



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:48 PM UTC

PDB ID : 1YVY / pdb_00001yvy
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

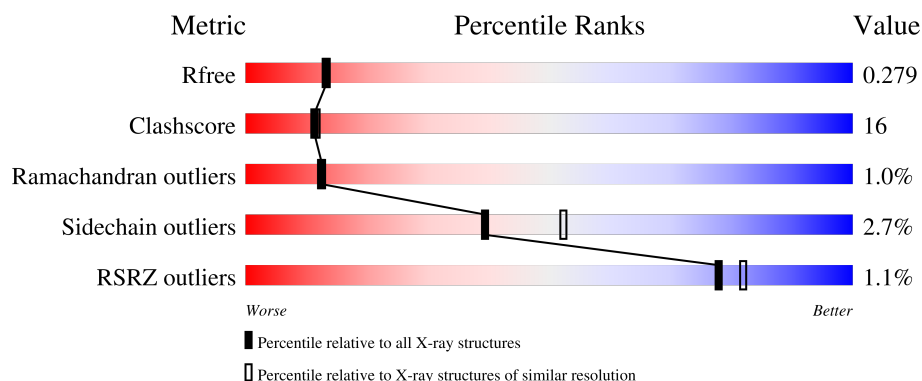
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

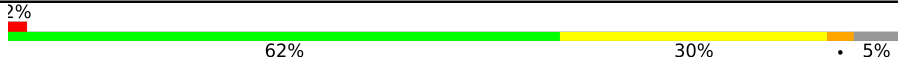
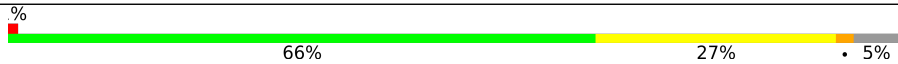
The reported resolution of this entry is 2.35 Å.

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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	532	
1	B	532	

2 Entry composition

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			

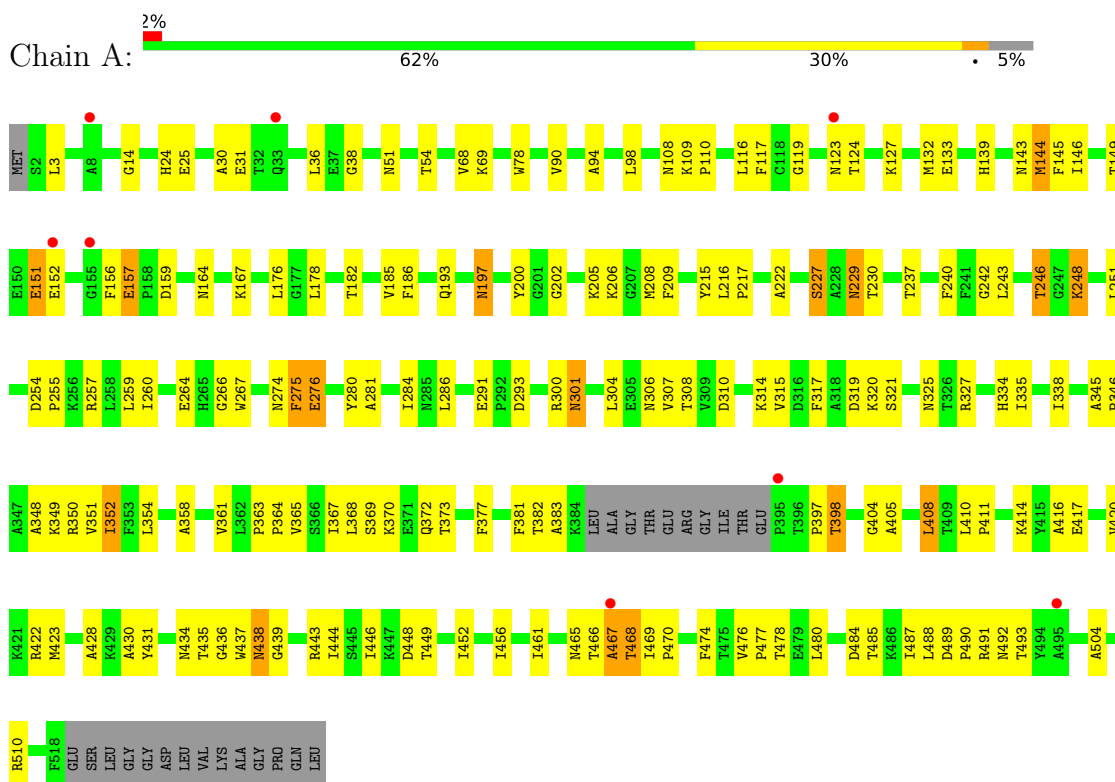
- Molecule 2 is water.

