Full wwPDB X-ray Structure Validation Report (i)

May 16, 2020 – 02:15 am BST

PDB ID	:	5U1S
Title	:	Crystal structure of the Saccharomyces cerevisiae separase-securin complex at 3.0 angstrom resolution
Authors	:	Luo, S.; Tong, L.
Deposited on	:	2016-11-29
Resolution	:	3.00 Å(reported)

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

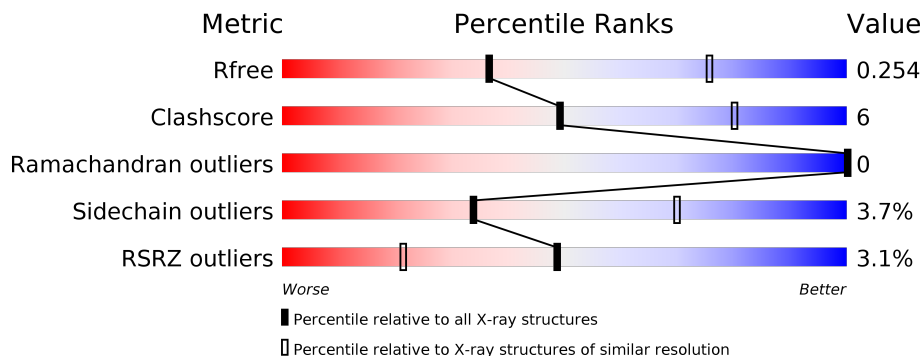|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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	Percentile Ranks	Value
Rfree		0.254
Clashscore		6
Ramachandran outliers		0
Sidechain outliers		3.7%
RSRZ outliers		3.1%

Worse ← → Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

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	1596	3% · 76% · 16% · 7%
2	B	117	% · 43% · 10% · 45%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12609 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 Separin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1488	12083	7817	1979	2219	68	0	0	0

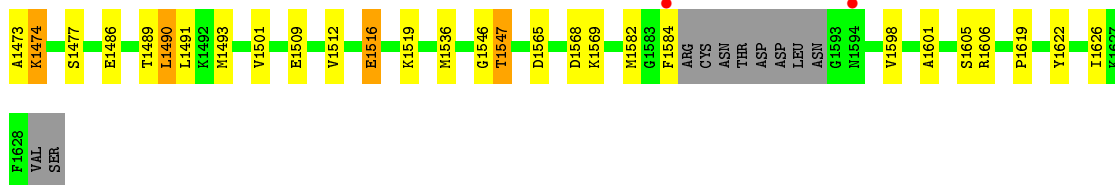There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	MET	-	expression tag	UNP Q03018
A	36	HIS	-	expression tag	UNP Q03018
A	37	HIS	-	expression tag	UNP Q03018
A	38	HIS	-	expression tag	UNP Q03018
A	39	HIS	-	expression tag	UNP Q03018
A	40	HIS	-	expression tag	UNP Q03018
A	41	HIS	-	expression tag	UNP Q03018
A	42	SER	-	expression tag	UNP Q03018
A	43	GLY	-	expression tag	UNP Q03018
A	44	GLY	-	expression tag	UNP Q03018
A	45	SER	-	expression tag	UNP Q03018
A	46	ARG	-	expression tag	UNP Q03018
A	47	SER	-	expression tag	UNP Q03018
A	48	GLU	-	expression tag	UNP Q03018
A	49	ALA	-	expression tag	UNP Q03018
A	50	HIS	-	expression tag	UNP Q03018

- Molecule 2 is a protein called Securin.

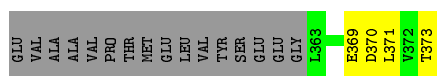| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	64	526	339	77	109	1	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	257	MET	-	initiating methionine	UNP P40316

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: Separin

A1473 K1474 S1477 E1486 T1489 L1490 L1491 K1492 M1493 V1501 E1509 V1512 E1516 K1519 M1536 G1546 T1547 D1565 D1568 K1569 M1582 G1583 F1584 ARG CYS ASN THR ASP ASP LEU ASN G1593 N1594 V1598 A1601 S1605 R1606 P1619 Y1622 I1626 K1627

F1628 VAL SER

• Molecule 2: Securin

Chain B:

43%   10% •   45%

M257 E260 L269 P270 Y276 D283 P293 Y294 K295 L296 D297 L298 GLU ASP GLU ASP ASP THR PRO D306 L311 P312 I316 ASP GLU GLU GLU LYS ASP GLU THR GLU CYS ILE THR ARG ASN GLN GLU GLU GLY ALA ALA LEU PRO LEU LEU SER LYS ASN PHE LYS

