



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 02:24 PM EST

PDB ID : 5U1T
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

<http://wwpdb.org/validation/2016/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
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

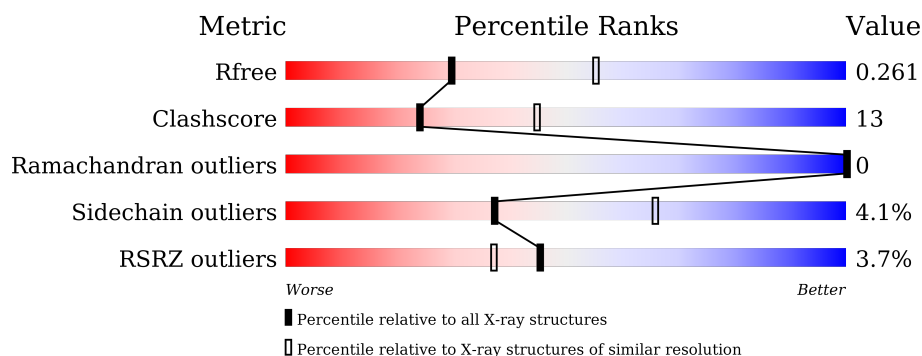
1 Overall quality at a glance

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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 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

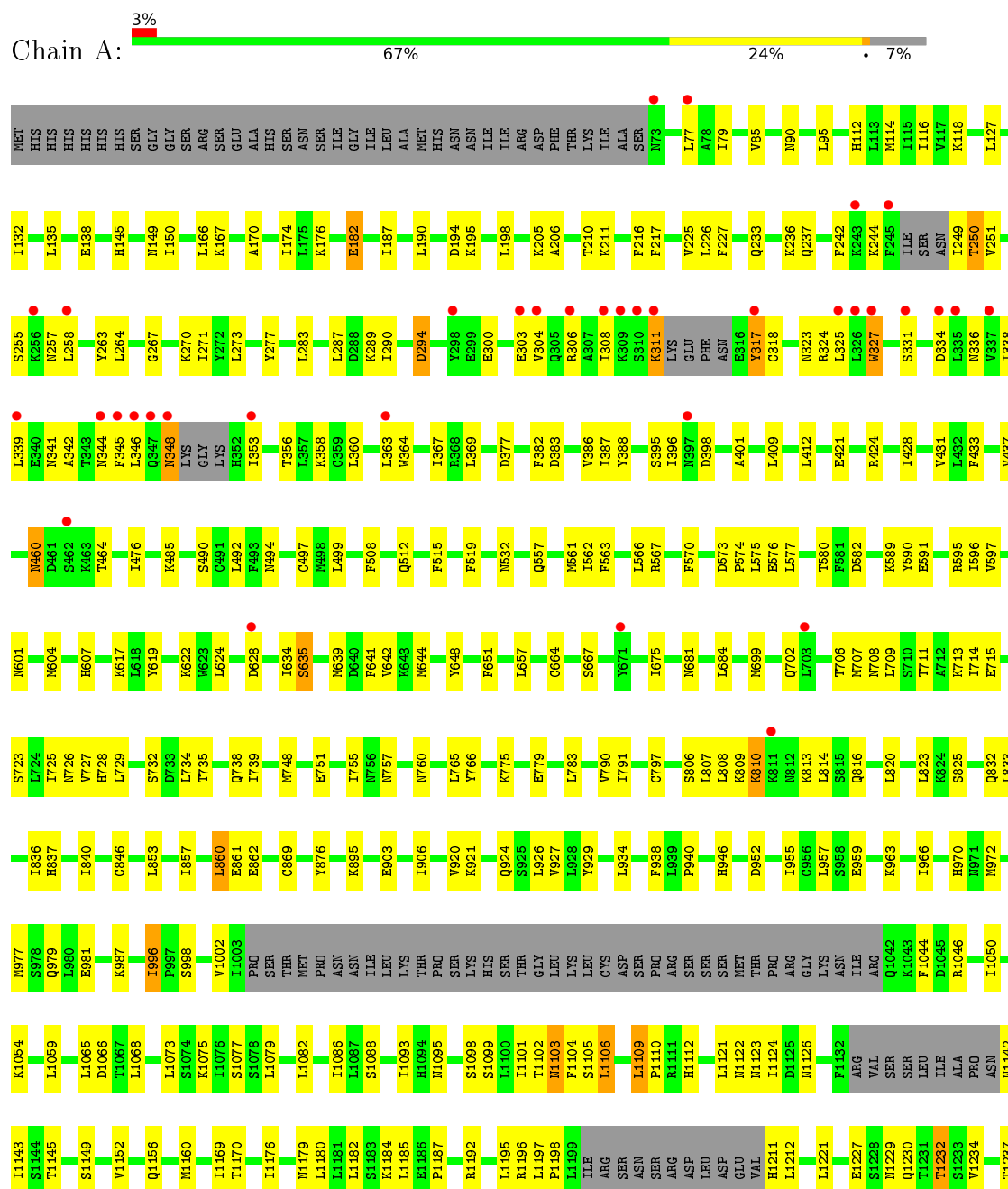
- Molecule 3 is water.

