



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 07:26 PM UTC

PDB ID : 5CS4 / pdb_00005cs4
Title : Crystal structure of domains AC3-AC5 of yeast acetyl-CoA carboxylase
Authors : Wei, J.; Tong, L.
Deposited on : 2015-07-23
Resolution : 3.19 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (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

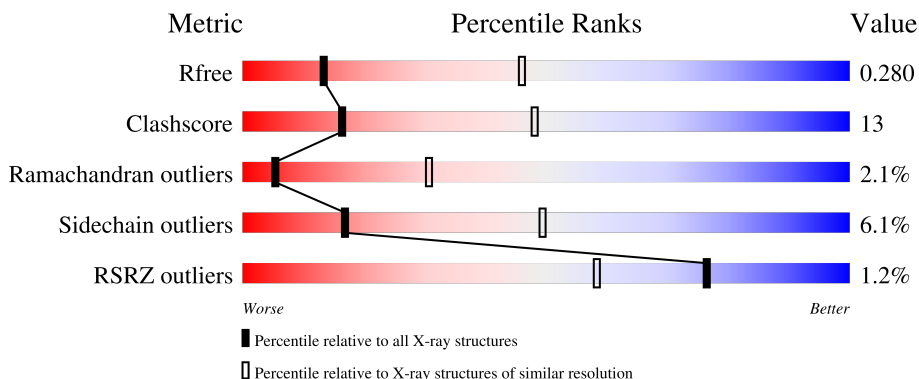
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	474	 53% 28% 15%
1	B	474	 59% 20% 19%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6353 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 Acetyl-CoA carboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	402	3235	2066	555	608	1	5	0	0	0
1	B	385	3118	1997	536	579	1	5	0	0	0

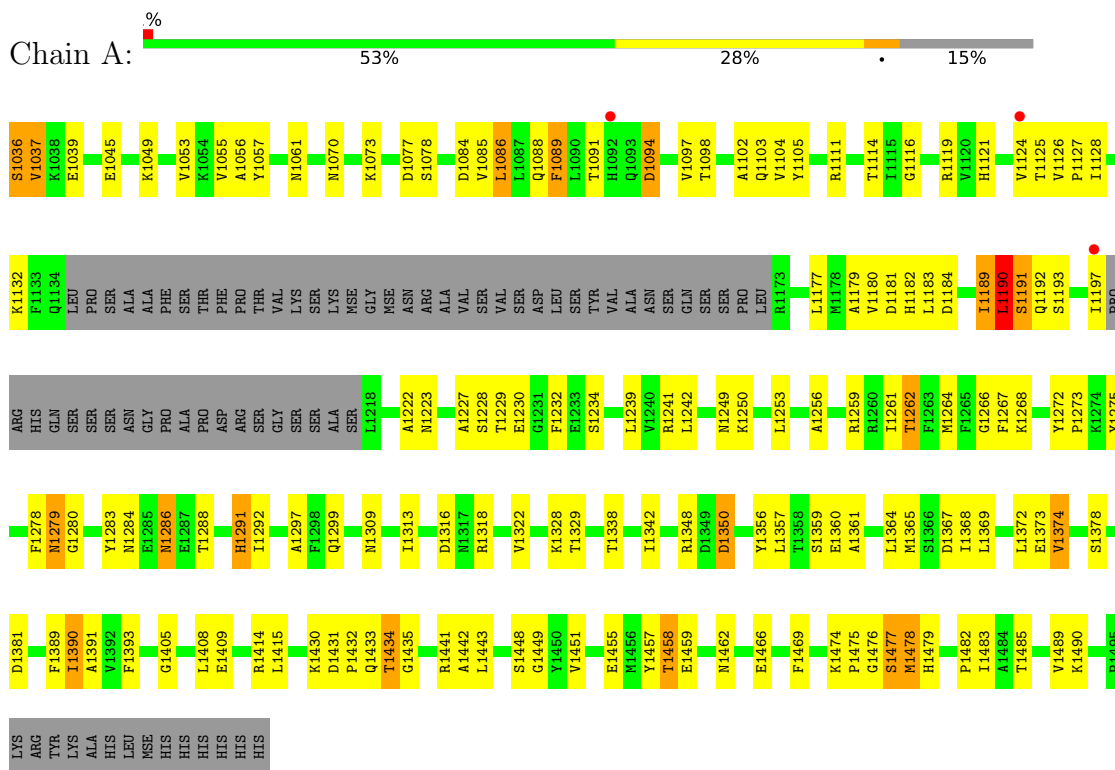
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1504	HIS	-	expression tag	UNP Q00955
A	1505	HIS	-	expression tag	UNP Q00955
A	1506	HIS	-	expression tag	UNP Q00955
A	1507	HIS	-	expression tag	UNP Q00955
A	1508	HIS	-	expression tag	UNP Q00955
A	1509	HIS	-	expression tag	UNP Q00955
B	1504	HIS	-	expression tag	UNP Q00955
B	1505	HIS	-	expression tag	UNP Q00955
B	1506	HIS	-	expression tag	UNP Q00955
B	1507	HIS	-	expression tag	UNP Q00955
B	1508	HIS	-	expression tag	UNP Q00955
B	1509	HIS	-	expression tag	UNP Q00955

