Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Feb 20, 2018 – 10:11 pm GMT

PDB ID	:	5OJS
EMDB ID:	:	EMD-3824
Title	:	Cryo-EM structure of the SAGA and NuA4 coactivator subunit Tra1
Authors	:	Diaz-Santin, L.M.; Lukoyanova, N.; Aciyan, E.; Cheung, A.C.M.
Deposited on	:	2017-07-24
Resolution	:	3.70 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

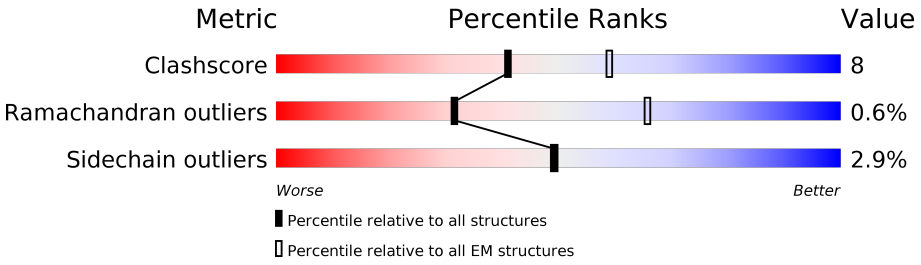
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30686

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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)	EM structures (#Entries)
Clashscore	136279	1886
Ramachandran outliers	132675	1663
Sidechain outliers	132484	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 <=5%

Mol	Chain	Length	Quality of chain
1	T	3767	69% 21% • 8%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 28407 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Transcription-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	T	3473	28407	18391	4718	5178	120	0	0

There are 23 discrepancies between the modelled and reference sequences:

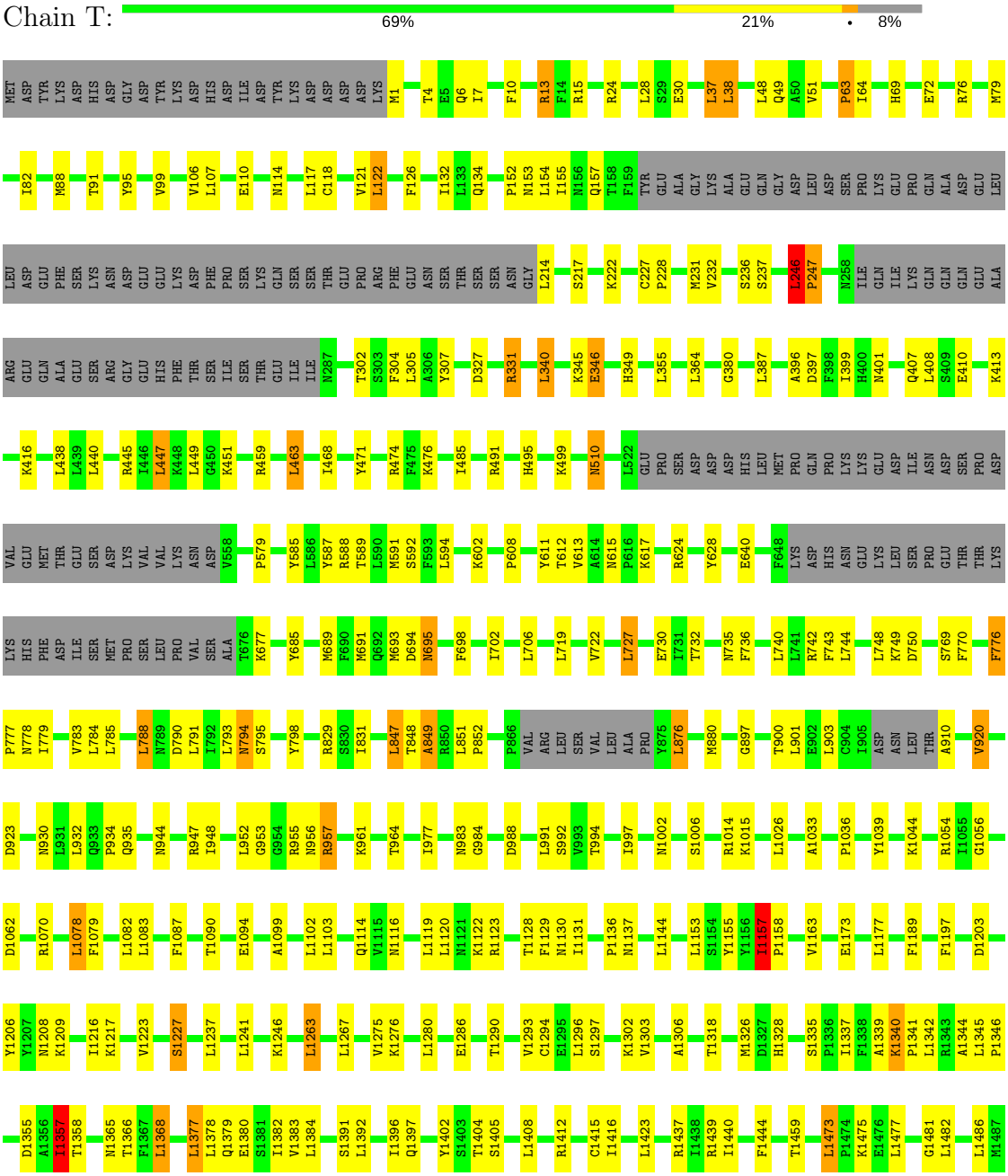
Chain	Residue	Modelled	Actual	Comment	Reference
T	-22	MET	-	initiating methionine	UNP P38811
T	-21	ASP	-	expression tag	UNP P38811
T	-20	TYR	-	expression tag	UNP P38811
