Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 02:22 am BST

PDB ID	:	5CSA
Title	:	Crystal structure of domains BT-BCCP-AC1-AC5 of yeast acetyl-CoA carboxylase
Authors	:	Wei, J.; Tong, L.
Deposited on	:	2015-07-23
Resolution	:	3.00 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:

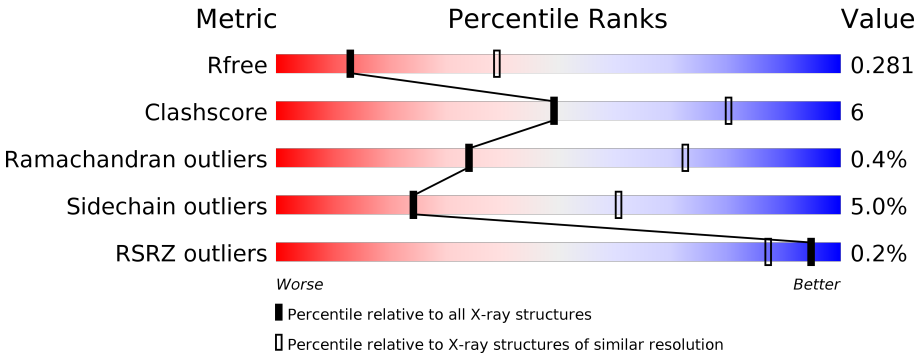
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	932	78% 14% • 6%
1	B	932	77% 13% • 9%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13699 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	872	Total	C	N	O	S	0	4	0
			6939	4440	1182	1296	21			
1	B	852	Total	C	N	O	S	0	0	0
			6760	4329	1146	1265	20			

There are 12 discrepancies between the modelled and reference sequences:

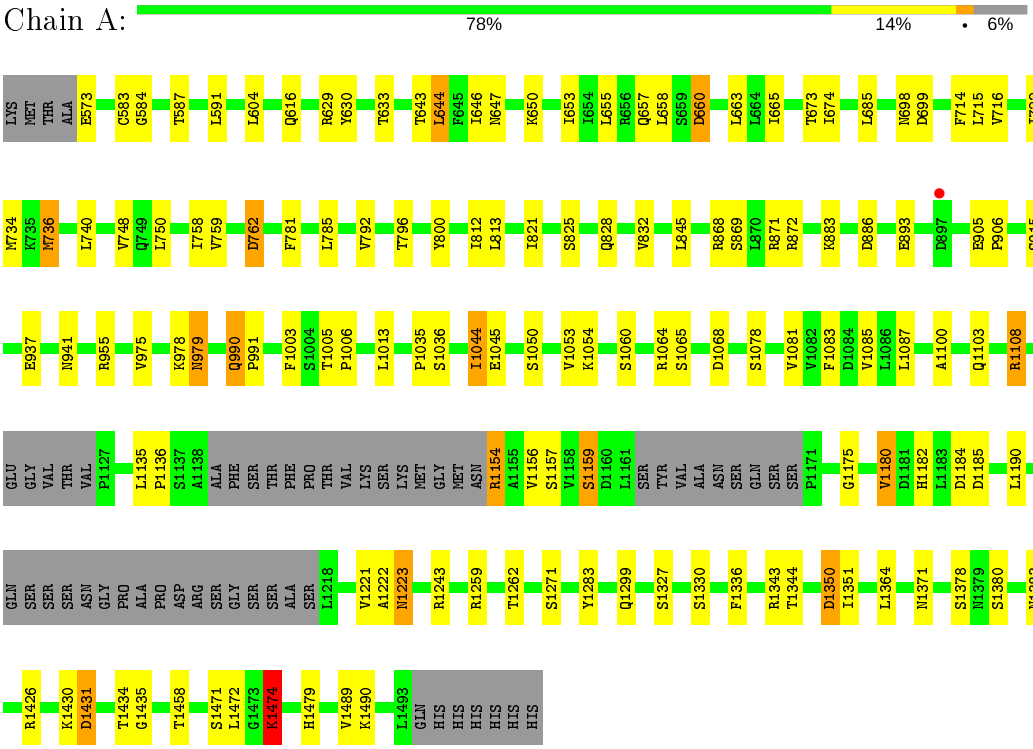
Chain	Residue	Modelled	Actual	Comment	Reference
A	1495	HIS	-	expression tag	UNP Q00955
A	1496	HIS	-	expression tag	UNP Q00955
A	1497	HIS	-	expression tag	UNP Q00955
A	1498	HIS	-	expression tag	UNP Q00955
A	1499	HIS	-	expression tag	UNP Q00955
A	1500	HIS	-	expression tag	UNP Q00955
B	1495	HIS	-	expression tag	UNP Q00955
B	1496	HIS	-	expression tag	UNP Q00955
B	1497	HIS	-	expression tag	UNP Q00955
B	1498	HIS	-	expression tag	UNP Q00955
B	1499	HIS	-	expression tag	UNP Q00955
B	1500	HIS	-	expression tag	UNP Q00955