GLU VAL ALA ALA VAL PRO THR MET GLU LEU VAL TYR SER GLU GLU GLY L363 E369 D370 L371 V372 T373

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	126.30Å 126.30Å 273.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.98 – 3.00 48.98 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.98-3.00) 99.5 (48.98-3.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.55 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.190 , 0.251 0.197 , 0.254	Depositor DCC
R_{free} test set	2633 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å²)	86.6	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.33 , 58.5	EDS
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12609	wwPDB-VP
Average B, all atoms (Å²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (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	0.25	0/12319	0.39	0/16621
2	B	0.22	0/536	0.39	0/728
All	All	0.24	0/12855	0.39	0/17349

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 (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	12083	0	12338	146	0
2	B	526	0	511	9	0
All	All	12609	0	12849	151	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 6.

All (151) 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:1273:ASN:OD1	1:A:1343:ASP:OD2	1.98	0.81
1:A:868:ARG:NH2	1:A:908:SER:OG	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1156:GLN:HE21	1:A:1192:ARG:NH1	1.86	0.72
1:A:236:LYS:HD2	1:A:284:TYR:CE2	2.26	0.70
1:A:1156:GLN:HE21	1:A:1192:ARG:HH11	1.40	0.68
1:A:1442:ILE:HD11	1:A:1584:PHE:HD1	1.60	0.67
1:A:786:LYS:NZ	1:A:959:GLU:OE2	2.27	0.67
1:A:727:VAL:HG13	1:A:779:GLU:OE2	1.96	0.66
1:A:1180:LEU:HB2	1:A:1199:LEU:HD21	1.79	0.65
1:A:1232:THR:HG21	1:A:1565:ASP:HB3	1.78	0.65
1:A:989:MET:HE1	1:A:1090:ILE:HD11	1.79	0.64
1:A:1509:GLU:OE2	1:A:1547:THR:HG21	1.98	0.63
1:A:1490:LEU:HA	1:A:1493:MET:HB2	1.81	0.63
1:A:1432:PHE:O	1:A:1435:GLN:HG2	1.99	0.63
1:A:1240:ILE:HG13	1:A:1245:GLU:HG3	1.80	0.63
1:A:1435:GLN:O	1:A:1435:GLN:HG3	1.97	0.62
1:A:604:MET:HE1	1:A:816:GLN:HG2	1.81	0.62
1:A:1569:LYS:HD2	2:B:260:GLU:HG2	1.82	0.62
1:A:60:HIS:HD2	1:A:88:SER:HA	1.64	0.61
1:A:695:ASP:OD1	1:A:936:LYS:HD3	2.00	0.61
1:A:1432:PHE:CG	1:A:1438:LEU:HD11	2.36	0.60
1:A:157:THR:HA	1:A:160:ASP:OD2	2.01	0.60
1:A:286:GLY:O	1:A:287:LEU:HG	2.02	0.58
1:A:1169:ILE:HG12	1:A:1184:LYS:HG3	1.86	0.57
1:A:228:GLY:HA3	1:A:258:LEU:HD21	1.87	0.57
1:A:1486:GLU:O	1:A:1489:THR:OG1	2.22	0.56
1:A:607:HIS:ND1	1:A:862:GLU:OE2	2.38	0.56
1:A:238:PHE:N	1:A:238:PHE:CD1	2.73	0.56
1:A:235:ILE:O	1:A:238:PHE:O	2.24	0.55
1:A:1458:ARG:NH2	1:A:1568:ASP:OD2	2.40	0.54
1:A:1443:GLU:HA	1:A:1474:LYS:HE3	1.89	0.54
1:A:226:LEU:HD21	1:A:273:LEU:HA	1.90	0.54
1:A:239:LYS:HD3	1:A:239:LYS:N	2.23	0.54
1:A:210:THR:HG22	1:A:234:TYR:HB3	1.89	0.54