T	-19	LYS	-	expression tag	UNP P38811
T	-18	ASP	-	expression tag	UNP P38811
T	-17	HIS	-	expression tag	UNP P38811
T	-16	ASP	-	expression tag	UNP P38811
T	-15	GLY	-	expression tag	UNP P38811
T	-14	ASP	-	expression tag	UNP P38811
T	-13	TYR	-	expression tag	UNP P38811
T	-12	LYS	-	expression tag	UNP P38811
T	-11	ASP	-	expression tag	UNP P38811
T	-10	HIS	-	expression tag	UNP P38811
T	-9	ASP	-	expression tag	UNP P38811
T	-8	ILE	-	expression tag	UNP P38811
T	-7	ASP	-	expression tag	UNP P38811
T	-6	TYR	-	expression tag	UNP P38811
T	-5	LYS	-	expression tag	UNP P38811
T	-4	ASP	-	expression tag	UNP P38811
T	-3	ASP	-	expression tag	UNP P38811
T	-2	ASP	-	expression tag	UNP P38811
T	-1	ASP	-	expression tag	UNP P38811
T	0	LYS	-	expression tag	UNP P38811

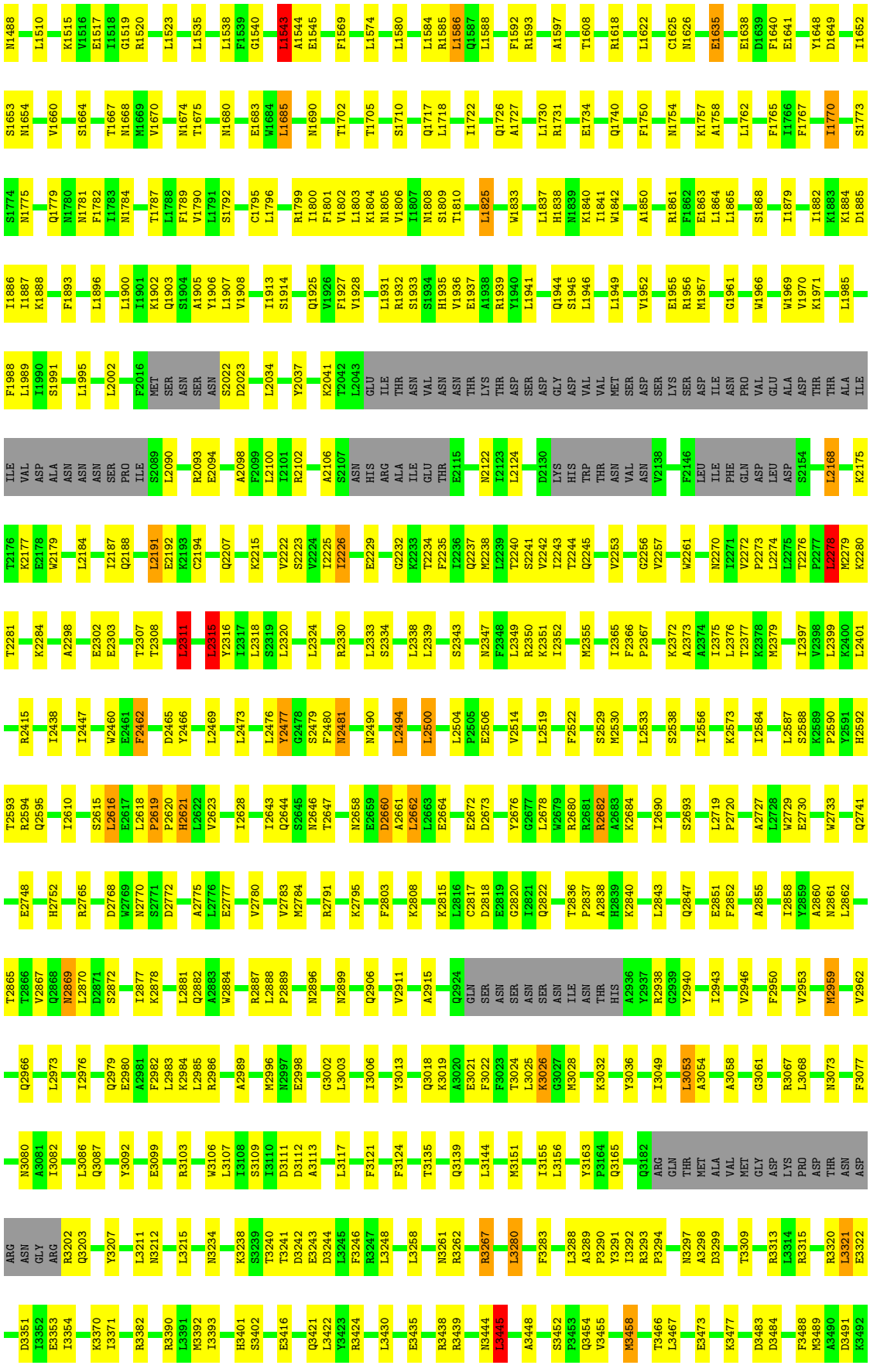
3 Residue-property plots (i)

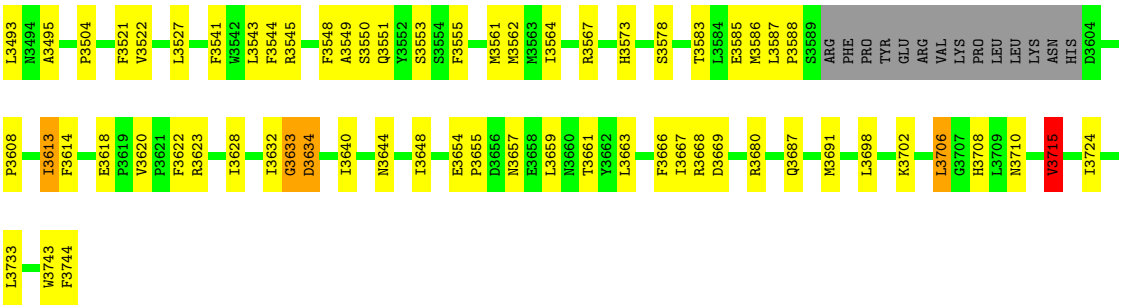
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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: Transcription-associated protein 1

Chain T:






L3493 N3494 A3495 P3504 F3521 V3522 L3527 F3541 W3542 L3543 F3544 R3545 F3548 A3549 S3550 Q3551 Y3552 S3553 S3554 F3555 M3561 M3562 M3563 I3564 R3567 H3573 S3578 T3583 L3584 E3585 M3586 L3587 P3588 S3589 ARG PHE PRO TYR GLU ARG VAL LYS PRO LEU LEU LYS ASN HIS D3604
