



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:46 AM UTC

PDB ID : 5U1T / pdb_00005u1t
Title : Crystal structure of the *Saccharomyces cerevisiae* separase-securin complex at 2.6 angstrom resolution
Authors : Luo, S.; Tong, L.
Deposited on : 2016-11-29
Resolution : 2.60 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

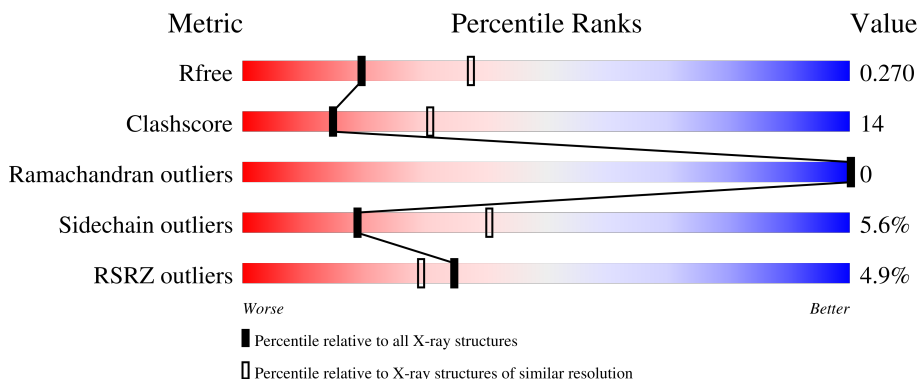
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

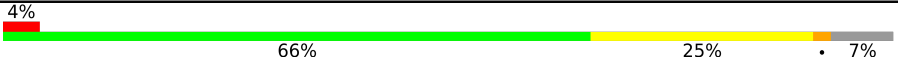
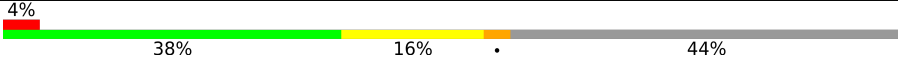
The reported resolution of this entry is 2.60 Å.

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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	 4% 66% 25% • 7%
2	B	117	 4% 38% 16% • 44%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12633 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	1486	Total	C	N	O	S	0	0	0
			12078	7811	1979	2220	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	66	Total	C	N	O	S	0	0	0
			539	346	79	113	1			

There is a discrepancy between the modelled and reference sequences:

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

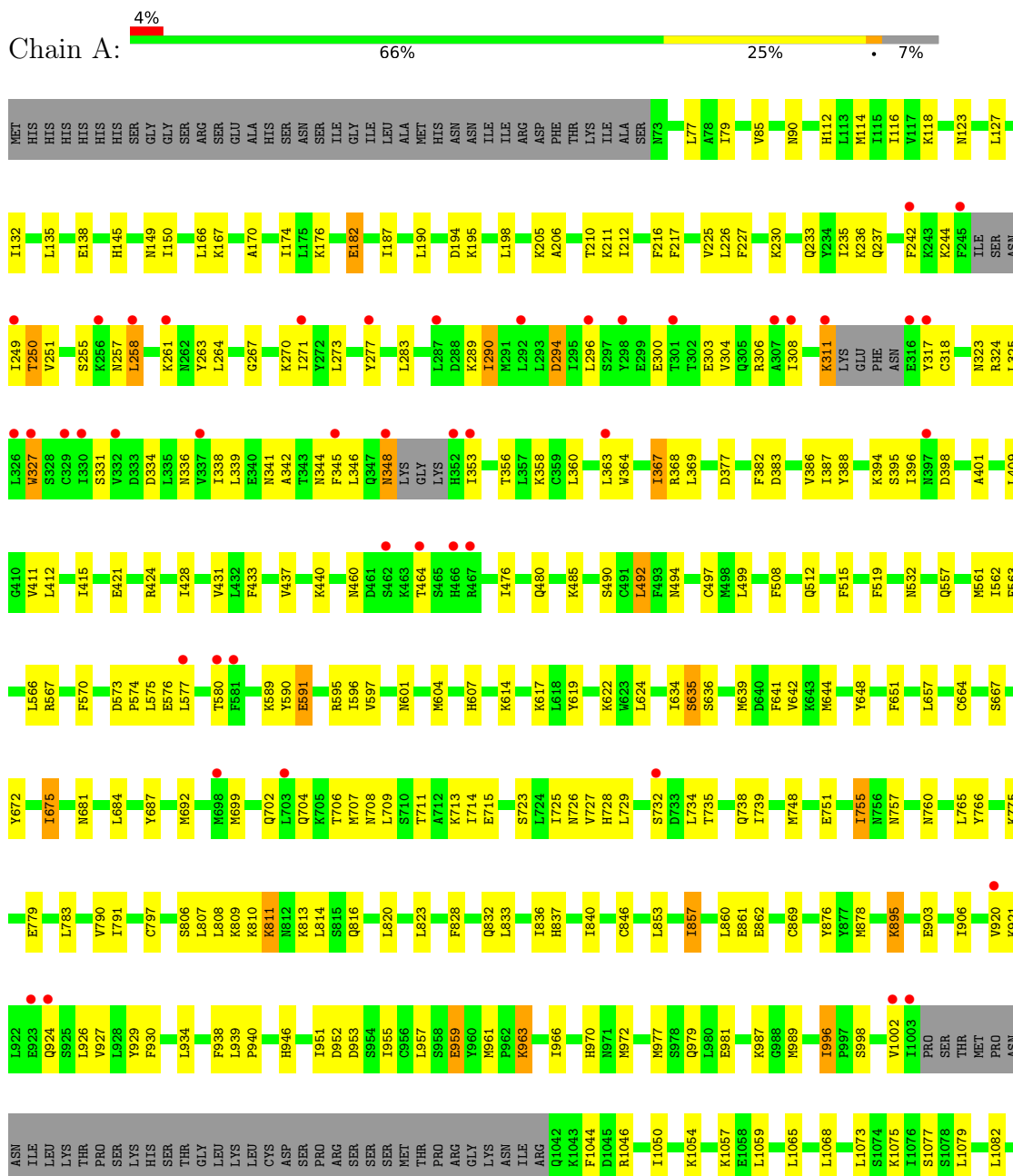
- Molecule 3 is water.