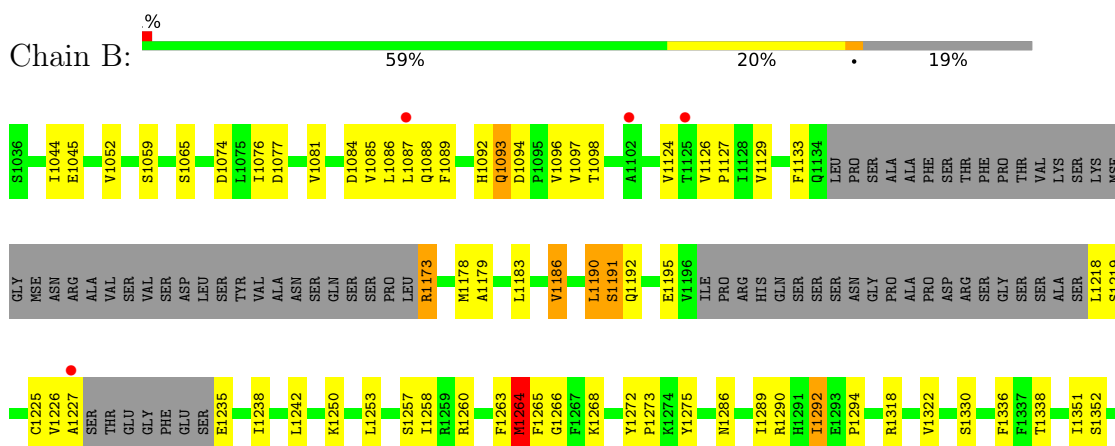
3 Residue-property plots

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: Acetyl-CoA carboxylase



- Molecule 1: Acetyl-CoA carboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.85Å 93.28Å 111.14Å 90.00° 100.62° 90.00°	Depositor
Resolution (Å)	42.90 – 3.19 42.90 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.8 (42.90-3.19) 99.8 (42.90-3.19)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.00 (at 3.19Å)	Xtrriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.234 , 0.287 0.233 , 0.280	Depositor DCC
R_{free} test set	980 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	74.6	Xtrriage
Anisotropy	0.206	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6353	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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	0.75	0/3294	1.00	5/4456 (0.1%)
1	B	0.69	2/3172 (0.1%)	0.96	4/4287 (0.1%)
All	All	0.72	2/6466 (0.0%)	0.98	9/8743 (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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1264	MSE	CA-C	-6.10	1.46	1.52
1	B	1478	MSE	CA-C	-5.53	1.46	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1478	MSE	CB-CA-C	-7.15	101.95	111.82
1	B	1445	ASN	N-CA-C	6.00	119.26	109.24
1	A	1478	MSE	CA-CB-CG	-5.71	102.68	114.10
1	A	1405	GLY	N-CA-C	-5.50	103.33	111.03
1	A	1448	SER	N-CA-C	-5.29	104.72	110.91
1	A	1280	GLY	CA-C-N	5.28	126.44	119.84
1	A	1280	GLY	C-N-CA	5.28	126.44	119.84
1	B	1264	MSE	CB-CA-C	-5.23	103.53	110.79
1	B	1186	VAL	N-CA-C	5.11	116.20	111.45

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1279	ASN	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	3235	0	3242	99	0
1	B	3118	0	3134	68	0
All	All	6353	0	6376	165	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 13.

