



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:56 AM UTC

PDB ID : 5U1S / pdb_00005u1s
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)

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

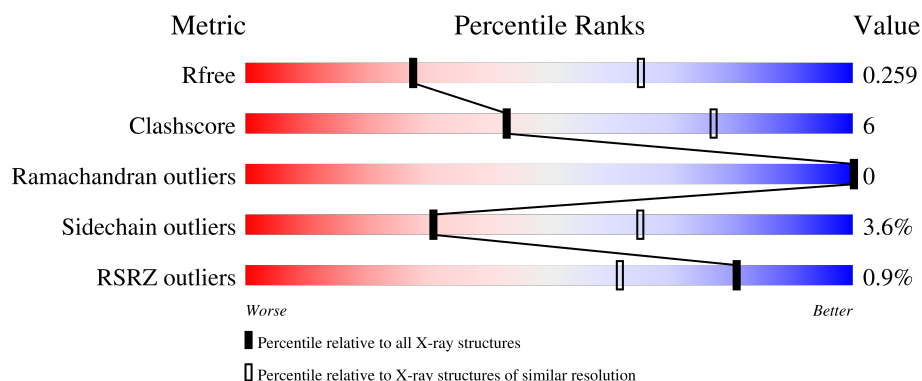
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

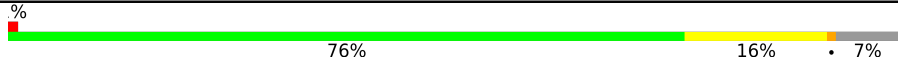
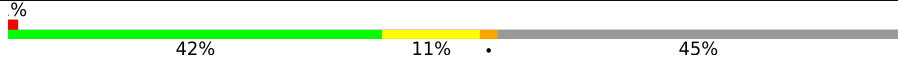
The reported resolution of this entry is 3.00 Å.

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 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	1596	
2	B	117	

2 Entry composition

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
1	A	1488	Total	C	N	O	S	0	0	0
			12083	7817	1979	2219	68			

There are 16 discrepancies between the modelled and reference sequences:

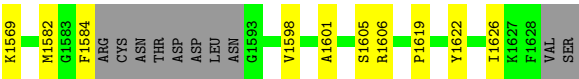
Chain	Residue	Modelled	Actual	Comment	Reference
A	35	MET	-	expression tag	UNP Q03018
A	36	HIS	-	expression tag	UNP Q03018
A	37	HIS	-	expression tag	UNP Q03018
A	38	HIS	-	expression tag	UNP Q03018
A	39	HIS	-	expression tag	UNP Q03018
A	40	HIS	-	expression tag	UNP Q03018
A	41	HIS	-	expression tag	UNP Q03018
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.

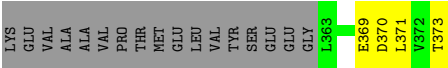
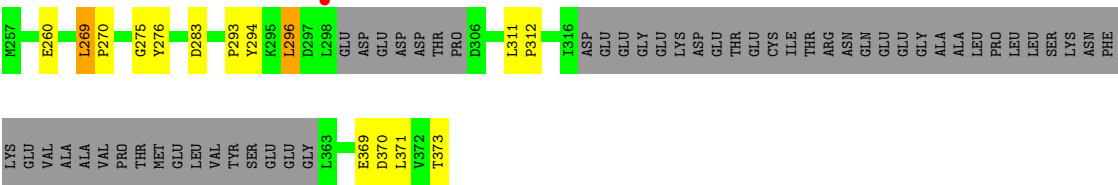
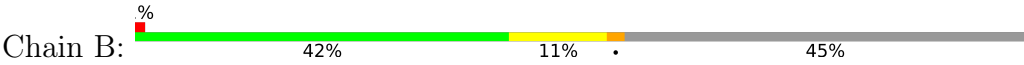
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	64	Total	C	N	O	S	0	0	0
			526	339	77	109	1			

There is a discrepancy between the modelled and reference sequences:

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



● Molecule 2: Securin



4 Data and refinement statistics

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) 99.4 (48.98-3.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.190 , 0.251 (Not available) , 0.259	Depositor DCC
R_{free} test set	2633 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	86.6	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 66.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 (Å ²)	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.*

