



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:52 PM GMT

PDB ID : 1HO1  
Title : CRYSTAL STRUCTURE OF PYRIDOXINE 5'-PHOSPHATE SYNTHASE  
Authors : Garrido-Franco, M.; Laber, B.; Huber, R.; Clausen, T.  
Deposited on : 2000-12-08  
Resolution : 2.00 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  
<http://wwpdb.org/validation/2016/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  
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

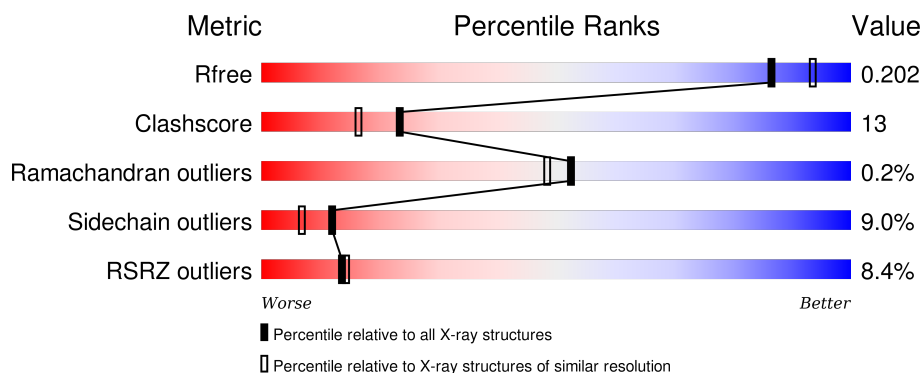
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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. 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	242	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>• •</div> </div> </div>
1	B	242	<div> <div>10%</div> <div> <div></div> <div>69%</div> <div>24%</div> <div>• •</div> </div> </div>
1	C	242	<div> <div>11%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>•</div> </div> </div>
1	D	242	<div> <div>9%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div>5%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7937 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 PYRIDOXINE 5'-PHOSPHATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	0	0	0
			1774	1101	325	336	12			
1	B	235	Total	C	N	O	S	0	0	0
			1778	1103	325	338	12			
1	C	242	Total	C	N	O	S	0	0	0
			1805	1120	332	341	12			
1	D	242	Total	C	N	O	S	0	0	0
			1833	1135	336	350	12			

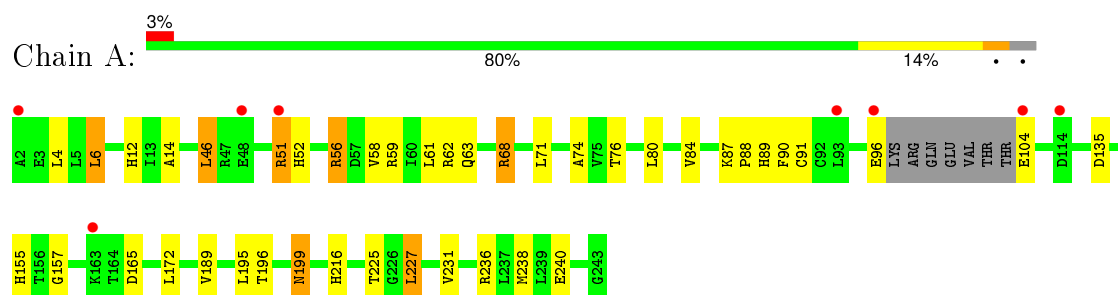
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	199	Total	O	0	0
			199	199		
2	B	170	Total	O	0	0
			170	170		
2	C	194	Total	O	0	0
			194	194		
2	D	184	Total	O	0	0
			184	184		