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.

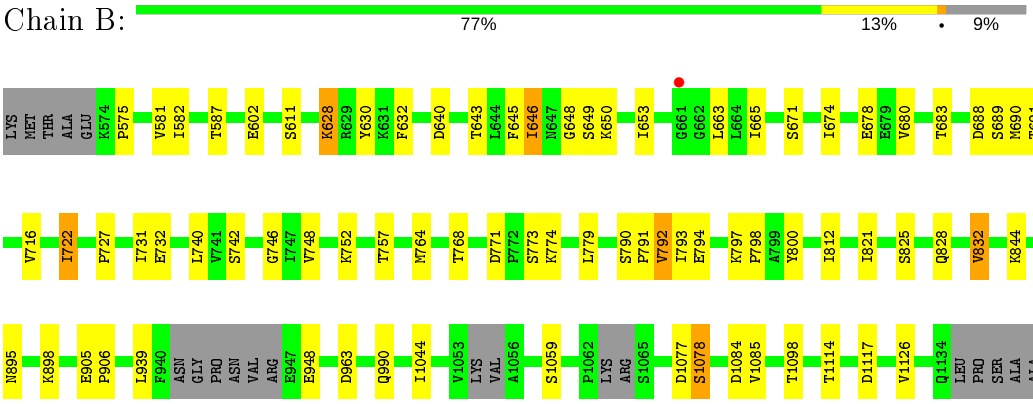
- Molecule 1: Acetyl-CoA carboxylase

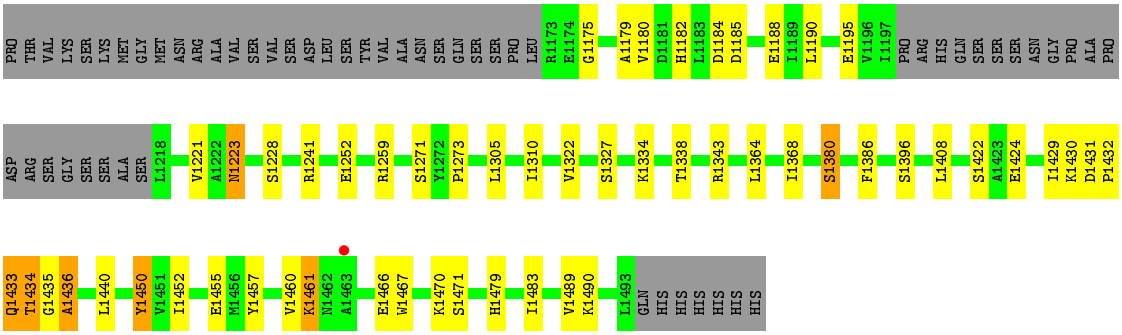
Chain A:



- Molecule 1: Acetyl-CoA carboxylase

Chain B:




PRO THR VAL LYS SER LYS MET GLY MET ASN ARG ALA VAL SER VAL SER SER ASP LEU SER TYR VAL ALA ASN SER GLN SER SER PRO LEU R1173 E1174 G1175 A1179 V1180 D1181 H1182 L1183 D1184 D1185 E1188 I1189 L1190 E1195 V1196 I1197 PRO ARG HIS GLN SER SER SER ASN GLY PRO ALA PRO
ASP ARG SER GLY SER SER ALA SER L1218 V1221 A1222 N1223 S1228 R1241 E1252 R1259 S1271 Y1272 P1273 L1305 I1310 V1322 S1327 K1334 T1338 R1343 L1364 I1368 S1380 F1386 S1396 L1408 S1422 A1423 E1424 I1429 K1430 D1431 P1432
Q1433 T1434 G1435 A1436 L1440 Y1450 V1451 I1452 E1455 M1456 Y1457 V1460 K1461 M1462 A1463 E1466 W1467 K1470 S1471 H1479 I1483 V1489 K1490 L1493 GLN 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	93.33Å 149.67Å 95.44Å 90.00° 118.39° 90.00°	Depositor
Resolution (Å)	42.63 – 3.00 42.64 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.8 (42.63-3.00) 97.9 (42.64-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.230 , 0.289 0.224 , 0.281	Depositor DCC
R_{free} test set	2290 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	60.3	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 17.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h-l,k,h 0.000 for l,k,-h-l 0.020 for h,-k,-h-l 0.023 for -h-l,-k,l 0.018 for l,-k,h	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13699	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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	0.52	1/7082 (0.0%)	0.68	3/9586 (0.0%)
1	B	0.58	6/6890 (0.1%)	0.66	1/9327 (0.0%)
All	All	0.55	7/13972 (0.1%)	0.67	4/18913 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1450	TYR	CE1-CZ	12.68	1.55	1.38
1	B	1466	GLU	CD-OE1	7.30	1.33	1.25
1	B	602	GLU	CD-OE2	7.02	1.33	1.25
1	B	602	GLU	CD-OE1	7.01	1.33	1.25
1	B	1450	TYR	CZ-OH	5.80	1.47	1.37
1	A	573	GLU	CD-OE2	5.62	1.31	1.25
1	B	1450	TYR	CG-CD2	5.30	1.46	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1474	LYS	CD-CE-NZ	7.50	128.95	111.70
1	B	1436	ALA	C-N-CD	5.39	139.72	128.40
1	A	660	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	1431	ASP	C-N-CD	5.02	138.95	128.40

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	6939	0	7077	82	6
1	B	6760	0	6877	87	6
All	All	13699	0	13954	164	6

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 6.