All (165) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1272:TYR:O	1:A:1318:ARG:NH1	1.93	1.01
1:B:1087:LEU:HD11	1:B:1264:MSE:HE2	1.54	0.89
1:B:1272:TYR:O	1:B:1318:ARG:NH2	2.08	0.86
1:A:1036:SER:O	1:A:1037:VAL:C	2.40	0.64
1:A:1124:VAL:HG23	1:A:1192:GLN:HG2	1.79	0.64
1:B:1253:LEU:HA	1:B:1258:ILE:HD12	1.79	0.62
1:B:1087:LEU:HD12	1:B:1273:PRO:HB3	1.82	0.62
1:A:1356:TYR:O	1:A:1357:LEU:C	2.43	0.61
1:B:1242:LEU:HD22	1:B:1263:PHE:CE2	2.34	0.61
1:A:1266:GLY:O	1:A:1267:PHE:CG	2.55	0.60
1:B:1126:VAL:HG13	1:B:1127:PRO:HD2	1.85	0.59
1:A:1433:GLN:HG2	1:A:1434:THR:H	1.66	0.59
1:A:1482:PRO:O	1:A:1485:THR:OG1	2.17	0.59
1:A:1124:VAL:HG12	1:A:1125:THR:HG23	1.85	0.58
1:A:1431:ASP:CG	1:A:1432:PRO:HD2	2.29	0.57
1:A:1469:PHE:O	1:A:1479:HIS:O	2.23	0.57
1:A:1190:LEU:O	1:A:1193:SER:OG	2.19	0.57
1:B:1322:VAL:HG22	1:B:1338:THR:HG23	1.85	0.57
1:B:1264:MSE:HE3	1:B:1275:TYR:CE1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1055:VAL:HG21	1:A:1061:ASN:HA	1.87	0.57
1:B:1088:GLN:HB2	1:B:1268:LYS:HE2	1.85	0.57
1:A:1091:THR:HG21	1:A:1180:VAL:O	2.05	0.56
1:B:1085:VAL:O	1:B:1087:LEU:N	2.39	0.56
1:A:1299:GLN:CD	1:A:1390:ILE:HD11	2.31	0.56
1:A:1391:ALA:HB3	1:A:1393:PHE:CE2	2.42	0.55
1:B:1084:ASP:OD1	1:B:1084:ASP:N	2.40	0.55
1:B:1359:SER:O	1:B:1363:ARG:HG3	2.07	0.55
1:A:1291:HIS:CD2	1:A:1318:ARG:HD3	2.41	0.55
1:B:1351:ILE:HG22	1:B:1352:SER:O	2.08	0.54
1:A:1182:HIS:CD2	1:A:1184:ASP:H	2.25	0.54
1:A:1124:VAL:HG23	1:A:1192:GLN:CG	2.37	0.54
1:B:1126:VAL:CG1	1:B:1127:PRO:HD2	2.37	0.54
1:B:1045:GLU:HA	1:B:1089:PHE:HE1	1.73	0.54
1:B:1124:VAL:HG12	1:B:1124:VAL:O	2.07	0.54
1:A:1126:VAL:HG13	1:A:1127:PRO:HD2	1.89	0.54
1:A:1474:LYS:O	1:A:1475:PRO:C	2.49	0.54
1:B:1400:VAL:HG21	1:B:1429:ILE:HD11	1.89	0.54
1:B:1044:ILE:O	1:B:1045:GLU:C	2.50	0.53
1:A:1222:ALA:O	1:A:1261:ILE:HA	2.08	0.53
1:B:1225:CYS:SG	1:B:1226:VAL:N	2.81	0.53
1:A:1433:GLN:HG2	1:A:1434:THR:N	2.24	0.52
1:B:1242:LEU:HD22	1:B:1263:PHE:CD2	2.44	0.52
1:B:1393:PHE:O	1:B:1429:ILE:HA	2.10	0.52
1:A:1055:VAL:HG12	1:A:1056:ALA:N	2.24	0.52
1:B:1378:SER:OG	1:B:1379:ASN:N	2.43	0.52
1:A:1097:VAL:O	1:A:1098:THR:C	2.53	0.51
1:A:1264:MSE:HG2	1:A:1275:TYR:CE1	2.45	0.51
1:B:1250:LYS:HA	1:B:1253:LEU:HD12	1.93	0.51
1:A:1056:ALA:HB1	1:B:1074:ASP:OD2	2.10	0.51
1:A:1372:LEU:C	1:A:1374:VAL:H	2.18	0.51
1:A:1322:VAL:HG22	1:A:1338:THR:HG23	1.91	0.51
1:B:1265:PHE:N	1:B:1265:PHE:CD2	2.76	0.50
1:B:1235:GLU:O	1:B:1238:ILE:N	2.45	0.50
1:A:1365:MSE:HE1	1:A:1415:LEU:HD21	1.94	0.50
1:A:1455:GLU:OE1	1:A:1457:TYR:OH	2.24	0.50
1:B:1356:TYR:O	1:B:1357:LEU:C	2.54	0.50
