



# Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 02:34 am BST

PDB ID : 6W0P  
Title : Putative kojibiose phosphorylase from human microbiome  
Authors : Dementiev, A.; Osipiuk, J.; Endres, M.; Wakatsuki, S.; Hess, M.; Joachimiak, A.  
Deposited on : 2020-03-02  
Resolution : 2.23 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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

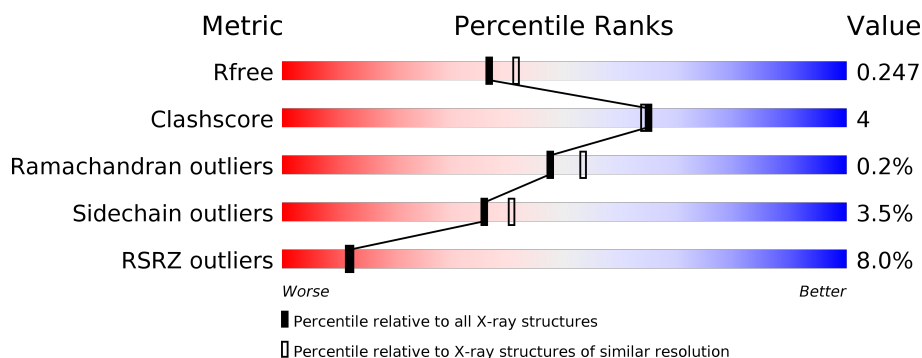
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.23 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))
$R_{free}$	130704	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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  $\geq 3$ , 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	760	<div> <div>3%</div> <div>91%</div> <div>8%</div> </div>
1	B	760	<div> <div>3%</div> <div>91%</div> <div>7%</div> </div>
1	C	760	<div> <div>13%</div> <div>78%</div> <div>16%</div> <div>5%</div> </div>
1	D	760	<div> <div>12%</div> <div>76%</div> <div>11%</div> <div>11%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25131 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 Kojibiose phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	752	Total	C	N	O	S	0	5	0
			6234	4014	1021	1166	33			
1	B	751	Total	C	N	O	S	0	5	0
			6220	4006	1021	1162	31			
1	C	719	Total	C	N	O	S	0	2	0
			5942	3829	978	1104	31			
1	D	677	Total	C	N	O	S	0	1	0
			5583	3594	923	1036	30			

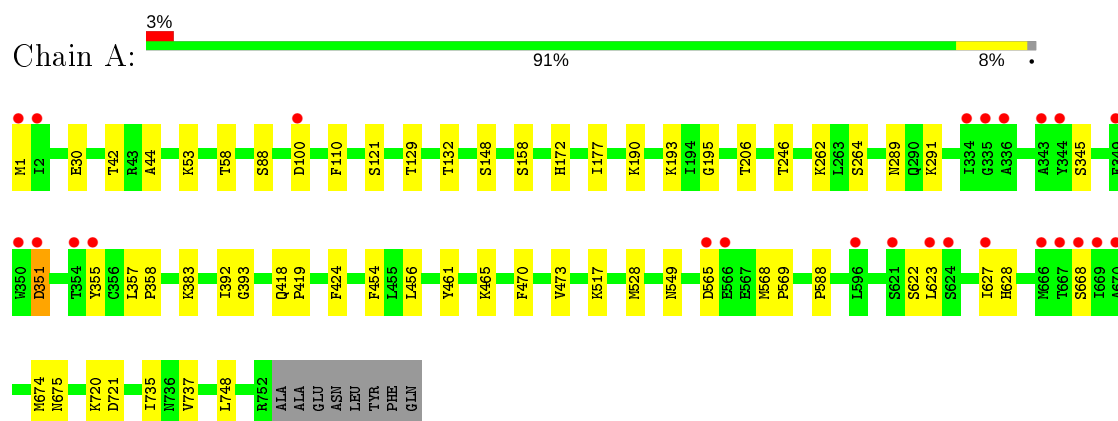
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	396	Total	O	0	0
			396	396		
2	B	444	Total	O	0	0
			444	444		
2	C	136	Total	O	0	0
			136	136		
2	D	176	Total	O	0	0
			176	176		