All (164) 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:1431:ASP:OD2	1:A:1434:THR:OG1	1.89	0.91
1:B:1461:LYS:HE2	1:B:1467:TRP:CD1	2.10	0.85
1:B:1432:PRO:HG2	1:B:1433:GLN:NE2	1.92	0.85
1:B:1432:PRO:HG2	1:B:1433:GLN:HE21	1.42	0.85
1:B:1431:ASP:OD2	1:B:1434:THR:OG1	2.00	0.79
1:A:872:ARG:NE	1:B:1188:GLU:HG2	2.00	0.77
1:B:1471:SER:HB2	1:B:1479:HIS:HD2	1.50	0.75
1:A:1154:ARG:NH2	1:A:1351:ILE:O	2.20	0.74
1:B:1327:SER:OG	1:B:1489:VAL:HG11	1.89	0.71
1:A:872:ARG:HE	1:B:1188:GLU:HG2	1.56	0.71
1:A:1371[B]:ASN:O	1:A:1371[B]:ASN:OD1	2.10	0.69
1:A:1431:ASP:OD2	1:A:1434:THR:N	2.21	0.69
1:A:722:ILE:HD12	1:A:748:VAL:HG21	1.75	0.68
1:A:1053:VAL:HG12	1:A:1054:LYS:O	1.94	0.67
1:B:1433:GLN:N	1:B:1433:GLN:HE21	1.93	0.67
1:A:1431:ASP:CG	1:A:1434:THR:HG1	1.95	0.66
1:A:1243:ARG:NH1	1:A:1283:TYR:O	2.26	0.66
1:A:1197:ILE:HG22	1:A:1197:ILE:O	1.96	0.64
1:A:716:VAL:HG21	1:A:722:ILE:HD11	1.79	0.64
1:B:731:ILE:HD11	1:B:740:LEU:HD11	1.80	0.64
1:B:792:VAL:HG11	1:B:800:TYR:CE2	2.34	0.63
1:A:872:ARG:CD	1:B:1188:GLU:HG2	2.29	0.63
1:A:1371[B]:ASN:OD1	1:A:1371[B]:ASN:C	2.37	0.61
1:B:1434:THR:HB	1:B:1436:ALA:H	1.64	0.61
1:A:868:ARG:HG2	1:A:871:ARG:NH1	2.16	0.61
1:B:1305:LEU:HB3	1:B:1310:ILE:HD11	1.83	0.61
1:B:1252:GLU:OE1	1:B:1252:GLU:N	2.32	0.61
1:B:828:GLN:O	1:B:832:VAL:HG23	2.01	0.59
1:A:1078:SER:O	1:A:1108:ARG:NH2	2.35	0.58
1:B:1180:VAL:HG13	1:B:1185:ASP:HB2	1.86	0.58
1:A:937:GLU:OE1	1:A:975:VAL:HG11	2.03	0.58
1:B:628:LYS:HA	1:B:779:LEU:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1458:THR:OG1	1:A:1472:LEU:HD21	2.04	0.58
1:B:1327:SER:OG	1:B:1489:VAL:CG1	2.51	0.58
1:A:1135:LEU:HB3	1:A:1136:PRO:CD	2.34	0.57
1:A:1197:ILE:CG2	1:A:1197:ILE:O	2.53	0.57
1:A:731:ILE:HD12	1:A:740:LEU:HD21	1.85	0.57
1:A:828:GLN:O	1:A:832:VAL:HG23	2.05	0.57
1:B:1455:GLU:OE1	1:B:1457:TYR:OH	2.19	0.57
1:B:792:VAL:HG11	1:B:800:TYR:HE2	1.70	0.57
1:A:1471:SER:HB2	1:A:1479:HIS:HD2	1.69	0.56
1:B:1182:HIS:CD2	1:B:1184:ASP:H	2.23	0.56
1:A:792:VAL:HG13	1:A:800:TYR:CE2	2.40	0.56
1:B:722:ILE:HD12	1:B:748:VAL:HG21	1.87	0.56
1:A:604:LEU:HG	1:A:955:ARG:HD3	1.88	0.56
1:A:587:THR:HG22	1:A:663:LEU:HD12	1.88	0.56
1:A:872:ARG:HD2	1:B:1188:GLU:HG2	1.88	0.56
1:A:1223:ASN:HB3	1:A:1262:THR:HB	1.89	0.55
1:A:698:ASN:OD1	1:A:699:ASP:N	2.39	0.55
1:A:655:LEU:HD22	1:A:663:LEU:HD22	1.89	0.55
1:A:583:CYS:SG	1:A:674:ILE:HD11	2.47	0.54
1:A:658:LEU:O	1:A:660:ASP:O	2.25	0.54
1:B:794:GLU:O	1:B:844:LYS:CD	2.55	0.54
1:B:632:PHE:CZ	1:B:646:ILE:HD11	2.43	0.53
1:A:792:VAL:HG12	1:A:796:THR:OG1	2.10	0.52
1:B:1126:VAL:HG11	1:B:1179:ALA:O	2.08	0.52