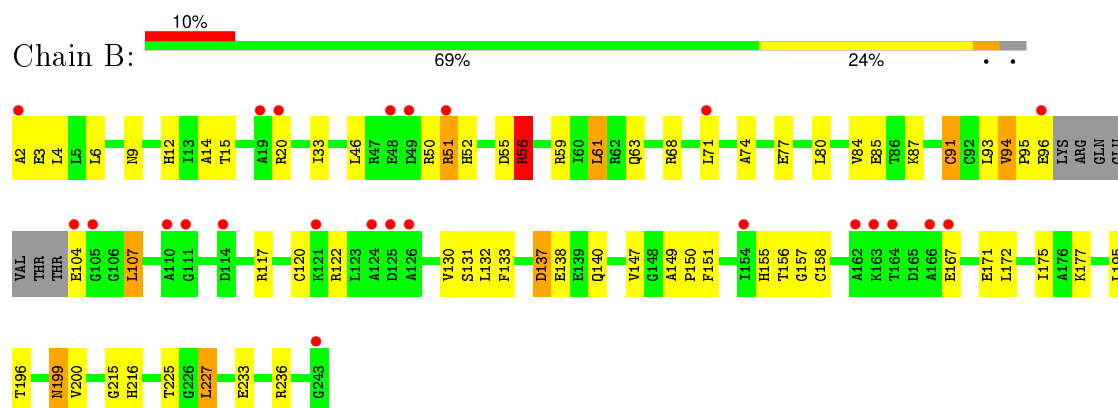
### 3 Residue-property plots [i](#)

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.

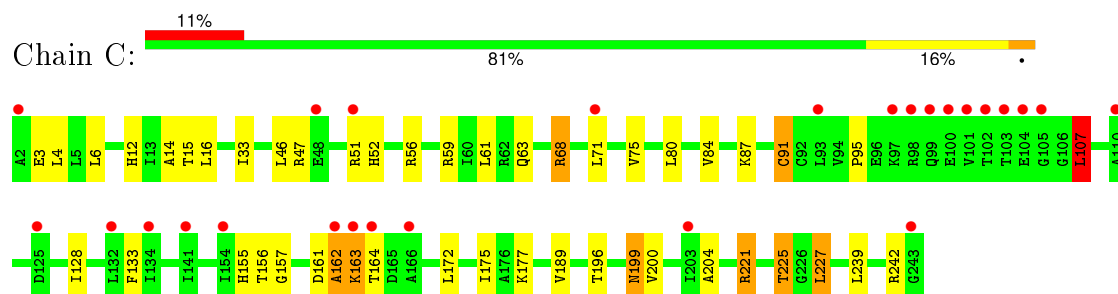
#### • Molecule 1: PYRIDOXINE 5'-PHOSPHATE SYNTHASE



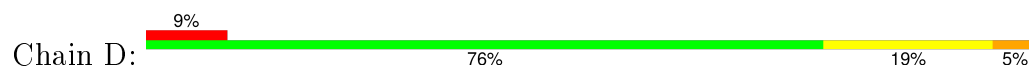
#### • Molecule 1: PYRIDOXINE 5'-PHOSPHATE SYNTHASE