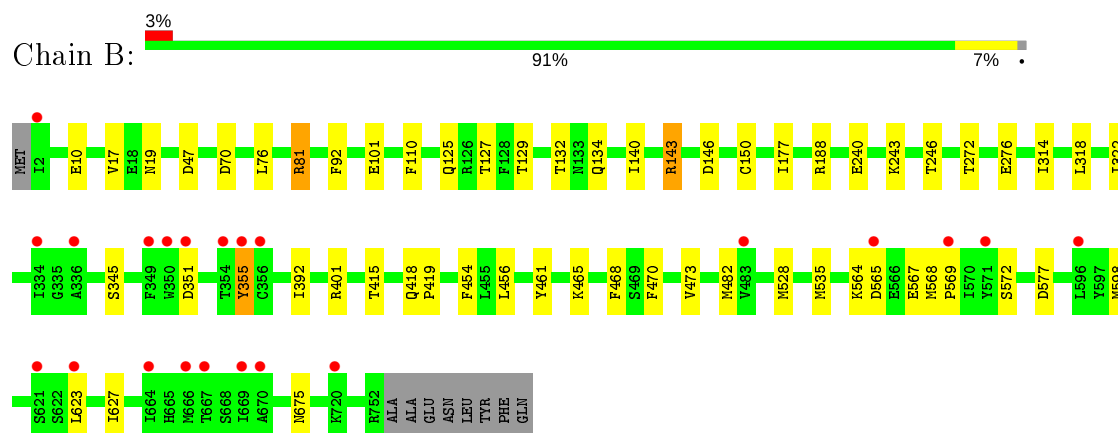
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

