Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 11:54 PM EDT

PDB ID	:	5CS4
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 (i) 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 (1)) were used in the production of this report:

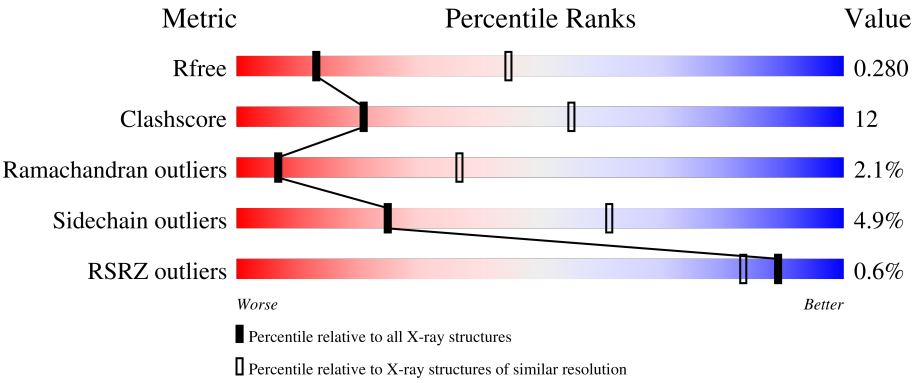
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (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 <=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	55% 27% . 15%
1	B	474	% 60% 19% . 19%

2 Entry composition (i)

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
1	A	402	Total	C	N	O	S	Se	0	0	0
			3235	2066	555	608	1	5			
1	B	385	Total	C	N	O	S	Se	0	0	0
			3118	1997	536	579	1	5			

There are 12 discrepancies between the modelled and reference sequences:

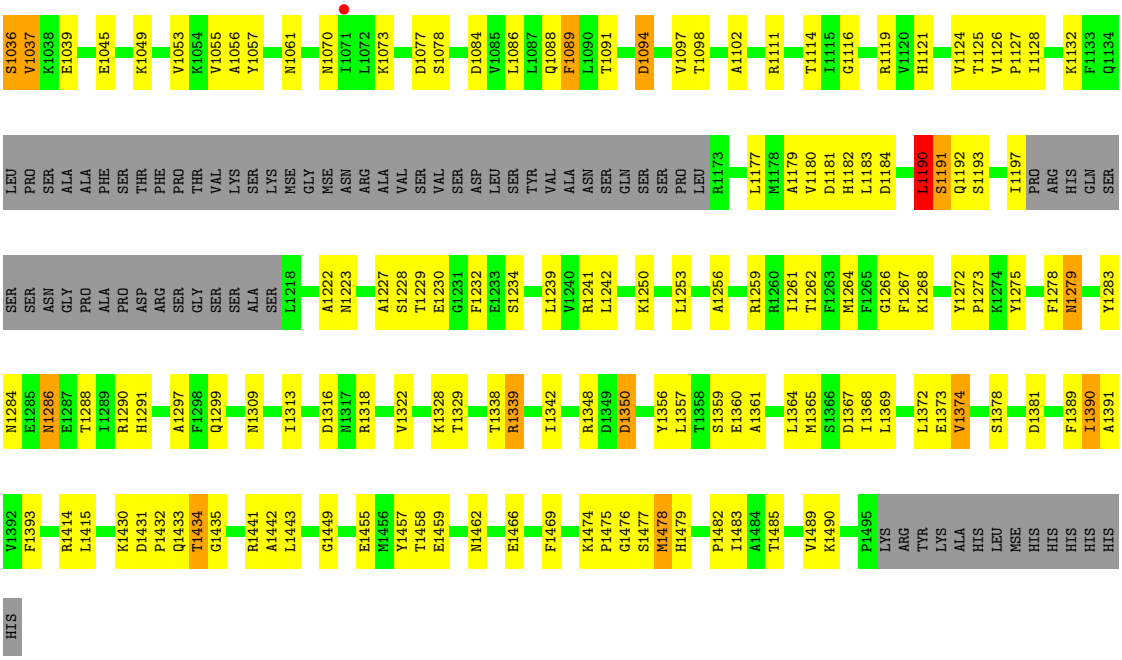
Chain	Residue	Modelled	Actual	Comment	Reference
A	1504	HIS	-	expression tag	UNP Q00955
A	1505	HIS	-	expression tag	UNP Q00955
A	1506	HIS	-	expression tag	UNP Q00955
A	1507	HIS	-	expression tag	UNP Q00955
A	1508	HIS	-	expression tag	UNP Q00955
A	1509	HIS	-	expression tag	UNP Q00955
B	1504	HIS	-	expression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