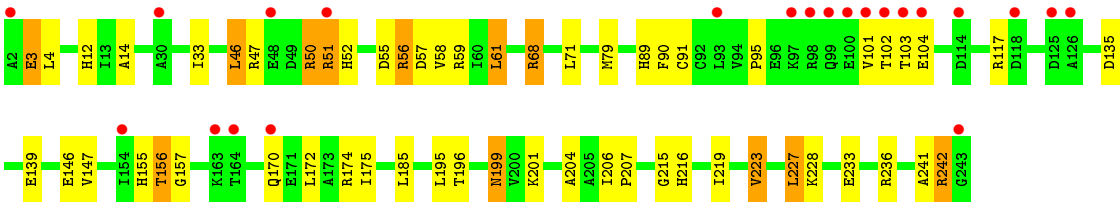


#### • Molecule 1: PYRIDOXINE 5'-PHOSPHATE SYNTHASE



#### • Molecule 1: PYRIDOXINE 5'-PHOSPHATE SYNTHASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.13Å 155.36Å 129.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.97 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.00) 98.4 (19.97-2.00)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.90 (at 2.01Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.206 , 0.253 0.209 , 0.202	Depositor DCC
$R_{free}$ test set	4401 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.3	Xtriage
Anisotropy	0.565	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 63.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 87859 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7937	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.12% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.53	0/1795	0.77	2/2422 (0.1%)
1	B	0.50	0/1799	0.73	2/2427 (0.1%)
1	C	0.52	0/1827	0.76	2/2469 (0.1%)
1	D	0.49	0/1855	0.73	1/2505 (0.0%)
All	All	0.51	0/7276	0.75	7/9823 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	ARG	NE-CZ-NH1	9.16	124.88	120.30
1	A	56	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	D	242	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	B	61	LEU	CA-CB-CG	5.61	128.20	115.30
1	C	221	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	C	107	LEU	CA-CB-CG	5.12	127.06	115.30
1	B	56	ARG	NE-CZ-NH1	5.09	122.84	120.30

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	1774	0	1786	33	0
1	B	1778	0	1790	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1805	0	1797	40	0
1	D	1833	0	1843	59	0
2	A	199	0	0	3	1
2	B	170	0	0	13	1
2	C	194	0	0	5	0
2	D	184	0	0	6	0
All	All	7937	0	7216	192	1

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 13.