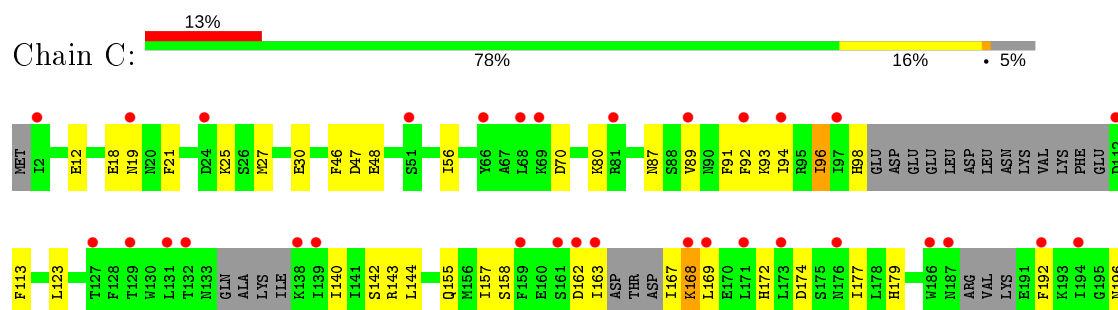
- Molecule 1: Kojibiose phosphorylase

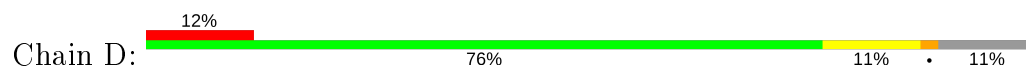


- Molecule 1: Kojibiose phosphorylase



- Molecule 1: Kojibiose phosphorylase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.22Å 200.45Å 293.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.44 – 2.23 49.40 – 2.23	Depositor EDS
% Data completeness (in resolution range)	92.6 (49.44-2.23) 92.7 (49.40-2.23)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.22 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, $R_{free}$	0.200 , 0.246 0.203 , 0.247	Depositor DCC
$R_{free}$ test set	12344 reflections (7.22%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.4	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 37.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	25131	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	0.68	0/6391	0.81	0/8615
1	B	0.68	0/6376	0.81	0/8596
1	C	0.71	2/6080 (0.0%)	0.80	1/8190 (0.0%)
1	D	0.70	2/5714 (0.0%)	0.79	0/7696
All	All	0.69	4/24561 (0.0%)	0.80	1/33097 (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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	18	GLU	CD-OE2	13.56	1.40	1.25
1	D	18	GLU	CD-OE2	8.44	1.34	1.25
1	C	18	GLU	CD-OE1	8.18	1.34	1.25
1	D	18	GLU	CD-OE1	5.73	1.31	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	18	GLU	OE1-CD-OE2	5.37	129.74	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	172	HIS	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	6234	0	6170	39	0
1	B	6220	0	6168	32	0
1	C	5942	0	5865	72	0
1	D	5583	0	5492	55	0
2	A	396	0	0	5	0
2	B	444	0	0	3	0
2	C	136	0	0	4	0
2	D	176	0	0	0	0
All	All	25131	0	23695	196	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 (196) 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:355[B]:TYR:CE1	1:A:627:ILE:HD11	2.17	0.79
1:C:91:PHE:HE1	1:C:92:PHE:CZ	2.05	0.74
1:C:529:LYS:O	1:C:533:ARG:HG3	1.88	0.73
1:A:355[A]:TYR:OH	1:A:623:LEU:HB3	1.90	0.71
1:D:355:TYR:CD1	1:D:623:LEU:HD21	2.26	0.71
1:C:355[A]:TYR:OH	1:C:623:LEU:HB3	1.91	0.70
1:C:696:SER:OG	1:C:720:LYS:HE3	1.91	0.70
1:C:568:MET:HG3	1:C:569:PRO:HA	1.73	0.69
1:D:263:LEU:O	1:D:267:ARG:HG3	1.95	0.67
1:C:91:PHE:CE1	1:C:92:PHE:CE2	2.81	0.67
1:A:735[B]:ILE:HD12	1:A:737:VAL:HG23	1.75	0.67
1:D:56:ILE:O	1:D:87:ASN:ND2	2.27	0.67
1:D:254:ILE:CD1	1:D:269:ILE:HG22	2.26	0.65
1:D:10:GLU:HB2	1:D:17:VAL:CG1	2.26	0.65
1:D:186:TRP:CE3	1:D:202:VAL:HG22	2.32	0.65
1:D:186:TRP:HE3	1:D:202:VAL:HG22	1.61	0.65
1:D:56:ILE:HD12	1:D:56:ILE:H	1.62	0.65
1:A:1:MET:HB2	1:A:565:ASP:OD2	1.97	0.65
1:D:355:TYR:CG	1:D:623:LEU:HD21	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355[B]:TYR:CD1	1:A:674:MET:HE2	2.32	0.64
1:A:735[B]:ILE:CD1	1:A:737:VAL:HG23	2.27	0.64
1:D:177:ILE:HD12	1:D:177:ILE:O	1.97	0.63
1:B:568:MET:HA	1:B:569:PRO:C	2.19	0.63
1:C:167:ILE:HG13	1:C:239:LEU:HD12	1.81	0.62
1:C:237:LEU:HD13	1:C:245:LYS:HE2	1.82	0.61
1:B:355:TYR:CE1	1:B:627:ILE:HD11	2.36	0.61
1:D:56:ILE:HD12	1:D:56:ILE:N	2.15	0.61
1:C:144:LEU:HD11	1:C:286:VAL:HA	1.83	0.61
1:A:351[B]:ASP:OD1	1:A:623:LEU:HD21	2.00	0.60
1:B:70:ASP:OD1	1:B:81:ARG:NE	2.32	0.60
1:C:167:ILE:HG13	1:C:239:LEU:CD1	2.32	0.60
1:A:355[B]:TYR:CE1	1:A:674:MET:HE2	2.38	0.59
1:B:482:MET:HA	1:B:482:MET:HE2	1.85	0.59
1:C:220:LYS:HE3	1:C:221:GLU:O	2.03	0.59
1:C:598:MET:HE3	2:C:928:HOH:O	2.03	0.58
1:A:735[B]:ILE:HD11	1:A:748:LEU:HD23	1.84	0.58
1:D:10:GLU:HB2	1:D:17:VAL:HG13	1.86	0.58
1:D:268:ASP:O	1:D:272:THR:OG1	2.17	0.58
1:D:42:THR:HG22	1:D:58:THR:HG23	1.85	0.57