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

3 Residue-property plots

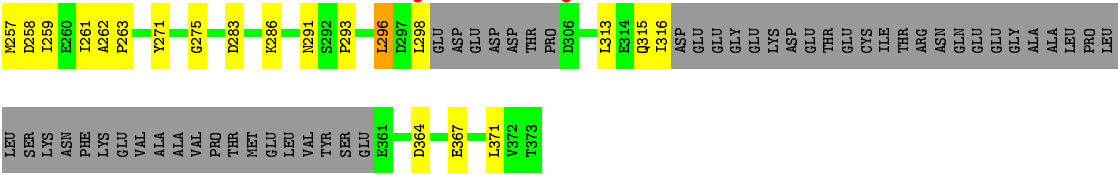
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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	1.86 (at 2.61Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.221 , 0.264 0.220 , 0.261	Depositor DCC
R_{free} test set	1836 reflections (2.59%)	DCC
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 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 [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	0.53	0/12316	0.59	2/16621 (0.0%)
2	B	0.56	0/549	0.61	0/745
All	All	0.53	0/12865	0.59	2/17366 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	813	LYS	N-CA-C	-5.18	97.02	111.00
1	A	860	LEU	CB-CG-CD1	-5.11	102.31	111.00

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 [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	12078	0	12320	325	0
2	B	539	0	518	21	0
3	A	16	0	0	1	0
All	All	12633	0	12838	333	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 13.

