Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2020 – 02:12 PM BST

PDB ID	:	1YVY
Title	:	Crystal structure of Anaerobiospirillum succiniciproducens phosphoenolpyruvate carboxykinase
Authors	:	Cotelesage, J.J.; Prasad, L.; Zeikus, J.G.; Laivenieks, M.; Delbaere, L.T.
Deposited on	:	2005-02-16
Resolution	:	2.35 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:

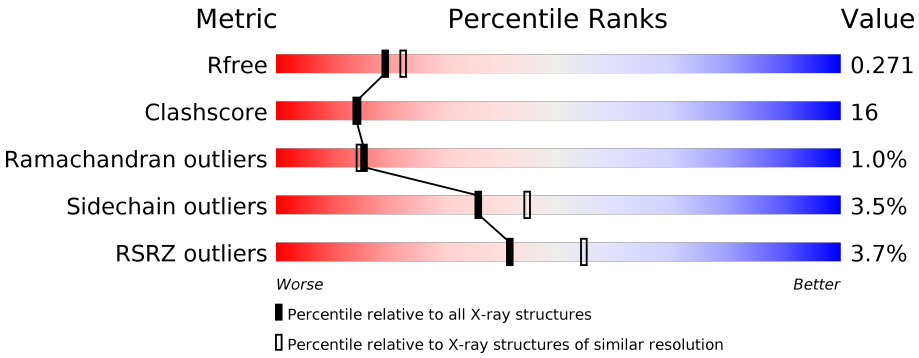
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.14.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.2

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 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	532	4% 64% 29% • 5%
1	B	532	3% 68% 24% • 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7817 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 Phosphoenolpyruvate carboxykinase [ATP].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	507	Total	C	N	O	S	0	0	0
			3815	2450	629	721	15			
1	B	504	Total	C	N	O	S	0	0	0
			3806	2443	633	715	15			

- Molecule 2 is water.

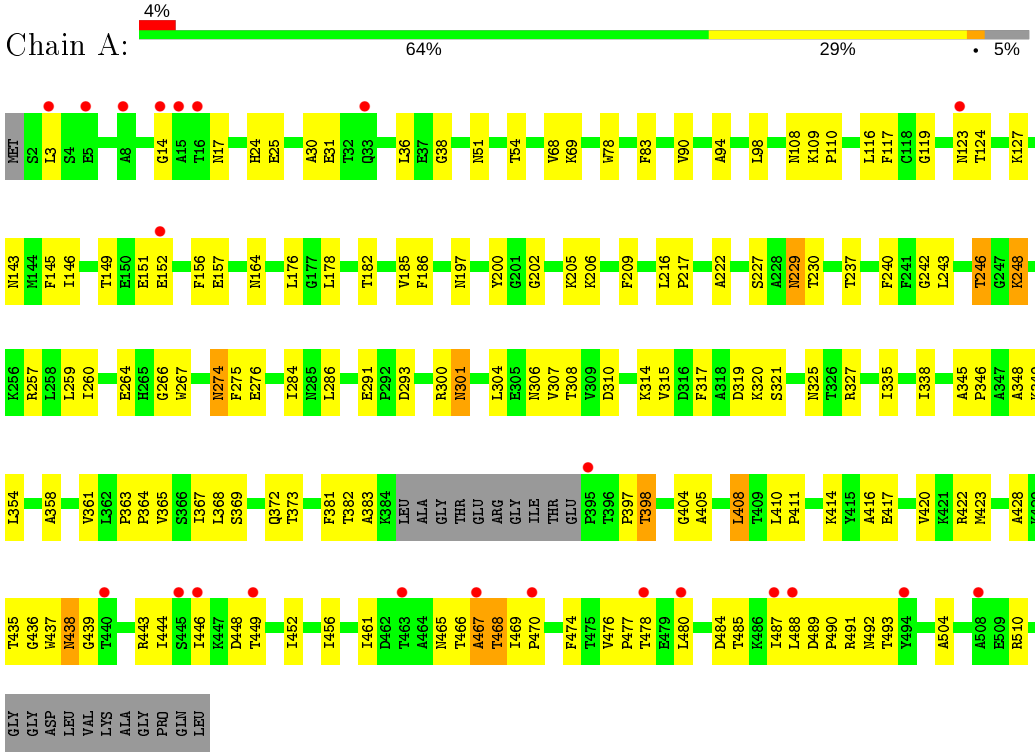
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	91	Total	O	0	0
			91	91		
2	B	105	Total	O	0	0
			105	105		

3 Residue-property plots (i)

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.