P3608 I3613 F3614 E3618 P3619 V3620 P3621 F3622 R3623 I3628 I3632 G3633 D3634 I3640 N3644 I3648 E3654 P3655 D3656 N3657 E3658 L3659 N3660 T3661 Y3662 L3663 F3666 I3667 R3668 D3669 R3680 Q3687 M3691 L3698 K3702 L3706 G3707 H3708 L3709 N3710 V3715 I3724
L3733 W3743 F3744

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	182285	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.4	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	T	0.37	0/29026	0.74	49/39323 (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	T	0	50

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	3053	LEU	CA-CB-CG	11.43	141.60	115.30
1	T	1825	LEU	CA-CB-CG	11.13	140.90	115.30
1	T	2278	LEU	CA-CB-CG	9.14	136.32	115.30
1	T	38	LEU	CA-CB-CG	8.63	135.14	115.30
1	T	876	LEU	CA-CB-CG	7.54	132.63	115.30
1	T	2494	LEU	CA-CB-CG	7.47	132.48	115.30
1	T	932	LEU	CA-CB-CG	7.41	132.35	115.30
1	T	2315	LEU	CA-CB-CG	7.37	132.26	115.30
1	T	2339	LEU	CA-CB-CG	7.31	132.11	115.30
1	T	3444	ASN	C-N-CA	7.15	139.56	121.70
1	T	2504	LEU	CA-CB-CG	6.97	131.34	115.30
1	T	3445	LEU	CA-CB-CG	6.90	131.18	115.30
1	T	246	LEU	CA-CB-CG	6.78	130.88	115.30
1	T	1368	LEU	CA-CB-CG	6.71	130.74	115.30
1	T	991	LEU	CA-CB-CG	6.68	130.66	115.30
1	T	788	LEU	CA-CB-CG	6.61	130.50	115.30
1	T	340	LEU	CA-CB-CG	6.55	130.36	115.30
1	T	3634	ASP	CB-CG-OD1	6.33	124.00	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	2618	LEU	CA-CB-CG	6.12	129.38	115.30