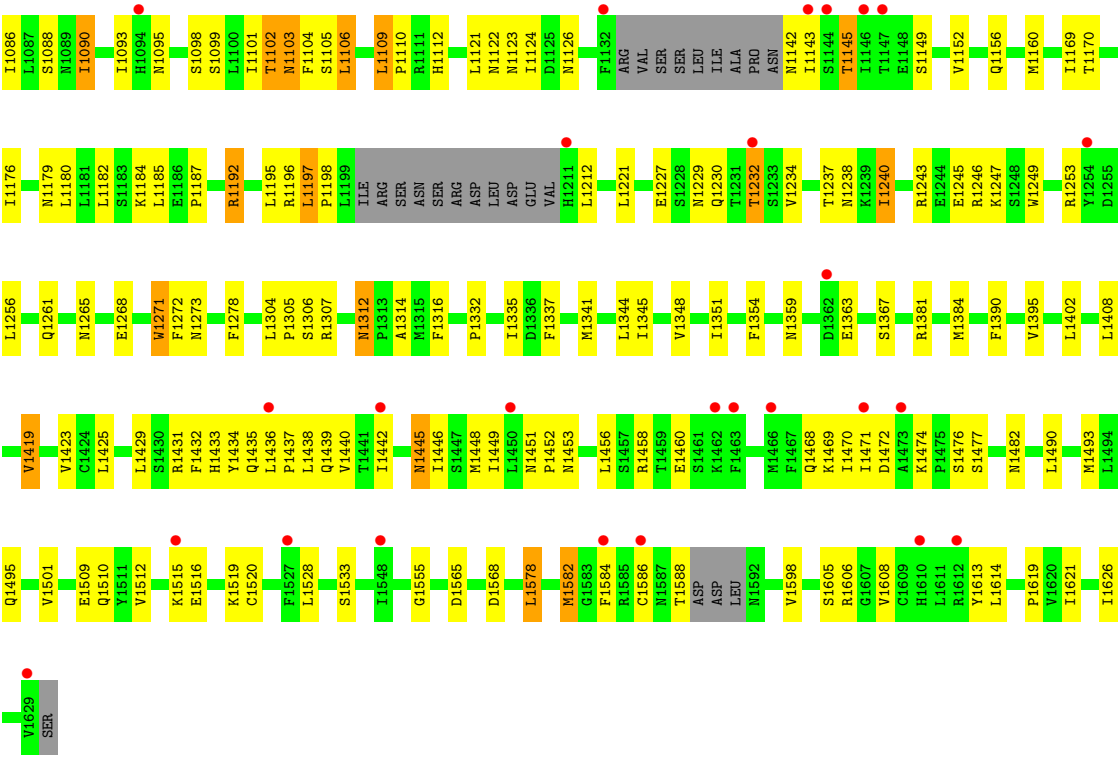
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		

3 Residue-property plots

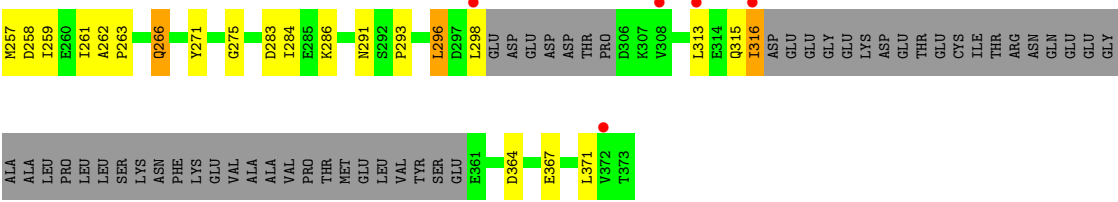
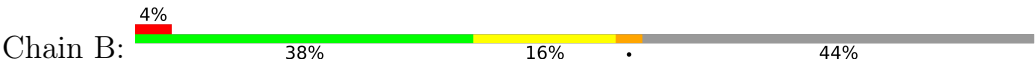
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Separin





● 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	125.86Å 125.86Å 271.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.67 – 2.60 48.67 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.67-2.60) 91.5 (48.67-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.221 , 0.264 0.228 , 0.270	Depositor DCC
R_{free} test set	2016 reflections (2.60%)	wwPDB-VP
Wilson B-factor (Å ²)	55.5	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12633	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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	0.67	0/12316	0.88	13/16621 (0.1%)
2	B	0.65	0/549	0.89	0/745
All	All	0.67	0/12865	0.88	13/17366 (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

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	939	LEU	CA-C-N	-6.55	112.95	119.56
1	A	939	LEU	C-N-CA	-6.55	112.95	119.56
1	A	857	ILE	CB-CA-C	-6.46	103.61	111.88
1	A	811	LYS	N-CA-C	6.10	119.83	112.38
1	A	591	GLU	N-CA-C	6.08	117.91	111.28
1	A	1312	ASN	CA-C-N	-5.91	113.73	119.87
1	A	1312	ASN	C-N-CA	-5.91	113.73	119.87
1	A	636	SER	N-CA-C	-5.88	104.82	112.23
1	A	1197	LEU	CA-C-N	5.58	124.93	118.85
1	A	1197	LEU	C-N-CA	5.58	124.93	118.85
1	A	813	LYS	N-CA-C	-5.44	97.02	107.57
1	A	1271	TRP	N-CA-C	5.42	118.10	111.82
1	A	963	LYS	N-CA-C	-5.08	105.83	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	996	ILE	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	12078	0	12320	343	0
2	B	539	0	518	23	0
3	A	16	0	0	1	0
All	All	12633	0	12838	351	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 14.

