Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 07:33 pm BST

PDB ID	:	6KD3
Title	:	Structural and catalytic analysis of two diverse uridine phosphorylases in the oomycete Phytophthora capsici.
Authors	:	Yang, C.C.; Zhang, X.G.
Deposited on	:	2019-06-30
Resolution	:	2.76 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 following versions of software and data (see references ⓘ) were used in the production of this report:

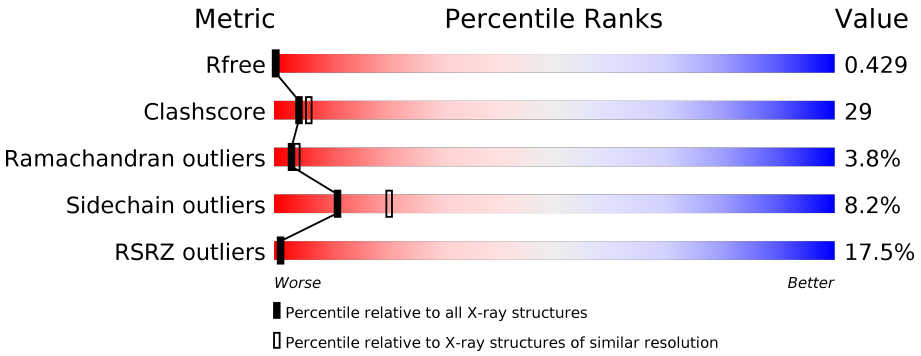
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 >=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 <=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	322	12% 49% 38% 9%
1	B	322	20% 59% 29% 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3894 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 Uridine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			1916	1202	338	367	9			
1	B	294	Total	C	N	O	S	0	0	0
			1916	1202	338	367	9			

- Molecule 2 is water.

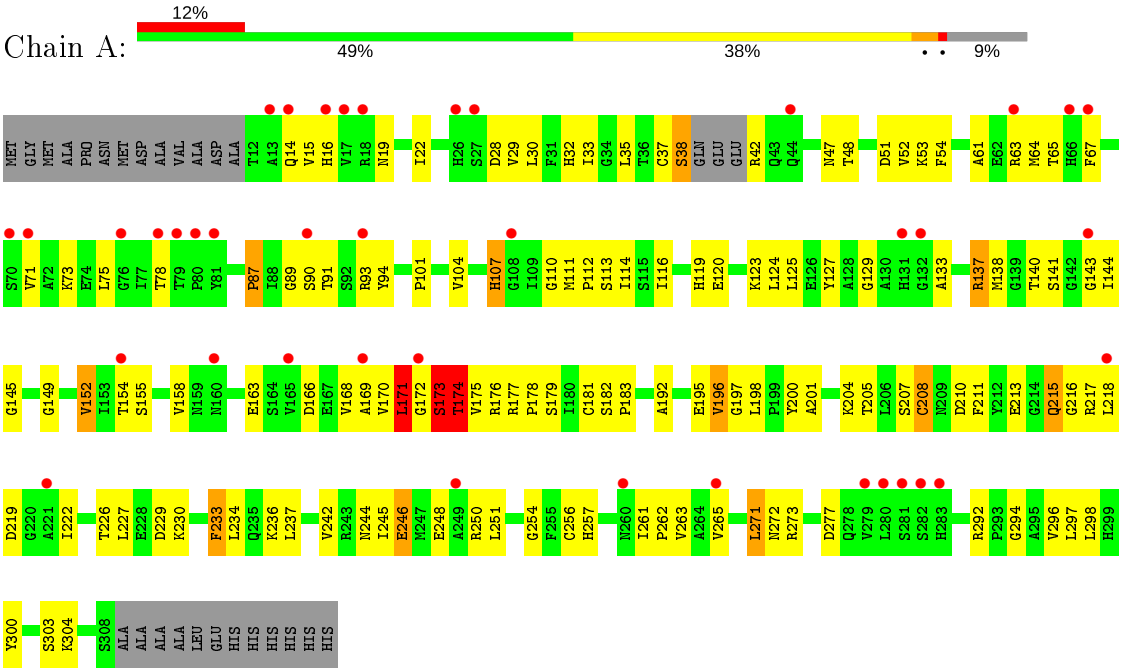
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	30	Total	O	0	0
			30	30		
2	B	32	Total	O	0	0
			32	32		

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.