All (192) 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:D:95:PRO:HB2	1:D:101:VAL:HG22	1.44	0.99
1:A:59:ARG:HH12	1:C:63:GLN:HE22	1.00	0.96
1:A:63:GLN:HE22	1:C:59:ARG:HH12	1.02	0.95
1:B:80:LEU:O	1:B:84:VAL:HG23	1.75	0.87
1:B:117:ARG:HA	1:B:147:VAL:HG13	1.57	0.86
1:B:33:ILE:HG23	2:B:407:HOH:O	1.75	0.85
1:D:50:ARG:HG3	1:D:50:ARG:HH11	1.40	0.85
1:D:47:ARG:O	1:D:50:ARG:HD2	1.78	0.84
1:B:63:GLN:HE22	1:D:59:ARG:HH12	1.32	0.78
1:B:199:ASN:HD22	1:B:199:ASN:C	1.87	0.76
1:D:12:HIS:CD2	1:D:216:HIS:HD2	2.05	0.74
1:D:47:ARG:NH1	1:D:51:ARG:HD2	2.02	0.74
1:C:199:ASN:C	1:C:199:ASN:HD22	1.92	0.73
1:A:59:ARG:HH12	1:C:63:GLN:NE2	1.83	0.73
1:D:117:ARG:HA	1:D:147:VAL:HG13	1.72	0.72
1:A:68:ARG:HG2	2:A:436:HOH:O	1.91	0.70
1:A:51:ARG:C	1:A:51:ARG:HD2	2.11	0.70
1:D:50:ARG:CG	1:D:50:ARG:HH11	2.04	0.70
1:B:63:GLN:HE22	1:D:59:ARG:NH1	1.91	0.69
1:D:199:ASN:HD22	1:D:199:ASN:C	1.97	0.68
1:A:199:ASN:C	1:A:199:ASN:HD22	1.96	0.68
1:B:12:HIS:CD2	1:B:216:HIS:HD2	2.12	0.68
1:B:155:HIS:CD2	1:B:157:GLY:H	2.12	0.67
1:C:12:HIS:HA	1:C:15:THR:HG23	1.75	0.67
1:A:225:THR:HG22	2:A:266:HOH:O	1.93	0.67
1:C:47:ARG:HH12	1:C:51:ARG:NH2	1.92	0.67
1:D:139:GLU:HG3	2:D:423:HOH:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:ARG:HA	1:D:147:VAL:CG1	2.24	0.67
1:B:225:THR:HG22	2:B:410:HOH:O	1.93	0.66
1:B:15:THR:HA	1:B:51:ARG:NH2	2.11	0.66
1:A:12:HIS:CD2	1:A:216:HIS:HD2	2.14	0.65
1:B:177:LYS:HG3	2:B:360:HOH:O	1.97	0.65
1:A:51:ARG:HD2	1:A:51:ARG:O	1.96	0.64
1:D:196:THR:H	1:D:199:ASN:ND2	1.96	0.64
1:C:155:HIS:CD2	1:C:157:GLY:H	2.16	0.64
1:A:196:THR:H	1:A:199:ASN:ND2	1.97	0.63
1:B:137:ASP:OD2	1:B:140:GLN:HG2	1.99	0.63
1:C:47:ARG:NH1	1:C:51:ARG:NH2	2.45	0.63
1:A:12:HIS:HD2	1:A:216:HIS:HD2	1.46	0.62
1:B:199:ASN:HD22	1:B:200:VAL:N	1.98	0.62
1:D:3:GLU:HA	1:D:3:GLU:OE2	2.00	0.62
1:C:177:LYS:HE3	2:C:357:HOH:O	1.99	0.61
1:B:12:HIS:HD2	1:B:216:HIS:HD2	1.49	0.61
1:C:68:ARG:NE	2:C:411:HOH:O	2.26	0.61
1:B:138:GLU:HG3	2:B:354:HOH:O	2.01	0.61
1:C:3:GLU:OE2	1:C:239:LEU:HD22	2.00	0.61
1:B:130:VAL:O	1:B:150:PRO:HD2	1.99	0.61
1:D:89:HIS:HD2	1:D:90:PHE:CE1	2.18	0.61
1:B:91:CYS:SG	2:B:403:HOH:O	2.56	0.60
1:A:59:ARG:NH1	1:C:63:GLN:HE22	1.84	0.60
1:C:15:THR:HG22	1:C:52:HIS:HB3	1.84	0.60
1:B:156:THR:HG22	1:B:175:ILE:HD13	1.84	0.59
1:D:156:THR:HG22	1:D:175:ILE:HD13	1.83	0.59
1:D:117:ARG:CA	1:D:147:VAL:HG13	2.32	0.59
1:C:91:CYS:HB2	1:C:128:ILE:HG21	1.84	0.59
1:C:80:LEU:O	1:C:84:VAL:HG23	2.03	0.58
1:A:56:ARG:HD2	2:C:365:HOH:O	2.03	0.58
1:A:196:THR:H	1:A:199:ASN:HD21	1.52	0.58
1:D:12:HIS:HD2	1:D:216:HIS:HD2	1.51	0.57
1:B:117:ARG:CA	1:B:147:VAL:HG13	2.32	0.57
1:D:3:GLU:CA	1:D:3:GLU:OE2	2.52	0.57
1:B:12:HIS:HA	1:B:15:THR:HG23	1.86	0.57
1:C:84:VAL:O	1:C:87:LYS:HD2	2.04	0.57
1:A:63:GLN:HE22	1:C:59:ARG:NH1	1.87	0.56