All (351) 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:353:ILE:CD1	1:A:395:SER:OG	1.66	1.43
1:A:734:LEU:HD11	1:A:738:GLN:NE2	1.42	1.33
1:A:353:ILE:HD12	1:A:395:SER:OG	1.12	1.28
1:A:591:GLU:OE2	1:A:595:ARG:NE	1.71	1.23
1:A:634:ILE:HG21	1:A:639:MET:HE3	1.28	1.12
1:A:255:SER:HB3	1:A:290:ILE:HD11	1.15	1.12
1:A:634:ILE:CG2	1:A:639:MET:HE3	1.90	1.01
1:A:860:LEU:HD12	1:A:861:GLU:H	1.22	1.00
1:A:255:SER:HB3	1:A:290:ILE:CD1	1.95	0.97
1:A:860:LEU:HD12	1:A:861:GLU:N	1.79	0.97
1:A:323:ASN:HD21	1:A:358:LYS:HZ2	1.10	0.96
1:A:734:LEU:HD11	1:A:738:GLN:HE21	0.86	0.96
1:A:734:LEU:CD1	1:A:738:GLN:NE2	2.29	0.95
1:A:336:ASN:ND2	1:A:377:ASP:OD2	1.99	0.95
1:A:634:ILE:HG21	1:A:639:MET:CE	1.97	0.94
1:A:317:TYR:OH	1:A:341:ASN:ND2	2.01	0.93
1:A:494:ASN:HD21	1:A:532:ASN:HD22	1.14	0.93
1:A:255:SER:CB	1:A:290:ILE:HD11	1.99	0.93
1:A:356:THR:O	1:A:360:LEU:HD13	1.70	0.92
1:A:607:HIS:CD2	1:A:862:GLU:OE2	2.23	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:728:HIS:ND1	1:A:959:GLU:OE1	2.04	0.90
1:A:187:ILE:HD13	1:A:216:PHE:HE2	1.38	0.88
1:A:494:ASN:HD21	1:A:532:ASN:ND2	1.72	0.88
1:A:1446:ILE:HD11	1:A:1470:ILE:HG21	1.53	0.88
1:A:323:ASN:HD21	1:A:358:LYS:NZ	1.70	0.88
1:A:860:LEU:CD1	1:A:861:GLU:H	1.87	0.87
1:A:277:TYR:OH	1:A:289:LYS:CE	2.22	0.86
1:A:1446:ILE:HD11	1:A:1470:ILE:CG2	2.06	0.85
1:A:145:HIS:H	1:A:149:ASN:HD22	1.27	0.82
1:A:557:GLN:HG3	1:A:580:THR:OG1	1.79	0.81
1:A:277:TYR:OH	1:A:289:LYS:HE2	1.82	0.78
1:A:734:LEU:CD1	1:A:738:GLN:HE21	1.83	0.77
1:A:604:MET:HE2	1:A:816:GLN:HE21	1.50	0.76
1:A:1490:LEU:HD11	1:A:1512:VAL:HB	1.68	0.75
1:A:271:ILE:HD11	1:A:324:ARG:NH1	2.02	0.75
2:B:316:ILE:N	2:B:316:ILE:HD12	2.02	0.74
1:A:323:ASN:ND2	1:A:358:LYS:NZ	2.35	0.73
1:A:303:GLU:HA	1:A:306:ARG:HB2	1.69	0.73
1:A:1490:LEU:HA	1:A:1493:MET:HB2	1.70	0.73
1:A:808:LEU:HD13	2:B:283:ASP:HB3	1.70	0.73
1:A:1046:ARG:NH2	1:A:1354:PHE:O	2.22	0.72
1:A:323:ASN:ND2	1:A:358:LYS:HZ2	1.85	0.72
1:A:857:ILE:HD11	1:A:869:CYS:HB3	1.72	0.72
1:A:1268:GLU:HG3	1:A:1408:LEU:HD22	1.70	0.72
1:A:1123:ASN:HD21	1:A:1519:LYS:HA	1.55	0.71
1:A:187:ILE:HD13	1:A:216:PHE:CE2	2.25	0.70
1:A:304:VAL:O	1:A:308:ILE:HG12	1.92	0.69
1:A:236:LYS:HG2	1:A:283:LEU:HB3	1.74	0.69
1:A:353:ILE:CD1	1:A:395:SER:CB	2.69	0.69
1:A:492:LEU:C	1:A:492:LEU:HD13	2.19	0.68
1:A:494:ASN:ND2	1:A:532:ASN:HD22	1.88	0.67
1:A:727:VAL:HG12	1:A:783:LEU:HG	1.77	0.67
1:A:353:ILE:HD13	1:A:395:SER:OG	1.84	0.67
1:A:258:LEU:HA	1:A:263:TYR:HD2	1.59	0.67
1:A:1432:PHE:CG	1:A:1438:LEU:HD11	2.30	0.66
1:A:267:GLY:O	1:A:270:LYS:HE2	1.95	0.66
1:A:806:SER:HA	1:A:809:LYS:HE2	1.77	0.66
1:A:604:MET:HE1	1:A:644:MET:SD	2.35	0.66
1:A:1170:THR:HG22	1:A:1395:VAL:HB	1.76	0.66
1:A:114:MET:HE3	1:A:118:LYS:HE2	1.78	0.66
1:A:1160:MET:HE3	1:A:1192:ARG:NH1	2.11	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1606:ARG:NH2	1:A:1619:PRO:O	2.29	0.65
1:A:382:PHE:HZ	1:A:428:ILE:HD11	1.61	0.65
1:A:494:ASN:ND2	1:A:532:ASN:ND2	2.42	0.65
1:A:356:THR:O	1:A:360:LEU:CD1	2.44	0.65
1:A:421:GLU:HB3	1:A:424:ARG:HB2	1.78	0.64
1:A:998:SER:HB2	1:A:1351:ILE:HD13	1.79	0.64
1:A:860:LEU:CD1	1:A:861:GLU:N	2.53	0.64
1:A:946:HIS:HD2	1:A:963:LYS:HE2	1.62	0.64
1:A:1470:ILE:HG13	1:A:1586:CYS:SG	2.38	0.64
1:A:1149:SER:O	1:A:1152:VAL:HG12	1.99	0.62
1:A:810:LYS:O	2:B:286:LYS:NZ	2.32	0.62
1:A:1431:ARG:NH2	1:A:1555:GLY:O	2.24	0.62
1:A:237:GLN:CB	1:A:283:LEU:HD21	2.30	0.62
1:A:1098:SER:O	1:A:1102:THR:HG23	1.98	0.62
1:A:1232:THR:HG21	1:A:1565:ASP:HB3	1.83	0.61
1:A:563:PHE:CZ	1:A:567:ARG:HD2	2.35	0.61
1:A:1470:ILE:HG23	1:A:1474:LYS:HD2	1.83	0.60
1:A:492:LEU:HD13	1:A:492:LEU:O	2.00	0.60
1:A:725:ILE:HG22	1:A:779:GLU:HG3	1.83	0.60
2:B:316:ILE:HG22	2:B:316:ILE:O	2.01	0.60
1:A:237:GLN:HB2	1:A:283:LEU:HD21	1.83	0.60
1:A:728:HIS:CE1	1:A:959:GLU:OE2	2.54	0.60
1:A:617:LYS:HE2	1:A:657:LEU:HD21	1.84	0.60
1:A:1306:SER:H	1:A:1359:ASN:HD21	1.48	0.60
1:A:1446:ILE:CD1	1:A:1470:ILE:HG21	2.28	0.59
1:A:311:LYS:HE2	1:A:317:TYR:HB3	1.84	0.59
1:A:591:GLU:OE2	1:A:595:ARG:CZ	2.46	0.59
1:A:277:TYR:OH	1:A:289:LYS:HE3	2.01	0.59