1:D:262:LYS:HE3	1:D:264:SER:OG	2.04	0.57
1:C:726:THR:HG22	1:C:747:LYS:HG3	1.88	0.56
1:A:355[B]:TYR:CE1	1:A:674:MET:CE	2.88	0.56
1:C:701:ASN:HB2	2:C:921:HOH:O	2.05	0.56
1:C:201:THR:HG21	1:C:263:LEU:HD12	1.87	0.56
1:D:64:TYR:HB2	1:D:84:PHE:O	2.05	0.56
1:C:91:PHE:HB2	1:C:251:VAL:HG11	1.86	0.56
1:D:186:TRP:HB3	1:D:202:VAL:HG21	1.87	0.56
1:B:246[B]:THR:HG22	2:B:948:HOH:O	2.05	0.55
1:C:96:ILE:O	1:C:96:ILE:HG13	2.06	0.55
1:C:691:ASN:HA	1:C:736:ASN:O	2.07	0.55
1:C:91:PHE:CE1	1:C:92:PHE:CZ	2.91	0.55
1:C:192:PHE:CE2	1:C:267:ARG:HD3	2.42	0.54
1:C:140:ILE:O	1:C:157:ILE:HA	2.07	0.54
1:C:46:PHE:HB3	1:C:48:GLU:OE2	2.08	0.54
1:D:186:TRP:HB3	1:D:202:VAL:CG2	2.38	0.53
1:D:250:TYR:OH	1:D:280:PHE:O	2.16	0.53
1:A:418:GLN:HG2	1:A:419:PRO:HD3	1.91	0.53
1:C:27:MET:HE1	2:C:859:HOH:O	2.09	0.53
1:D:116:ILE:HG23	1:D:125:GLN:HB3	1.91	0.53
1:A:735[B]:ILE:HD11	1:A:748:LEU:CD2	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ASP:CG	1:B:143:ARG:HH21	2.13	0.52
1:C:179:HIS:NE2	1:C:342:GLU:HB3	2.25	0.52
1:D:21:PHE:CE1	1:D:46:PHE:CZ	2.98	0.52
1:D:9:LEU:N	1:D:9:LEU:HD22	2.25	0.52
1:D:146:ASP:OD2	1:D:288:LYS:NZ	2.42	0.52
1:D:8:TYR:CE1	1:D:9:LEU:HD21	2.44	0.52
1:B:127[A]:THR:HG22	1:B:140:ILE:HG23	1.92	0.51
1:C:214:VAL:HG23	1:C:274:LEU:HD22	1.93	0.51
1:D:8:TYR:CZ	1:D:9:LEU:HD21	2.46	0.51
1:D:21:PHE:CE1	1:D:46:PHE:HZ	2.29	0.51
1:C:355[A]:TYR:CE2	1:C:623:LEU:HD23	2.46	0.51
1:C:355[B]:TYR:CE1	1:C:627:ILE:HD11	2.46	0.50
1:C:510:LYS:HE2	1:C:513:LYS:HE3	1.93	0.50
1:C:177:ILE:HD12	1:C:177:ILE:O	2.11	0.50
1:C:302:ILE:HA	1:C:704:GLN:O	2.12	0.50
1:C:199:GLY:HA3	1:C:214:VAL:HG12	1.94	0.50
1:C:719:ASP:O	1:C:752:ARG:NH1	2.45	0.50
1:D:29:SER:O	1:D:33:PHE:HB2	2.11	0.50
1:D:725:ILE:HD13	1:D:735:ILE:CD1	2.42	0.50
1:D:154:TYR:CE2	1:D:285:LEU:HD13	2.47	0.50
1:D:725:ILE:HD13	1:D:735:ILE:HD11	1.94	0.50
1:A:392:ILE:O	1:A:454:PHE:HA	2.11	0.49
1:C:355[B]:TYR:CE1	1:C:674:MET:HE3	2.47	0.49
1:D:586:LYS:HG3	1:D:620:GLU:HB3	1.94	0.49
1:C:724:ILE:HG12	1:C:749:GLU:HG2	1.95	0.49
1:D:47:ASP:OD2	1:D:155:GLN:NE2	2.46	0.48
1:D:254:ILE:HD13	1:D:269:ILE:HG22	1.95	0.48
1:C:199:GLY:CA	1:C:214:VAL:HG12	2.43	0.48
1:A:193:LYS:NZ	1:A:195:GLY:O	2.46	0.48
1:B:110:PHE:HA	1:B:129:THR:O	2.11	0.48
1:C:167:ILE:CG1	1:C:239:LEU:HD12	2.41	0.48
1:D:271:LEU:HD11	1:D:275:LYS:NZ	2.28	0.48
1:D:39:TYR:CE2	1:D:151:GLU:HA	2.48	0.48
1:C:357:LEU:HB3	1:C:358:PRO:HD3	1.94	0.48
1:B:240:GLU:HB2	1:B:243:LYS:HD3	1.95	0.48
1:B:76:LEU:HB3	2:B:1106:HOH:O	2.13	0.48
1:C:500:LEU:O	1:C:504:LEU:HG	2.13	0.48
1:D:70:ASP:OD1	1:D:81:ARG:HD3	2.13	0.48
1:C:213:SER:OG	1:C:253:ASN:ND2	2.46	0.48
1:B:272:THR:O	1:B:276:GLU:HG3	2.13	0.48
1:C:265:GLN:O	1:C:269:ILE:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:634:LYS:HD3	2:C:925:HOH:O	2.14	0.48
1:C:568:MET:HA	1:C:569:PRO:C	2.33	0.47
1:B:418:GLN:HG2	1:B:419:PRO:HD3	1.96	0.47
1:D:443:TYR:O	1:D:447:MET:HG3	2.14	0.47
1:C:337:LYS:HE2	1:C:344:TYR:CD2	2.50	0.47
1:A:622:SER:HB2	1:A:668:SER:HB2	1.98	0.46
1:A:262:LYS:HE3	1:A:264:SER:HB3	1.97	0.46
1:B:345:SER:HA	2:B:893:HOH:O	2.16	0.46
1:D:121:SER:O	1:D:289:ASN:HB3	2.16	0.46
1:C:463:GLN:NE2	1:D:555:MET:O	2.46	0.46
1:D:311:GLN:CA	1:D:311:GLN:HE21	2.29	0.46
1:B:92:PHE:CE2	1:B:143:ARG:HD3	2.51	0.46
1:C:47:ASP:OD2	1:C:155:GLN:NE2	2.48	0.46
1:D:216:ARG:HD2	1:D:278:SER:OG	2.16	0.46
1:A:177:ILE:HG22	2:A:1178:HOH:O	2.15	0.46
1:D:355:TYR:CE1	1:D:623:LEU:HD21	2.50	0.46
1:C:634:LYS:HE2	1:C:684:MET:HE1	1.97	0.46
1:A:110:PHE:HA	1:A:129:THR:O	2.16	0.45
1:A:355[B]:TYR:CE1	1:A:627:ILE:CD1	2.94	0.45
1:A:720:LYS:HG3	1:A:721:ASP:OD1	2.15	0.45