1	T	1157	ILE	C-N-CD	-6.09	107.19	120.60
1	T	2660	ASP	CB-CG-OD1	6.05	123.74	118.30
1	T	37	LEU	CA-CB-CG	5.90	128.87	115.30
1	T	785	LEU	CA-CB-CG	5.82	128.69	115.30
1	T	107	LEU	CA-CB-CG	5.76	128.55	115.30
1	T	3706	LEU	CA-CB-CG	5.72	128.47	115.30
1	T	1907	LEU	CA-CB-CG	5.66	128.32	115.30
1	T	2959	MET	CA-CB-CG	5.64	122.89	113.30
1	T	1510	LEU	CA-CB-CG	5.59	128.16	115.30
1	T	847	LEU	CA-CB-CG	5.52	128.00	115.30
1	T	2662	LEU	CA-CB-CG	5.51	127.97	115.30
1	T	1263	LEU	CB-CG-CD1	-5.45	101.74	111.00
1	T	122	LEU	CA-CB-CG	5.38	127.67	115.30
1	T	2339	LEU	CB-CG-CD2	-5.36	101.88	111.00
1	T	3715	VAL	C-N-CA	5.35	135.07	121.70
1	T	3430	LEU	CA-CB-CG	5.33	127.55	115.30
1	T	1586	LEU	CA-CB-CG	5.32	127.53	115.30
1	T	1083	LEU	CA-CB-CG	5.31	127.50	115.30
1	T	1384	LEU	CA-CB-CG	5.29	127.46	115.30
1	T	3633	GLY	C-N-CA	5.27	134.88	121.70
1	T	3543	LEU	CA-CB-CG	5.26	127.40	115.30
1	T	1588	LEU	CA-CB-CG	5.24	127.35	115.30
1	T	748	LEU	CA-CB-CG	5.18	127.20	115.30
1	T	2311	LEU	CA-CB-CG	5.14	127.13	115.30
1	T	727	LEU	CA-CB-CG	5.14	127.13	115.30
1	T	1296	LEU	CA-CB-CG	5.12	127.09	115.30
1	T	2616	LEU	CA-CB-CG	5.11	127.04	115.30
1	T	3613	ILE	CG1-CB-CG2	-5.06	100.28	111.40
1	T	1357	ILE	CG1-CB-CG2	-5.05	100.28	111.40
1	T	1078	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (50) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	T	1070	ARG	Peptide