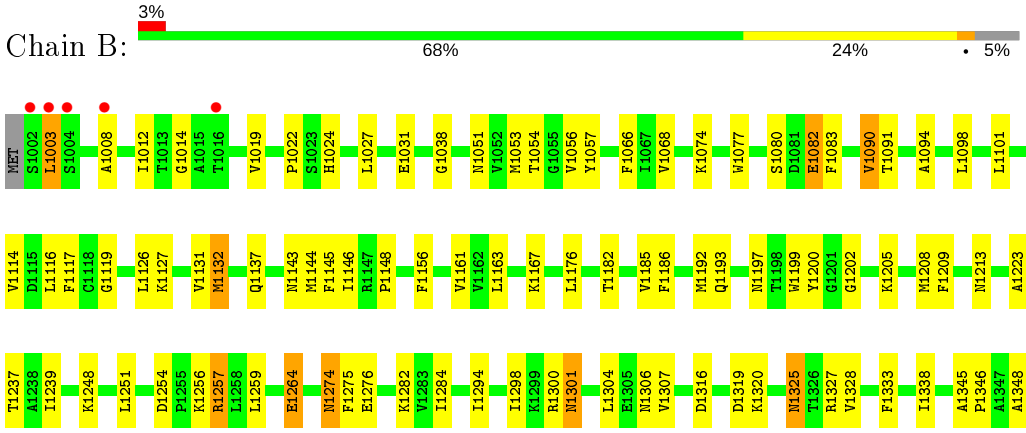
- Molecule 1: Phosphoenolpyruvate carboxykinase [ATP]

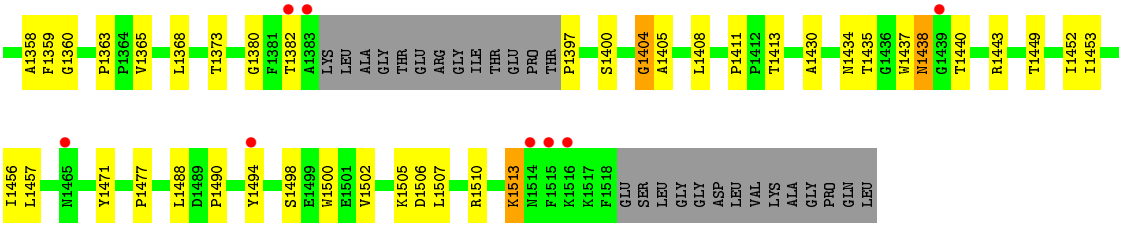
Chain A:



- Molecule 1: Phosphoenolpyruvate carboxykinase [ATP]

Chain B:




A1358
F1359
G1360
P1363
P1364
V1365
L1368
T1373
G1380
F1381
T1382
A1383
LYS
LEU
ALA
GLY
THR
GLU
ARG
GLY
ILE
THR
GLU
PRO
THR
P1397
S1400
G1404
A1405
L1408
P1411
P1412
T1413
A1430
N1434
T1435
G1436
W1437
N1438
G1439
T1440
R1443
T1449
I1452
I1453
I1456
L1457
N1465
Y1471
P1477
L1488
D1489
P1490
Y1494
S1498
E1499
W1500
E1501
V1502
K1505
D1506
L1507
R1510
K1513
N1514
F1515
K1516
K1517
F1518
GLU
SER
LEU
GLY
GLY
ASP
LEU
VAL
LYS
ALA
GLY
PRO
GLN
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	129.66Å 55.73Å 139.40Å 90.00° 93.77° 90.00°	Depositor
Resolution (Å)	10.00 – 2.35 41.75 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.35) 98.3 (41.75-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 2.20Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.221 , 0.263 0.227 , 0.271	Depositor DCC
R_{free} test set	2499 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	43.0	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 48.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7817	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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	0.39	0/3903	0.59	0/5312
1	B	0.40	0/3893	0.60	0/5291
All	All	0.40	0/7796	0.59	0/10603

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3815	0	3647	127	0
1	B	3806	0	3664	106	0
2	A	91	0	0	4	0
2	B	105	0	0	6	0
All	All	7817	0	7311	233	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 16.