1:B:84:VAL:O	1:B:87:LYS:HD2	2.04	0.56
1:B:63:GLN:NE2	1:D:59:ARG:HH12	2.01	0.56
1:C:47:ARG:NH1	1:C:51:ARG:HH21	2.03	0.56
1:A:155:HIS:CD2	1:A:157:GLY:H	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:THR:HG21	2:C:253:HOH:O	2.05	0.56
1:D:33:ILE:HG21	1:D:227:LEU:HB3	1.88	0.56
1:A:84:VAL:O	1:A:87:LYS:HD2	2.06	0.56
1:C:95:PRO:HG3	1:C:107:LEU:HA	1.88	0.56
1:D:51:ARG:HH11	1:D:51:ARG:HB2	1.70	0.55
1:D:196:THR:H	1:D:199:ASN:HD21	1.53	0.55
1:C:155:HIS:HD2	1:C:157:GLY:H	1.54	0.55
1:B:95:PRO:HG3	1:B:107:LEU:HA	1.89	0.55
1:B:196:THR:H	1:B:199:ASN:ND2	2.05	0.55
1:B:2:ALA:HA	2:B:385:HOH:O	2.04	0.55
1:D:102:THR:HG22	1:D:103:THR:N	2.22	0.54
1:B:15:THR:HA	1:B:51:ARG:HH22	1.71	0.54
1:B:117:ARG:HA	1:B:147:VAL:CG1	2.34	0.54
1:B:104:GLU:O	1:B:104:GLU:HG2	2.08	0.53
1:B:199:ASN:C	1:B:199:ASN:ND2	2.61	0.53
1:B:131:SER:HA	1:B:151:PHE:O	2.10	0.52
1:A:14:ALA:HB3	1:A:52:HIS:HB2	1.90	0.52
1:D:146:GLU:HG2	2:D:314:HOH:O	2.09	0.52
1:B:91:CYS:HB3	2:B:403:HOH:O	2.09	0.52
1:A:80:LEU:O	1:A:84:VAL:HG23	2.09	0.52
1:C:161:ASP:O	1:C:163:LYS:HE2	2.09	0.52
1:A:74:ALA:HB1	1:A:96:GLU:HG3	1.91	0.52
1:B:56:ARG:HD2	2:D:350:HOH:O	2.10	0.52
1:D:101:VAL:HG12	1:D:102:THR:N	2.25	0.52
1:D:50:ARG:N	1:D:50:ARG:CD	2.72	0.52
1:B:77:GLU:CD	1:B:122:ARG:HH12	2.14	0.51
1:B:12:HIS:HD2	1:B:216:HIS:CD2	2.28	0.51
1:B:91:CYS:CB	2:B:403:HOH:O	2.57	0.51
1:D:57:ASP:O	1:D:61:LEU:HB2	2.11	0.51
1:C:204:ALA:O	1:C:242:ARG:HD3	2.10	0.51
1:B:15:THR:HG22	1:B:51:ARG:CZ	2.40	0.51
1:C:161:ASP:O	1:C:162:ALA:C	2.49	0.51
1:B:33:ILE:HG21	1:B:227:LEU:HB3	1.90	0.51
1:D:233:GLU:CD	1:D:236:ARG:HH21	2.15	0.51
1:B:15:THR:HG22	1:B:51:ARG:NH1	2.26	0.50
1:B:196:THR:H	1:B:199:ASN:HD21	1.59	0.50
1:D:117:ARG:NH1	1:D:146:GLU:OE2	2.42	0.50
1:B:15:THR:CB	1:B:51:ARG:HH22	2.24	0.50
1:C:196:THR:H	1:C:199:ASN:ND2	2.10	0.50
1:D:204:ALA:O	1:D:242:ARG:HD3	2.12	0.50
1:A:104:GLU:HB2	1:A:135:ASP:OD1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:ARG:HD3	1:D:56:ARG:C	2.32	0.49
1:B:147:VAL:O	1:B:147:VAL:HG12	2.12	0.49
1:D:102:THR:HG21	1:D:135:ASP:OD2	2.12	0.49
1:D:79:MET:CE	1:D:79:MET:HA	2.42	0.49
1:B:155:HIS:HD2	1:B:157:GLY:H	1.61	0.49
1:C:3:GLU:CD	1:C:239:LEU:HD22	2.33	0.48
1:C:91:CYS:HB2	1:C:128:ILE:CG2	2.42	0.48
1:A:87:LYS:N	1:A:88:PRO:HD3	2.29	0.48
1:B:233:GLU:CD	1:B:236:ARG:HH21	2.16	0.48
1:D:14:ALA:HB3	1:D:52:HIS:HB2	1.95	0.48
1:A:6:LEU:HG	1:A:238:MET:SD	2.54	0.48
1:C:199:ASN:C	1:C:199:ASN:ND2	2.65	0.48
1:D:195:LEU:HA	1:D:199:ASN:HD21	1.78	0.48
1:D:102:THR:HG22	1:D:104:GLU:H	1.78	0.48
1:C:196:THR:H	1:C:199:ASN:HD21	1.62	0.47
1:B:59:ARG:NH2	2:B:340:HOH:O	2.47	0.47
1:B:120:CYS:HB3	2:B:278:HOH:O	2.14	0.47
1:D:147:VAL:HG12	1:D:147:VAL:O	2.13	0.47
1:D:242:ARG:NH2	2:D:418:HOH:O	2.45	0.47
1:C:163:LYS:HD2	1:C:163:LYS:H	1.80	0.47