1	T	1136	PRO	Peptide
1	T	1157	ILE	Peptide
1	T	1227	SER	Peptide
1	T	1297	SER	Peptide
1	T	1346	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	T	1357	ILE	Peptide
1	T	1473	LEU	Peptide
1	T	1543	LEU	Peptide
1	T	1635	GLU	Peptide
1	T	1660	VAL	Peptide
1	T	1710	SER	Peptide
1	T	1770	ILE	Peptide
1	T	1773	SER	Peptide
1	T	1795	CYS	Peptide
1	T	1850	ALA	Peptide
1	T	1900	LEU	Peptide
1	T	2225	ILE	Peptide
1	T	2226	ILE	Peptide
1	T	227	CYS	Peptide
1	T	2315	LEU	Peptide
1	T	2343	SER	Peptide
1	T	2366	PHE	Peptide
1	T	246	LEU	Peptide
1	T	2462	PHE	Peptide
1	T	2615	SER	Peptide
1	T	2619	PRO	Peptide
1	T	2888	LEU	Peptide
1	T	2973	LEU	Peptide
1	T	2976	ILE	Peptide
1	T	3163	TYR	Peptide
1	T	3238	LYS	Peptide
1	T	3290	PRO	Peptide
1	T	346	GLU	Peptide
1	T	3504	PRO	Peptide
1	T	3608	PRO	Peptide
1	T	3618	GLU	Peptide
1	T	3633	GLY	Peptide
1	T	3654	GLU	Peptide
1	T	3680	ARG	Peptide
1	T	3715	VAL	Peptide
1	T	380	GLY	Peptide
1	T	693	MET	Peptide
1	T	694	ASP	Peptide
1	T	72	GLU	Peptide
1	T	750	ASP	Peptide
1	T	776	PHE	Peptide
1	T	847	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	T	851	LEU	Peptide
1	T	935	GLN	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	T	28407	0	28803	463	0
All	All	28407	0	28803	463	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 8.