1:B:771:ASP:OD1	1:B:773:SER:OG	2.28	0.52
1:A:1350:ASP:N	1:A:1350:ASP:OD1	2.43	0.52
1:B:731:ILE:HG22	1:B:732:GLU:N	2.25	0.52
1:B:1460:VAL:HG21	1:B:1470:LYS:HD3	1.91	0.51
1:A:587:THR:HG22	1:A:663:LEU:CD1	2.40	0.51
1:B:587:THR:HG22	1:B:663:LEU:HD12	1.93	0.51
1:A:715:LEU:O	1:A:716:VAL:HG23	2.11	0.50
1:A:714:PHE:CD1	1:A:750:LEU:HD22	2.46	0.50
1:B:752:LYS:HG2	1:B:764:MET:HA	1.93	0.50
1:A:941:ASN:HD21	1:A:1013:LEU:HA	1.75	0.50
1:B:1322:VAL:HG22	1:B:1338:THR:HG23	1.93	0.50
1:A:1064:ARG:HD2	1:A:1068:ASP:HB2	1.94	0.50
1:B:1431:ASP:O	1:B:1435:GLY:N	2.41	0.49
1:B:1432:PRO:CG	1:B:1433:GLN:HE21	2.19	0.49
1:B:794:GLU:O	1:B:844:LYS:HD2	2.11	0.49
1:B:1430:LYS:HE3	1:B:1435:GLY:HA2	1.94	0.49
1:B:1467:TRP:HB3	1:B:1483:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:665:ILE:HD12	1:B:674:ILE:CD1	2.43	0.49
1:B:1334:LYS:O	1:B:1380:SER:HA	2.12	0.49
1:A:584:GLY:HA2	1:A:685:LEU:HD11	1.95	0.49
1:B:895:ASN:OD1	1:B:898:LYS:HA	2.12	0.49
1:A:630:TYR:CE1	1:A:781:PHE:CD1	3.01	0.49
1:A:905:GLU:HB3	1:A:906:PRO:HD3	1.95	0.48
1:B:794:GLU:O	1:B:844:LYS:HD3	2.14	0.48
1:A:1115:ILE:HD12	1:A:1159:SER:HB3	1.94	0.47
1:A:644:LEU:O	1:A:650:LYS:HA	2.14	0.47
1:A:759:VAL:O	1:A:762:ASP:HB2	2.15	0.47
1:B:1433:GLN:N	1:B:1433:GLN:NE2	2.60	0.47
1:B:1180:VAL:CG1	1:B:1185:ASP:HB2	2.44	0.47
1:B:793:ILE:HG22	1:B:794:GLU:N	2.30	0.47
1:A:1156:VAL:HG12	1:A:1157:SER:O	2.15	0.47
1:B:1182:HIS:HD2	1:B:1184:ASP:H	1.62	0.47
1:B:792:VAL:HG21	1:B:800:TYR:CE2	2.50	0.47
1:A:990:GLN:HG3	1:A:991:PRO:N	2.30	0.47
1:B:1175:GLY:HA2	1:B:1221:VAL:O	2.15	0.47
1:B:1432:PRO:CG	1:B:1433:GLN:NE2	2.73	0.46
1:A:1044:ILE:HD12	1:A:1085:VAL:HG23	1.97	0.46
1:A:734:MET:O	1:A:736:MET:N	2.47	0.46
1:B:705:THR:HG22	1:B:740:LEU:HD11	1.97	0.46
1:A:1489:VAL:HG12	1:A:1490:LYS:N	2.31	0.46
1:A:1221:VAL:HG12	1:A:1222:ALA:N	2.31	0.46
1:A:1182:HIS:CD2	1:A:1184:ASP:H	2.34	0.46
1:A:933:TYR:OH	1:A:979:ASN:ND2	2.49	0.46
1:B:1433:GLN:HE21	1:B:1433:GLN:H	1.60	0.46
1:B:1429:ILE:HD12	1:B:1440:LEU:CD1	2.46	0.45
1:B:731:ILE:CD1	1:B:740:LEU:HD21	2.46	0.45
1:A:1135:LEU:HB3	1:A:1136:PRO:HD3	1.98	0.45
1:A:665:ILE:HG13	1:A:674:ILE:HD12	1.98	0.45
1:B:575:PRO:HB3	1:B:690:MET:HE3	1.99	0.45
1:A:587:THR:HG21	1:A:674:ILE:HG21	1.99	0.45
1:B:582:ILE:CG2	1:B:653:ILE:HD11	2.46	0.45
1:A:734:MET:C	1:A:736:MET:H	2.20	0.45
1:A:731:ILE:HD11	1:A:740:LEU:HD11	1.99	0.45
1:A:1336:PHE:N	1:A:1383:ASN:OD1	2.47	0.44
1:A:1431:ASP:O	1:A:1435:GLY:N	2.47	0.44
1:A:1035:PRO:HB3	1:B:1059:SER:O	2.17	0.44
1:B:821:ILE:CG2	1:B:825:SER:HB3	2.47	0.44