1:C:168:LYS:HG3	1:C:168:LYS:O	2.15	0.45
1:C:418:GLN:N	1:C:419:PRO:CD	2.79	0.45
1:A:517:LYS:NZ	2:A:813:HOH:O	2.47	0.45
1:C:144:LEU:HD23	1:C:144:LEU:HA	1.83	0.45
1:A:190:LYS:HE2	2:A:811:HOH:O	2.16	0.45
1:C:27:MET:O	1:C:30:GLU:HB2	2.17	0.45
1:A:568:MET:HG3	1:A:569:PRO:HA	1.98	0.45
1:C:56:ILE:O	1:C:87:ASN:ND2	2.49	0.45
1:B:470:PHE:HB3	1:B:473:VAL:HG11	1.99	0.45
1:B:318:LEU:O	1:B:322:ILE:HG13	2.16	0.44
1:B:10:GLU:HB2	1:B:17:VAL:HB	1.99	0.44
1:C:92:PHE:CE2	1:C:143:ARG:HD3	2.52	0.44
1:D:694:PRO:HD2	1:D:738:TYR:CZ	2.52	0.44
1:B:415:THR:HG22	1:B:482:MET:CE	2.47	0.44
1:C:418:GLN:HG2	1:C:419:PRO:HD3	1.99	0.44
1:C:142:SER:O	1:C:155:GLN:HA	2.18	0.44
1:D:44:ALA:HA	1:D:143:ARG:HH21	1.83	0.44
1:A:735[B]:ILE:CD1	1:A:737:VAL:CG2	2.94	0.44
1:B:146:ASP:O	1:B:150:CYS:HA	2.17	0.44
1:A:121:SER:O	1:A:289:ASN:HB3	2.18	0.43
1:C:614:GLU:HB3	1:C:615:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:THR:HG22	1:A:58:THR:HG23	2.00	0.43
1:B:461:TYR:HB3	1:B:465:LYS:HA	1.99	0.43
1:B:101:GLU:OE1	1:B:132:THR:OG1	2.29	0.43
1:A:158:SER:CB	1:A:246:THR:HG22	2.48	0.43
1:A:470:PHE:HB3	1:A:473:VAL:HG11	2.01	0.43
1:D:43:ARG:NH1	1:D:55:LEU:HB3	2.34	0.43
1:B:127[A]:THR:HG22	1:B:140:ILE:HG12	2.00	0.43
1:C:726:THR:HA	1:C:746:ASP:O	2.18	0.43
1:A:30:GLU:HA	1:A:44:ALA:HB3	2.00	0.43
1:A:1:MET:CB	1:A:565:ASP:OD2	2.66	0.43
1:B:392:ILE:O	1:B:454:PHE:HA	2.19	0.43
1:D:599:GLU:HB2	1:D:686:LYS:HG3	2.00	0.43
1:C:732:ILE:HG21	1:C:743:GLU:HG3	2.00	0.43
1:C:98:HIS:CG	1:C:98:HIS:O	2.72	0.43
1:C:12:GLU:O	1:C:312:GLN:HG3	2.19	0.42
1:A:158:SER:HB2	1:A:246:THR:HG22	2.01	0.42
1:D:18:GLU:HB3	1:D:115:ARG:HB3	2.00	0.42
1:A:461:TYR:HB3	1:A:465:LYS:HA	2.01	0.42
1:C:744:LEU:HD13	1:C:748:LEU:HD22	2.00	0.42
1:D:271:LEU:HD11	1:D:275:LYS:HZ2	1.84	0.42
1:A:345:SER:HA	2:A:991:HOH:O	2.20	0.42
1:A:588:PRO:HG3	1:A:628:HIS:CE1	2.55	0.42
1:B:314:ILE:HD12	1:B:314:ILE:HA	1.92	0.42
1:B:468:PHE:O	1:B:535:MET:HA	2.20	0.42
1:B:565:ASP:C	1:B:567:GLU:H	2.23	0.42
1:C:472:GLY:C	1:C:482:MET:HE2	2.40	0.42
1:D:623:LEU:HA	1:D:623:LEU:HD23	1.89	0.42
1:D:44:ALA:HA	1:D:143:ARG:NH2	2.34	0.42
1:B:456:LEU:HD21	1:B:528:MET:HA	2.02	0.42
1:C:415:THR:HG22	1:C:482:MET:HE1	2.01	0.42
1:A:456:LEU:HD21	1:A:528:MET:HA	2.02	0.41
1:D:697:ASN:ND2	1:D:700:TRP:CZ2	2.88	0.41
1:A:88:SER:O	1:A:177:ILE:HG12	2.20	0.41
1:B:401:ARG:HA	1:B:401:ARG:HD2	1.84	0.41
1:D:379:LEU:HA	1:D:379:LEU:HD23	1.92	0.41
1:C:212:THR:N	1:C:266:GLN:OE1	2.53	0.41
1:D:65:GLU:HB2	1:D:86:ILE:HG21	2.01	0.41
1:C:295:HIS:NE2	1:C:299:LYS:HE3	2.34	0.41
1:A:383:LYS:HA	1:A:393:GLY:O	2.21	0.41
1:C:21:PHE:HB2	1:C:113:PHE:CD1	2.56	0.41
1:C:355[B]:TYR:HE2	1:C:671:ALA:CB	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:GLU:HA	1:C:94:ILE:O	2.21	0.41
1:C:379:LEU:HA	1:C:379:LEU:HD23	1.87	0.41
1:B:623:LEU:O	1:B:627:ILE:HG12	2.22	0.41
1:B:134:GLN:NE2	1:D:600:GLU:HA	2.36	0.40
1:B:415:THR:CG2	1:B:482:MET:HE3	2.51	0.40
1:C:163:ILE:HG22	1:C:163:ILE:O	2.21	0.40
1:C:211:LEU:C	1:C:211:LEU:HD23	2.41	0.40
1:C:93:LYS:HD3	1:C:174:ASP:CB	2.51	0.40
1:A:262:LYS:HD3	2:A:1170:HOH:O	2.21	0.40
1:C:392:ILE:O	1:C:454:PHE:HA	2.21	0.40
1:D:32:ILE:HD13	1:D:653:LEU:HA	2.03	0.40
1:A:357:LEU:N	1:A:358:PRO:CD	2.84	0.40
1:B:418:GLN:N	1:B:419:PRO:CD	2.85	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	755/760 (99%)	722 (96%)	33 (4%)	0	100	100
1	B	754/760 (99%)	725 (96%)	29 (4%)	0	100	100
1	C	709/760 (93%)	662 (93%)	44 (6%)	3 (0%)	34	35
1	D	666/760 (88%)	628 (94%)	36 (5%)	2 (0%)	41	44
All	All	2884/3040 (95%)	2737 (95%)	142 (5%)	5 (0%)	47	53

