	0.11	0/5503	0.25	0/7492
All	All	0.12	0/12126	0.26	0/16453

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	6504	0	6370	15	0
1	B	5424	0	4761	12	0
2	A	10	0	2	0	0
2	B	10	0	2	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	11950	0	11135	25	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 1.

All (25) 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:658:ASN:O	1:B:787:LYS:NZ	2.22	0.73
1:A:601:ARG:NH1	1:A:690:GLN:OE1	2.27	0.66
1:A:319:ASP:OD1	1:A:320:MET:N	2.34	0.60
1:B:305:GLU:O	1:B:309:ASN:ND2	2.34	0.58
1:A:129:ARG:NH1	1:A:173:LEU:O	2.36	0.58
1:B:369:VAL:O	1:B:871:GLN:NE2	2.37	0.58
1:A:787:LYS:NZ	1:B:658:ASN:O	2.34	0.57
1:B:317:TYR:HB2	1:B:321:MET:HE3	1.91	0.53
1:B:143:GLY:O	1:B:148:GLY:N	2.39	0.52
1:B:318:LYS:O	1:B:368:ARG:NH1	2.41	0.52
1:A:479:ASP:N	1:A:479:ASP:OD1	2.45	0.49
1:A:754:LEU:O	1:A:821:LYS:NZ	2.45	0.49
1:B:319:ASP:OD1	1:B:320:MET:N	2.46	0.48
1:A:573:ARG:NH1	1:A:603:ASP:OD2	2.41	0.47
1:B:398:PRO:O	1:B:453:MET:HE1	2.14	0.47
1:A:225:ARG:O	1:A:229:GLN:N	2.44	0.45
1:B:37:LEU:HD21	1:B:312:ILE:HG21	2.00	0.44
1:A:1:LYS:N	1:A:4:VAL:O	2.52	0.43
1:B:833:ILE:HG23	1:B:855:VAL:HA	2.02	0.42
1:A:388:TYR:CD1	1:A:388:TYR:C	2.98	0.42
1:A:219:PRO:O	1:A:220:ARG:CB	2.68	0.41
1:A:520:ASN:O	1:A:524:ILE:HG12	2.21	0.41
1:B:530:ASP:OD1	1:B:866:ARG:HD2	2.21	0.41
1:A:369:VAL:HB	1:A:525:PHE:CZ	2.56	0.40
1:A:429:ARG:O	1:A:448:THR:HA	2.21	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	861/874 (98%)	832 (97%)	28 (3%)	1 (0%)	48	77
1	B	775/874 (89%)	752 (97%)	22 (3%)	1 (0%)	48	77
All	All	1636/1748 (94%)	1584 (97%)	50 (3%)	2 (0%)	48	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	279	GLY
1	A	229	GLN

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	675/715 (94%)	672 (100%)	3 (0%)	84	94
1	B	467/715 (65%)	465 (100%)	2 (0%)	84	94
All	All	1142/1430 (80%)	1137 (100%)	5 (0%)	84	94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	476	ARG
1	A	631	GLU
1	A	833	ILE
1	B	795	GLN
1	B	833	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	626	HIS
1	B	565	HIS
1	B	626	HIS
1	B	658	ASN

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Mol	Chain	Res	Type
1	B	800	HIS

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 ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	PEP	B	901	3	9,9,9	1.59	2 (22%)	11,13,13	2.28	2 (18%)
2	PEP	A	901	3	9,9,9	0.68	0	11,13,13	0.70	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	PEP	B	901	3	-	0/9/9/9	-
2	PEP	A	901	3	-	3/9/9/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	PEP	O1-C1	3.43	1.31	1.22
2	B	901	PEP	O2'-C1	-2.82	1.22	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	PEP	O1-C1-C2	-5.22	113.92	121.79
2	B	901	PEP	O2'-C1-C2	4.92	122.30	113.91

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	PEP	C1-C2-O2-P
2	A	901	PEP	C3-C2-O2-P
2	A	901	PEP	C2-O2-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

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	865/874 (98%)	0.45	78 (9%) 15 13	11, 34, 100, 133	2 (0%)
1	B	797/874 (91%)	1.65	284 (35%) 1 0	32, 80, 118, 156	0
All	All	1662/1748 (95%)	1.03	362 (21%) 2 2	11, 61, 114, 156	2 (0%)