1:A:1438:LEU:O	1:A:1440:VAL:HG23	2.02	0.59
1:A:607:HIS:HD2	1:A:862:GLU:OE2	1.85	0.58
1:A:713:LYS:HZ2	1:A:715:GLU:H	1.52	0.58
1:A:972:MET:SD	1:A:1059:LEU:CD2	2.91	0.58
1:A:1432:PHE:CD1	1:A:1438:LEU:HD11	2.38	0.58
1:A:353:ILE:HD11	1:A:395:SER:OG	1.92	0.58
1:A:1341:MET:O	1:A:1345:ILE:HG12	2.04	0.58
2:B:315:GLN:C	2:B:316:ILE:HD12	2.29	0.58
1:A:249:ILE:HG22	1:A:250:THR:H	1.69	0.57
1:A:346:LEU:HD22	1:A:388:TYR:CD2	2.39	0.57
1:A:573:ASP:HB3	1:A:576:GLU:HG2	1.86	0.57
1:A:267:GLY:O	1:A:270:LYS:HG2	2.05	0.57
1:A:1433:HIS:O	1:A:1435:GLN:HG3	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:952:ASP:HB3	1:A:955:ILE:HG12	1.86	0.56
1:A:1442:ILE:HD11	1:A:1584:PHE:HD1	1.70	0.56
2:B:296:LEU:CD2	2:B:296:LEU:H	2.18	0.56
1:A:972:MET:SD	1:A:1059:LEU:HD22	2.46	0.56
1:A:714:ILE:HD12	1:A:751:GLU:HG3	1.88	0.56
1:A:226:LEU:HD21	1:A:273:LEU:HA	1.88	0.56
1:A:684:LEU:HD13	1:A:699:MET:HB3	1.87	0.56
1:A:205:LYS:HG3	2:B:371:LEU:HD12	1.87	0.56
1:A:271:ILE:HG21	1:A:369:LEU:HD13	1.87	0.56
1:A:1182:LEU:HD12	1:A:1195:LEU:HD11	1.88	0.56
1:A:237:GLN:HB2	1:A:283:LEU:CD2	2.36	0.56
1:A:639:MET:HE1	1:A:672:TYR:CD1	2.42	0.55
1:A:1232:THR:HG23	2:B:262:ALA:CB	2.37	0.55
1:A:1306:SER:H	1:A:1359:ASN:ND2	2.04	0.55
1:A:570:PHE:HZ	1:A:601:ASN:HB3	1.71	0.55
1:A:727:VAL:N	1:A:779:GLU:OE2	2.40	0.55
1:A:1234:VAL:O	1:A:1238:ASN:HB2	2.07	0.55
1:A:604:MET:HE3	1:A:648:TYR:CD1	2.41	0.55
1:A:996:ILE:HD12	1:A:1088:SER:OG	2.07	0.55
1:A:1179:ASN:HD22	1:A:1196:ARG:NH1	2.05	0.54
1:A:1442:ILE:HD11	1:A:1584:PHE:CD1	2.43	0.54
2:B:296:LEU:H	2:B:296:LEU:HD23	1.71	0.54
1:A:1445:ASN:ND2	1:A:1476:SER:OG	2.41	0.54
1:A:331:SER:HB2	1:A:334:ASP:HB2	1.88	0.54
1:A:725:ILE:HD12	1:A:775:LYS:HD3	1.90	0.54
1:A:79:ILE:HD13	1:A:85:VAL:HG21	1.90	0.54
1:A:236:LYS:HE2	1:A:283:LEU:O	2.08	0.54
1:A:727:VAL:HG13	1:A:779:GLU:OE2	2.07	0.54
1:A:713:LYS:HZ1	1:A:715:GLU:HB2	1.73	0.53
1:A:989:MET:HE1	1:A:1090:ILE:HG12	1.90	0.53
1:A:1073:LEU:HD21	1:A:1109:LEU:HB3	1.89	0.53
1:A:308:ILE:HD12	1:A:338:ILE:HD11	1.90	0.53
1:A:574:PRO:HA	1:A:577:LEU:HD23	1.91	0.53
1:A:1227:GLU:O	1:A:1230:GLN:HB3	2.09	0.53
1:A:1598:VAL:HG13	1:A:1621:ILE:HD13	1.90	0.53
1:A:1246:ARG:HG2	2:B:257:MET:O	2.09	0.53
1:A:145:HIS:H	1:A:149:ASN:ND2	2.03	0.52
1:A:681:ASN:ND2	1:A:723:SER:HB3	2.24	0.52
2:B:296:LEU:CD2	2:B:296:LEU:N	2.72	0.52
1:A:277:TYR:CZ	1:A:289:LYS:HE3	2.44	0.52
1:A:692:MET:HE2	1:A:930:PHE:HE1	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1180:LEU:HD23	1:A:1197:LEU:HD12	1.92	0.52
1:A:237:GLN:N	1:A:283:LEU:HD23	2.25	0.52
1:A:1169:ILE:HG12	1:A:1184:LYS:HG3	1.91	0.52
1:A:267:GLY:O	1:A:270:LYS:CG	2.58	0.52
1:A:1449:ILE:HG22	1:A:1452:PRO:HG3	1.92	0.52
1:A:364:TRP:CZ3	1:A:367:ILE:HD12	2.46	0.51
1:A:833:LEU:O	1:A:837:HIS:HD2	1.94	0.51
1:A:1495:GLN:NE2	1:A:1520:CYS:SG	2.83	0.51
1:A:1509:GLU:H	1:A:1509:GLU:CD	2.19	0.51
1:A:242:PHE:CD2	1:A:251:VAL:HB	2.46	0.51
1:A:1605:SER:O	1:A:1608:VAL:HG22	2.10	0.51
1:A:257:ASN:O	1:A:263:TYR:CD2	2.64	0.51
1:A:1082:LEU:O	1:A:1086:ILE:HG12	2.11	0.51
1:A:1195:LEU:HD13	1:A:1197:LEU:HD21	1.93	0.51
1:A:211:LYS:NZ	2:B:367:GLU:OE1	2.40	0.50
1:A:492:LEU:C	1:A:492:LEU:CD1	2.85	0.50
1:A:1256:LEU:HB2	1:A:1614:LEU:HD11	1.93	0.50
1:A:294:ASP:OD1	1:A:294:ASP:N	2.42	0.50
1:A:924:GLN:O	1:A:927:VAL:HG22	2.12	0.50
1:A:979:GLN:HB3	1:A:1044:PHE:HE2	1.76	0.50
1:A:1446:ILE:HD11	1:A:1470:ILE:HG22	1.88	0.50
1:A:596:ILE:HD12	1:A:619:TYR:HB2	1.94	0.50
1:A:926:LEU:HD13	1:A:940:PRO:HA	1.94	0.50
1:A:132:ILE:HG23	1:A:166:LEU:HD11	1.93	0.50
1:A:382:PHE:O	1:A:386:VAL:HG13	2.12	0.49
1:A:116:ILE:HD13	1:A:132:ILE:HG12	1.93	0.49
1:A:972:MET:SD	1:A:1059:LEU:HD23	2.52	0.49
1:A:589:LYS:HE2	1:A:590:TYR:OH	2.12	0.49
1:A:460:ASN:HD22	1:A:499:LEU:HD13	1.77	0.49
1:A:1073:LEU:HG	1:A:1110:PRO:HG3	1.94	0.49
1:A:860:LEU:CG	1:A:861:GLU:N	2.75	0.49
1:A:1419:VAL:HG11	1:A:1425:LEU:HB2	1.95	0.49
1:A:570:PHE:CZ	1:A:601:ASN:HB3	2.48	0.49
1:A:644:MET:HE3	2:B:293:PRO:HB3	1.94	0.49
1:A:966:ILE:O	1:A:970:HIS:HD2	1.96	0.49
1:A:597:VAL:HG22	1:A:641:PHE:CD1	2.48	0.48