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	465	LYS
1	D	89	VAL

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Mol	Chain	Res	Type
1	C	462	ASN
1	D	646	GLY
1	C	89	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	689/690 (100%)	678 (98%)	11 (2%)	62	70
1	B	688/690 (100%)	675 (98%)	13 (2%)	57	64
1	C	654/690 (95%)	619 (95%)	35 (5%)	22	20
1	D	611/690 (89%)	577 (94%)	34 (6%)	21	19
All	All	2642/2760 (96%)	2549 (96%)	93 (4%)	36	40

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LYS
1	A	100	ASP
1	A	132	THR
1	A	148	SER
1	A	206	THR
1	A	291	LYS
1	A	351[A]	ASP
1	A	351[B]	ASP
1	A	424	PHE
1	A	549	ASN
1	A	675	ASN
1	B	19	ASN
1	B	81	ARG
1	B	125	GLN
1	B	143	ARG
1	B	177	ILE
1	B	188	ARG
1	B	351	ASP

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Mol	Chain	Res	Type
1	B	355	TYR
1	B	564	LYS
1	B	572	SER
1	B	577	ASP
1	B	598	MET
1	B	675	ASN
1	C	19	ASN
1	C	25	LYS
1	C	70	ASP
1	C	80	LYS
1	C	96	ILE
1	C	123	LEU
1	C	158	SER
1	C	162	ASP
1	C	168	LYS
1	C	169	LEU
1	C	172	HIS
1	C	196	ASN
1	C	219	LEU
1	C	221	GLU
1	C	225	GLN
1	C	261	GLN
1	C	276	GLU
1	C	290	GLN
1	C	342	GLU
1	C	369	LYS
1	C	424	PHE
1	C	457	SER
1	C	513	LYS
1	C	516	ASP
1	C	529	LYS
1	C	541	LYS
1	C	549	ASN
1	C	568	MET
1	C	598	MET
1	C	600	GLU
1	C	675	ASN
1	C	696	SER
1	C	720	LYS
1	C	748	LEU
1	C	751	LYS
1	D	7	ARG