1:B:131:SER:HB2	1:B:151:PHE:HB2	1.97	0.47
1:D:206:ILE:HA	1:D:207:PRO:HD3	1.80	0.47
1:B:12:HIS:CD2	1:B:216:HIS:CD2	2.97	0.46
1:A:62:ARG:HD2	2:A:428:HOH:O	2.15	0.46
1:D:47:ARG:NH2	1:D:51:ARG:NH1	2.63	0.46
1:D:50:ARG:CG	1:D:50:ARG:NH1	2.70	0.46
1:D:102:THR:CG2	1:D:103:THR:N	2.78	0.45
1:D:50:ARG:HH12	1:D:55:ASP:CG	2.19	0.45
1:C:47:ARG:CZ	1:C:51:ARG:HH21	2.29	0.45
1:B:74:ALA:HB2	1:B:96:GLU:HB2	1.97	0.45
1:D:104:GLU:OE2	1:D:174:ARG:NH2	2.50	0.45
1:B:107:LEU:HB2	1:B:133:PHE:O	2.17	0.45
1:D:219:ILE:O	1:D:223:VAL:HG23	2.16	0.45
1:A:46:LEU:HG	1:A:58:VAL:HG21	1.98	0.45
1:B:225:THR:CG2	2:B:251:HOH:O	2.65	0.45
1:B:51:ARG:C	1:B:51:ARG:HE	2.20	0.44
1:B:147:VAL:CG1	1:B:147:VAL:O	2.64	0.44
1:C:163:LYS:HD2	1:C:163:LYS:N	2.32	0.44
1:C:14:ALA:HB3	1:C:52:HIS:HB2	2.00	0.44
1:D:155:HIS:CD2	1:D:157:GLY:H	2.34	0.44
1:B:9:ASN:HB3	1:B:215:GLY:HA3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LEU:HA	1:A:199:ASN:HD21	1.82	0.44
1:B:14:ALA:HB3	1:B:52:HIS:HB2	1.99	0.44
1:B:94:VAL:HG12	1:B:95:PRO:O	2.17	0.44
1:D:56:ARG:HD2	1:D:57:ASP:OD2	2.18	0.44
1:A:199:ASN:C	1:A:199:ASN:ND2	2.69	0.43
1:A:12:HIS:HD2	1:A:216:HIS:CD2	2.30	0.43
1:B:195:LEU:HA	1:B:199:ASN:HD21	1.83	0.43
1:D:46:LEU:HG	1:D:58:VAL:HG21	2.00	0.43
1:D:56:ARG:HD3	1:D:57:ASP:N	2.33	0.43
1:C:199:ASN:HD22	1:C:200:VAL:N	2.17	0.43
1:A:76:THR:O	1:A:80:LEU:HG	2.19	0.43
1:B:20:ARG:O	1:B:20:ARG:HG3	2.18	0.43
1:D:95:PRO:CB	1:D:101:VAL:HG22	2.31	0.43
1:B:104:GLU:CG	1:B:158:CYS:SG	3.07	0.42
1:A:236:ARG:NH1	1:A:240:GLU:OE2	2.49	0.42
1:B:15:THR:CA	1:B:51:ARG:HH22	2.30	0.42
1:C:47:ARG:NH2	1:C:51:ARG:HH21	2.17	0.42
1:A:227:LEU:HD22	1:A:231:VAL:HG23	2.01	0.42
1:B:74:ALA:HA	1:B:94:VAL:O	2.19	0.42
1:D:117:ARG:NH2	1:D:146:GLU:OE2	2.53	0.42
1:B:149:ALA:HA	1:B:150:PRO:HD3	1.90	0.42
1:C:156:THR:HG22	1:C:175:ILE:HD13	2.02	0.42
1:B:50:ARG:HE	1:B:55:ASP:CG	2.22	0.42
1:D:201:LYS:HG2	1:D:241:ALA:HB2	2.00	0.42
1:C:75:VAL:HG23	2:C:382:HOH:O	2.20	0.42
1:C:12:HIS:HA	1:C:15:THR:CG2	2.48	0.42
1:D:68:ARG:HG2	2:D:365:HOH:O	2.19	0.42
1:A:89:HIS:HD2	1:A:90:PHE:CE1	2.38	0.41
1:B:15:THR:HB	1:B:51:ARG:HH22	1.85	0.41
1:A:12:HIS:CD2	1:A:216:HIS:CD2	3.02	0.41
1:C:33:ILE:HG21	1:C:227:LEU:HB3	2.02	0.41
1:D:228:LYS:HE2	1:D:228:LYS:HB3	1.81	0.41
1:D:89:HIS:CD2	1:D:90:PHE:CE1	3.05	0.41
1:B:167:GLU:O	1:B:171:GLU:HG2	2.21	0.41
1:B:150:PRO:HG3	2:B:372:HOH:O	2.21	0.40
1:D:50:ARG:N	1:D:50:ARG:HD2	2.36	0.40
1:D:51:ARG:HH11	1:D:51:ARG:CB	2.34	0.40
1:D:68:ARG:NH1	2:D:388:HOH:O	2.54	0.40
1:B:46:LEU:HD11	1:B:50:ARG:CZ	2.51	0.40
1:B:177:LYS:HE3	2:B:360:HOH:O	2.21	0.40
1:C:107:LEU:HB2	1:C:133:PHE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:LEU:HD12	1:B:132:LEU:CD2	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:295:HOH:O	2:B:341:HOH:O[4_555]	2.10	0.10