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

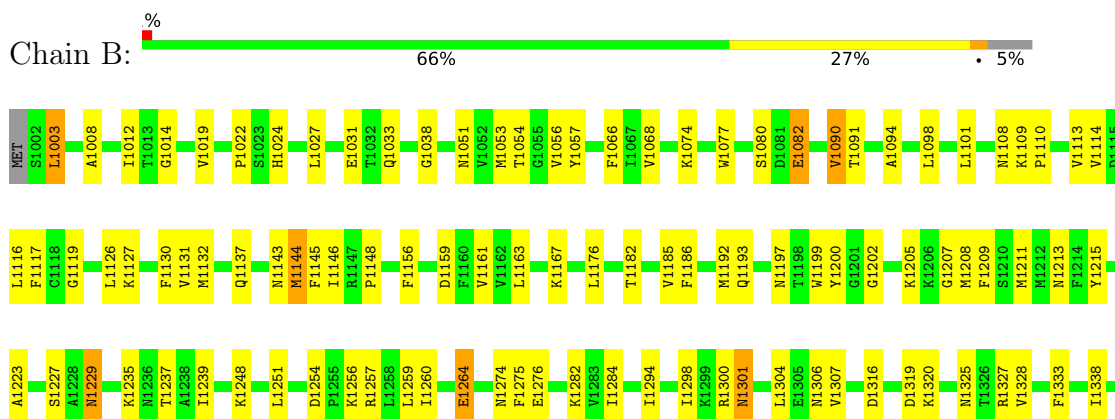
3 Residue-property plots

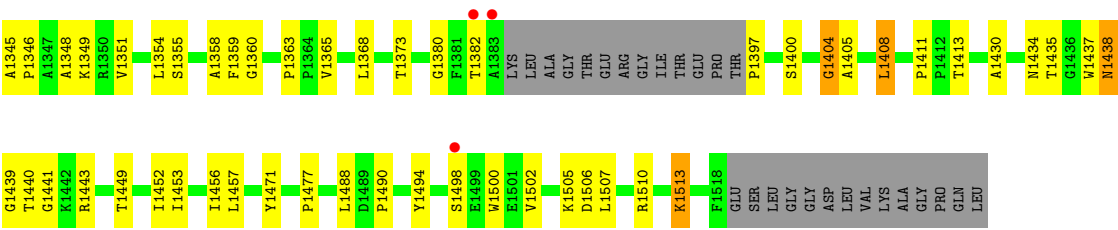
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Phosphoenolpyruvate carboxykinase [ATP]