All (362) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	697	ASN	6.3
1	B	701	THR	6.1
1	A	645	THR	5.7
1	B	699	GLY	5.5
1	B	640	GLU	5.3
1	B	700	VAL	4.8
1	B	585	THR	4.8
1	A	281	ASP	4.7
1	B	82	SER	4.6
1	B	417	THR	4.4
1	B	454	THR	4.4
1	B	380	PRO	4.4
1	B	642	ALA	4.4
1	A	175	ALA	4.4
1	B	297	THR	4.3
1	A	284	ALA	4.3
1	B	215	SER	4.2
1	B	161	MET	4.2
1	B	189	TYR	4.2
1	B	423	LYS	4.2
1	B	782	ARG	4.1
1	B	638	VAL	4.1
1	B	608	PHE	4.1
1	B	210	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	9	LYS	4.1
1	B	728	ALA	4.0
1	B	641	LEU	4.0
1	B	28	ASN	4.0
1	B	517	ALA	4.0
1	B	383	GLU	4.0
1	B	398	PRO	4.0
1	B	23	GLY	3.9
1	B	639	ASN	3.9
1	B	171	THR	3.9
1	B	499	LEU	3.9
1	B	512	LEU	3.9
1	A	282	VAL	3.9
1	B	516	PRO	3.9
1	B	11	ARG	3.8
1	B	467	CYS	3.8
1	B	625	LEU	3.8
1	A	866	ARG	3.7
1	A	170	ASP	3.7
1	B	644	ASP	3.7
1	B	237	ALA	3.7
1	B	607	ILE	3.7
1	B	468	CYS	3.7
1	B	397	LEU	3.7
1	A	176	ALA	3.7
1	B	254	THR	3.7
1	B	66	ASP	3.6
1	B	469	VAL	3.6
1	B	133	ASP	3.6
1	B	514	ALA	3.6
1	B	431	GLU	3.6
1	B	115	ASN	3.6
1	B	128	ALA	3.6
1	B	473	ALA	3.6
1	B	8	GLY	3.6
1	A	161	MET	3.6
1	B	492	LYS	3.5
1	B	483	ILE	3.5
1	B	741	TYR	3.5
1	B	643	VAL	3.5
1	B	630	PRO	3.5
1	B	301	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	587	GLU	3.4
1	B	544	PRO	3.4
1	B	456	HIS	3.4
1	B	160	GLN	3.4
1	B	114	LEU	3.4
1	A	236	THR	3.4
1	B	520	ASN	3.3
1	B	429	ARG	3.3
1	B	653	TYR	3.3
1	B	183	GLU	3.3
1	B	424	SER	3.3
1	B	203	LYS	3.3
1	B	633	ASP	3.3
1	B	486	ILE	3.3
1	A	163	ALA	3.3
1	B	199	THR	3.3
1	A	637	ILE	3.2
1	B	568	PHE	3.2
1	B	93	SER	3.2
1	B	695	MET	3.2
1	B	573	ARG	3.2
1	A	154	PHE	3.2
1	B	119	VAL	3.2
1	B	212	VAL	3.2
1	A	1	LYS	3.2
1	B	409	CYS	3.2
1	B	660	SER	3.2
1	B	144	ASN	3.2
1	B	330	ASN	3.2
1	A	189	TYR	3.2
1	A	177	ASP	3.2
1	B	287	ARG	3.2
1	B	413	GLU	3.2
1	B	588	GLN	3.1
1	A	279	GLY	3.1
1	B	493	GLU	3.1
1	B	637	ILE	3.1
1	B	80	SER	3.1
1	B	169	LEU	3.1
1	B	155	ASP	3.1
1	B	295	MET	3.1
1	B	481	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	606	GLY	3.1
1	B	703	ILE	3.1
1	B	408	VAL	3.1
1	B	737	VAL	3.1
1	B	275	ILE	3.1
1	A	226	SER	3.0
1	B	187	ASN	3.0
1	B	470	SER	3.0
1	B	45	ILE	3.0
1	B	167	ILE	3.0
1	B	688	ILE	3.0
1	B	92	LEU	3.0
1	B	110	LEU	3.0
1	A	649	ALA	3.0
1	B	708	VAL	3.0