All (463) 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:T:118:CYS:O	1:T:122:LEU:HB2	1.70	0.91
1:T:2188:GLN:O	1:T:2192:GLU:HB3	1.71	0.89
1:T:3293:ARG:O	1:T:3297:ASN:HB2	1.73	0.89
1:T:3258:LEU:O	1:T:3262:ARG:HB2	1.72	0.89
1:T:1902:LYS:O	1:T:1906:TYR:HB2	1.74	0.87
1:T:1404:THR:O	1:T:1408:LEU:HB2	1.73	0.87
1:T:3541:PHE:O	1:T:3544:PHE:HB3	1.80	0.82
1:T:1173:GLU:O	1:T:1177:LEU:HB2	1.82	0.80
1:T:702:ILE:O	1:T:706:LEU:HB2	1.81	0.80
1:T:2473:LEU:O	1:T:2477:TYR:HB2	1.82	0.78
1:T:3473:GLU:O	1:T:3477:LYS:HB2	1.84	0.78
1:T:2372:LYS:O	1:T:2376:LEU:HB2	1.84	0.77
1:T:1838:HIS:O	1:T:1842:TRP:HB2	1.85	0.77
1:T:2590:PRO:HG2	1:T:2592:HIS:HB3	1.70	0.73
1:T:1335:SER:O	1:T:1339:ALA:HB2	1.89	0.73
1:T:2238:MET:O	1:T:2241:SER:HB2	1.90	0.72
1:T:1114:GLN:HG3	1:T:1189:PHE:HD1	1.56	0.71
1:T:397:ASP:O	1:T:401:ASN:HB2	1.92	0.70
1:T:246:LEU:HD12	1:T:247:PRO:HD2	1.75	0.69
1:T:685:TYR:O	1:T:689:MET:HB2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:1099:ALA:O	1:T:1103:LEU:HB2	1.94	0.68
1:T:1726:GLN:HE21	1:T:1762:LEU:HB2	1.59	0.68
1:T:1988:PHE:HA	1:T:1991:SER:HB3	1.75	0.68
1:T:695:ASN:HD21	1:T:1540:GLY:HA2	1.59	0.67
1:T:10:PHE:HB2	1:T:13:ARG:HE	1.60	0.67
1:T:2168:LEU:O	1:T:2215:LYS:NZ	2.27	0.67
1:T:3211:LEU:O	1:T:3215:LEU:HB2	1.94	0.67
1:T:447:LEU:O	1:T:451:LYS:HB2	1.95	0.67
1:T:2397:ILE:O	1:T:2401:LEU:HB2	1.94	0.66
1:T:3024:THR:O	1:T:3028:MET:N	2.29	0.66
1:T:476:LYS:HG3	1:T:640:GLU:HG2	1.78	0.65
1:T:1939:ARG:HE	1:T:1985:LEU:HD13	1.59	0.65
1:T:1750:PHE:O	1:T:1799:ARG:NH2	2.30	0.65
1:T:1730:LEU:HD11	1:T:1765:PHE:HB2	1.78	0.64
1:T:3491:ASP:O	1:T:3495:ALA:HB2	1.98	0.64
1:T:2094:GLU:O	1:T:2098:ALA:HB3	1.97	0.64
1:T:3687:GLN:O	1:T:3691:MET:HB2	1.98	0.64
1:T:1293:VAL:HG21	1:T:1326:MET:HG2	1.79	0.64
1:T:730:GLU:HB3	1:T:732:THR:H	1.63	0.64
1:T:1805:ASN:O	1:T:1809:SER:HB2	1.98	0.63
1:T:2980:GLU:O	1:T:2984:LYS:HB2	1.97	0.63
1:T:3315:ARG:NH1	1:T:3483:ASP:OD1	2.32	0.63
1:T:3309:THR:O	1:T:3313:ARG:HB2	1.99	0.62
1:T:76:ARG:HD3	1:T:117:LEU:HD21	1.80	0.62
1:T:2316:TYR:O	1:T:2320:LEU:HB2	2.00	0.62
1:T:3036:TYR:O	1:T:3067:ARG:NH2	2.34	0.61
1:T:1805:ASN:O	1:T:1809:SER:CB	2.48	0.61
1:T:2469:LEU:HB2	1:T:2556:ILE:HD11	1.82	0.61