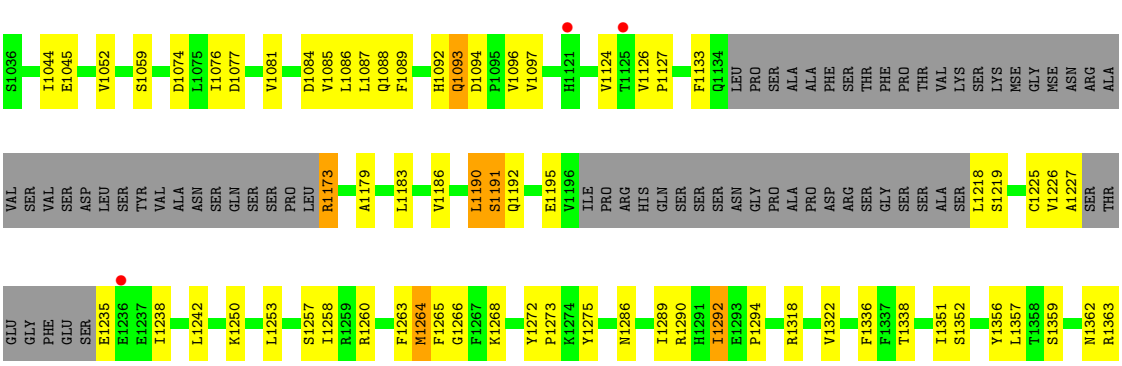
• Molecule 1: Acetyl-CoA carboxylase

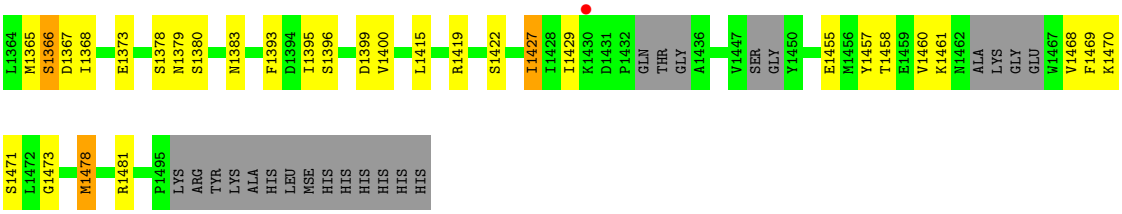
Chain A:



• Molecule 1: Acetyl-CoA carboxylase

Chain B:




L1364
M1365
S1366
D1367
I1368
E1373
S1378
N1379
S1380
N1383
F1393
D1394
I1395
S1396
D1399
V1400
L1415
R1419
S1422
I1427
I1428
I1429
K1430
D1431
P1432
GLN
THR
GLY
A1436
V1447
SER
GLY
Y1450
E1455
M1456
Y1457
T1458
E1459
V1460
K1461
N1462
ALA
LYS
GLY
GLU
W1467
V1468
F1469
K1470
S1471
L1472
G1473
M1478
R1481
P1495
LYS
ARG
TYR
LYS
ALA
HIS
LEU
MSE
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

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) 99.9 (42.90-3.19)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.00 (at 3.19Å)	Xtriage
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 (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	74.6	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 46.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6353	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage'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.*

[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	0.54	0/3294	0.78	3/4456 (0.1%)
1	B	0.50	0/3172	0.74	0/4287
All	All	0.52	0/6466	0.76	3/8743 (0.0%)

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1478	MSE	CA-CB-CG	-6.25	102.68	113.30
1	A	1339	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	1339	ARG	NE-CZ-NH2	-5.25	117.67	120.30

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

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	92	0
1	B	3118	0	3134	65	0
All	All	6353	0	6376	155	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 12.