1:A:1160:MET:HE3	1:A:1192:ARG:CZ	2.43	0.48
1:A:1515:LYS:HD3	2:B:271:TYR:CE1	2.48	0.48
1:A:755:ILE:O	1:A:766:TYR:OH	2.24	0.48
1:A:1065:LEU:HB2	1:A:1145:THR:HG21	1.95	0.48
1:A:398:ASP:OD1	1:A:398:ASP:N	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:791:ILE:HB	1:A:1142:ASN:OD1	2.13	0.48
1:A:604:MET:HE3	1:A:648:TYR:CG	2.49	0.48
1:A:216:PHE:HB3	1:A:227:PHE:CE2	2.48	0.48
1:A:814:LEU:O	2:B:291:ASN:ND2	2.43	0.48
1:A:1249:TRP:CZ2	1:A:1253:ARG:HD2	2.48	0.48
1:A:1307:ARG:HG2	1:A:1316:PHE:CE2	2.49	0.48
1:A:664:CYS:O	1:A:667:SER:HB3	2.14	0.48
1:A:1436:LEU:N	1:A:1436:LEU:HD12	2.29	0.48
1:A:557:GLN:HG3	1:A:580:THR:HG1	1.77	0.48
1:A:1271:TRP:N	1:A:1271:TRP:CD1	2.80	0.48
2:B:316:ILE:N	2:B:316:ILE:CD1	2.72	0.48
1:A:1184:LYS:HE2	1:A:1278:PHE:O	2.13	0.47
1:A:1442:ILE:O	1:A:1474:LYS:HD3	2.14	0.47
1:A:1243:ARG:HH12	1:A:1247:LYS:HZ2	1.61	0.47
1:A:300:GLU:O	1:A:304:VAL:HG23	2.15	0.47
1:A:934:LEU:HD11	1:A:940:PRO:HG3	1.96	0.47
2:B:364:ASP:OD1	2:B:367:GLU:HG3	2.14	0.47
1:A:242:PHE:CG	1:A:251:VAL:HB	2.49	0.47
1:A:966:ILE:HD13	1:A:966:ILE:HA	1.73	0.47
1:A:1077:SER:CB	1:A:1106:LEU:HD22	2.44	0.47
1:A:1468:GLN:O	1:A:1471:ILE:HG12	2.14	0.47
1:A:832:GLN:O	1:A:836:ILE:HG13	2.15	0.47
1:A:382:PHE:CZ	1:A:428:ILE:HD11	2.47	0.47
1:A:687:TYR:HE2	1:A:699:MET:HE3	1.80	0.47
1:A:112:HIS:CG	1:A:135:LEU:HD12	2.50	0.47
1:A:233:GLN:O	1:A:283:LEU:HD22	2.14	0.47
1:A:1160:MET:HE1	1:A:1185:LEU:HG	1.97	0.47
1:A:1578:LEU:CD1	1:A:1582:MET:HE1	2.45	0.47
1:A:790:VAL:HG11	1:A:840:ILE:HG21	1.97	0.47
1:A:708:ASN:HD21	1:A:711:THR:HG23	1.79	0.47
1:A:194:ASP:OD2	1:A:230:LYS:NZ	2.41	0.46
1:A:1469:LYS:O	1:A:1472:ASP:HB2	2.16	0.46
1:A:895:LYS:HB2	1:A:895:LYS:HE3	1.55	0.46
1:A:1240:ILE:HG23	1:A:1245:GLU:HB3	1.97	0.46
1:A:1456:LEU:HD21	2:B:263:PRO:HD3	1.98	0.46
1:A:237:GLN:CA	1:A:283:LEU:HD21	2.46	0.46
1:A:757:ASN:HB2	1:A:766:TYR:CE1	2.51	0.46
1:A:1101:ILE:HG12	1:A:1192:ARG:NH2	2.31	0.46
1:A:1105:SER:HB2	1:A:1152:VAL:HG13	1.98	0.46
1:A:1077:SER:HB2	1:A:1106:LEU:HD22	1.97	0.46
1:A:1515:LYS:O	1:A:1519:LYS:HG3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1578:LEU:HD13	1:A:1582:MET:CE	2.46	0.46
1:A:114:MET:O	1:A:118:LYS:HG3	2.16	0.45
1:A:283:LEU:N	1:A:283:LEU:HD12	2.30	0.45
1:A:735:THR:O	1:A:739:ILE:HG12	2.16	0.45
1:A:1179:ASN:HD22	1:A:1196:ARG:HH11	1.63	0.45
1:A:702:GLN:O	1:A:706:THR:HG23	2.16	0.45
1:A:1390:PHE:HZ	1:A:1437:PRO:HD3	1.81	0.45
1:A:190:LEU:HD11	1:A:198:LEU:HD23	1.99	0.45
1:A:409:LEU:HD11	1:A:431:VAL:HG12	1.98	0.45
1:A:709:LEU:HD12	1:A:748:MET:HE3	1.97	0.45
1:A:857:ILE:CD1	1:A:869:CYS:HB3	2.44	0.45
1:A:1458:ARG:NH2	1:A:1568:ASP:OD2	2.48	0.45
1:A:1344:LEU:HD23	1:A:1344:LEU:HA	1.78	0.45
1:A:1429:LEU:HB3	1:A:1434:TYR:CD1	2.51	0.45
1:A:1474:LYS:HZ1	1:A:1588:THR:HG23	1.81	0.45
1:A:635:SER:O	1:A:639:MET:HG2	2.16	0.45
1:A:977:MET:O	1:A:981:GLU:HB2	2.17	0.45
1:A:1460:GLU:OE1	1:A:1482:ASN:HB2	2.17	0.45
1:A:217:PHE:HB2	1:A:227:PHE:HB3	1.99	0.45
1:A:713:LYS:NZ	1:A:715:GLU:HB2	2.31	0.45
1:A:807:LEU:C	1:A:807:LEU:HD23	2.42	0.45
1:A:353:ILE:HD13	1:A:395:SER:CB	2.44	0.45
1:A:966:ILE:HD11	1:A:1068:LEU:HD21	1.99	0.45
1:A:1451:ASN:C	1:A:1453:ASN:H	2.25	0.45
1:A:562:ILE:O	1:A:566:LEU:HD23	2.16	0.44
1:A:1510:GLN:HG3	2:B:266:GLN:CD	2.42	0.44
1:A:409:LEU:HD23	1:A:409:LEU:HA	1.81	0.44
1:A:692:MET:HE2	1:A:930:PHE:CE1	2.52	0.44
1:A:1104:PHE:HB2	1:A:1156:GLN:HE22	1.83	0.44
1:A:622:LYS:HA	1:A:622:LYS:HD2	1.80	0.44
1:A:1221:LEU:HD23	1:A:1402:LEU:HD12	1.99	0.44
1:A:325:LEU:HD11	1:A:363:LEU:HD12	1.98	0.44
1:A:938:PHE:CD2	1:A:957:LEU:HD12	2.52	0.44
1:A:1079:LEU:HD13	1:A:1176:ILE:HD13	1.98	0.44
1:A:1095:ASN:HB3	1:A:1098:SER:OG	2.17	0.44
1:A:644:MET:HG2	2:B:293:PRO:HG3	1.99	0.44
1:A:1109:LEU:HD23	1:A:1109:LEU:HA	1.78	0.44
1:A:1232:THR:O	2:B:262:ALA:HB3	2.18	0.44
1:A:1272:PHE:CD1	1:A:1272:PHE:N	2.86	0.44
1:A:1470:ILE:CG1	1:A:1586:CYS:SG	3.06	0.44
1:A:687:TYR:CE2	1:A:699:MET:HE3	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:ILE:O	1:A:485:LYS:HG2	2.18	0.43
1:A:1446:ILE:HG13	1:A:1477:SER:OG	2.18	0.43