1:A:1606:ARG:NH2	1:A:1619:PRO:O	2.41	0.53
1:A:725:ILE:HG22	1:A:779:GLU:HG3	1.89	0.53
1:A:1491:LEU:HD21	1:A:1516:GLU:HB3	1.91	0.52
1:A:1490:LEU:HD11	1:A:1512:VAL:HB	1.91	0.52
1:A:220:THR:OG1	1:A:222:SER:O	2.23	0.51
1:A:1474:LYS:NZ	1:A:1474:LYS:HA	2.25	0.51
1:A:600:LEU:O	1:A:604:MET:HG3	2.11	0.51
1:A:1331:ASN:HD22	1:A:1334:GLU:HG3	1.76	0.50
1:A:190:LEU:HD11	1:A:198:LEU:HD23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:LYS:HG3	2:B:371:LEU:HD12	1.92	0.50
1:A:542:TYR:HB3	1:A:550:ILE:HD13	1.92	0.50
1:A:1285:ASP:OD2	1:A:1288:LEU:HG	2.11	0.50
1:A:1043:LYS:NZ	1:A:1043:LYS:HB2	2.26	0.49
1:A:1330:LEU:HD11	1:A:1344:LEU:HD12	1.94	0.49
1:A:382:PHE:HZ	1:A:428:ILE:HD11	1.77	0.49
1:A:1085:THR:HG21	1:A:1196:ARG:HD2	1.93	0.49
1:A:912:PHE:O	1:A:916:ASN:ND2	2.43	0.49
2:B:370:ASP:HA	2:B:373:THR:HG22	1.95	0.49
1:A:1307:ARG:NH1	1:A:1316:PHE:HB3	2.28	0.49
1:A:1473:ALA:O	1:A:1474:LYS:NZ	2.33	0.49
1:A:220:THR:HG23	1:A:224:LYS:HG2	1.95	0.48
1:A:1449:ILE:HG22	1:A:1452:PRO:HG3	1.95	0.48
1:A:271:ILE:HG21	1:A:369:LEU:HD13	1.96	0.48
1:A:1401:HIS:CE1	1:A:1622:TYR:HH	2.32	0.47
1:A:1079:LEU:HD13	1:A:1176:ILE:HD13	1.96	0.47
1:A:79:ILE:HG23	1:A:127:LEU:HD11	1.97	0.47
1:A:158:TRP:CZ2	1:A:496:TYR:HA	2.50	0.47
1:A:790:VAL:HG11	1:A:840:ILE:HG21	1.95	0.46
1:A:871:HIS:ND1	1:A:915:ASP:OD2	2.42	0.46
1:A:364:TRP:CE3	1:A:367:ILE:HD12	2.50	0.46
2:B:293:PRO:HG2	2:B:294:TYR:CD1	2.51	0.46
1:A:206:ALA:O	1:A:210:THR:HG23	2.16	0.46
1:A:1448:MET:HB3	1:A:1501:VAL:HG22	1.97	0.46
1:A:270:LYS:NZ	1:A:328:SER:OG	2.49	0.46
1:A:433:PHE:CE2	1:A:474:LYS:HE3	2.51	0.46
1:A:643:LYS:HD2	1:A:675:ILE:HD11	1.97	0.46
1:A:1419:VAL:HG11	1:A:1425:LEU:HB2	1.97	0.46
1:A:1432:PHE:CD1	1:A:1438:LEU:HD11	2.51	0.46
1:A:159:ASN:HA	1:A:162:TYR:CE2	2.51	0.46
1:A:698:MET:O	1:A:702:GLN:HG2	2.15	0.46
1:A:195:LYS:HA	1:A:199:LEU:HB2	1.98	0.45
1:A:1403:PHE:O	1:A:1418:ARG:NH2	2.48	0.45
1:A:714:ILE:HD12	1:A:751:GLU:HG3	1.99	0.45
1:A:1341:MET:O	1:A:1345:ILE:HG12	2.16	0.45
1:A:1536:MET:HG2	1:A:1546:GLY:HA3	1.98	0.45
1:A:1582:MET:HE1	1:A:1598:VAL:HG23	1.98	0.45
1:A:255:SER:HB3	1:A:290:ILE:HD11	1.98	0.45
1:A:718:LEU:HD23	1:A:772:LEU:HD22	1.99	0.45
1:A:1336:ASP:OD1	1:A:1336:ASP:N	2.47	0.45
1:A:1470:ILE:O	1:A:1474:LYS:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:VAL:HG23	1:A:532:ASN:O	2.17	0.44
1:A:973:TRP:CD2	1:A:1079:LEU:HD11	2.53	0.44
1:A:1174:CYS:HB2	1:A:1181:LEU:HD11	2.00	0.44
1:A:1402:LEU:HD23	1:A:1402:LEU:H	1.82	0.44
1:A:1598:VAL:HG12	1:A:1626:ILE:H	1.83	0.44
1:A:1601:ALA:O	1:A:1605:SER:OG	2.25	0.44
1:A:472:PHE:O	1:A:476:ILE:HG13	2.18	0.44
1:A:798:ARG:NH1	2:B:276:TYR:HA	2.33	0.44
1:A:356:THR:HG23	1:A:357:LEU:HD12	2.00	0.43
1:A:735:THR:O	1:A:739:ILE:HG12	2.18	0.43
1:A:1170:THR:HG22	1:A:1395:VAL:HB	2.00	0.43
1:A:236:LYS:HB3	1:A:283:LEU:HD21	2.00	0.43