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

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	0.31	0/12319	0.69	3/16621 (0.0%)
2	B	0.29	0/536	0.72	2/728 (0.3%)
All	All	0.31	0/12855	0.69	5/17349 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	PHE	N-CA-C	-5.54	99.69	108.73
1	A	1304	LEU	CA-C-N	5.16	125.20	119.32
1	A	1304	LEU	C-N-CA	5.16	125.20	119.32
2	B	269	LEU	CA-C-N	5.03	125.03	119.90
2	B	269	LEU	C-N-CA	5.03	125.03	119.90

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	12083	0	12338	153	0
2	B	526	0	511	12	0
All	All	12609	0	12849	158	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 (158) 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:604:MET:HE2	1:A:816:GLN:HE21	1.44	0.81
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
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:644:MET:HE3	2:B:293:PRO:HB3	1.75	0.68
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: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: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:989:MET:HE1	1:A:1090:ILE:HD11	1.81	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:607:HIS:ND1	1:A:862:GLU:OE2	2.38	0.56
1:A:1486:GLU:O	1:A:1489:THR:OG1	2.22	0.56
1:A:238:PHE:CD1	1:A:238:PHE:N	2.73	0.56
1:A:433:PHE:O	1:A:436:SER:OG	2.22	0.55
1:A:604:MET:HE1	1:A:644:MET:SD	2.47	0.55
1:A:235:ILE:O	1:A:238:PHE:O	2.24	0.55
1:A:220:THR:OG1	1:A:222:SER:O	2.23	0.55
1:A:1458:ARG:NH2	1:A:1568:ASP:OD2	2.40	0.54
1:A:226:LEU:HD21	1:A:273:LEU:HA	1.90	0.54
1:A:1443:GLU:HA	1:A:1474:LYS:HE3	1.89	0.54
1:A:239:LYS:N	1:A:239:LYS:HD3	2.23	0.54
1:A:210:THR:HG22	1:A:234:TYR:HB3	1.89	0.54
1:A:1582:MET:HE2	1:A:1598:VAL:HA	1.89	0.53
1:A:725:ILE:HG22	1:A:779:GLU:HG3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1606:ARG:NH2	1:A:1619:PRO:O	2.41	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:1474:LYS:HA	1:A:1474:LYS:NZ	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
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:172:GLN:HE21	1:A:176:LYS:HZ2	1.59	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: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:1079:LEU:HD13	1:A:1176:ILE:HD13	1.96	0.47
1:A:1401:HIS:CD2	1:A:1536:MET:HE2	2.50	0.46
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:232:LEU:O	1:A:284:TYR:OH	2.25	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:1448:MET:HB3	1:A:1501:VAL:HG22	1.97	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:159:ASN:HA	1:A:162:TYR:CE2	2.51	0.46
1:A:1432:PHE:CD1	1:A:1438:LEU:HD11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:604:MET:HE3	1:A:648:TYR:CD1	2.52	0.45
1:A:714:ILE:HD12	1:A:751:GLU:HG3	1.99	0.45
1:A:1403:PHE:O	1:A:1418:ARG:NH2	2.48	0.45
1:A:1341:MET:O	1:A:1345:ILE:HG12	2.16	0.45
1:A:1401:HIS:ND1	1:A:1622:TYR:OH	2.45	0.45
1:A:1536:MET:HG2	1:A:1546:GLY:HA3	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:1601:ALA:O	1:A:1605:SER:OG	2.25	0.45
1:A:1336:ASP:OD1	1:A:1336:ASP:N	2.47	0.45
1:A:1569:LYS:HB2	2:B:260:GLU:CD	2.41	0.45
1:A:495:VAL:HG23	1:A:532:ASN:O	2.17	0.44
1:A:1470:ILE:O	1:A:1474:LYS:HB2	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:H	1:A:1402:LEU:HD23	1.82	0.44
1:A:1446:ILE:HD11	1:A:1448:MET:HE3	2.00	0.44
1:A:1598:VAL:HG12	1:A:1626:ILE:H	1.83	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:236:LYS:HB3	1:A:283:LEU:HD21	2.00	0.43
1:A:1170:THR:HG22	1:A:1395:VAL:HB	2.00	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:1180:LEU:HD22	1:A:1180:LEU:HA	1.89	0.43
1:A:839:ARG:HG3	1:A:1069:ASP:HA	2.01	0.43
1:A:921:LYS:HE3	1:A:921:LYS:HB2	1.86	0.43
1:A:366:THR:HA	1:A:369:LEU:HD12	2.01	0.43
1:A:584:LEU:HD23	1:A:584:LEU:HA	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:808:LEU:HD13	2:B:283:ASP:HB3	2.02	0.42
1:A:385:THR:O	1:A:389:ILE:HG13	2.19	0.42
1:A:1057:LYS:HE2	1:A:1057:LYS:HB3	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:PHE:N	1:A:238:PHE:HD1	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:1160:MET:HE3	1:A:1192:ARG:CZ	2.49	0.41
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:67:PHE:CD1	1:A:85:VAL:HG21	2.56	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:OD1	1:A:628:ASP:N	2.54	0.41
1:A:854:SER:HA	1:A:857:ILE:HD12	2.02	0.41
1:A:597:VAL:HG22	1:A:641:PHE:CD1	2.55	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: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: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:798:ARG:NH1	2:B:275:GLY:C	2.78	0.41
1:A:67:PHE:CE1	1:A:78:ALA:HB1	2.55	0.41
1:A:116:ILE:O	1:A:120:ILE:HG13	2.20	0.41
1:A:217:PHE:HB2	1:A:227:PHE:HB3	2.03	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:336:ASN:ND2	1:A:377:ASP:OD2	2.54	0.40
1:A:1179:ASN:HD22	1:A:1196:ARG:NH1	2.18	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
1:A:1267:ILE:HG23	1:A:1271:TRP:CE3	2.56	0.40
2:B:269:LEU:HA	2:B:270:PRO:HD3	1.89	0.40
1:A:749:LYS:HD2	1:A:749:LYS:HA	1.83	0.40
1:A:1073:LEU:HD21	1:A:1109:LEU:HB3	2.04	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