1:A:494:ASN:O	1:A:497:CYS:HB2	2.18	0.43
1:A:1578:LEU:HD11	1:A:1582:MET:HE1	2.00	0.43
1:A:906:ILE:HB	1:A:929:TYR:CD2	2.53	0.43
1:A:1261:GLN:HB2	1:A:1613:TYR:CE1	2.54	0.43
1:A:619:TYR:CZ	1:A:624:LEU:HD13	2.54	0.43
1:A:1528:LEU:HD23	1:A:1533:SER:HB2	2.00	0.43
1:A:396:ILE:HG23	1:A:401:ALA:HB3	2.01	0.43
1:A:440:LYS:C	1:A:480:GLN:NE2	2.77	0.43
1:A:807:LEU:HD23	1:A:807:LEU:O	2.18	0.43
1:A:604:MET:HE2	1:A:816:GLN:NE2	2.25	0.43
1:A:1121:LEU:HD23	1:A:1124:ILE:HD11	2.00	0.43
1:A:639:MET:HE1	1:A:672:TYR:HD1	1.84	0.43
1:A:846:CYS:HB3	1:A:876:TYR:CE1	2.53	0.43
1:A:387:ILE:HD12	2:B:313:LEU:HD13	2.01	0.42
1:A:182:GLU:OE2	1:A:182:GLU:N	2.47	0.42
1:A:421:GLU:OE1	1:A:424:ARG:NH1	2.51	0.42
1:A:1438:LEU:HA	1:A:1438:LEU:HD12	1.84	0.42
1:A:237:GLN:CA	1:A:283:LEU:CD2	2.97	0.42
1:A:651:PHE:CD2	1:A:820:LEU:HB3	2.55	0.42
1:A:1312:ASN:OD1	1:A:1314:ALA:N	2.48	0.42
1:A:190:LEU:HD11	1:A:198:LEU:CD2	2.49	0.42
1:A:809:LYS:HE2	1:A:809:LYS:HB2	1.84	0.42
1:A:823:LEU:HD23	1:A:823:LEU:HA	1.92	0.42
1:A:853:LEU:HD11	1:A:869:CYS:SG	2.60	0.42
1:A:251:VAL:O	1:A:251:VAL:HG22	2.17	0.42
1:A:356:THR:C	1:A:360:LEU:HD13	2.40	0.42
1:A:589:LYS:HE2	1:A:590:TYR:CZ	2.55	0.42
1:A:1075:LYS:HB2	1:A:1075:LYS:HE3	1.93	0.42
1:A:1104:PHE:HB3	1:A:1156:GLN:OE1	2.20	0.42
1:A:1381:ARG:O	1:A:1384:MET:HG2	2.20	0.42
1:A:604:MET:HE3	1:A:648:TYR:HB2	2.00	0.42
1:A:728:HIS:CE1	1:A:959:GLU:CD	2.97	0.42
1:A:1332:PRO:HA	1:A:1337:PHE:CD1	2.55	0.42
1:A:1185:LEU:O	1:A:1187:PRO:HD3	2.20	0.41
1:A:1197:LEU:HA	1:A:1198:PRO:HD3	1.80	0.41
1:A:634:ILE:CG2	1:A:639:MET:CE	2.73	0.41
1:A:946:HIS:CD2	1:A:963:LYS:HE2	2.48	0.41
1:A:515:PHE:HA	1:A:519:PHE:HB3	2.01	0.41
1:A:575:LEU:HD12	1:A:575:LEU:HA	1.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:828:PHE:CD1	1:A:828:PHE:C	2.99	0.41
1:A:1436:LEU:N	1:A:1436:LEU:CD1	2.84	0.41
1:A:1237:THR:HA	1:A:1240:ILE:HG13	2.02	0.41
1:A:1305:PRO:HD2	1:A:1359:ASN:ND2	2.35	0.41
1:A:1123:ASN:ND2	1:A:1519:LYS:HA	2.30	0.41
1:A:176:LYS:HA	1:A:176:LYS:HD2	1.65	0.41
1:A:557:GLN:CG	1:A:580:THR:OG1	2.62	0.41
1:A:170:ALA:O	1:A:174:ILE:HG13	2.21	0.41
1:A:336:ASN:HA	1:A:339:LEU:HB2	2.03	0.41
1:A:734:LEU:CG	1:A:738:GLN:NE2	2.83	0.41
1:A:1112:HIS:CE1	1:A:1423:VAL:HG11	2.56	0.41
1:A:1126:ASN:ND2	2:B:275:GLY:HA3	2.36	0.41
1:A:1229:ASN:O	1:A:1232:THR:HB	2.20	0.41
1:A:726:ASN:O	1:A:729:LEU:HB2	2.20	0.41
1:A:921:LYS:HE2	1:A:921:LYS:HB2	1.78	0.41
1:A:953:ASP:CG	1:A:961:MET:HE1	2.46	0.41
1:A:1256:LEU:CB	1:A:1614:LEU:HD11	2.51	0.41
1:A:348:ASN:N	1:A:348:ASN:HD22	2.19	0.41
1:A:1232:THR:HG21	1:A:1565:ASP:CB	2.49	0.41
1:A:1344:LEU:O	1:A:1348:VAL:HG23	2.21	0.41
1:A:1402:LEU:H	1:A:1402:LEU:HD23	1.86	0.41
1:A:323:ASN:HD22	1:A:323:ASN:HA	1.68	0.41
1:A:1273:ASN:OD1	1:A:1273:ASN:N	2.52	0.41
1:A:112:HIS:HB3	1:A:135:LEU:HD12	2.03	0.40
1:A:242:PHE:O	1:A:244:LYS:N	2.54	0.40
1:A:342:ALA:HA	1:A:345:PHE:HB2	2.04	0.40
1:A:561:MET:CE	1:A:595:ARG:HA	2.51	0.40
1:A:206:ALA:O	1:A:210:THR:HG23	2.21	0.40
1:A:382:PHE:CE2	1:A:412:LEU:HD22	2.55	0.40
1:A:642:VAL:HB	1:A:675:ILE:HD11	2.04	0.40
1:A:90:ASN:ND2	1:A:138:GLU:OE2	2.52	0.40
1:A:304:VAL:HG22	1:A:327:TRP:HB3	2.02	0.40
1:A:364:TRP:CE3	1:A:367:ILE:HD12	2.57	0.40
1:A:878:MET:HE2	1:A:878:MET:HB3	1.88	0.40
1:A:1099:SER:O	1:A:1103:ASN:HB2	2.21	0.40
1:A:1468:GLN:NE2	3:A:1701:HOH:O	2.54	0.40
1:A:433:PHE:O	1:A:437:VAL:HG23	2.21	0.40
1:A:715:GLU:HG3	1:A:765:LEU:HD21	2.04	0.40
1:A:150:ILE:O	1:A:167:LYS:HE2	2.22	0.40
1:A:194:ASP:OD1	1:A:195:LYS:N	2.55	0.40
1:A:383:ASP:O	1:A:387:ILE:HD13	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:734:LEU:HA	1:A:783:LEU:HD13	2.04	0.40
1:A:1050:ILE:HG22	1:A:1054:LYS:HD2	2.04	0.40
1:A:1438:LEU:HB3	1:A:1626:ILE:HG22	2.03	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%)	1394 (95%)	76 (5%)	0	100	100
2	B	60/117 (51%)	58 (97%)	2 (3%)	0	100	100
All	All	1530/1713 (89%)	1452 (95%)	78 (5%)	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	1391/1491 (93%)	1318 (95%)	73 (5%)	21	44
2	B	63/108 (58%)	55 (87%)	8 (13%)	4	9
All	All	1454/1599 (91%)	1373 (94%)	81 (6%)	19	40