1:A:1180:LEU:HA	1:A:1180:LEU:HD22	1.89	0.43
1:A:57:LEU:HD22	1:A:584:LEU:HD11	2.00	0.43
1:A:757:ASN:HB2	1:A:766:TYR:CE1	2.53	0.43
1:A:996:ILE:HG12	1:A:1100:LEU:HD13	2.00	0.43
1:A:839:ARG:HG3	1:A:1069:ASP:HA	2.01	0.43
1:A:921:LYS:HB2	1:A:921:LYS:HE3	1.86	0.43
1:A:366:THR:HA	1:A:369:LEU:HD12	2.01	0.43
1:A:584:LEU:HA	1:A:584:LEU:HD23	1.89	0.43
1:A:1108:ASP:OD2	1:A:1422:TYR:HB2	2.18	0.43
1:A:1199:LEU:HD22	1:A:1271:TRP:CG	2.54	0.43
1:A:67:PHE:CG	1:A:85:VAL:HG21	2.53	0.42
1:A:56:ILE:O	1:A:60:HIS:ND1	2.51	0.42
1:A:604:MET:HE2	1:A:816:GLN:HE21	1.83	0.42
1:A:808:LEU:HD13	2:B:283:ASP:HB3	2.02	0.42
1:A:1057:LYS:HE2	1:A:1057:LYS:HB3	1.89	0.42
1:A:385:THR:O	1:A:389:ILE:HG13	2.19	0.42
1:A:433:PHE:O	1:A:436:SER:OG	2.22	0.42
1:A:1195:LEU:HD13	1:A:1197:LEU:HD21	2.02	0.42
1:A:1359:ASN:HB3	1:A:1364:ILE:HD11	2.01	0.42
1:A:238:PHE:HD1	1:A:238:PHE:N	2.16	0.42
1:A:258:LEU:HA	1:A:263:TYR:HD2	1.85	0.42
1:A:684:LEU:HD23	1:A:723:SER:HB2	2.02	0.42
1:A:1474:LYS:HB3	1:A:1477:SER:OG	2.20	0.41
2:B:296:LEU:HD12	2:B:296:LEU:HA	1.79	0.41
1:A:169:LEU:O	1:A:173:ILE:HG13	2.20	0.41
1:A:249:ILE:HD12	1:A:249:ILE:H	1.84	0.41
1:A:628:ASP:N	1:A:628:ASP:OD1	2.54	0.41
1:A:67:PHE:CD1	1:A:85:VAL:HG21	2.56	0.41
1:A:854:SER:HA	1:A:857:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:GLN:HE21	1:A:176:LYS:HZ2	1.67	0.41
1:A:597:VAL:HG22	1:A:641:PHE:CD1	2.55	0.41
1:A:1292:PHE:CG	1:A:1328:LEU:HD21	2.55	0.41
1:A:1347:PHE:O	1:A:1351:ILE:HG13	2.20	0.41
1:A:275:SER:OG	1:A:369:LEU:O	2.39	0.41
1:A:412:LEU:HA	1:A:415:ILE:HD12	2.02	0.41
1:A:1460:GLU:O	1:A:1464:LYS:HB2	2.20	0.41
1:A:765:LEU:HD23	1:A:765:LEU:HA	1.89	0.41
1:A:217:PHE:HB2	1:A:227:PHE:HB3	2.03	0.41
1:A:116:ILE:O	1:A:120:ILE:HG13	2.20	0.41
1:A:250:THR:OG1	1:A:251:VAL:N	2.54	0.41
1:A:67:PHE:CE1	1:A:78:ALA:HB1	2.55	0.41
1:A:993:THR:HG23	1:A:1197:LEU:HD23	2.03	0.41
1:A:287:LEU:HB3	1:A:288:ASP:H	1.69	0.41
1:A:331:SER:HB2	1:A:334:ASP:OD2	2.21	0.41
1:A:479:ALA:HB3	1:A:485:LYS:HG3	2.02	0.40
1:A:1179:ASN:HD22	1:A:1196:ARG:NH1	2.18	0.40
1:A:336:ASN:ND2	1:A:377:ASP:OD2	2.54	0.40
1:A:1267:ILE:HG23	1:A:1271:TRP:CE3	2.56	0.40
1:A:253:CYS:O	1:A:257:ASN:HB2	2.21	0.40
1:A:846:CYS:HB3	1:A:876:TYR:CE1	2.57	0.40
1:A:923:GLU:O	1:A:927:VAL:HG13	2.22	0.40
2:B:269:LEU:HA	2:B:270:PRO:HD3	1.89	0.40
1:A:1073:LEU:HD21	1:A:1109:LEU:HB3	2.04	0.40
1:A:749:LYS:HD2	1:A:749:LYS:HA	1.83	0.40
2:B:311:LEU:HA	2:B:312:PRO:HD3	1.84	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	1470/1596 (92%)	1428 (97%)	42 (3%)	0	100	100
2	B	58/117 (50%)	58 (100%)	0	0	100	100
All	All	1528/1713 (89%)	1486 (97%)	42 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	1390/1491 (93%)	1340 (96%)	50 (4%)	35	70
2	B	62/108 (57%)	59 (95%)	3 (5%)	25	62
All	All	1452/1599 (91%)	1399 (96%)	53 (4%)	34	70