All (233) 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:1325:ASN:HD21	1:B:1327:ARG:HE	1.11	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ASN:ND2	1:A:307:VAL:HG22	1.86	0.90
1:A:284:ILE:HD11	1:A:320:LYS:HG2	1.61	0.82
1:A:242:GLY:HA3	1:A:246:THR:HG21	1.60	0.81
1:B:1363:PRO:HB3	1:B:1490:PRO:HD3	1.59	0.81
1:B:1054:THR:H	1:B:1306:ASN:HD21	1.25	0.81
1:B:1325:ASN:ND2	1:B:1327:ARG:HE	1.84	0.76
1:A:485:THR:HA	1:A:488:LEU:HD23	1.69	0.74
1:A:274:ASN:ND2	1:A:276:GLU:H	1.84	0.74
1:B:1345:ALA:HB1	1:B:1346:PRO:HD2	1.69	0.73
1:B:1094:ALA:HA	1:B:1176:LEU:HD22	1.72	0.72
1:A:274:ASN:HD22	1:A:275:PHE:N	1.87	0.72
1:A:368:LEU:HD23	1:A:373:THR:HA	1.72	0.71
1:A:229:ASN:HD22	1:A:229:ASN:C	1.92	0.71
1:A:68:VAL:HA	1:A:90:VAL:HG12	1.70	0.71
1:A:358:ALA:H	1:A:383:ALA:HB3	1.55	0.70
1:A:94:ALA:HA	1:A:176:LEU:HD22	1.75	0.69
1:B:1091:THR:HG21	2:B:83:HOH:O	1.92	0.69
1:B:1068:VAL:HA	1:B:1090:VAL:HG23	1.75	0.68
1:B:1053:MET:HA	1:B:1306:ASN:ND2	2.08	0.68
1:A:127:LYS:HD2	1:A:157:GLU:O	1.93	0.68
1:A:54:THR:H	1:A:306:ASN:HD21	1.40	0.68
1:B:1325:ASN:HD21	1:B:1327:ARG:NE	1.89	0.67
1:B:1205:LYS:HE3	1:B:1276:GLU:OE1	1.94	0.66
1:B:1091:THR:HG23	1:B:1094:ALA:H	1.60	0.65
1:B:1437:TRP:NE1	1:B:1443:ARG:HG2	2.12	0.65
1:A:3:LEU:O	1:A:3:LEU:HD23	1.96	0.64
1:A:51:ASN:HD21	1:A:307:VAL:H	1.44	0.64
1:B:1003:LEU:HD11	1:B:1113:VAL:HG21	1.79	0.64
1:B:1200:TYR:CE2	1:B:1202:GLY:HA3	2.33	0.64
1:B:1229:ASN:ND2	1:B:1257:ARG:HH11	1.95	0.64
1:A:484:ASP:O	1:A:487:ILE:HG22	1.99	0.63
1:A:405:ALA:HA	1:A:408:LEU:HD22	1.81	0.62
1:B:1316:ASP:OD1	1:B:1319:ASP:HB2	1.98	0.62
1:A:149:THR:C	1:A:151:GLU:H	2.02	0.62
1:B:1513:LYS:HB2	1:B:1513:LYS:NZ	2.13	0.62
1:A:363:PRO:HB3	1:A:490:PRO:HD3	1.81	0.62
1:B:1254:ASP:OD1	1:B:1256:LYS:HG2	2.00	0.62
1:A:30:ALA:O	1:A:36:LEU:HD11	2.00	0.62
1:A:308:THR:OG1	1:A:319:ASP:HB3	2.00	0.61
1:B:1506:ASP:O	1:B:1510:ARG:HG2	1.98	0.61
1:A:439:GLY:H	1:A:493:THR:CG2	2.12	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:THR:HA	1:A:474:PHE:O	2.01	0.60
1:A:365:VAL:O	1:A:476:VAL:HG12	2.01	0.60
1:B:1438:ASN:HD22	1:B:1438:ASN:H	1.49	0.60
1:A:243:LEU:O	1:A:246:THR:HB	2.01	0.60
1:B:1057:TYR:HE1	1:B:1182:THR:HG1	1.48	0.60
1:B:1116:LEU:HD13	1:B:1145:PHE:HB2	1.84	0.59
1:A:351:VAL:O	1:A:430:ALA:HA	2.02	0.59
1:A:465:ASN:O	1:A:477:PRO:HA	2.02	0.59
1:A:14:GLY:O	1:A:108:ASN:HA	2.02	0.59
1:A:24:HIS:HB3	1:A:301:ASN:OD1	2.02	0.59
1:A:90:VAL:HG22	1:A:94:ALA:HB3	1.85	0.58
1:A:117:PHE:HE2	1:A:152:GLU:OE1	1.86	0.58
1:B:1051:ASN:ND2	1:B:1307:VAL:HG22	2.19	0.58
1:B:1024:HIS:HE1	1:B:1143:ASN:ND2	2.02	0.57
1:B:1117:PHE:HB2	1:B:1146:ILE:HB	1.85	0.57
1:B:1282:LYS:HE3	1:B:1325:ASN:ND2	2.20	0.56