All (333) 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:255:SER:HB3	1:A:290:ILE:HD11	1.15	1.12
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: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
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:634:ILE:HG21	1:A:639:MET:HE3	1.63	0.81
1:A:323:ASN:HD21	1:A:358:LYS:HZ2	1.27	0.79
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:634:ILE:HG21	1:A:639:MET:HE2	1.66	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: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:634:ILE:CG2	1:A:639:MET:HE2	2.20	0.71
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: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:1170:THR:HG22	1:A:1395:VAL:HB	1.76	0.66
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:634:ILE:CG2	1:A:639:MET:CE	2.73	0.65
1:A:356:THR:O	1:A:360:LEU:CD1	2.44	0.65
1:A:323:ASN:ND2	1:A:358:LYS:HZ1	1.95	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:1160:MET:HE3	1:A:1192:ARG:NH1	2.13	0.64
1:A:1470:ILE:HG13	1:A:1586:CYS:SG	2.38	0.64
1:A:492:LEU:HD13	1:A:492:LEU:C	2.19	0.63
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1098:SER:O	1:A:1102:THR:HG23	1.98	0.62
1:A:237:GLN:CB	1:A:283:LEU:HD21	2.30	0.62
1:A:1232:THR:HG21	1:A:1565:ASP:HB3	1.83	0.61
1:A:713:LYS:HZ2	1:A:715:GLU:H	1.48	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:O	1:A:492:LEU:HD13	2.00	0.60
1:A:725:ILE:HG22	1:A:779:GLU:HG3	1.83	0.60
2:B:316:ILE:O	2:B:316:ILE:HG22	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:1306:SER:H	1:A:1359:ASN:HD21	1.48	0.60
1:A:617:LYS:HE2	1:A:657:LEU:HD21	1.84	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:1160:MET:HE2	1:A:1185:LEU:HD21	1.83	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:1432:PHE:CD1	1:A:1438:LEU:HD11	2.38	0.58
1:A:972:MET:SD	1:A:1059:LEU:CD2	2.91	0.58
1:A:1341:MET:O	1:A:1345:ILE:HG12	2.04	0.58
1:A:353:ILE:HD11	1:A:395:SER:OG	1.92	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
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:H	2:B:296:LEU:CD2	2.18	0.56
1:A:709:LEU:HD12	1:A:748:MET:HE3	1.87	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:1182:LEU:HD12	1:A:1195:LEU:HD11	1.88	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:237:GLN:HB2	1:A:283:LEU:CD2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1306:SER:H	1:A:1359:ASN:ND2	2.04	0.55
1:A:1232:THR:HG23	2:B:262:ALA:CB	2.37	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: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:HD23	2:B:296:LEU:H	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: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:79:ILE:HD13	1:A:85:VAL:HG21	1.90	0.54
1:A:1073:LEU:HD21	1:A:1109:LEU:HB3	1.89	0.53
1:A:294:ASP:N	1:A:294:ASP:OD1	2.42	0.53
2:B:315:GLN:C	2:B:316:ILE:HD12	2.29	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: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: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:604:MET:HE2	1:A:648:TYR:CD1	2.44	0.52
1:A:681:ASN:ND2	1:A:723:SER:HB3	2.24	0.52
2:B:296:LEU:N	2:B:296:LEU:CD2	2.72	0.52
1:A:277:TYR:CZ	1:A:289:LYS:HE3	2.44	0.52
1:A:1180:LEU:HD23	1:A:1197:LEU:HD12	1.92	0.52
1:A:1169:ILE:HG12	1:A:1184:LYS:HG3	1.91	0.52
1:A:237:GLN:N	1:A:283:LEU:HD23	2.25	0.52
1:A:1449:ILE:HG22	1:A:1452:PRO:HG3	1.92	0.52
1:A:267:GLY:O	1:A:270:LYS:CG	2.58	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:1605:SER:O	1:A:1608:VAL:HG22	2.10	0.51
1:A:242:PHE:CD2	1:A:251:VAL:HB	2.46	0.51
1:A:1082:LEU:O	1:A:1086:ILE:HG12	2.11	0.51
1:A:257:ASN:O	1:A:263:TYR:CD2	2.64	0.51
1:A:1195:LEU:HD13	1:A:1197:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:LYS:NZ	2:B:367:GLU:OE1	2.40	0.50
1:A:1256:LEU:HB2	1:A:1614:LEU:HD11	1.93	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:323:ASN:HD21	1:A:358:LYS:HZ1	1.51	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:972:MET:SD	1:A:1059:LEU:HD23	2.52	0.49
1:A:116:ILE:HD13	1:A:132:ILE:HG12	1.93	0.49
1:A:589:LYS:HE2	1:A:590:TYR:OH	2.12	0.49
1:A:1073:LEU:HG	1:A:1110:PRO:HG3	1.94	0.49
1:A:460:ASN:HD22	1:A:499:LEU:HD13	1.77	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: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:1515:LYS:HD3	2:B:271:TYR:CE1	2.48	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
1:A:713:LYS:HZ1	1:A:715:GLU:HB2	1.78	0.48
1:A:791:ILE:HB	1:A:1142:ASN:OD1	2.13	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: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:1436:LEU:HD12	1:A:1436:LEU:N	2.29	0.48
1:A:664:CYS:O	1:A:667:SER:HB3	2.14	0.48
1:A:1271:TRP:CD1	1:A:1271:TRP:N	2.80	0.48