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LEU
1	A	123	ASN
1	A	127	LEU
1	A	182	GLU
1	A	212	ILE
1	A	225	VAL
1	A	235	ILE
1	A	250	THR
1	A	258	LEU
1	A	261	LYS
1	A	264	LEU
1	A	290	ILE
1	A	294	ASP
1	A	296	LEU
1	A	311	LYS
1	A	318	CYS
1	A	327	TRP
1	A	344	ASN
1	A	348	ASN
1	A	367	ILE
1	A	368	ARG
1	A	394	LYS
1	A	411	VAL
1	A	415	ILE
1	A	464	THR
1	A	490	SER
1	A	492	LEU
1	A	508	PHE
1	A	512	GLN
1	A	614	LYS
1	A	635	SER
1	A	675	ILE
1	A	704	GLN
1	A	707	MET
1	A	732	SER
1	A	755	ILE
1	A	760	ASN
1	A	797	CYS
1	A	811	LYS
1	A	895	LYS
1	A	903	GLU
1	A	920	VAL
1	A	951	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	959	GLU
1	A	987	LYS
1	A	1002	VAL
1	A	1057	LYS
1	A	1090	ILE
1	A	1093	ILE
1	A	1102	THR
1	A	1103	ASN
1	A	1106	LEU
1	A	1109	LEU
1	A	1122	ASN
1	A	1143	ILE
1	A	1145	THR
1	A	1192	ARG
1	A	1212	LEU
1	A	1232	THR
1	A	1240	ILE
1	A	1265	ASN
1	A	1304	LEU
1	A	1335	ILE
1	A	1363	GLU
1	A	1367	SER
1	A	1419	VAL
1	A	1439	GLN
1	A	1445	ASN
1	A	1448	MET
1	A	1501	VAL
1	A	1516	GLU
1	A	1578	LEU
1	A	1582	MET
2	B	258	ASP
2	B	259	ILE
2	B	261	ILE
2	B	266	GLN
2	B	284	ILE
2	B	296	LEU
2	B	298	LEU
2	B	316	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	HIS
1	A	111	GLN
1	A	143	GLN
1	A	149	ASN
1	A	165	ASN
1	A	207	HIS
1	A	269	ASN
1	A	323	ASN
1	A	341	ASN
1	A	348	ASN
1	A	381	GLN
1	A	392	ASN
1	A	442	HIS
1	A	460	ASN
1	A	466	HIS
1	A	480	GLN
1	A	532	ASN
1	A	557	GLN
1	A	578	ASN
1	A	607	HIS
1	A	625	GLN
1	A	652	ASN
1	A	681	ASN
1	A	701	ASN
1	A	704	GLN
1	A	708	ASN
1	A	716	GLN
1	A	720	HIS
1	A	738	GLN
1	A	773	ASN
1	A	812	ASN
1	A	837	HIS
1	A	946	HIS
1	A	1070	ASN
1	A	1071	HIS
1	A	1095	ASN
1	A	1123	ASN
1	A	1126	ASN
1	A	1128	ASN
1	A	1179	ASN
1	A	1303	ASN
1	A	1359	ASN
1	A	1372	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1445	ASN
1	A	1495	GLN
1	A	1496	ASN
1	A	1498	ASN
1	A	1562	ASN
2	B	280	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 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