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Mol	Chain	Res	Type
1	D	24	ASP
1	D	43	ARG
1	D	47	ASP
1	D	55	LEU
1	D	69	LYS
1	D	117	LEU
1	D	128	PHE
1	D	148	SER
1	D	177	ILE
1	D	184	CYS
1	D	188	ARG
1	D	196	ASN
1	D	206	THR
1	D	208	ASN
1	D	216	ARG
1	D	220	LYS
1	D	225	GLN
1	D	262	LYS
1	D	265	GLN
1	D	289	ASN
1	D	291	LYS
1	D	298	GLN
1	D	299	LYS
1	D	311	GLN
1	D	355	TYR
1	D	424	PHE
1	D	507	LYS
1	D	549	ASN
1	D	572	SER
1	D	623	LEU
1	D	675	ASN
1	D	686	LYS
1	D	757	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	134	GLN
1	B	225	GLN
1	C	54	GLN
1	C	133	ASN
1	C	225	GLN

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Mol	Chain	Res	Type
1	C	253	ASN
1	C	265	GLN
1	C	290	GLN
1	D	187	ASN
1	D	258	ASN
1	D	437	HIS

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	752/760 (98%)	-0.13	25 (3%)	46	46	25, 36, 56, 81	0
1	B	751/760 (98%)	-0.26	22 (2%)	51	52	22, 34, 54, 86	0
1	C	719/760 (94%)	0.55	95 (13%)	3	2	36, 56, 96, 110	0
1	D	677/760 (89%)	0.50	90 (13%)	3	2	30, 52, 89, 122	0
All	All	2899/3040 (95%)	0.15	232 (8%)	12	12	22, 43, 84, 122	0