2:B:316:ILE:CD1	2:B:316:ILE:N	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: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: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:242:PHE:CG	1:A:251:VAL:HB	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:966:ILE:HD13	1:A:966:ILE:HA	1.73	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: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: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:1469:LYS:O	1:A:1472:ASP:HB2	2.16	0.46
1:A:1509:GLU:H	1:A:1509:GLU:CD	2.19	0.46
1:A:1240:ILE:HG23	1:A:1245:GLU:HB3	1.97	0.46
1:A:895:LYS:HB2	1:A:895:LYS:HE3	1.55	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:1578:LEU:CD1	1:A:1582:MET:HE1	2.46	0.46
1:A:604:MET:CE	1:A:816:GLN:HE21	2.29	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
1:A:1578:LEU:HD13	1:A:1582:MET:CE	2.46	0.46
1:A:492:LEU:C	1:A:492:LEU:CD1	2.85	0.46
1:A:604:MET:HE3	1:A:648:TYR:HB2	1.98	0.45
1:A:114:MET:O	1:A:118:LYS:HG3	2.16	0.45
1:A:1179:ASN:HD22	1:A:1196:ARG:HH11	1.63	0.45
1:A:283:LEU:HD12	1:A:283:LEU:N	2.30	0.45
1:A:735:THR:O	1:A:739:ILE:HG12	2.16	0.45
1:A:702:GLN:O	1:A:706:THR:HG23	2.16	0.45
1:A:1160:MET:HE3	1:A:1192:ARG:HH11	1.80	0.45
1:A:1390:PHE:HZ	1:A:1437:PRO:HD3	1.81	0.45
1:A:1458:ARG:NH2	1:A:1568:ASP:OD2	2.48	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:857:ILE:CD1	1:A:869:CYS:HB3	2.44	0.45
1:A:1344:LEU:HA	1:A:1344:LEU:HD23	1.78	0.45
1:A:1429:LEU:HB3	1:A:1434:TYR:CD1	2.51	0.45
1:A:1460:GLU:OE1	1:A:1482:ASN:HB2	2.17	0.45
1:A:557:GLN:HG3	1:A:580:THR:HG1	1.79	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:217:PHE:HB2	1:A:227:PHE:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:LYS:NZ	1:A:715:GLU:HB2	2.31	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:562:ILE:O	1:A:566:LEU:HD23	2.16	0.44
1:A:1104:PHE:HB2	1:A:1156:GLN:HE22	1.83	0.44
1:A:409:LEU:HA	1:A:409:LEU:HD23	1.81	0.44
1:A:1221:LEU:HD23	1:A:1402:LEU:HD12	1.99	0.44
1:A:622:LYS:HD2	1:A:622:LYS:HA	1.80	0.44
1:A:325:LEU:HD11	1:A:363:LEU:HD12	1.98	0.44
1:A:1095:ASN:HB3	1:A:1098:SER:OG	2.17	0.44
1:A:1079:LEU:HD13	1:A:1176:ILE:HD13	1.98	0.44
1:A:634:ILE:HG22	1:A:639:MET:HE2	1.99	0.44
1:A:755:ILE:O	1:A:766:TYR:OH	2.24	0.44
1:A:938:PHE:CD2	1:A:957:LEU:HD12	2.52	0.44
1:A:1109:LEU:HA	1:A:1109:LEU:HD23	1.78	0.44
1:A:1232:THR:O	2:B:262:ALA:HB3	2.18	0.44
1:A:644:MET:HG2	2:B:293:PRO:HG3	1.99	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:1446:ILE:HG13	1:A:1477:SER:OG	2.18	0.43
1:A:476:ILE:O	1:A:485:LYS:HG2	2.18	0.43
1:A:1493:MET:O	1:A:1497:SER:OG	2.26	0.43
1:A:494:ASN:O	1:A:497:CYS:HB2	2.18	0.43
1:A:1261:GLN:HB2	1:A:1613:TYR:CE1	2.54	0.43
1:A:906:ILE:HB	1:A:929:TYR:CD2	2.53	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:807:LEU:HD23	1:A:807:LEU:O	2.18	0.43
1:A:1121:LEU:HD23	1:A:1124:ILE:HD11	2.00	0.43
1:A:1578:LEU:HD11	1:A:1582:MET:HE1	2.01	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:1438:LEU:HD12	1:A:1438:LEU:HA	1.84	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:1312:ASN:OD1	1:A:1314:ALA:N	2.48	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:1243:ARG:HH12	1:A:1247:LYS:HZ2	1.65	0.42
1:A:190:LEU:HD11	1:A:198:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1160:MET:HE2	1:A:1185:LEU:CD2	2.50	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: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:946:HIS:CD2	1:A:963:LYS:HE2	2.48	0.41
1:A:1436:LEU:CD1	1:A:1436:LEU:N	2.84	0.41
1:A:515:PHE:HA	1:A:519:PHE:HB3	2.01	0.41
1:A:575:LEU:HA	1:A:575:LEU:HD12	1.89	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:1229:ASN:O	1:A:1232:THR:HB	2.20	0.41
1:A:1112:HIS:CE1	1:A:1423:VAL:HG11	2.56	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:1126:ASN:ND2	2:B:275:GLY:HA3	2.36	0.41
1:A:1256:LEU:CB	1:A:1614:LEU:HD11	2.51	0.41
1:A:726:ASN:O	1:A:729:LEU:HB2	2.20	0.41
1:A:921:LYS:HB2	1:A:921:LYS:HE2	1.78	0.41
1:A:1232:THR:HG21	1:A:1565:ASP:CB	2.49	0.41
1:A:1402:LEU:H	1:A:1402:LEU:HD23	1.86	0.41
1:A:348:ASN:HD22	1:A:348:ASN:N	2.19	0.41
1:A:1344:LEU:O	1:A:1348:VAL:HG23	2.21	0.41
1:A:1273:ASN:N	1:A:1273:ASN:OD1	2.52	0.41
1:A:323:ASN:HD22	1:A:323:ASN:HA	1.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1099:SER:O	1:A:1103:ASN:HB2	2.21	0.40
1:A:90:ASN:ND2	1:A:138:GLU:OE2	2.52	0.40
1:A:1468:GLN:NE2	3:A:1701:HOH:O	2.54	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: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: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
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
1:A:734:LEU:HA	1:A:783:LEU:HD13	2.04	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%)	1337 (96%)	54 (4%)	39	68
2	B	63/108 (58%)	58 (92%)	5 (8%)	15	30
All	All	1454/1599 (91%)	1395 (96%)	59 (4%)	37	66