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	75	ILE
1	A	87	HIS
1	A	176	LYS
1	A	198	LEU
1	A	238	PHE
1	A	292	LEU
1	A	327	TRP
1	A	332	VAL
1	A	374	LYS
1	A	460	ASN
1	A	628	ASP
1	A	699	MET
1	A	704	GLN
1	A	735	THR
1	A	748	MET
1	A	760	ASN
1	A	860	LEU

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Mol	Chain	Res	Type
1	A	864	ILE
1	A	868	ARG
1	A	900	LEU
1	A	996	ILE
1	A	1043	LYS
1	A	1063	LEU
1	A	1087	LEU
1	A	1091	THR
1	A	1093	ILE
1	A	1104	PHE
1	A	1106	LEU
1	A	1141	ASN
1	A	1151	ARG
1	A	1164	LEU
1	A	1180	LEU
1	A	1230	GLN
1	A	1232	THR
1	A	1255	ASP
1	A	1301	HIS
1	A	1302	GLN
1	A	1370	HIS
1	A	1383	THR
1	A	1419	VAL
1	A	1428	LEU
1	A	1436	LEU
1	A	1446	ILE
1	A	1453	ASN
1	A	1474	LYS
1	A	1490	LEU
1	A	1516	GLU
1	A	1519	LYS
1	A	1547	THR
2	B	283	ASP
2	B	296	LEU
2	B	369	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	GLN
1	A	704	GLN
1	A	1042	GLN

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Mol	Chain	Res	Type
1	A	1128	ASN
1	A	1156	GLN
1	A	1179	ASN
1	A	1230	GLN
1	A	1273	ASN
1	A	1331	ASN
1	A	1439	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 carbohydrates 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(Å²)	Q<0.9
1	A	1488/1596 (93%)	-0.01	47 (3%)	47	20	49, 86, 164, 240	0
2	B	64/117 (54%)	0.02	1 (1%)	72	44	65, 103, 150, 161	0
All	All	1552/1713 (90%)	-0.01	48 (3%)	49	21	49, 86, 164, 240	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	299	GLU	7.3
1	A	296	LEU	4.6
1	A	300	GLU	4.5
1	A	292	LEU	4.3
1	A	340	GLU	4.2
1	A	377	ASP	4.1
1	A	254	PHE	3.9
1	A	308	ILE	3.6
1	A	258	LEU	3.6
1	A	286	GLY	3.2
1	A	388	TYR	3.2
1	A	419	TYR	3.1
1	A	306	ARG	3.0
1	A	1385	THR	3.0
1	A	330	ILE	2.9
1	A	1594	ASN	2.9
1	A	305	GLN	2.8
1	A	216	PHE	2.7
1	A	295	ILE	2.6
1	A	76	ASP	2.6
1	A	54	ILE	2.6
1	A	232	LEU	2.6
1	A	294	ASP	2.5
1	A	298	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1125	ASP	2.5
1	A	78	ALA	2.5
1	A	73	ASN	2.4
1	A	253	CYS	2.4
1	A	343	THR	2.4
1	A	376	LYS	2.4
1	A	395	SER	2.3
1	A	80	GLU	2.3
1	A	1584	PHE	2.3
1	A	372	LEU	2.3
1	A	1384	MET	2.2
1	A	225	VAL	2.2
1	A	1130	ARG	2.2
1	A	341	ASN	2.2
1	A	260	HIS	2.2
1	A	398	ASP	2.2
1	A	309	LYS	2.2
1	A	1383	THR	2.2
1	A	1386	THR	2.1
1	A	671	TYR	2.1
2	B	306	ASP	2.1
1	A	370	GLU	2.1
1	A	374	LYS	2.1
1	A	297	SER	2.1

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 carbohydrates 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.