4 Data and refinement statistics

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 10.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.35) 97.5 (10.00-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.20Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.221 , 0.263 0.233 , 0.279	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)	0.42 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.46	0/3903	0.90	13/5312 (0.2%)
1	B	0.46	0/3893	0.89	7/5291 (0.1%)
All	All	0.46	0/7796	0.89	20/10603 (0.2%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1260	ILE	N-CA-C	-7.78	105.12	111.81
1	A	144	MET	N-CA-C	7.13	121.81	113.18
1	A	276	GLU	N-CA-C	6.79	120.57	110.52
1	B	1207	GLY	N-CA-C	-6.72	104.36	112.49
1	B	1159	ASP	N-CA-C	-6.52	105.48	113.50
1	A	151	GLU	N-CA-C	-6.51	103.40	112.45
1	B	1227	SER	N-CA-C	-6.06	101.23	110.14
1	B	1215	TYR	N-CA-C	5.92	117.41	111.07
1	A	215	TYR	N-CA-C	5.79	117.67	111.36
1	B	1144	MET	N-CA-C	5.75	120.02	112.89
1	A	157	GLU	CA-C-N	5.74	126.07	119.93
1	A	157	GLU	C-N-CA	5.74	126.07	119.93
1	A	197	ASN	N-CA-C	5.68	119.51	112.24
1	A	159	ASP	N-CA-C	-5.63	105.53	112.90
1	A	275	PHE	N-CA-C	-5.36	105.10	111.69
1	A	377	PHE	N-CA-C	-5.34	105.37	111.14
1	B	1349	LYS	N-CA-C	-5.27	106.98	113.41
1	A	227	SER	N-CA-C	-5.24	102.01	110.14
1	A	334	HIS	N-CA-C	-5.11	107.00	113.18
1	A	281	ALA	N-CA-C	5.09	118.41	110.32

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	130	0
1	B	3806	0	3664	112	0
2	A	91	0	0	4	0
2	B	105	0	0	6	0
All	All	7817	0	7311	242	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 (242) 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
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:A:229:ASN:C	1:A:229:ASN:HD22	1.92	0.77
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:1130:PHE:HB3	1:B:1132:MET:HE1	1.69	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1325:ASN:HD21	1:B:1327:ARG:NE	1.89	0.67
1:A:149:THR:C	1:A:151:GLU:H	2.02	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:HD23	1:A:3:LEU:O	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:B:1513:LYS:NZ	1:B:1513:LYS:HB2	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
1:A:468:THR:HA	1:A:474:PHE:O	2.01	0.60
1:B:1229:ASN:C	1:B:1229:ASN:HD22	2.08	0.60
1:A:365:VAL:O	1:A:476:VAL:HG12	2.01	0.60
1:B:1438:ASN:H	1:B:1438:ASN:HD22	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:B:1193:GLN:NE2	1:B:1208:MET:HE3	2.17	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:1211:MET:HE2	1:B:1211:MET:HA	1.86	0.56
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:68:VAL:HA	1:A:90:VAL:CG1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:ARG:HD3	2:A:617:HOH:O	2.05	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:A:144:MET:HE2	1:A:280:TYR:HB2	1.89	0.54
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:A:254:ASP:CG	1:A:255:PRO:HD2	2.32	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
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:397:PRO:HG3	1:A:510:ARG:HD3	1.92	0.52
1:A:438:ASN:HB3	1:A:493:THR:HG21	1.91	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:B:1082:GLU:CD	1:B:1082:GLU:H	2.17	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:B:1438:ASN:ND2	2.11	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:B:1248:LYS:NZ	2:B:271:HOH:O	2.42	0.48
1:A:31:GLU:OE1	1:A:139:HIS:CD2	2.66	0.48
1:A:117:PHE:HE1	1:A:127:LYS:HG2	1.78	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:A:229:ASN:C	1:A:229:ASN:ND2	2.64	0.48
1:B:1365:VAL:HB	1:B:1452:ILE:HG21	1.94	0.48
1:A:438:ASN:CG	1:A:493:THR:HG21	2.38	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:B:1438:ASN:HD22	1:B:1438:ASN:C	2.21	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
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:A:149:THR:C	1:A:151:GLU:N	2.69	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:A:444:ILE:HG23	1:A:487:ILE:HD11	1.97	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ILE:HD12	1:A:431:TYR:HE1	1.81	0.46
1:B:1328:VAL:O	1:B:1328:VAL:HG13	2.15	0.46
1:A:267:TRP:CE2	1:A:422:ARG:HB3	2.51	0.45
1:A:414:LYS:HD2	1:A:417:GLU:OE2	2.17	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:HD23	1:B:1126:LEU:HA	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:B:1439:GLY:C	1:B:1441:GLY:H	2.25	0.44
1:B:1193:GLN:HE21	1:B:1208:MET:HE3	1.83	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:B:1014:GLY:O	1:B:1108:ASN:HA	2.18	0.43
1:B:1208:MET:HE2	1:B:1208:MET:HA	1.99	0.43
1:B:1404:GLY:O	1:B:1408:LEU:HD13	2.17	0.43
1:B:1438:ASN:ND2	1:B:1438:ASN:N	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:69:LYS:HD2	1:A:78:TRP:CZ2	2.54	0.43
1:A:382:THR:CG2	1:A:398:THR:HG23	2.48	0.43
1:A:461:ILE:HG12	1:A:461:ILE:O	2.18	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:HD22	1:B:1438:ASN:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ASN:HD22	1:A:274:ASN:C	2.27	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: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:B:1471:TYR:HE2	1:B:1505:LYS:HZ3	1.68	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
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:A:117:PHE:CE2	1:A:152:GLU:OE1	2.71	0.41
1:A:361:VAL:HG11	1:A:504:ALA:HA	2.02	0.41
1:A:465:ASN:HB2	1:A:478:THR:OG1	2.20	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:B:1438:ASN:ND2	1:B:1438:ASN:C	2.78	0.41
1:A:51:ASN:HD22	1:A:304:LEU:CB	2.34	0.41
1:A:68:VAL:HG23	1:A:186:PHE:O	2.21	0.41
1:A:133:GLU:CD	1:A:167:LYS:HD3	2.46	0.41
1:A:364:PRO:HB3	1:A:452:ILE:CD1	2.51	0.41
1:A:365:VAL:HB	1:A:452:ILE:HG21	2.02	0.41
1:A:434:ASN:O	1:A:444:ILE:HD12	2.21	0.41
1:B:1131:VAL:HB	1:B:1163:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ALA:O	1:A:420:VAL:HG23	2.21	0.40
1:A:248:LYS:NZ	1:A:248:LYS:HB3	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
1:A:193:GLN:NE2	1:A:208:MET:HE3	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%)	12	12
1	B	500/532 (94%)	474 (95%)	21 (4%)	5 (1%)	12	12
All	All	1003/1064 (94%)	939 (94%)	54 (5%)	10 (1%)	12	12