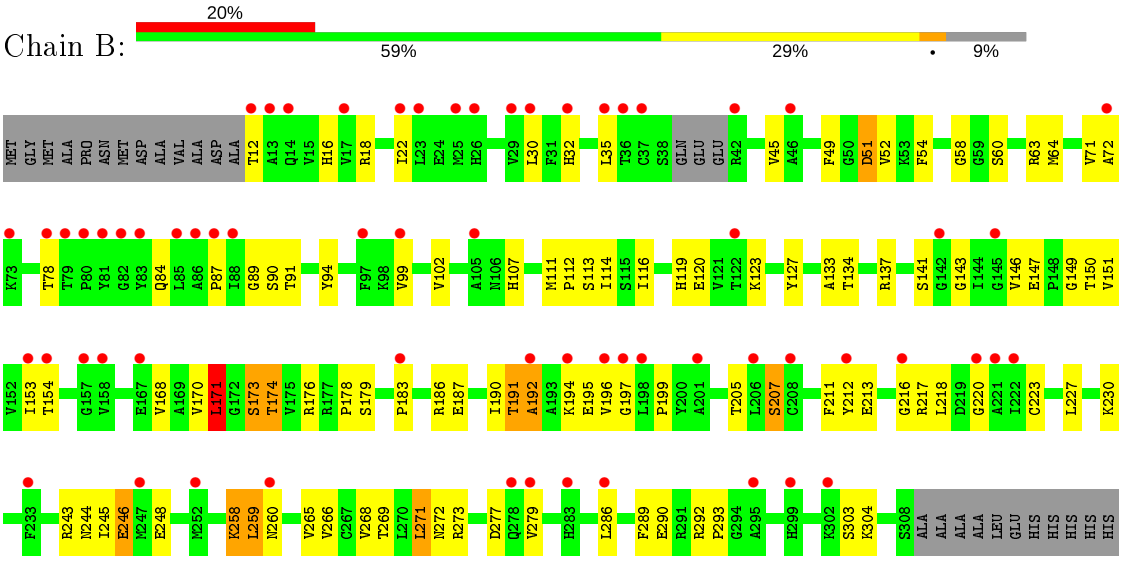
- Molecule 1: Uridine phosphorylase

Chain A:



- Molecule 1: Uridine phosphorylase

Chain B:



HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	105.84Å 66.39Å 261.06Å 90.00° 96.77° 90.00°	Depositor
Resolution (Å)	47.45 – 2.76 47.45 – 2.76	Depositor EDS
% Data completeness (in resolution range)	67.8 (47.45-2.76) 56.3 (47.45-2.76)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.386 , 0.428 0.387 , 0.429	Depositor DCC
R_{free} test set	1585 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	44.0	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 52.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.61	EDS
Total number of atoms	3894	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.51	0/1930	0.73	2/2596 (0.1%)
1	B	0.45	0/1930	0.76	5/2596 (0.2%)
All	All	0.48	0/3860	0.75	7/5192 (0.1%)

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
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	173	SER	N-CA-C	8.58	134.18	111.00
1	B	174	THR	N-CA-C	8.22	133.19	111.00
1	B	171	LEU	CA-CB-CG	7.47	132.48	115.30
1	B	271	LEU	CA-CB-CG	6.52	130.30	115.30
1	B	243	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	A	173	SER	N-CA-C	5.80	126.65	111.00
1	A	174	THR	N-CA-C	5.55	125.99	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	216	GLY	Peptide
1	B	192	ALA	Peptide

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	1916	0	1640	118	0
1	B	1916	0	1640	99	0
2	A	30	0	0	26	0
2	B	32	0	0	16	0
All	All	3894	0	3280	205	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 29.