## 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	231/242 (96%)	222 (96%)	9 (4%)	0	100	100
1	B	231/242 (96%)	225 (97%)	6 (3%)	0	100	100
1	C	240/242 (99%)	232 (97%)	7 (3%)	1 (0%)	39	33
1	D	240/242 (99%)	230 (96%)	9 (4%)	1 (0%)	39	33
All	All	942/968 (97%)	909 (96%)	31 (3%)	2 (0%)	52	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	162	ALA
1	D	215	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	177/185 (96%)	164 (93%)	13 (7%)	17	11
1	B	178/185 (96%)	162 (91%)	16 (9%)	12	7
1	C	176/185 (95%)	158 (90%)	18 (10%)	9	5
1	D	184/185 (100%)	167 (91%)	17 (9%)	11	6
All	All	715/740 (97%)	651 (91%)	64 (9%)	12	7

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	6	LEU
1	A	46	LEU
1	A	51	ARG
1	A	61	LEU
1	A	68	ARG
1	A	71	LEU
1	A	91	CYS
1	A	165	ASP
1	A	172	LEU
1	A	189	VAL
1	A	199	ASN
1	A	227	LEU
1	B	3	GLU
1	B	4	LEU
1	B	6	LEU
1	B	51	ARG
1	B	56	ARG
1	B	61	LEU
1	B	68	ARG
1	B	71	LEU
1	B	85	GLU
1	B	91	CYS
1	B	94	VAL
1	B	107	LEU
1	B	137	ASP
1	B	172	LEU
1	B	199	ASN
1	B	227	LEU
1	C	4	LEU