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LEU
1	A	95	LEU
1	A	127	LEU
1	A	182	GLU
1	A	225	VAL
1	A	250	THR
1	A	264	LEU
1	A	287	LEU
1	A	294	ASP
1	A	311	LYS
1	A	317	TYR
1	A	318	CYS
1	A	327	TRP
1	A	344	ASN
1	A	348	ASN
1	A	460	ASN
1	A	464	THR
1	A	490	SER
1	A	508	PHE
1	A	512	GLN
1	A	582	ASP
1	A	628	ASP
1	A	635	SER
1	A	707	MET
1	A	732	SER
1	A	760	ASN
1	A	797	CYS
1	A	810	LYS
1	A	825	SER
1	A	903	GLU
1	A	920	VAL

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Mol	Chain	Res	Type
1	A	987	LYS
1	A	1002	VAL
1	A	1066	ASP
1	A	1093	ILE
1	A	1103	ASN
1	A	1106	LEU
1	A	1109	LEU
1	A	1122	ASN
1	A	1143	ILE
1	A	1211	HIS
1	A	1212	LEU
1	A	1232	THR
1	A	1240	ILE
1	A	1265	ASN
1	A	1363	GLU
1	A	1367	SER
1	A	1419	VAL
1	A	1448	MET
1	A	1490	LEU
1	A	1516	GLU
1	A	1568	ASP
1	A	1570	ASP
1	A	1582	MET
2	B	258	ASP
2	B	259	ILE
2	B	261	ILE
2	B	296	LEU
2	B	298	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	143	GLN
1	A	149	ASN
1	A	323	ASN
1	A	341	ASN
1	A	348	ASN
1	A	392	ASN
1	A	442	HIS
1	A	460	ASN
1	A	466	HIS