1:A:1342:ILE:HD12	1:A:1389:PHE:CZ	2.47	0.49
1:B:1289:ILE:O	1:B:1290:ARG:C	2.55	0.49
1:A:1469:PHE:CE2	1:A:1483:ILE:HA	2.47	0.49
1:A:1181:ASP:HA	1:A:1227:ALA:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1084:ASP:HA	1:A:1273:PRO:HD3	1.94	0.49
1:A:1381:ASP:CG	1:A:1381:ASP:O	2.56	0.49
1:A:1348:ARG:NH2	1:A:1350:ASP:OD2	2.46	0.48
1:A:1232:PHE:HE1	1:A:1241:ARG:HG3	1.78	0.48
1:B:1124:VAL:HB	1:B:1192:GLN:HE22	1.78	0.48
1:B:1468:VAL:HG12	1:B:1469:PHE:O	2.13	0.48
1:B:1365:MSE:HE1	1:B:1415:LEU:HD21	1.95	0.48
1:A:1364:LEU:O	1:A:1365:MSE:C	2.55	0.48
1:B:1087:LEU:HD21	1:B:1264:MSE:CE	2.43	0.48
1:A:1442:ALA:C	1:A:1443:LEU:HD12	2.39	0.47
1:A:1373:GLU:OE1	1:A:1414:ARG:NH2	2.45	0.47
1:B:1124:VAL:O	1:B:1124:VAL:CG1	2.62	0.47
1:B:1190:LEU:O	1:B:1191:SER:C	2.57	0.47
1:A:1286:ASN:OD1	1:A:1288:THR:OG1	2.32	0.47
1:A:1441:ARG:HB2	1:A:1457:TYR:HB2	1.95	0.47
1:B:1264:MSE:HB3	1:B:1275:TYR:CD1	2.49	0.47
1:A:1462:ASN:HB2	1:A:1466:GLU:O	2.14	0.47
1:B:1367:ASP:O	1:B:1368:ILE:C	2.57	0.47
1:A:1359:SER:O	1:A:1360:GLU:C	2.58	0.46
1:A:1430:LYS:HE2	1:A:1435:GLY:CA	2.45	0.46
1:A:1223:ASN:HB3	1:A:1262:THR:HB	1.97	0.46
1:B:1092:HIS:CG	1:B:1093:GLN:N	2.84	0.46
1:A:1489:VAL:HG12	1:A:1490:LYS:N	2.30	0.46
1:B:1336:PHE:N	1:B:1383:ASN:OD1	2.48	0.46
1:B:1351:ILE:CG2	1:B:1352:SER:O	2.64	0.46
1:A:1057:TYR:HE2	1:B:1081:VAL:O	1.99	0.46
1:B:1478:MSE:CG	1:B:1481:ARG:HG3	2.46	0.46
1:A:1360:GLU:O	1:A:1361:ALA:C	2.59	0.46
1:A:1430:LYS:HE3	1:A:1435:GLY:O	2.16	0.46
1:A:1190:LEU:O	1:A:1191:SER:C	2.59	0.45
1:A:1458:THR:CG2	1:A:1459:GLU:N	2.79	0.45
1:A:1036:SER:O	1:A:1039:GLU:N	2.49	0.45
1:A:1297:ALA:C	1:A:1299:GLN:N	2.74	0.45
1:B:1460:VAL:HG12	1:B:1461:LYS:H	1.80	0.45
1:A:1367:ASP:O	1:A:1368:ILE:C	2.59	0.45
1:B:1396:SER:O	1:B:1399:ASP:N	2.50	0.45
1:A:1077:ASP:OD1	1:A:1111:ARG:NE	2.38	0.45
1:A:1094:ASP:HB3	1:A:1097:VAL:HG23	1.99	0.45
1:A:1279:ASN:O	1:A:1283:TYR:HA	2.16	0.45
1:B:1260:ARG:NH1	1:B:1294:PRO:HB2	2.32	0.45
1:A:1088:GLN:HB3	1:A:1089:PHE:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1089:PHE:CD2	1:A:1089:PHE:N	2.85	0.44
1:A:1183:LEU:HD23	1:A:1232:PHE:CZ	2.52	0.44
1:B:1087:LEU:HD21	1:B:1264:MSE:HE1	2.00	0.44
1:A:1313:ILE:HG22	1:A:1313:ILE:O	2.16	0.44
1:A:1049:LYS:O	1:A:1053:VAL:HG23	2.18	0.44
1:A:1239:LEU:O	1:A:1242:LEU:N	2.51	0.43
1:A:1431:ASP:OD1	1:A:1432:PRO:HD2	2.18	0.43
1:A:1085:VAL:O	1:A:1086:LEU:C	2.62	0.43
1:B:1357:LEU:HD11	1:B:1395:ILE:HD12	2.00	0.43
1:A:1128:ILE:HD13	1:A:1193:SER:HA	2.00	0.43
1:A:1180:VAL:HG12	1:A:1181:ASP:N	2.33	0.43
1:A:1408:LEU:O	1:A:1409:GLU:C	2.62	0.43