1:A:345:ALA:HB1	1:A:346:PRO:HD2	1.87	0.56
1:A:350:ARG:HD3	2:A:617:HOH:O	2.05	0.56
1:A:68:VAL:HA	1:A:90:VAL:CG1	2.35	0.56
1:B:1229:ASN:C	1:B:1229:ASN:HD22	2.08	0.56
1:B:1380:GLY:HA3	1:B:1400:SER:O	2.05	0.55
1:B:1274:ASN:ND2	1:B:1276:GLU:H	2.04	0.55
1:B:1498:SER:O	1:B:1502:VAL:HG23	2.07	0.55
1:B:1027:LEU:O	1:B:1031:GLU:HG2	2.07	0.55
1:A:352:ILE:HG13	1:A:352:ILE:O	2.05	0.55
1:A:237:THR:HB	1:A:348:ALA:HA	1.89	0.55
1:B:1351:VAL:O	1:B:1430:ALA:HA	2.08	0.54
1:A:274:ASN:HD22	1:A:275:PHE:H	1.56	0.54
1:B:1167:LYS:HG2	1:B:1199:TRP:CZ2	2.43	0.54
1:B:1054:THR:N	1:B:1306:ASN:HD21	2.02	0.53
1:B:1098:LEU:HD13	1:B:1185:VAL:HG21	1.90	0.53
1:B:1109:LYS:HB2	1:B:1110:PRO:HD2	1.91	0.53
1:A:230:THR:O	1:A:257:ARG:HD3	2.08	0.53
1:B:1513:LYS:HB2	1:B:1513:LYS:HZ2	1.72	0.53
1:A:489:ASP:OD1	1:A:491:ARG:HG3	2.09	0.53
1:B:1182:THR:HA	1:B:1197:ASN:HB3	1.91	0.52
1:A:117:PHE:HB2	1:A:146:ILE:HB	1.91	0.52
1:A:300:ARG:O	1:A:301:ASN:HB2	2.08	0.52
1:B:1251:LEU:HD11	1:B:1435:THR:HG21	1.91	0.52
1:A:489:ASP:HB3	1:A:492:ASN:OD1	2.09	0.52
1:B:1368:LEU:HD23	1:B:1373:THR:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ASP:OD2	1:A:314:LYS:HB3	2.09	0.52
1:B:1300:ARG:O	1:B:1301:ASN:HB2	2.10	0.52
1:A:438:ASN:HB3	1:A:493:THR:HG21	1.91	0.52
1:A:397:PRO:HG3	1:A:510:ARG:HD3	1.92	0.52
1:B:1355:SER:O	1:B:1434:ASN:HA	2.09	0.51
1:B:1358:ALA:HA	1:B:1437:TRP:CE3	2.45	0.51
1:A:286:LEU:HD12	1:A:291:GLU:OE1	2.11	0.51
1:A:467:ALA:O	1:A:468:THR:HB	2.10	0.51
1:B:1057:TYR:HE1	1:B:1182:THR:OG1	1.93	0.51
1:B:1114:VAL:HG12	1:B:1116:LEU:HG	1.92	0.51
1:A:382:THR:HG23	1:A:398:THR:HG23	1.92	0.51
1:B:1453:ILE:O	1:B:1457:LEU:HG	2.11	0.51
1:A:480:LEU:HD12	1:A:488:LEU:HD11	1.93	0.51
1:A:229:ASN:C	1:A:229:ASN:ND2	2.64	0.51
1:A:410:LEU:HB3	1:A:411:PRO:HD2	1.92	0.50
1:A:417:GLU:HG2	2:A:620:HOH:O	2.11	0.50
1:A:51:ASN:HD22	1:A:304:LEU:HB3	1.76	0.50
1:A:448:ASP:O	1:A:452:ILE:HG13	2.11	0.50
1:A:182:THR:HA	1:A:197:ASN:HB3	1.93	0.50
1:A:466:THR:HA	1:A:476:VAL:O	2.12	0.50
1:B:1117:PHE:CE2	1:B:1148:PRO:HB3	2.47	0.50
1:A:251:LEU:HD11	1:A:435:THR:HG21	1.93	0.49
1:B:1274:ASN:HD22	1:B:1275:PHE:N	2.11	0.49
1:A:438:ASN:CB	1:A:493:THR:HG21	2.43	0.49
1:A:444:ILE:HG23	1:A:487:ILE:CD1	2.43	0.49
1:B:1132:MET:HB2	1:B:1137:GLN:NE2	2.28	0.49
1:B:1438:ASN:ND2	1:B:1438:ASN:H	2.11	0.48
1:A:254:ASP:CG	1:A:255:PRO:HD2	2.32	0.48
1:B:1235:LYS:HE3	2:B:274:HOH:O	2.12	0.48
1:A:123:ASN:O	1:A:124:THR:CB	2.61	0.48
1:A:117:PHE:HE1	1:A:127:LYS:HG2	1.78	0.48
1:A:31:GLU:OE1	1:A:139:HIS:CD2	2.66	0.48
1:A:205:LYS:HE3	1:A:206:LYS:HE2	1.95	0.48
1:A:149:THR:O	1:A:151:GLU:N	2.45	0.48
1:B:1365:VAL:HB	1:B:1452:ILE:HG21	1.94	0.48