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Mol	Chain	Res	Type
1	A	480	GLN
1	A	532	ASN
1	A	578	ASN
1	A	601	ASN
1	A	607	HIS
1	A	625	GLN
1	A	708	ASN
1	A	720	HIS
1	A	738	GLN
1	A	773	ASN
1	A	837	HIS
1	A	882	GLN
1	A	886	GLN
1	A	946	HIS
1	A	1095	ASN
1	A	1123	ASN
1	A	1126	ASN
1	A	1128	ASN
1	A	1179	ASN
1	A	1261	GLN
1	A	1301	HIS
1	A	1359	ASN
1	A	1445	ASN
1	A	1495	GLN
1	A	1498	ASN
2	B	280	GLN

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 ⓘ

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, 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%)	0.13	55 (3%) 45 37	42, 67, 107, 139	0
2	B	66/117 (56%)	0.30	2 (3%) 54 47	57, 79, 101, 119	0
All	All	1552/1713 (90%)	0.14	57 (3%) 45 37	42, 68, 108, 139	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	308	ILE	6.6
1	A	245	PHE	5.5
1	A	348	ASN	5.3
1	A	1594	ASN	4.9
1	A	1471	ILE	4.8
1	A	311	LYS	4.5
1	A	73	ASN	4.2
1	A	347	GLN	4.1
1	A	337	VAL	3.9
1	A	298	TYR	3.5
1	A	334	ASP	3.5
1	A	345	PHE	3.4
1	A	306	ARG	3.3
1	A	628	ASP	3.1
1	A	303	GLU	3.1
1	A	310	SER	3.0
1	A	1586	CYS	3.0
1	A	1241	LYS	2.9
1	A	258	LEU	2.9
1	A	317	TYR	2.8
2	B	298	LEU	2.7
1	A	353	ILE	2.7
1	A	243	LYS	2.7
1	A	671	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	304	VAL	2.6
1	A	346	LEU	2.6
1	A	1470	ILE	2.6
1	A	325	LEU	2.5
1	A	256	LYS	2.5
1	A	811	LYS	2.5
1	A	1588	THR	2.5
1	A	339	LEU	2.5
1	A	1443	GLU	2.5
1	A	1467	PHE	2.5
1	A	1387	ASN	2.4
1	A	1592	ASN	2.4
1	A	462	SER	2.4
1	A	327	TRP	2.4
1	A	1585	ARG	2.4
1	A	1629	VAL	2.3
1	A	1385	THR	2.3
1	A	397	ASN	2.2
1	A	335	LEU	2.2
1	A	1473	ALA	2.2
1	A	331	SER	2.2
1	A	1584	PHE	2.2
1	A	77	LEU	2.2
1	A	344	ASN	2.2
1	A	1468	GLN	2.2
1	A	363	LEU	2.1
1	A	1474	LYS	2.1
1	A	1463	PHE	2.1
1	A	309	LYS	2.1
2	B	306	ASP	2.1
1	A	326	LEU	2.1
1	A	703	LEU	2.1
1	A	1254	TYR	2.0

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.