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, 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	1486/1596 (93%)	0.48	71 (4%) 35 30	42, 67, 107, 139	0
2	B	66/117 (56%)	0.89	5 (7%) 20 16	57, 79, 101, 119	0
All	All	1552/1713 (90%)	0.49	76 (4%) 35 29	42, 68, 108, 139	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	298	LEU	5.6
1	A	249	ILE	4.5
1	A	245	PHE	4.5
2	B	316	ILE	4.4
1	A	1003	ILE	4.2
1	A	311	LYS	4.0
1	A	298	TYR	3.8
1	A	317	TYR	3.7
1	A	345	PHE	3.6
1	A	316	GLU	3.5
1	A	352	HIS	3.4
1	A	1471	ILE	3.2
1	A	397	ASN	3.1
1	A	363	LEU	3.1
1	A	258	LEU	3.0
1	A	1094	HIS	3.0
1	A	271	ILE	3.0
1	A	330	ILE	3.0
1	A	1002	VAL	3.0
1	A	277	TYR	2.9
1	A	1254	TYR	2.9
1	A	1462	LYS	2.8
1	A	327	TRP	2.8
1	A	292	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	332	VAL	2.8
1	A	1584	PHE	2.7
1	A	1132	PHE	2.7
1	A	287	LEU	2.6
1	A	326	LEU	2.6
1	A	703	LEU	2.6
1	A	1147	THR	2.6
1	A	296	LEU	2.6
1	A	466	HIS	2.6
1	A	698	MET	2.5
1	A	308	ILE	2.5
1	A	329	CYS	2.5
1	A	1612	ARG	2.5
1	A	1211	HIS	2.4
1	A	1143	ILE	2.4
2	B	372	VAL	2.4
1	A	1629	VAL	2.4
1	A	1442	ILE	2.4
1	A	1146	ILE	2.3
1	A	920	VAL	2.3
1	A	1527	PHE	2.3
1	A	577	LEU	2.3
1	A	242	PHE	2.3
1	A	256	LYS	2.3
1	A	1463	PHE	2.3
1	A	462	SER	2.3
1	A	1232	THR	2.2
1	A	301	THR	2.2
1	A	580	THR	2.2
1	A	1436	LEU	2.2
1	A	581	PHE	2.2
1	A	307	ALA	2.2
1	A	1473	ALA	2.2
1	A	1515	LYS	2.2
1	A	1450	LEU	2.2
1	A	732	SER	2.2
1	A	1610	HIS	2.2
1	A	1586	CYS	2.1
1	A	1466	MET	2.1
1	A	353	ILE	2.1
1	A	1548	ILE	2.1
1	A	337	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1144	SER	2.1
2	B	313	LEU	2.1
1	A	1362	ASP	2.1
1	A	467	ARG	2.1
1	A	261	LYS	2.1
1	A	464	THR	2.1
1	A	924	GLN	2.1
1	A	348	ASN	2.1
1	A	923	GLU	2.0
2	B	308	VAL	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.