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

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Mol	Chain	Res	Type
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 ⓘ

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%)	378 (98%)	9 (2%)	44	58
1	B	388/443 (88%)	376 (97%)	12 (3%)	35	47
All	All	775/886 (88%)	754 (97%)	21 (3%)	39	52

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLU
1	A	229	ASN
1	A	246	THR
1	A	248	LYS
1	A	352	ILE
1	A	370	LYS
1	A	398	THR
1	A	408	LEU
1	A	438	ASN
1	B	1003	LEU
1	B	1033	GLN
1	B	1082	GLU
1	B	1090	VAL
1	B	1101	LEU
1	B	1229	ASN
1	B	1259	LEU
1	B	1264	GLU

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Mol	Chain	Res	Type
1	B	1408	LEU
1	B	1413	THR
1	B	1438	ASN
1	B	1513	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) 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	137	GLN
1	A	143	ASN
1	A	179	ASN
1	A	193	GLN
1	A	219	GLN
1	A	229	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
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	1285	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 [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 oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	507/532 (95%)	0.03	8 (1%) 70 76	26, 46, 69, 78	0
1	B	504/532 (94%)	-0.14	3 (0%) 85 89	24, 43, 61, 78	0
All	All	1011/1064 (95%)	-0.05	11 (1%) 78 82	24, 44, 65, 78	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	ASN	4.5
1	A	152	GLU	2.8
1	A	155	GLY	2.5
1	B	1382	THR	2.4
1	B	1383	ALA	2.4
1	A	8	ALA	2.3
1	A	467	ALA	2.3
1	A	33	GLN	2.2
1	A	495	ALA	2.2
1	A	395	PRO	2.1
1	B	1498	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.