1:B:1489:VAL:HG12	1:B:1490:LYS:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1431:ASP:O	1:A:1435:GLY:HA2	2.16	0.44
1:B:581:VAL:HG21	1:B:630:TYR:CZ	2.53	0.44
1:B:746:GLY:HA3	1:B:768:THR:O	2.18	0.44
1:B:1044:ILE:HD12	1:B:1085:VAL:HG23	2.00	0.44
1:B:1431:ASP:OD1	1:B:1432:PRO:HD2	2.17	0.44
1:A:1100:ALA:O	1:A:1103:GLN:HB2	2.18	0.44
1:A:1175:GLY:HA2	1:A:1221:VAL:O	2.18	0.43
1:A:813:LEU:HA	1:A:978:LYS:HG2	2.00	0.43
1:A:733:VAL:N	1:A:736:MET:O	2.45	0.43
1:A:1344:THR:HG21	1:A:1393:PHE:HZ	1.84	0.43
1:A:646:ILE:HG23	1:A:647:ASN:N	2.33	0.43
1:B:1386:PHE:HA	1:B:1424:GLU:O	2.18	0.43
1:B:792:VAL:HG11	1:B:800:TYR:OH	2.18	0.43
1:A:665:ILE:HD12	1:A:674:ILE:CD1	2.50	0.42
1:B:1195:GLU:O	1:B:1195:GLU:CD	2.57	0.42
1:B:688:ASP:O	1:B:689:SER:OG	2.29	0.42
1:A:1327:SER:OG	1:A:1489:VAL:HG11	2.19	0.42
1:A:812:ILE:HD11	1:A:821:ILE:HD11	2.01	0.42
1:B:1077:ASP:O	1:B:1078:SER:C	2.57	0.42
1:B:727:PRO:HA	1:B:740:LEU:O	2.20	0.42
1:A:1005:THR:HB	1:A:1006:PRO:HD3	2.02	0.42
1:B:628:LYS:HG3	1:B:630:TYR:CZ	2.53	0.42
1:B:1408:LEU:HD22	1:B:1452:ILE:HD13	2.02	0.42
1:B:678:GLU:HG2	1:B:683:THR:HG22	2.02	0.42
1:B:797:LYS:HB2	1:B:798:PRO:HD3	2.00	0.42
1:A:1083:PHE:O	1:A:1087:LEU:HG	2.20	0.42
1:B:790:SER:HB2	1:B:791:PRO:CD	2.50	0.42
1:B:1338:THR:HG21	1:B:1368:ILE:HG23	2.02	0.42
1:A:1180:VAL:HG13	1:A:1185:ASP:HB2	2.02	0.42
1:A:587:THR:O	1:A:591:LEU:HG	2.20	0.42
1:B:645:PHE:HA	1:B:649:SER:O	2.20	0.42
1:A:714:PHE:CG	1:A:750:LEU:HD22	2.55	0.41
1:A:1299:GLN:O	1:A:1388:ASN:ND2	2.46	0.41
1:A:792:VAL:HG13	1:A:800:TYR:HE2	1.84	0.41
1:B:1223:ASN:OD1	1:B:1223:ASN:N	2.53	0.41
1:B:792:VAL:C	1:B:793:ILE:HG13	2.41	0.41
1:A:1050:SER:HA	1:A:1053:VAL:HG23	2.02	0.41
1:B:812:ILE:HD11	1:B:821:ILE:HD11	2.03	0.41
1:B:771:ASP:OD2	1:B:774:LYS:HE3	2.20	0.41
1:A:646:ILE:HG21	1:A:785:LEU:HG	2.03	0.41
1:B:716:VAL:HG21	1:B:722:ILE:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:905:GLU:HB3	1:B:906:PRO:HD3	2.01	0.41
1:B:1431:ASP:O	1:B:1435:GLY:HA2	2.20	0.41
1:B:632:PHE:CE1	1:B:646:ILE:CG1	3.04	0.41
1:B:1461:LYS:HE2	1:B:1467:TRP:CG	2.53	0.40
1:A:1003:PHE:C	1:A:1006:PRO:HD2	2.42	0.40
1:A:657:GLN:HA	1:A:663:LEU:HD23	2.03	0.40
1:B:1489:VAL:CG1	1:B:1490:LYS:N	2.84	0.40
1:B:1084:ASP:HA	1:B:1273:PRO:HD3	2.04	0.40
1:B:646:ILE:C	1:B:648:GLY:H	2.24	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1474:LYS:CD	1:B:1450:TYR:CE1[2_546]	1.72	0.48
1:A:1474:LYS:CE	1:B:1450:TYR:CE1[2_546]	1.85	0.35
1:A:1474:LYS:CE	1:B:1450:TYR:OH[2_546]	2.05	0.15
1:A:1474:LYS:CE	1:B:1450:TYR:CZ[2_546]	2.09	0.11
1:A:1474:LYS:NZ	1:B:1450:TYR:CE1[2_546]	2.10	0.10
1:A:1474:LYS:CD	1:B:1450:TYR:CZ[2_546]	2.17	0.03