1:T:790:ASP:O	1:T:794:ASN:HB2	2.01	0.61
1:T:2257:VAL:O	1:T:2261:TRP:HB2	2.00	0.60
1:T:719:LEU:O	1:T:722:VAL:HB	2.00	0.60
1:T:3550:SER:O	1:T:3553:SER:HB2	2.01	0.60
1:T:3698:LEU:O	1:T:3702:LYS:HB2	2.01	0.60
1:T:2690:ILE:HG13	1:T:3715:VAL:HA	1.82	0.60
1:T:1841:ILE:HG21	1:T:1885:ASP:HB3	1.83	0.60
1:T:2660:ASP:HB3	1:T:2682:ARG:HH22	1.66	0.60
1:T:3109:SER:OG	1:T:3668:ARG:NH1	2.35	0.60
1:T:1913:ILE:O	1:T:1956:ARG:NH1	2.35	0.59
1:T:3068:LEU:O	1:T:3073:ASN:ND2	2.35	0.59
1:T:2983:LEU:HA	1:T:2986:ARG:HB3	1.85	0.59
1:T:1217:LYS:HB3	1:T:1263:LEU:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:1006:SER:O	1:T:1014:ARG:NH2	2.36	0.59
1:T:1033:ALA:HB1	1:T:2530:MET:HB3	1.84	0.59
1:T:1740:GLN:HE22	1:T:1781:ASN:HB2	1.68	0.59
1:T:1936:VAL:HG22	1:T:1939:ARG:HD2	1.85	0.59
1:T:1945:SER:O	1:T:1949:LEU:HB2	2.03	0.59
1:T:1750:PHE:HZ	1:T:1802:VAL:HG21	1.68	0.58
1:T:2270:ASN:HB3	1:T:2272:VAL:HG23	1.84	0.58
1:T:1801:PHE:HA	1:T:1804:LYS:HG3	1.85	0.58
1:T:3452:SER:HB2	1:T:3455:VAL:H	1.69	0.58
1:T:2729:TRP:O	1:T:2733:TRP:HB2	2.02	0.58
1:T:2836:THR:HG22	1:T:2838:ALA:H	1.68	0.58
1:T:953:GLY:O	1:T:957:ARG:NH1	2.37	0.58
1:T:117:LEU:O	1:T:121:VAL:HB	2.04	0.58
1:T:3622:PHE:HZ	1:T:3724:ILE:HG22	1.68	0.58
1:T:1648:TYR:O	1:T:1652:ILE:HB	2.03	0.57
1:T:2768:ASP:OD1	1:T:2770:ASN:ND2	2.37	0.57
1:T:1966:TRP:HA	1:T:1969:TRP:HD1	1.70	0.57
1:T:2852:PHE:O	1:T:2855:ALA:HB3	2.05	0.57
1:T:2817:CYS:SG	1:T:2818:ASP:N	2.78	0.56
1:T:153:ASN:OD1	1:T:157:GLN:NE2	2.37	0.56
1:T:3424:ARG:NH1	1:T:3445:LEU:O	2.37	0.56
1:T:2465:ASP:OD1	1:T:2465:ASP:N	2.36	0.56
1:T:1952:VAL:HA	1:T:1955:GLU:HG2	1.87	0.56
1:T:3567:ARG:NH1	1:T:3585:GLU:OE1	2.38	0.56
1:T:3561:MET:HG2	1:T:3562:MET:HG3	1.87	0.56
1:T:3628:ILE:O	1:T:3632:ILE:HB	2.06	0.56
1:T:956:ASN:HD21	1:T:2843:LEU:HD12	1.70	0.56
1:T:2783:VAL:O	1:T:2791:ARG:NH2	2.36	0.56
1:T:1971:LYS:HD3	1:T:2002:LEU:HD23	1.88	0.56
1:T:3299:ASP:HB3	1:T:3313:ARG:HD2	1.87	0.56
1:T:49:GLN:NE2	1:T:91:THR:OG1	2.39	0.56
1:T:1380:GLU:HA	1:T:1383:VAL:HG12	1.88	0.55
1:T:1790:VAL:HG23	1:T:1800:ILE:HG23	1.88	0.55
1:T:1054:ARG:NH1	1:T:2506:GLU:OE2	2.39	0.55
1:T:3435:GLU:O	1:T:3439:ARG:NH1	2.39	0.55