1:B:1074:LYS:HA	2:B:252:HOH:O	2.13	0.48
1:B:1437:TRP:CE2	1:B:1443:ARG:HG2	2.48	0.48
1:B:1127:LYS:HB3	1:B:1156:PHE:CZ	2.49	0.48
1:A:119:GLY:HA2	1:A:275:PHE:HA	1.96	0.47
1:A:358:ALA:HA	1:A:437:TRP:CE3	2.49	0.47
1:A:109:LYS:HB2	1:A:110:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LYS:HB3	1:A:156:PHE:CZ	2.49	0.47
1:B:1300:ARG:O	1:B:1301:ASN:CB	2.62	0.47
1:B:1360:GLY:HA2	1:B:1437:TRP:O	2.14	0.47
1:B:1110:PRO:HG2	2:B:50:HOH:O	2.15	0.47
1:B:1405:ALA:HA	1:B:1408:LEU:HD22	1.96	0.47
1:B:1248:LYS:HA	1:B:1354:LEU:CD1	2.44	0.47
1:B:1082:GLU:H	1:B:1082:GLU:CD	2.17	0.46
1:A:444:ILE:HG23	1:A:487:ILE:HD11	1.97	0.46
1:B:1471:TYR:HE2	1:B:1505:LYS:HZ3	1.62	0.46
1:A:116:LEU:HD13	1:A:145:PHE:HB2	1.96	0.46
1:B:1024:HIS:HE1	1:B:1143:ASN:HD21	1.62	0.46
1:B:1248:LYS:NZ	2:B:271:HOH:O	2.42	0.46
1:B:1284:ILE:HD11	1:B:1320:LYS:HB3	1.98	0.46
1:A:98:LEU:HD13	1:A:185:VAL:HG21	1.98	0.46
1:A:325:ASN:HD21	1:A:327:ARG:HE	1.62	0.46
1:A:467:ALA:O	1:A:468:THR:CB	2.63	0.46
1:A:367:ILE:HD12	1:A:431:TYR:HE1	1.81	0.46
1:B:1328:VAL:HG13	1:B:1328:VAL:O	2.15	0.46
1:A:414:LYS:HD2	1:A:417:GLU:OE2	2.17	0.45
1:A:267:TRP:CE2	1:A:422:ARG:HB3	2.51	0.45
1:B:1294:ILE:O	1:B:1298:ILE:HG13	2.16	0.45
1:A:51:ASN:HA	1:A:304:LEU:O	2.16	0.45
1:B:1490:PRO:HB2	1:B:1500:TRP:HE1	1.82	0.45
1:A:242:GLY:CA	1:A:246:THR:HG21	2.38	0.45
1:B:1144:MET:O	1:B:1276:GLU:HB3	2.17	0.45
1:B:1126:LEU:HA	1:B:1126:LEU:HD23	1.82	0.45
1:A:300:ARG:O	1:A:301:ASN:CB	2.65	0.45
1:A:230:THR:HG23	1:A:260:ILE:HD11	1.98	0.44
1:A:315:VAL:HG11	1:A:317:PHE:CZ	2.51	0.44
1:A:487:ILE:HD12	2:A:564:HOH:O	2.17	0.44
1:B:1012:ILE:CD1	1:B:1131:VAL:HG11	2.47	0.44
1:B:1477:PRO:O	1:B:1488:LEU:HD13	2.17	0.44
1:B:1239:ILE:HD11	1:B:1351:VAL:HG22	2.00	0.44
1:B:1359:PHE:CE1	1:B:1397:PRO:HG3	2.52	0.44
1:A:149:THR:C	1:A:151:GLU:N	2.69	0.44
1:B:1507:LEU:O	1:B:1510:ARG:HB2	2.17	0.44
1:A:227:SER:OG	1:A:240:PHE:HB2	2.18	0.44
1:B:1209:PHE:CE1	1:B:1264:GLU:HB3	2.53	0.44
1:A:438:ASN:CG	1:A:493:THR:HG21	2.38	0.43
1:B:1014:GLY:O	1:B:1108:ASN:HA	2.18	0.43
1:B:1404:GLY:O	1:B:1408:LEU:HD13	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1438:ASN:N	1:B:1438:ASN:ND2	2.66	0.43
1:A:431:TYR:CD2	1:A:456:ILE:HD12	2.53	0.43
1:B:1117:PHE:HE1	1:B:1127:LYS:HG2	1.83	0.43
1:B:1213:ASN:OD1	1:B:1223:ALA:HB1	2.18	0.43
1:A:382:THR:CG2	1:A:398:THR:HG23	2.48	0.43
1:A:461:ILE:O	1:A:461:ILE:HG12	2.18	0.43
1:A:69:LYS:HD2	1:A:78:TRP:CZ2	2.54	0.43
1:A:439:GLY:H	1:A:493:THR:HG21	1.81	0.43
1:A:94:ALA:O	1:A:98:LEU:HG	2.18	0.43
1:B:1490:PRO:HB2	1:B:1500:TRP:NE1	2.33	0.43
1:A:423:MET:HB3	1:A:428:ALA:HB3	2.01	0.43
1:B:1119:GLY:HA2	1:B:1275:PHE:HA	2.00	0.43
1:B:1438:ASN:N	1:B:1438:ASN:HD22	2.09	0.43