All (155) 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: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: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:A:1036:SER:O	1:A:1037:VAL:C	2.40	0.59
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:1190:LEU:O	1:A:1193:SER:OG	2.19	0.58
1:A:1469:PHE:O	1:A:1479:HIS:O	2.23	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
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:A:1356:TYR:O	1:A:1357:LEU:C	2.43	0.56
1:B:1085:VAL:O	1:B:1087:LEU:N	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1400:VAL:HG21	1:B:1429:ILE:HD11	1.89	0.54
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:1431:ASP:CG	1:A:1432:PRO:HD2	2.29	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: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: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:1299:GLN:CD	1:A:1390:ILE:HD11	2.31	0.50
1:A:1365:MSE:HE1	1:A:1415:LEU:HD21	1.94	0.50
1:A:1342:ILE:HD12	1:A:1389:PHE:CZ	2.47	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
1:A:1084:ASP:HA	1:A:1273:PRO:HD3	1.94	0.49
1:A:1474:LYS:O	1:A:1475:PRO:C	2.49	0.49
1:B:1044:ILE:O	1:B:1045:GLU:C	2.50	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:B:1087:LEU:HD21	1:B:1264:MSE:CE	2.43	0.48
1:A:1373:GLU:OE1	1:A:1414:ARG:NH2	2.45	0.47
1:A:1489:VAL:HG12	1:A:1490:LYS:N	2.30	0.47
1:B:1124:VAL:O	1:B:1124:VAL:CG1	2.62	0.47
1:A:1097:VAL:O	1:A:1098:THR:C	2.53	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:A:1430:LYS:HE2	1:A:1435:GLY:CA	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1223:ASN:HB3	1:A:1262:THR:HB	1.97	0.46
1:A:1372:LEU:C	1:A:1374:VAL:H	2.18	0.46
1:B:1092:HIS:CG	1:B:1093:GLN:N	2.84	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:1430:LYS:HE3	1:A:1435:GLY:O	2.16	0.46
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:B:1460:VAL:HG12	1:B:1461:LYS:H	1.80	0.45
1:B:1356:TYR:O	1:B:1357:LEU:C	2.54	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:B:1289:ILE:O	1:B:1290:ARG:C	2.55	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
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:A:1381:ASP:O	1:A:1381:ASP:CG	2.56	0.44
1:A:1455:GLU:OE1	1:A:1457:TYR:OH	2.24	0.44
1:A:1364:LEU:O	1:A:1365:MSE:C	2.55	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: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:1070:ASN:HA	1:A:1073:LYS:HG2	2.00	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:A:1442:ALA:C	1:A:1443:LEU:HD12	2.39	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:A:1088:GLN:HB3	1:A:1089:PHE:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1238:ILE:O	1:B:1242:LEU:HG	2.18	0.42
1:B:1190:LEU:O	1:B:1191:SER:C	2.57	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: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:1362:ASN:O	1:B:1366:SER:OG	2.36	0.42
1:B:1367:ASP:O	1:B:1368:ILE:C	2.57	0.42
1:A:1359:SER:O	1:A:1360:GLU:C	2.58	0.42
1:B:1455:GLU:OE1	1:B:1457:TYR:OH	2.34	0.42
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
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:1190:LEU:O	1:A:1191:SER:C	2.59	0.41
1:A:1360:GLU:O	1:A:1361:ALA:C	2.59	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: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:1367:ASP:O	1:A:1368:ILE:C	2.59	0.40
1:A:1458:THR:HG22	1:A:1459:GLU:N	2.36	0.40
1:A:1116:GLY:N	1:A:1132:LYS:O	2.44	0.40
1:A:1297:ALA:C	1:A:1299:GLN:N	2.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	6 34
1	B	371/474 (78%)	314 (85%)	50 (14%)	7 (2%)	8 39
All	All	767/948 (81%)	644 (84%)	107 (14%)	16 (2%)	7 37

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%)	341 (95%)	19 (5%)	22 58
1	B	348/414 (84%)	332 (95%)	16 (5%)	27 63
All	All	708/828 (86%)	673 (95%)	35 (5%)	25 61

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1036	SER
1	A	1078	SER
1	A	1089	PHE
1	A	1094	ASP
1	A	1114	THR
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	1268	LYS
1	A	1290	ARG
1	A	1316	ASP
1	A	1329	THR
1	A	1339	ARG
1	A	1350	ASP
1	A	1390	ILE
1	A	1434	THR
1	B	1059	SER
1	B	1093	GLN
1	B	1094	ASP
1	B	1173	ARG
1	B	1191	SER
1	B	1264	MSE
1	B	1292	ILE
1	B	1366	SER

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Mol	Chain	Res	Type
1	B	1373	GLU
1	B	1380	SER
1	B	1419	ARG
1	B	1422	SER
1	B	1427	ILE
1	B	1458	THR
1	B	1471	SER
1	B	1478	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1121	HIS
1	A	1182	HIS
1	A	1291	HIS
1	A	1309	ASN
1	A	1354	GLN
1	B	1092	HIS
1	B	1192	GLN

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 monosaccharides 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

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	397/474 (83%)	-0.25	1 (0%)	94	92	28, 72, 112, 136	0
1	B	380/474 (80%)	-0.12	4 (1%)	80	69	47, 85, 121, 148	0
All	All	777/948 (81%)	-0.19	5 (0%)	89	83	28, 78, 117, 148	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1125	THR	3.4
1	B	1430	LYS	2.9
1	B	1236	GLU	2.7
1	B	1121	HIS	2.6
1	A	1071	ILE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides 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.