5.3.1 Protein backbone

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

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%)	31	65
2	B	62/108 (57%)	60 (97%)	2 (3%)	34	67
All	All	1452/1599 (91%)	1400 (96%)	52 (4%)	31	65

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	75	ILE
1	A	182	GLU
1	A	198	LEU
1	A	235	ILE
1	A	238	PHE
1	A	289	LYS
1	A	292	LEU

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Mol	Chain	Res	Type
1	A	332	VAL
1	A	360	LEU
1	A	387	ILE
1	A	675	ILE
1	A	699	MET
1	A	704	GLN
1	A	735	THR
1	A	748	MET
1	A	760	ASN
1	A	860	LEU
1	A	864	ILE
1	A	900	LEU
1	A	903	GLU
1	A	972	MET
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	1143	ILE
1	A	1164	LEU
1	A	1180	LEU
1	A	1219	LYS
1	A	1232	THR
1	A	1255	ASP
1	A	1265	ASN
1	A	1302	GLN
1	A	1383	THR
1	A	1419	VAL
1	A	1428	LEU
1	A	1436	LEU
1	A	1440	VAL
1	A	1446	ILE
1	A	1453	ASN
1	A	1474	LYS
1	A	1501	VAL
1	A	1516	GLU
1	A	1519	LYS
1	A	1547	THR

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Mol	Chain	Res	Type
2	B	296	LEU
2	B	369	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	111	GLN
1	A	172	GLN
1	A	186	HIS
1	A	494	ASN
1	A	532	ASN
1	A	544	ASN
1	A	621	ASN
1	A	652	ASN
1	A	704	GLN
1	A	886	GLN
1	A	924	GLN
1	A	1042	GLN
1	A	1071	HIS
1	A	1112	HIS
1	A	1156	GLN
1	A	1179	ASN
1	A	1230	GLN
1	A	1265	ASN
1	A	1273	ASN
1	A	1331	ASN
1	A	1355	HIS
1	A	1439	GLN
1	A	1496	ASN
2	B	291	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	1488/1596 (93%)	-0.21	13 (0%) 81 61	49, 86, 164, 240	0
2	B	64/117 (54%)	0.01	1 (1%) 70 47	65, 103, 150, 161	0
All	All	1552/1713 (90%)	-0.20	14 (0%) 81 61	49, 86, 164, 240	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	258	LEU	4.0
1	A	353	ILE	2.8
1	A	1200	ILE	2.8
1	A	310	SER	2.7
1	A	216	PHE	2.6
1	A	374	LYS	2.5
1	A	254	PHE	2.3
1	A	264	LEU	2.3
1	A	292	LEU	2.2
1	A	359	CYS	2.2
1	A	330	ILE	2.2
1	A	345	PHE	2.2
1	A	317	TYR	2.2
2	B	298	LEU	2.2

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.