All (205) 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:217:ARG:HG2	1:B:273:ARG:HH22	1.27	0.96
1:A:256:CYS:O	2:A:402:HOH:O	1.91	0.89
1:A:263:VAL:O	2:A:401:HOH:O	1.91	0.88
1:A:213:GLU:O	2:A:403:HOH:O	1.93	0.86
1:A:170:VAL:O	1:A:172:GLY:N	2.12	0.82
1:A:170:VAL:C	1:A:172:GLY:H	1.83	0.82
1:B:147:GLU:OE1	2:B:401:HOH:O	1.98	0.81
1:A:37:CYS:O	1:A:42:ARG:N	2.14	0.81
1:B:150:THR:HA	1:B:199:PRO:HB2	1.63	0.81
1:A:51:ASP:O	2:A:404:HOH:O	1.98	0.81
1:B:30:LEU:HD23	1:B:120:GLU:HB2	1.64	0.80
1:A:127:TYR:O	2:A:405:HOH:O	2.00	0.79
1:A:155:SER:O	2:A:406:HOH:O	2.00	0.79
1:A:195:GLU:O	2:A:407:HOH:O	2.00	0.79
1:B:217:ARG:HG2	1:B:273:ARG:NH2	1.98	0.79
1:A:215:GLN:OE1	2:A:408:HOH:O	2.01	0.79
1:A:94:TYR:OH	1:A:113:SER:O	2.00	0.78
1:A:196:VAL:N	2:A:411:HOH:O	2.16	0.78
1:B:90:SER:O	2:B:403:HOH:O	2.02	0.78
1:A:168:VAL:O	1:A:173:SER:O	2.04	0.76
1:B:245:ILE:HD12	1:B:273:ARG:HD3	1.68	0.75
1:A:179:SER:O	2:A:409:HOH:O	2.05	0.75
1:A:230:LYS:NZ	1:A:277:ASP:OD2	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:GLN:O	1:A:273:ARG:NH2	2.20	0.75
1:B:147:GLU:O	2:B:404:HOH:O	2.04	0.74
1:B:119:HIS:NE2	2:B:407:HOH:O	2.19	0.74
1:B:271:LEU:HD12	1:B:273:ARG:HG2	1.68	0.73
1:A:222:ILE:HA	1:B:18:ARG:HB2	1.71	0.72
1:A:192:ALA:O	2:A:411:HOH:O	2.07	0.71
1:A:48:THR:O	2:A:414:HOH:O	2.09	0.71
1:A:179:SER:OG	2:A:413:HOH:O	2.09	0.71
2:A:403:HOH:O	1:B:171:LEU:HG	1.90	0.70
1:B:149:GLY:H	1:B:269:THR:HG23	1.55	0.70
1:A:226:THR:OG1	1:A:229:ASP:OD2	2.08	0.70
1:A:141:SER:OG	1:A:244:ASN:ND2	2.25	0.69
1:A:28:ASP:N	1:A:37:CYS:SG	2.62	0.69
1:A:107:HIS:HE1	1:A:248:GLU:HG2	1.56	0.69
1:B:151:VAL:HG22	1:B:268:VAL:HG22	1.75	0.69
1:B:84:GLN:O	2:B:405:HOH:O	2.10	0.68
1:A:32:HIS:ND1	1:A:120:GLU:OE1	2.27	0.68
1:B:170:VAL:HB	1:B:173:SER:HB3	1.75	0.67
1:A:30:LEU:HD12	1:A:124:LEU:HD13	1.77	0.67
1:B:119:HIS:NE2	2:B:411:HOH:O	2.27	0.67
1:A:192:ALA:HB1	1:A:200:TYR:CG	2.30	0.67
1:A:233:PHE:CB	1:B:171:LEU:HD22	2.24	0.67
1:A:137:ARG:NH2	1:A:248:GLU:OE1	2.28	0.66
1:A:33:ILE:O	1:A:89:GLY:N	2.28	0.66
1:B:217:ARG:CG	1:B:273:ARG:HH22	2.07	0.66
1:B:205:THR:OG1	1:B:244:ASN:OD1	2.09	0.65
1:A:158:VAL:HG22	1:A:205:THR:O	1.97	0.65
1:B:192:ALA:O	2:B:406:HOH:O	2.14	0.65
1:A:101:PRO:HB3	2:A:404:HOH:O	1.96	0.65
1:B:271:LEU:O	2:B:402:HOH:O	2.13	0.65
1:B:153:ILE:HG12	1:B:266:VAL:HG22	1.79	0.64
1:A:107:HIS:CE1	1:A:248:GLU:HG2	2.32	0.64
1:A:141:SER:CB	1:A:244:ASN:HD21	2.11	0.64
1:A:233:PHE:O	1:A:236:LYS:N	2.31	0.63
1:B:192:ALA:HA	1:B:195:GLU:HB2	1.80	0.63
1:A:210:ASP:OD2	2:A:415:HOH:O	2.15	0.63
1:A:30:LEU:HD13	1:A:120:GLU:HB3	1.80	0.63
1:B:268:VAL:CG2	1:B:292:ARG:HB2	2.28	0.63
1:B:170:VAL:HG12	1:B:170:VAL:O	1.99	0.63
1:B:187:GLU:OE1	1:B:304:LYS:NZ	2.20	0.62
1:A:35:LEU:HD13	1:A:124:LEU:HD11	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:THR:HG21	2:B:404:HOH:O	1.98	0.62
1:A:64:MET:HB3	1:A:104:VAL:HG12	1.82	0.62
1:A:233:PHE:CG	1:B:171:LEU:HD23	2.35	0.61
1:A:166:ASP:HB2	1:A:250:ARG:HB2	1.81	0.61
1:A:169:ALA:HA	1:A:172:GLY:O	2.00	0.61