1	B	654	SER	3.0
1	B	94	VAL	3.0
1	A	160	GLN	3.0
1	B	137	ARG	3.0
1	B	381	GLN	3.0
1	B	412	ALA	3.0
1	B	3	ARG	3.0
1	B	135	TYR	3.0
1	B	609	ARG	3.0
1	A	49	ALA	3.0
1	B	39	VAL	3.0
1	B	95	ARG	2.9
1	B	286	ILE	2.9
1	B	402	GLY	2.9
1	B	88	LYS	2.9
1	B	185	TYR	2.9
1	B	146	VAL	2.9
1	B	410	PHE	2.9
1	B	151	HIS	2.9
1	B	593	LEU	2.9
1	B	132	TYR	2.9
1	B	214	ASP	2.9
1	B	176	ALA	2.9
1	A	159	GLU	2.8
1	B	117	GLU	2.8
1	B	415	ALA	2.8
1	B	382	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	180	ASP	2.8
1	B	598	PRO	2.8
1	B	698	GLN	2.8
1	B	15	ASN	2.8
1	B	636	HIS	2.8
1	B	519	SER	2.8
1	B	14	GLY	2.8
1	B	162	LYS	2.8
1	B	487	GLY	2.8
1	A	156	GLU	2.8
1	B	686	ARG	2.8
1	B	411	SER	2.8
1	A	235	GLY	2.8
1	B	129	ARG	2.7
1	A	188	VAL	2.7
1	A	569	ALA	2.7
1	B	173	LEU	2.7
1	B	278	GLN	2.7
1	B	690	GLN	2.7
1	B	335	LEU	2.7
1	B	170	ASP	2.7
1	A	289	PRO	2.7
1	B	315	ARG	2.7
1	A	283	VAL	2.7
1	A	230	ILE	2.7
1	B	157	LYS	2.7
1	A	57	GLY	2.7
1	B	614	LEU	2.7
1	B	277	ALA	2.7
1	A	185	TYR	2.7
1	A	250	ASN	2.7
1	B	511	GLN	2.7
1	B	145	VAL	2.7
1	B	449	ALA	2.6
1	B	418	TRP	2.6
1	A	23	GLY	2.6
1	A	635	GLU	2.6
1	A	519	SER	2.6
1	B	302	ALA	2.6
1	B	763	ALA	2.6
1	B	597	LEU	2.6
1	B	68	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	217	ASP	2.6
1	B	569	ALA	2.6
1	A	151	HIS	2.6
1	A	626	HIS	2.6
1	B	726	GLY	2.6
1	B	696	THR	2.6
1	A	149	ILE	2.6
1	B	111	ASN	2.6
1	B	290	GLU	2.6
1	B	99	ALA	2.6
1	B	96	SER	2.6
1	A	150	PRO	2.6
1	A	219	PRO	2.6
1	B	4	VAL	2.6
1	B	474	ASP	2.6
1	B	396	GLY	2.5
1	A	214	ASP	2.5
1	B	78	GLU	2.5
1	B	213	PHE	2.5
1	B	17	ASP	2.5
1	B	304	LYS	2.5
1	B	10	GLY	2.5
1	B	79	MET	2.5
1	B	453	MET	2.5
1	A	653	TYR	2.5
1	B	432	THR	2.5
1	A	158	LEU	2.5
1	B	188	VAL	2.5
1	B	311	GLU	2.5
1	B	81	ALA	2.5
1	B	29	LEU	2.4
1	B	384	ASP	2.4
1	B	513	LEU	2.4
1	A	630	PRO	2.4
1	B	400	SER	2.4
1	B	329	GLU	2.4
1	B	503	THR	2.4
1	A	173	LEU	2.4
1	B	147	MET	2.4
1	B	739	LEU	2.4
1	B	201	PRO	2.4
1	B	574	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	471	GLY	2.4
1	B	723	VAL	2.4
1	B	168	HIS	2.4
1	B	172	ASP	2.4
1	B	279	GLY	2.4
1	B	736	GLY	2.4
1	A	234	LYS	2.4
1	B	331	ARG	2.4
1	B	738	THR	2.4
1	B	647	MET	2.4
1	B	91	LEU	2.4
1	B	238	VAL	2.4
1	A	2	LYS	2.4
1	B	505	GLU	2.4
1	A	288	THR	2.4
1	B	596	LEU	2.4
1	B	2	LYS	2.3