1:A:38:GLY:HA3	2:A:582:HOH:O	2.19	0.43
1:B:1282:LYS:HG2	1:B:1327:ARG:CZ	2.49	0.43
1:B:1438:ASN:HD22	1:B:1438:ASN:C	2.21	0.43
1:A:259:LEU:HB3	1:A:338:ILE:HG22	2.00	0.43
1:B:1345:ALA:HB1	1:B:1346:PRO:CD	2.45	0.43
1:A:200:TYR:CE2	1:A:202:GLY:HA3	2.54	0.42
1:A:349:LYS:O	1:A:428:ALA:HA	2.20	0.42
1:A:423:MET:CB	1:A:428:ALA:HB3	2.49	0.42
1:B:1298:ILE:HG21	1:B:1304:LEU:HD21	2.01	0.42
1:B:1435:THR:HG22	1:B:1449:THR:HG21	2.02	0.42
1:A:446:ILE:HA	1:A:449:THR:HG22	2.02	0.42
1:B:1094:ALA:O	1:B:1098:LEU:HG	2.20	0.42
1:B:1161:VAL:O	1:B:1192:MET:HA	2.20	0.42
1:A:205:LYS:NZ	1:A:276:GLU:OE1	2.52	0.41
1:B:1077:TRP:HB2	1:B:1411:PRO:HD3	2.01	0.41
1:B:1237:THR:HB	1:B:1348:ALA:HA	2.02	0.41
1:A:98:LEU:HD21	1:A:178:LEU:HD11	2.03	0.41
1:A:438:ASN:OD1	1:A:487:ILE:HG13	2.19	0.41
1:A:452:ILE:O	1:A:456:ILE:HG12	2.20	0.41
1:A:209:PHE:CD1	1:A:264:GLU:HG2	2.55	0.41
1:A:369:SER:OG	1:A:372:GLN:HG3	2.20	0.41
1:A:436:GLY:O	1:A:443:ARG:HG3	2.20	0.41
1:B:1066:PHE:O	1:B:1185:VAL:HA	2.20	0.41
1:A:437:TRP:CD1	1:A:443:ARG:HA	2.54	0.41
1:B:1452:ILE:O	1:B:1456:ILE:HG13	2.21	0.41
1:B:1494:TYR:CD2	1:B:1500:TRP:HB2	2.55	0.41
1:A:132:MET:HB3	1:A:164:ASN:HB3	2.03	0.41
1:A:438:ASN:HD22	1:A:438:ASN:HA	1.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1008:ALA:HA	1:B:1012:ILE:O	2.20	0.41
1:A:438:ASN:HB3	1:A:439:GLY:H	1.65	0.41
1:B:1193:GLN:NE2	1:B:1208:MET:HE2	2.35	0.41
1:A:117:PHE:CE2	1:A:152:GLU:OE1	2.71	0.41
1:A:465:ASN:HB2	1:A:478:THR:OG1	2.20	0.41
1:A:361:VAL:HG11	1:A:504:ALA:HA	2.02	0.41
1:B:1298:ILE:CG2	1:B:1304:LEU:HD21	2.51	0.41
1:B:1333:PHE:HA	1:B:1338:ILE:HD13	2.03	0.41
1:A:68:VAL:HG23	1:A:186:PHE:O	2.21	0.41
1:A:364:PRO:HB3	1:A:452:ILE:CD1	2.51	0.41
1:A:434:ASN:O	1:A:444:ILE:HD12	2.21	0.41
1:A:365:VAL:HB	1:A:452:ILE:HG21	2.02	0.41
1:A:51:ASN:HD22	1:A:304:LEU:CB	2.34	0.41
1:B:1131:VAL:HB	1:B:1163:LEU:HD23	2.03	0.41
1:A:416:ALA:O	1:A:420:VAL:HG23	2.21	0.40
1:A:248:LYS:HB3	1:A:248:LYS:NZ	2.36	0.40
1:A:293:ASP:HB3	1:A:335:ILE:HD12	2.03	0.40
1:B:1019:VAL:CG1	1:B:1022:PRO:HB3	2.51	0.40
1:A:24:HIS:HE1	1:A:143:ASN:ND2	2.20	0.40
1:A:216:LEU:HB2	1:A:217:PRO:HD3	2.03	0.40
1:A:222:ALA:O	1:A:266:GLY:HA2	2.21	0.40
1:B:1038:GLY:HA3	2:B:61:HOH:O	2.21	0.40
1:A:352:ILE:CD1	1:A:354:LEU:HD21	2.51	0.40
1:A:381:PHE:CG	1:A:382:THR:N	2.89	0.40
1:A:469:ILE:HA	1:A:470:PRO:HD3	1.92	0.40
1:B:1080:SER:OG	1:B:1082:GLU:HG2	2.21	0.40
1:B:1185:VAL:HG12	1:B:1186:PHE:N	2.36	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	503/532 (94%)	465 (92%)	33 (7%)	5 (1%)	15	15
1	B	500/532 (94%)	474 (95%)	21 (4%)	5 (1%)	15	15
All	All	1003/1064 (94%)	939 (94%)	54 (5%)	10 (1%)	15	15