1:A:234:LEU:HD21	1:A:273:ARG:HH21	1.65	0.61
1:A:213:GLU:OE1	2:A:415:HOH:O	2.16	0.60
1:A:141:SER:CB	1:A:244:ASN:ND2	2.65	0.60
1:B:72:ALA:HB2	1:B:99:VAL:HG21	1.83	0.60
1:A:211:PHE:O	1:A:217:ARG:HD3	2.03	0.59
1:A:257:HIS:HA	2:A:402:HOH:O	2.01	0.58
1:A:35:LEU:CD1	1:A:124:LEU:HD11	2.33	0.58
1:B:32:HIS:CD2	1:B:116:ILE:HG21	2.38	0.58
1:B:303:SER:OG	1:B:303:SER:O	2.22	0.58
1:B:146:VAL:O	2:B:404:HOH:O	2.17	0.58
1:A:233:PHE:HB2	1:B:171:LEU:HD22	1.83	0.58
1:A:219:ASP:OD1	1:A:219:ASP:N	2.35	0.58
1:B:168:VAL:HG11	1:B:176:ARG:NH1	2.18	0.57
1:B:137:ARG:NH2	1:B:248:GLU:OE1	2.36	0.57
1:B:141:SER:O	1:B:269:THR:HA	2.04	0.57
1:A:137:ARG:NH1	1:A:138:MET:O	2.38	0.56
1:B:211:PHE:CE2	1:B:217:ARG:NH1	2.74	0.56
1:A:37:CYS:SG	1:A:38:SER:N	2.78	0.56
1:A:53:LYS:O	1:A:133:ALA:HA	2.06	0.55
1:A:107:HIS:CG	1:A:114:ILE:HG13	2.42	0.55
1:A:233:PHE:CB	1:B:171:LEU:CD2	2.84	0.55
1:B:143:GLY:O	1:B:272:ASN:HA	2.06	0.55
1:A:32:HIS:HE1	1:B:211:PHE:CZ	2.24	0.55
1:A:257:HIS:CA	2:A:402:HOH:O	2.54	0.54
1:A:149:GLY:O	1:A:292:ARG:NH1	2.40	0.54
1:B:146:VAL:H	1:B:272:ASN:ND2	2.06	0.54
1:A:144:ILE:HD11	1:A:245:ILE:HD11	1.90	0.54
1:A:192:ALA:HB2	1:A:296:VAL:HG11	1.89	0.54
1:B:271:LEU:HD12	1:B:273:ARG:CG	2.38	0.54
1:A:19:ASN:HD22	1:B:223:CYS:HB2	1.74	0.53
1:B:154:THR:HG23	2:B:409:HOH:O	2.08	0.53
1:B:114:ILE:HD12	1:B:248:GLU:HB3	1.89	0.53
1:B:268:VAL:HG21	1:B:292:ARG:HB2	1.90	0.53
1:B:107:HIS:CE1	1:B:248:GLU:OE2	2.62	0.53
1:A:158:VAL:HA	1:A:163:GLU:O	2.08	0.53
1:A:154:THR:OG1	1:A:265:VAL:HB	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:HIS:CE1	2:B:411:HOH:O	2.62	0.52
1:A:179:SER:HA	2:A:406:HOH:O	2.10	0.52
1:B:195:GLU:O	1:B:197:GLY:N	2.42	0.52
1:B:286:LEU:O	1:B:290:GLU:N	2.39	0.52
1:A:67:PHE:CE1	1:A:71:VAL:HB	2.45	0.52
1:A:256:CYS:HB3	1:A:261:ILE:O	2.09	0.52
1:A:32:HIS:HE1	1:B:211:PHE:CE2	2.28	0.52
1:A:170:VAL:C	1:A:171:LEU:HG	2.31	0.51
1:A:257:HIS:C	2:A:402:HOH:O	2.48	0.51
1:B:207:SER:HA	1:B:246:GLU:O	2.11	0.50
1:B:63:ARG:NH1	2:B:412:HOH:O	2.30	0.50
1:B:123:LYS:O	1:B:127:TYR:HD1	1.95	0.50
1:A:181:CYS:N	2:A:401:HOH:O	2.13	0.50
1:A:63:ARG:HH22	1:A:140:THR:HG23	1.77	0.50
1:B:107:HIS:HE1	1:B:248:GLU:OE2	1.95	0.50
1:A:141:SER:HB2	1:A:245:ILE:O	2.12	0.50
1:B:137:ARG:NH1	1:B:248:GLU:HB2	2.26	0.50
1:A:107:HIS:O	1:A:107:HIS:ND1	2.44	0.49
1:B:60:SER:N	2:B:416:HOH:O	2.46	0.49
1:B:137:ARG:HG2	1:B:265:VAL:HG13	1.94	0.49
1:B:71:VAL:HG21	1:B:102:VAL:HG21	1.95	0.49
1:B:168:VAL:HG11	1:B:176:ARG:HH12	1.76	0.49
1:A:273:ARG:NH1	1:A:277:ASP:OD1	2.46	0.49
1:B:51:ASP:OD1	1:B:52:VAL:HG13	2.13	0.48
1:A:218:LEU:HD11	1:A:227:LEU:HB2	1.95	0.48
1:A:177:ARG:O	1:A:254:GLY:HA2	2.13	0.48
1:A:271:LEU:HG	1:A:272:ASN:N	2.27	0.48
1:B:54:PHE:HA	1:B:134:THR:O	2.14	0.48
1:A:218:LEU:HD21	1:A:226:THR:C	2.34	0.47
1:B:154:THR:HA	2:B:409:HOH:O	2.13	0.47
1:A:198:LEU:O	1:A:200:TYR:CG	2.67	0.47
1:B:22:ILE:HG23	1:B:127:TYR:OH	2.14	0.47
1:B:212:TYR:O	1:B:216:GLY:N	2.34	0.47
1:A:304:LYS:HB3	1:A:304:LYS:HE3	1.68	0.47