1	B	184	LYS	2.3
1	B	702	VAL	2.3
1	B	107	ASP	2.3
1	A	221	ALA	2.3
1	A	59	SER	2.3
1	B	181	LEU	2.3
1	B	502	THR	2.3
1	A	157	LYS	2.3
1	B	182	VAL	2.3
1	B	127	GLY	2.3
1	A	99	ALA	2.3
1	A	280	GLU	2.3
1	A	517	ALA	2.3
1	B	734	GLU	2.3
1	A	636	HIS	2.3
1	B	428	VAL	2.3
1	B	521	ASP	2.3
1	B	735	MET	2.3
1	B	570	SER	2.3
1	B	40	PRO	2.3
1	B	693	VAL	2.3
1	A	639	ASN	2.3
1	B	404	ALA	2.3
1	B	825	ALA	2.3
1	A	229	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	6	THR	2.3
1	A	143	GLY	2.3
1	B	557	GLY	2.3
1	A	625	LEU	2.2
1	B	389	LYS	2.2
1	A	227	ILE	2.2
1	A	237	ALA	2.2
1	B	98	ALA	2.2
1	B	443	ALA	2.2
1	B	75	VAL	2.2
1	B	300	PRO	2.2
1	B	348	VAL	2.2
1	B	395	THR	2.2
1	A	215	SER	2.2
1	B	69	SER	2.2
1	B	67	GLU	2.2
1	B	634	LEU	2.2
1	A	228	ASN	2.2
1	B	589	ARG	2.2
1	B	89	PRO	2.2
1	B	150	PRO	2.2
1	B	393	VAL	2.2
1	B	288	THR	2.2
1	B	464	TRP	2.2
1	A	631	GLU	2.2
1	B	555	ALA	2.2
1	B	307	VAL	2.2
1	A	518	MET	2.2
1	B	362	THR	2.2
1	A	298	CYS	2.2
1	B	130	PHE	2.2
1	B	484	PHE	2.2
1	B	722	SER	2.2
1	A	286	ILE	2.1
1	B	426	ILE	2.1
1	B	446	ILE	2.1
1	B	724	ILE	2.1
1	A	874	VAL	2.1
1	B	244	VAL	2.1
1	B	289	PRO	2.1
1	B	73	ASP	2.1
1	B	177	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	63	GLY	2.1
1	A	171	THR	2.1
1	B	31	GLU	2.1
1	B	441	HIS	2.1
1	B	490	VAL	2.1
1	B	580	MET	2.1
1	B	709	PRO	2.1
1	B	71	GLY	2.1
1	B	174	THR	2.1
1	B	251	THR	2.1
1	B	706	ILE	2.1
1	A	102	MET	2.1
1	A	181	LEU	2.1
1	B	142	PHE	2.1
1	B	732	PHE	2.1
1	B	462	ARG	2.1
1	B	33	SER	2.1
1	B	34	SER	2.1
1	B	579	LYS	2.1
1	A	153	LEU	2.1
1	B	140	ASP	2.1
1	B	594	ASP	2.1
1	B	583	ALA	2.1
1	B	610	ALA	2.1
1	A	96	SER	2.0
1	A	218	SER	2.0
1	B	141	MET	2.0
1	B	874	VAL	2.0
1	B	422	GLY	2.0
1	B	501	GLY	2.0
1	A	192	ALA	2.0
1	B	248	MET	2.0
1	B	299	MET	2.0
1	B	684	GLN	2.0
1	B	112	LEU	2.0
1	B	153	LEU	2.0
1	B	113	GLY	2.0
1	B	504	GLY	2.0
1	B	567	PHE	2.0
1	B	652	ILE	2.0
1	B	27	ALA	2.0
1	B	131	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	592	ALA	2.0
1	B	622	ASP	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(Å ²)	Q<0.9
2	PEP	B	901	10/10	0.94	0.10	39,41,43,44	0
2	PEP	A	901	10/10	0.96	0.09	13,19,23,24	0
3	MG	A	902	1/1	0.97	0.07	23,23,23,23	0
3	MG	B	902	1/1	0.99	0.03	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.