All (232) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	219	LEU	7.3
1	C	355[A]	TYR	6.2
1	C	226	LEU	6.1
1	D	128	PHE	6.0
1	D	8	TYR	6.0
1	D	213	SER	5.4
1	D	226	LEU	5.0
1	D	566	GLU	4.8
1	C	204	THR	4.8
1	C	2	ILE	4.8
1	C	97	ILE	4.8
1	D	26	SER	4.8
1	A	355[A]	TYR	4.8
1	D	207	THR	4.7
1	C	169	LEU	4.6
1	C	187	ASN	4.6
1	C	202	VAL	4.6
1	C	214	VAL	4.6
1	C	237	LEU	4.6
1	C	251	VAL	4.5
1	D	198	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	224	TYR	4.5
1	C	243	LYS	4.3
1	D	46	PHE	4.3
1	C	350	TRP	4.3
1	D	195	GLY	4.3
1	D	189	VAL	4.2
1	D	214	VAL	4.1
1	D	23	PRO	4.1
1	D	200	LEU	4.1
1	C	201	THR	4.1
1	B	2	ILE	4.0
1	A	623	LEU	4.0
1	A	670	ALA	4.0
1	D	569	PRO	4.0
1	A	2	ILE	4.0
1	C	198	ILE	3.9
1	D	2	ILE	3.9
1	C	199	GLY	3.8
1	D	212	THR	3.8
1	D	573	HIS	3.8
1	C	667	THR	3.7
1	D	285	LEU	3.7
1	A	1	MET	3.7
1	D	116	ILE	3.7
1	D	283	ALA	3.6
1	C	192	PHE	3.6
1	C	623	LEU	3.6
1	D	9	LEU	3.5
1	D	757	LEU	3.5
1	D	221	GLU	3.4
1	D	571	TYR	3.4
1	D	623	LEU	3.4
1	C	129	THR	3.4
1	D	44	ALA	3.4
1	C	670	ALA	3.3
1	D	91	PHE	3.3
1	D	222	ASP	3.3
1	A	100	ASP	3.3
1	C	596	LEU	3.3
1	D	68	LEU	3.3
1	C	168	LYS	3.2
1	D	199	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	92	PHE	3.2
1	D	253	ASN	3.2
1	A	667	THR	3.2
1	D	127	THR	3.1
1	D	24	ASP	3.1
1	C	336	ALA	3.1
1	D	21	PHE	3.1
1	C	666	MET	3.1
1	C	207	THR	3.1
1	B	569	PRO	3.0
1	C	89	VAL	3.0
1	B	355	TYR	3.0
1	C	250	TYR	3.0
1	D	670	ALA	3.0
1	C	356	CYS	3.0
1	C	132	THR	3.0
1	C	161	SER	3.0
1	D	564	LYS	3.0
1	C	354	THR	3.0
1	C	19	ASN	2.9
1	D	210	THR	2.9
1	A	666	MET	2.9
1	C	349	PHE	2.9
1	C	203	LYS	2.9
1	C	139	ILE	2.9
1	C	262	LYS	2.9
1	C	344	TYR	2.9
1	D	192	PHE	2.9
1	B	623	LEU	2.9
1	B	670	ALA	2.9
1	A	350	TRP	2.9
1	C	112	ASP	2.9
1	D	356	CYS	2.8
1	D	666	MET	2.8
1	C	206	THR	2.8
1	D	572	SER	2.8
1	C	671	ALA	2.8
1	D	181	GLY	2.8
1	D	16	ILE	2.8
1	D	92	PHE	2.8
1	D	117	LEU	2.8
1	C	566	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	17	VAL	2.8
1	D	27	MET	2.8
1	C	138	LYS	2.8
1	C	194	ILE	2.8
1	B	483	VAL	2.8
1	C	176	ASN	2.8
1	D	125	GLN	2.8
1	C	247	ILE	2.8
1	C	260	ASN	2.7
1	D	280	PHE	2.7
1	C	68	LEU	2.7
1	B	621	SER	2.7
1	B	669	ILE	2.7
1	D	197	SER	2.7
1	A	351[A]	ASP	2.7
1	D	69	LYS	2.7
1	D	563	ILE	2.7
1	C	210	THR	2.7
1	D	596	LEU	2.7
1	D	667	THR	2.7
1	D	215	MET	2.7
1	A	334	ILE	2.6
1	D	354	THR	2.6
1	D	350	TRP	2.6
1	C	522	LYS	2.6
1	A	349	PHE	2.6
1	C	66	TYR	2.6
1	C	352	ASN	2.6
1	C	387[A]	LYS	2.6
1	D	336	ALA	2.6
1	B	356	CYS	2.6
1	B	666	MET	2.6
1	A	336	ALA	2.6
1	C	222	ASP	2.6
1	D	284	ASP	2.6
1	A	343	ALA	2.6
1	D	194	ILE	2.6
1	D	29	SER	2.5
1	D	269	ILE	2.5
1	A	565	ASP	2.5
1	B	336	ALA	2.5
1	C	627	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	20	ASN	2.5
1	C	595	PHE	2.5
1	C	267	ARG	2.5
1	A	354	THR	2.5
1	D	567	GLU	2.5
1	C	351	ASP	2.5
1	C	533	ARG	2.4
1	C	699	ASN	2.4
1	D	25	LYS	2.4
1	C	259	GLY	2.4
1	C	213	SER	2.4
1	C	127	THR	2.4
1	D	22	HIS	2.4
1	C	357	LEU	2.4
1	B	667	THR	2.4
1	C	238	THR	2.4
1	D	627	ILE	2.4
1	B	596	LEU	2.4
1	D	144	LEU	2.4
1	B	351	ASP	2.4
1	B	565	ASP	2.4
1	C	81	ARG	2.4
1	D	568	MET	2.4
1	C	51	SER	2.4
1	A	627	ILE	2.3
1	D	355	TYR	2.3
1	C	205	LEU	2.3
1	C	244	GLU	2.3
1	B	354	THR	2.3
1	C	646	GLY	2.3
1	C	488	TYR	2.3
1	D	153	ALA	2.3
1	A	596	LEU	2.3
1	C	215	MET	2.3
1	D	19	ASN	2.3
1	A	668	SER	2.3
1	D	152	ASN	2.3
1	A	621	SER	2.3
1	D	206	THR	2.2
1	C	620	GLU	2.2
1	D	184	CYS	2.2
1	C	69	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	186	TRP	2.2
1	A	344	TYR	2.2
1	C	492	MET	2.2
1	C	730	LYS	2.2
1	D	204	THR	2.2
1	D	182	SER	2.2
1	B	350	TRP	2.2
1	A	669	ILE	2.2
1	B	664	ILE	2.2
1	A	624	SER	2.2
1	B	720	LYS	2.2
1	C	211	LEU	2.2
1	C	159	PHE	2.2
1	C	225	GLN	2.2
1	B	334	ILE	2.2
1	C	197	SER	2.2
1	C	425	TYR	2.1
1	B	349	PHE	2.1
1	C	24	ASP	2.1
1	C	162	ASP	2.1
1	C	565	ASP	2.1
1	D	173	LEU	2.1
1	D	252	THR	2.1
1	C	94	ILE	2.1
1	C	334	ILE	2.1
1	D	4	ILE	2.1
1	C	131	LEU	2.1
1	D	196	ASN	2.1
1	C	173	LEU	2.1
1	D	351	ASP	2.1
1	C	163	ILE	2.1
1	C	514	ILE	2.1
1	C	171	LEU	2.1
1	B	571	TYR	2.1
1	D	276	GLU	2.1
1	D	249	ARG	2.1
1	D	176	ASN	2.0
1	A	335	GLY	2.0
1	D	250	TYR	2.0
1	A	566	GLU	2.0
1	D	273	LYS	2.0
1	C	219	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	265	GLN	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.