1:A:1070:ASN:HA	1:A:1073:LYS:HG2	2.00	0.43
1:A:1103:GLN:O	1:A:1104:VAL:C	2.61	0.43
1:A:1102:ALA:HB1	1:A:1177:LEU:HD23	2.01	0.43
1:B:1084:ASP:HA	1:B:1273:PRO:HD3	2.00	0.43
1:A:1266:GLY:O	1:A:1267:PHE:CD1	2.72	0.43
1:B:1126:VAL:HG11	1:B:1179:ALA:O	2.19	0.43
1:B:1364:LEU:O	1:B:1365:MSE:C	2.62	0.43
1:A:1197:ILE:HG21	1:A:1256:ALA:CB	2.48	0.42
1:B:1087:LEU:HD12	1:B:1266:GLY:HA2	2.01	0.42
1:B:1362:ASN:O	1:B:1366:SER:OG	2.36	0.42
1:A:1088:GLN:HB3	1:A:1089:PHE:HD2	1.84	0.42
1:A:1189:ILE:O	1:A:1190:LEU:C	2.60	0.42
1:B:1238:ILE:O	1:B:1242:LEU:HG	2.18	0.42
1:A:1091:THR:HG22	1:A:1179:ALA:HB1	2.02	0.42
1:A:1125:THR:OG1	1:A:1126:VAL:N	2.52	0.42
1:A:1249:ASN:O	1:A:1250:LYS:C	2.61	0.42
1:B:1218:LEU:HA	1:B:1257:SER:HB2	2.02	0.42
1:A:1278:PHE:HA	1:A:1284:ASN:O	2.20	0.42
1:B:1183:LEU:O	1:B:1186:VAL:HG23	2.19	0.42
1:B:1264:MSE:HE3	1:B:1275:TYR:CZ	2.54	0.42
1:A:1391:ALA:HB3	1:A:1393:PHE:CZ	2.55	0.42
1:B:1455:GLU:OE1	1:B:1457:TYR:OH	2.34	0.42
1:A:1476:GLY:O	1:A:1477:SER:C	2.62	0.41
1:B:1085:VAL:C	1:B:1087:LEU:N	2.76	0.41
1:A:1476:GLY:O	1:A:1478:MSE:N	2.53	0.41
1:B:1087:LEU:HD11	1:B:1264:MSE:CE	2.38	0.41
1:A:1055:VAL:CG1	1:A:1056:ALA:N	2.83	0.41
1:A:1441:ARG:NE	1:A:1459:GLU:OE2	2.44	0.41
1:B:1226:VAL:HG12	1:B:1227:ALA:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1232:PHE:CD2	1:A:1232:PHE:N	2.89	0.41
1:A:1250:LYS:O	1:A:1253:LEU:HB2	2.20	0.41
1:A:1264:MSE:HG2	1:A:1275:TYR:CD1	2.56	0.41
1:B:1292:ILE:O	1:B:1294:PRO:HD3	2.21	0.41
1:B:1357:LEU:HD22	1:B:1427:ILE:HD11	2.03	0.41
1:A:1350:ASP:OD1	1:A:1350:ASP:N	2.44	0.41
1:A:1045:GLU:HG3	1:A:1089:PHE:CE1	2.55	0.41
1:A:1119:ARG:CD	1:A:1121:HIS:HE1	2.34	0.41
1:A:1489:VAL:CG1	1:A:1490:LYS:N	2.84	0.41
1:B:1133:PHE:O	1:B:1173:ARG:HG3	2.21	0.41
1:B:1092:HIS:CD2	1:B:1097:VAL:HG11	2.56	0.41
1:A:1365:MSE:CE	1:A:1369:LEU:HD11	2.50	0.40
1:A:1430:LYS:HE2	1:A:1435:GLY:HA2	2.03	0.40
1:B:1097:VAL:O	1:B:1098:THR:C	2.64	0.40
1:B:1289:ILE:O	1:B:1289:ILE:HG22	2.20	0.40
1:A:1365:MSE:HE3	1:A:1369:LEU:HD11	2.03	0.40
1:A:1458:THR:HG22	1:A:1459:GLU:N	2.36	0.40
1:A:1104:VAL:O	1:A:1105:TYR:C	2.65	0.40
1:A:1116:GLY:N	1:A:1132:LYS:O	2.44	0.40
1:B:1286:ASN:ND2	1:B:1289:ILE:HD12	2.36	0.40
1:B:1460:VAL:HG21	1:B:1470:LYS:HD2	2.03	0.40
1:A:1309:ASN:ND2	1:A:1328:LYS:HG2	2.36	0.40
1:B:1052:VAL:HG22	1:B:1096:VAL:HG12	2.02	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	396/474 (84%)	330 (83%)	57 (14%)	9 (2%)	5 29
1	B	371/474 (78%)	314 (85%)	50 (14%)	7 (2%)	6 33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	767/948 (81%)	644 (84%)	107 (14%)	16 (2%)	5	31