1:A:233:PHE:CG	1:B:171:LEU:CD2	2.97	0.47
1:A:111:MET:HB2	1:A:112:PRO:HD3	1.96	0.46
1:A:93:ARG:NH2	2:A:420:HOH:O	2.47	0.46
1:B:94:TYR:OH	1:B:113:SER:O	2.30	0.46
1:B:107:HIS:O	1:B:113:SER:OG	2.19	0.46
1:A:120:GLU:O	1:A:124:LEU:HB2	2.16	0.46
1:A:28:ASP:OD1	1:A:29:VAL:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:GLN:O	1:A:16:HIS:N	2.48	0.46
1:B:217:ARG:HG2	1:B:273:ARG:HH12	1.80	0.46
1:A:52:VAL:HA	1:A:101:PRO:HA	1.98	0.46
1:B:191:THR:O	1:B:194:LYS:HB3	2.16	0.46
1:A:54:PHE:CE1	1:A:304:LYS:HD3	2.51	0.46
1:B:89:GLY:O	1:B:91:THR:N	2.48	0.46
1:B:58:GLY:N	1:B:64:MET:SD	2.89	0.45
1:A:110:GLY:HA3	1:B:112:PRO:HB2	1.98	0.45
1:B:72:ALA:C	1:B:78:THR:OG1	2.55	0.45
1:A:125:LEU:O	1:A:129:GLY:N	2.47	0.45
1:A:47:ASN:N	2:A:412:HOH:O	2.08	0.45
1:B:16:HIS:O	1:B:259:LEU:HB3	2.16	0.45
1:B:268:VAL:HG23	1:B:293:PRO:HG3	1.98	0.45
1:A:205:THR:HG23	1:A:244:ASN:O	2.17	0.45
1:B:289:PHE:HA	1:B:292:ARG:HG3	1.98	0.45
1:A:32:HIS:O	1:A:91:THR:OG1	2.34	0.45
1:B:147:GLU:H	1:B:147:GLU:CD	2.20	0.45
1:A:143:GLY:O	1:A:272:ASN:HA	2.17	0.45
1:B:227:LEU:O	1:B:230:LYS:N	2.50	0.45
1:B:22:ILE:HA	1:B:22:ILE:HD13	1.79	0.44
1:A:171:LEU:HD23	1:A:171:LEU:N	2.32	0.44
1:A:218:LEU:HD21	1:A:226:THR:O	2.17	0.44
1:B:186:ARG:O	1:B:190:ILE:N	2.45	0.44
1:A:233:PHE:O	1:A:237:LEU:N	2.47	0.44
1:B:258:LYS:C	1:B:260:ASN:H	2.21	0.44
1:A:204:LYS:HB2	1:A:242:VAL:HA	1.99	0.43
1:A:208:CYS:SG	1:A:215:GLN:NE2	2.92	0.43
1:B:268:VAL:HG22	1:B:292:ARG:HB2	1.98	0.43
1:A:294:GLY:O	1:A:298:LEU:N	2.38	0.43
1:B:51:ASP:OD1	1:B:52:VAL:N	2.50	0.43
1:A:73:LYS:HA	1:A:78:THR:OG1	2.19	0.43
1:A:207:SER:HB2	1:A:246:GLU:OE2	2.19	0.43
1:A:296:VAL:O	1:A:300:TYR:HB3	2.19	0.42
1:B:45:VAL:HA	1:B:49:PHE:HD1	1.83	0.42
1:A:116:ILE:O	1:A:119:HIS:N	2.51	0.42
1:B:218:LEU:HG	1:B:277:ASP:OD2	2.20	0.42
1:B:30:LEU:N	1:B:30:LEU:HD12	2.34	0.42
1:A:42:ARG:NH1	2:A:410:HOH:O	2.07	0.42
1:A:233:PHE:HB3	1:B:171:LEU:CD2	2.50	0.42
1:B:116:ILE:O	1:B:120:GLU:HG2	2.20	0.42
1:B:217:ARG:HG2	1:B:273:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:GLY:O	1:B:273:ARG:NH2	2.53	0.42
1:B:212:TYR:CE2	1:B:217:ARG:NH2	2.88	0.42
1:B:111:MET:HA	1:B:114:ILE:HG22	2.02	0.42
1:A:294:GLY:HA2	1:A:297:LEU:HB3	2.02	0.41
1:A:75:LEU:HD13	2:A:423:HOH:O	2.20	0.41
1:A:152:VAL:HA	1:A:201:ALA:O	2.20	0.41
1:A:35:LEU:HA	1:A:35:LEU:HD23	1.89	0.41
1:B:271:LEU:CD2	1:B:279:VAL:HG22	2.49	0.41
1:B:217:ARG:HD2	1:B:273:ARG:HH12	1.85	0.41
1:B:220:GLY:N	2:B:410:HOH:O	2.53	0.41
1:B:217:ARG:HG2	1:B:273:ARG:CZ	2.49	0.41
1:A:123:LYS:HE2	1:A:123:LYS:HB2	1.84	0.41
1:A:54:PHE:CZ	1:A:304:LYS:HB2	2.56	0.41
1:A:226:THR:HB	1:A:227:LEU:H	1.74	0.40
1:A:94:TYR:OH	1:A:116:ILE:HB	2.22	0.40
1:A:22:ILE:HA	1:A:22:ILE:HD13	1.68	0.40
1:A:145:GLY:N	1:A:272:ASN:OD1	2.49	0.40
1:A:170:VAL:HG13	1:B:213:GLU:HB3	2.04	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	290/322 (90%)	228 (79%)	45 (16%)	17 (6%)	1 1
1	B	290/322 (90%)	249 (86%)	36 (12%)	5 (2%)	9 16
All	All	580/644 (90%)	477 (82%)	81 (14%)	22 (4%)	3 4