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	866/932 (93%)	792 (92%)	73 (8%)	1 (0%)	51 85
1	B	840/932 (90%)	775 (92%)	60 (7%)	5 (1%)	25 64
All	All	1706/1864 (92%)	1567 (92%)	133 (8%)	6 (0%)	34 72

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	680	VAL
1	A	1378	SER
1	B	939	LEU
1	B	948	GLU
1	B	646	ILE
1	B	792	VAL

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	774/821 (94%)	731 (94%)	43 (6%)	21	56
1	B	752/821 (92%)	719 (96%)	33 (4%)	28	65
All	All	1526/1642 (93%)	1450 (95%)	76 (5%)	24	60

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	616	GLN
1	A	629	ARG
1	A	633	THR
1	A	643	THR
1	A	644	LEU
1	A	653	ILE
1	A	673	THR
1	A	736	MET
1	A	758	ILE
1	A	762	ASP
1	A	825	SER
1	A	845	LEU
1	A	869	SER
1	A	883	LYS
1	A	886	ASP
1	A	893	GLU
1	A	915	SER
1	A	924	SER

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Mol	Chain	Res	Type
1	A	979	ASN
1	A	990	GLN
1	A	1036	SER
1	A	1044	ILE
1	A	1045	GLU
1	A	1060	SER
1	A	1065	SER
1	A	1081	VAL
1	A	1108	ARG
1	A	1114	THR
1	A	1154	ARG
1	A	1159	SER
1	A	1180	VAL
1	A	1190	LEU
1	A	1223	ASN
1	A	1259	ARG
1	A	1271	SER
1	A	1330	SER
1	A	1343	ARG
1	A	1350	ASP
1	A	1364	LEU
1	A	1380	SER
1	A	1426	ARG
1	A	1430	LYS
1	A	1474	LYS
1	B	611	SER
1	B	628	LYS
1	B	640	ASP
1	B	643	THR
1	B	650	LYS
1	B	671	SER
1	B	691	THR
1	B	707	SER
1	B	722	ILE
1	B	742	SER
1	B	757	THR
1	B	832	VAL
1	B	882	SER
1	B	963	ASP
1	B	990	GLN
1	B	1078	SER
1	B	1098	THR

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Mol	Chain	Res	Type
1	B	1114	THR
1	B	1117	ASP
1	B	1190	LEU
1	B	1223	ASN
1	B	1228	SER
1	B	1241	ARG
1	B	1259	ARG
1	B	1271	SER
1	B	1343	ARG
1	B	1364	LEU
1	B	1380	SER
1	B	1396	SER
1	B	1422	SER
1	B	1433	GLN
1	B	1434	THR
1	B	1461	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	721	HIS
1	A	835	ASN
1	A	846	HIS
1	A	979	ASN
1	A	1182	HIS
1	A	1479	HIS
1	B	1182	HIS
1	B	1371	ASN
1	B	1384	HIS
1	B	1433	GLN
1	B	1479	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

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	872/932 (93%)	-0.41	1 (0%)	95	89	40, 71, 105, 142	0
1	B	852/932 (91%)	-0.37	3 (0%)	92	79	44, 75, 111, 151	0
All	All	1724/1864 (92%)	-0.39	4 (0%)	95	87	40, 73, 109, 151	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	853	ARG	2.7
1	A	897	ASP	2.6
1	B	661	GLY	2.3
1	B	1463	ALA	2.2

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 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.