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1190	LEU
1	A	1449	GLY
1	B	1086	LEU
1	B	1190	LEU
1	A	1230	GLU
1	A	1477	SER
1	A	1086	LEU
1	A	1378	SER
1	B	1195	GLU
1	B	1219	SER
1	A	1037	VAL
1	A	1286	ASN
1	A	1374	VAL
1	B	1077	ASP
1	B	1473	GLY
1	B	1076	ILE

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	360/414 (87%)	337 (94%)	23 (6%)	16	48
1	B	348/414 (84%)	328 (94%)	20 (6%)	18	51
All	All	708/828 (86%)	665 (94%)	43 (6%)	17	49

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1036	SER
1	A	1078	SER

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Mol	Chain	Res	Type
1	A	1089	PHE
1	A	1094	ASP
1	A	1114	THR
1	A	1189	ILE
1	A	1190	LEU
1	A	1191	SER
1	A	1228	SER
1	A	1229	THR
1	A	1234	SER
1	A	1259	ARG
1	A	1262	THR
1	A	1268	LYS
1	A	1291	HIS
1	A	1292	ILE
1	A	1316	ASP
1	A	1329	THR
1	A	1350	ASP
1	A	1390	ILE
1	A	1434	THR
1	A	1451	VAL
1	A	1458	THR
1	B	1059	SER
1	B	1065	SER
1	B	1093	GLN
1	B	1094	ASP
1	B	1129	VAL
1	B	1173	ARG
1	B	1178	MSE
1	B	1191	SER
1	B	1264	MSE
1	B	1292	ILE
1	B	1330	SER
1	B	1366	SER
1	B	1373	GLU
1	B	1380	SER
1	B	1422	SER
1	B	1427	ILE
1	B	1458	THR
1	B	1460	VAL
1	B	1471	SER
1	B	1478	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	1121	HIS
1	A	1182	HIS
1	A	1249	ASN
1	A	1291	HIS
1	A	1309	ASN
1	B	1046	HIS
1	B	1192	GLN
1	B	1299	GLN
1	B	1346	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	397/474 (83%)	-0.07	3 (0%) 82 67	28, 72, 112, 136	0
1	B	380/474 (80%)	0.08	6 (1%) 70 51	47, 85, 121, 148	0
All	All	777/948 (81%)	0.00	9 (1%) 76 58	28, 78, 117, 148	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1447	VAL	4.2
1	A	1124	VAL	3.1
1	B	1087	LEU	2.9
1	A	1092	HIS	2.6
1	A	1197	ILE	2.4
1	B	1102	ALA	2.1
1	B	1462	ASN	2.1
1	B	1125	THR	2.1
1	B	1227	ALA	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.