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	VAL
1	A	173	SER
1	A	178	PRO
1	B	178	PRO
1	B	196	VAL
1	A	15	VAL
1	A	174	THR
1	A	182	SER
1	A	215	GLN
1	A	251	LEU
1	B	133	ALA
1	B	258	LYS
1	A	61	ALA
1	A	90	SER
1	A	171	LEU
1	A	271	LEU
1	B	259	LEU
1	A	197	GLY
1	A	233	PHE
1	A	107	HIS
1	A	196	VAL
1	A	87	PRO

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	147/262 (56%)	134 (91%)	13 (9%)	10 17
1	B	144/262 (55%)	133 (92%)	11 (8%)	13 23
All	All	291/524 (56%)	267 (92%)	24 (8%)	11 20

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	65	THR

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Mol	Chain	Res	Type
1	A	87	PRO
1	A	137	ARG
1	A	171	LEU
1	A	174	THR
1	A	175	VAL
1	A	176	ARG
1	A	183	PRO
1	A	208	CYS
1	A	246	GLU
1	A	262	PRO
1	A	303	SER
1	B	12	THR
1	B	35	LEU
1	B	51	ASP
1	B	87	PRO
1	B	171	LEU
1	B	174	THR
1	B	179	SER
1	B	183	PRO
1	B	191	THR
1	B	207	SER
1	B	246	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	ASN
1	B	272	ASN