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	321	SER
1	B	1301	ASN
1	A	301	ASN
1	A	467	ALA
1	A	468	THR
1	B	1056	VAL
1	B	1382	THR
1	B	1440	THR
1	A	404	GLY
1	B	1404	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	387/443 (87%)	375 (97%)	12 (3%)	40	48
1	B	388/443 (88%)	373 (96%)	15 (4%)	32	40
All	All	775/886 (88%)	748 (96%)	27 (4%)	36	44

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	25	GLU
1	A	83	PHE
1	A	132	MET
1	A	229	ASN
1	A	246	THR

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Mol	Chain	Res	Type
1	A	248	LYS
1	A	274	ASN
1	A	352	ILE
1	A	398	THR
1	A	408	LEU
1	A	438	ASN
1	B	1003	LEU
1	B	1082	GLU
1	B	1083	PHE
1	B	1090	VAL
1	B	1101	LEU
1	B	1132	MET
1	B	1229	ASN
1	B	1257	ARG
1	B	1259	LEU
1	B	1264	GLU
1	B	1274	ASN
1	B	1325	ASN
1	B	1413	THR
1	B	1438	ASN
1	B	1513	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	24	HIS
1	A	51	ASN
1	A	87	ASN
1	A	121	ASN
1	A	137	GLN
1	A	139	HIS
1	A	143	ASN
1	A	193	GLN
1	A	229	ASN
1	A	236	ASN
1	A	274	ASN
1	A	306	ASN
1	A	325	ASN
1	A	438	ASN
1	B	1024	HIS
1	B	1051	ASN