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Mol	Chain	Res	Type
1	C	6	LEU
1	C	16	LEU
1	C	46	LEU
1	C	56	ARG
1	C	61	LEU
1	C	68	ARG
1	C	71	LEU
1	C	91	CYS
1	C	107	LEU
1	C	163	LYS
1	C	164	THR
1	C	172	LEU
1	C	189	VAL
1	C	199	ASN
1	C	221	ARG
1	C	225	THR
1	C	227	LEU
1	D	3	GLU
1	D	4	LEU
1	D	46	LEU
1	D	50	ARG
1	D	51	ARG
1	D	56	ARG
1	D	61	LEU
1	D	68	ARG
1	D	71	LEU
1	D	91	CYS
1	D	156	THR
1	D	170	GLN
1	D	172	LEU
1	D	185	LEU
1	D	199	ASN
1	D	223	VAL
1	D	227	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	63	GLN
1	A	89	HIS
1	A	155	HIS

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Mol	Chain	Res	Type
1	A	199	ASN
1	A	216	HIS
1	B	12	HIS
1	B	63	GLN
1	B	89	HIS
1	B	155	HIS
1	B	193	HIS
1	B	199	ASN
1	B	216	HIS
1	C	63	GLN
1	C	89	HIS
1	C	155	HIS
1	C	199	ASN
1	D	12	HIS
1	D	63	GLN
1	D	89	HIS
1	D	155	HIS
1	D	199	ASN
1	D	216	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 carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 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, 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	235/242 (97%)	0.13	8 (3%) 49 50	19, 33, 56, 87	0
1	B	235/242 (97%)	0.42	24 (10%) 9 9	22, 39, 63, 87	0
1	C	242/242 (100%)	0.57	26 (10%) 8 8	21, 36, 62, 94	0
1	D	242/242 (100%)	0.41	22 (9%) 11 12	21, 36, 62, 88	0
All	All	954/968 (98%)	0.38	80 (8%) 14 14	19, 36, 62, 94	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	103	THR	12.1
1	C	104	GLU	8.3
1	C	102	THR	8.3
1	C	99	GLN	8.3
1	D	103	THR	8.0
1	C	98	ARG	7.3
1	B	104	GLU	7.0
1	C	101	VAL	6.9
1	B	2	ALA	6.6
1	C	97	LYS	6.4
1	D	101	VAL	6.3
1	D	2	ALA	6.2
1	D	98	ARG	5.9
1	C	100	GLU	5.8
1	D	104	GLU	5.5
1	A	104	GLU	5.3
1	A	96	GLU	4.4
1	B	163	LYS	4.4
1	D	97	LYS	4.3
1	C	2	ALA	4.3
1	A	48	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	105	GLY	4.1
1	D	102	THR	4.1
1	D	164	THR	4.1
1	C	243	GLY	3.9
1	C	166	ALA	3.9
1	D	126	ALA	3.8
1	D	99	GLN	3.7
1	C	105	GLY	3.6
1	C	163	LYS	3.5
1	B	48	GLU	3.3
1	B	162	ALA	3.3
1	B	125	ASP	3.3
1	D	163	LYS	3.2
1	B	96	GLU	3.2
1	B	154	ILE	3.2
1	B	114	ASP	3.2
1	C	48	GLU	3.1
1	A	2	ALA	3.1
1	D	48	GLU	3.1
1	D	100	GLU	3.1
1	D	243	GLY	3.0
1	B	111	GLY	2.9
1	C	125	ASP	2.9
1	B	110	ALA	2.9
1	D	93	LEU	2.8
1	C	51	ARG	2.8
1	C	71	LEU	2.8
1	A	93	LEU	2.7
1	B	164	THR	2.7
1	C	93	LEU	2.6
1	A	163	LYS	2.5
1	D	125	ASP	2.5
1	B	124	ALA	2.5
1	B	166	ALA	2.5
1	B	167	GLU	2.4
1	B	51	ARG	2.4
1	A	114	ASP	2.4
1	C	132	LEU	2.4
1	B	126	ALA	2.4
1	D	114	ASP	2.4
1	B	20	ARG	2.4
1	C	164	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	118	ASP	2.3
1	D	51	ARG	2.3
1	C	162	ALA	2.3
1	C	203	ILE	2.3
1	B	19	ALA	2.2
1	D	30	ALA	2.2
1	B	121	LYS	2.2
1	B	71	LEU	2.2
1	C	134	ILE	2.1
1	D	170	GLN	2.1
1	B	243	GLY	2.1
1	C	154	ILE	2.0
1	C	141	ILE	2.0
1	C	110	ALA	2.0
1	A	51	ARG	2.0
1	B	49	ASP	2.0
1	D	154	ILE	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.