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^{th} 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	294/322 (91%)	0.93	39 (13%)	3 4	12, 24, 46, 66	0
1	B	294/322 (91%)	1.36	64 (21%)	0 0	16, 34, 66, 97	0
All	All	588/644 (91%)	1.14	103 (17%)	1 1	12, 30, 59, 97	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	80	PRO	11.4
1	B	23	LEU	7.8
1	A	16	HIS	7.5
1	B	279	VAL	7.5
1	B	81	TYR	7.1
1	B	87	PRO	6.5
1	A	281	SER	6.2
1	B	83	TYR	6.2
1	B	79	THR	6.1
1	B	25	MET	6.1
1	B	221	ALA	5.8
1	B	26	HIS	5.7
1	A	131	HIS	5.4
1	A	132	GLY	5.3
1	B	105	ALA	5.0
1	B	13	ALA	4.9
1	A	279	VAL	4.6
1	A	79	THR	4.5
1	A	90	SER	4.3
1	B	14	GLN	4.3
1	A	14	GLN	4.3
1	B	252	MET	4.1
1	B	36	THR	4.0
1	B	32	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	143	GLY	3.8
1	A	81	TYR	3.7
1	A	80	PRO	3.7
1	A	282	SER	3.7
1	B	295	ALA	3.7
1	A	218	LEU	3.7
1	B	142	GLY	3.7
1	A	44	GLN	3.5
1	B	22	ILE	3.4
1	B	88	ILE	3.4
1	A	66	HIS	3.4
1	B	196	VAL	3.4
1	B	194	LYS	3.2
1	B	78	THR	3.2
1	B	198	LEU	3.2
1	B	220	GLY	3.1
1	B	46	ALA	3.1
1	A	221	ALA	3.1
1	B	99	VAL	3.0
1	A	78	THR	3.0
1	B	158	VAL	3.0
1	B	183	PRO	3.0
1	B	283	HIS	3.0
1	B	37	CYS	3.0
1	A	169	ALA	2.9
1	B	35	LEU	2.9
1	A	71	VAL	2.9
1	B	12	THR	2.9
1	B	233	PHE	2.8
1	B	72	ALA	2.8
1	B	302	LYS	2.8
1	A	260	ASN	2.8
1	A	13	ALA	2.8
1	A	63	ARG	2.8
1	A	26	HIS	2.7
1	B	85	LEU	2.7
1	B	278	GLN	2.7
1	A	93	ARG	2.7
1	A	280	LEU	2.7
1	B	212	TYR	2.6
1	B	192	ALA	2.6
1	A	76	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	154	THR	2.5
1	B	222	ILE	2.5
1	B	208	CYS	2.5
1	B	247	MET	2.5
1	A	18	ARG	2.5
1	A	160	ASN	2.5
1	B	197	GLY	2.4
1	B	86	ALA	2.4
1	B	30	LEU	2.4
1	B	286	LEU	2.4
1	B	206	LEU	2.3
1	B	260	ASN	2.3
1	B	157	GLY	2.3
1	A	249	ALA	2.3
1	A	17	VAL	2.3
1	B	17	VAL	2.2
1	A	27	SER	2.2
1	B	201	ALA	2.2
1	B	73	LYS	2.2
1	B	153	ILE	2.2
1	A	283	HIS	2.2
1	A	108	GLY	2.2
1	A	165	VAL	2.1
1	A	265	VAL	2.1
1	B	167	GLU	2.1
1	B	42	ARG	2.1
1	B	299	HIS	2.1
1	A	67	PHE	2.1
1	B	145	GLY	2.1
1	B	97	PHE	2.1
1	A	70	SER	2.0
1	A	172	GLY	2.0
1	B	122	THR	2.0
1	B	154	THR	2.0
1	B	216	GLY	2.0
1	B	29	VAL	2.0
1	B	82	GLY	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.