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Mol	Chain	Res	Type
1	B	1087	ASN
1	B	1121	ASN
1	B	1137	GLN
1	B	1143	ASN
1	B	1193	GLN
1	B	1219	GLN
1	B	1229	ASN
1	B	1236	ASN
1	B	1274	ASN
1	B	1290	ASN
1	B	1306	ASN
1	B	1325	ASN
1	B	1372	GLN
1	B	1438	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 monosaccharides 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	507/532 (95%)	0.37	23 (4%) 33 46	26, 46, 69, 78	0
1	B	504/532 (94%)	0.27	14 (2%) 53 64	24, 43, 61, 78	0
All	All	1011/1064 (95%)	0.32	37 (3%) 41 54	24, 44, 65, 78	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	487	ILE	4.4
1	B	1003	LEU	4.1
1	A	446	ILE	4.0
1	A	494	TYR	3.8
1	B	1002	SER	3.8
1	A	14	GLY	3.6
1	A	463	THR	3.3
1	A	123	ASN	2.9
1	A	5	GLU	2.8
1	A	15	ALA	2.7
1	B	1514	ASN	2.7
1	A	467	ALA	2.6
1	A	470	PRO	2.6
1	A	3	LEU	2.6
1	B	1016	THR	2.5
1	B	1465	ASN	2.5
1	A	445	SER	2.4
1	A	480	LEU	2.4
1	B	1108	ASN	2.4
1	B	1008	ALA	2.3
1	A	449	THR	2.3
1	B	1382	THR	2.3
1	A	395	PRO	2.3
1	B	1494	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1516	LYS	2.2
1	A	16	THR	2.2
1	A	152	GLU	2.2
1	B	1515	PHE	2.1
1	A	478	THR	2.1
1	B	1004	SER	2.1
1	A	440	THR	2.1
1	A	8	ALA	2.1
1	A	508	ALA	2.1
1	B	1383	ALA	2.1
1	A	33	GLN	2.0
1	A	488	LEU	2.0
1	B	1439	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 (i)

There are no monosaccharides 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.