1:T:2741:GLN:OE1	1:T:2765:ARG:NH2	2.39	0.55
1:T:3156:LEU:HD13	1:T:3211:LEU:HD11	1.89	0.55
1:T:1203:ASP:OD2	1:T:1208:ASN:ND2	2.40	0.55
1:T:355:LEU:HD21	1:T:364:LEU:HD13	1.89	0.55
1:T:445:ARG:O	1:T:449:LEU:HB2	2.06	0.55
1:T:1337:ILE:HG21	1:T:1357:ILE:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:1477:LEU:O	1:T:1481:GLY:N	2.38	0.55
1:T:910:ALA:O	1:T:955:ARG:NH2	2.40	0.55
1:T:1015:LYS:NZ	1:T:1094:GLU:O	2.39	0.55
1:T:1416:ILE:HG23	1:T:1444:PHE:HE1	1.71	0.55
1:T:3351:ASP:HB3	1:T:3370:LYS:HG2	1.89	0.55
1:T:222:LYS:NZ	1:T:237:SER:OG	2.40	0.54
1:T:122:LEU:O	1:T:126:PHE:HB2	2.07	0.54
1:T:3058:ALA:O	1:T:3061:GLY:N	2.41	0.54
1:T:3640:ILE:O	1:T:3644:ASN:ND2	2.40	0.54
1:T:1664:SER:O	1:T:1668:ASN:ND2	2.41	0.54
1:T:1391:SER:OG	1:T:1397:GLN:NE2	2.41	0.54
1:T:2593:THR:OG1	1:T:2595:GLN:NE2	2.40	0.54
1:T:1517:GLU:HA	1:T:1520:ARG:HD3	1.89	0.54
1:T:1991:SER:HB2	1:T:2034:LEU:HD11	1.90	0.54
1:T:3521:PHE:HB3	1:T:3522:VAL:HG23	1.89	0.54
1:T:2587:LEU:O	1:T:2594:ARG:NH2	2.41	0.54
1:T:3454:GLN:HG3	1:T:3455:VAL:HG23	1.90	0.54
1:T:1625:CYS:SG	1:T:1675:THR:OG1	2.60	0.54
1:T:2473:LEU:HD23	1:T:2476:LEU:HD11	1.90	0.54
1:T:3135:THR:O	1:T:3421:GLN:NE2	2.40	0.54
1:T:2102:ARG:O	1:T:2106:ALA:HB2	2.07	0.54
1:T:3139:GLN:NE2	1:T:3669:ASP:OD2	2.40	0.54
1:T:1099:ALA:O	1:T:1103:LEU:CB	2.55	0.53
1:T:3422:LEU:HD11	1:T:3666:PHE:HB3	1.90	0.53
1:T:934:PRO:HB3	1:T:2822:GLN:HE21	1.74	0.53
1:T:106:VAL:HG21	1:T:117:LEU:HB2	1.89	0.53
1:T:3545:ARG:HA	1:T:3548:PHE:HB3	1.90	0.53
1:T:1519:GLY:O	1:T:1523:LEU:CB	2.55	0.53
1:T:1580:LEU:HD22	1:T:1592:PHE:HZ	1.73	0.53
1:T:1757:LYS:HE3	1:T:1802:VAL:HG13	1.90	0.53
1:T:1925:GLN:HA	1:T:1928:VAL:HB	1.88	0.53
1:T:1122:LYS:HE3	1:T:1123:ARG:HH12	1.74	0.53
1:T:1683:GLU:HG3	1:T:1685:LEU:H	1.74	0.53
1:T:1734:GLU:HB3	1:T:1765:PHE:HE1	1.73	0.53
1:T:474:ARG:NH2	1:T:474:ARG:O	2.40	0.53
1:T:1957:MET:HG3	1:T:1961:GLY:HA3	1.90	0.53
1:T:510:ASN:ND2	1:T:2207:GLN:OE1	2.42	0.53
1:T:2784:MET:HG3	1:T:2795:LYS:HD3	1.91	0.53
1:T:2529:SER:O	1:T:2533:LEU:N	2.41	0.53
1:T:1593:ARG:O	1:T:1597:ALA:N	2.40	0.53
1:T:3564:ILE:HA	1:T:3588:PRO:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:468:ILE:HA	1:T:471:TYR:HD2	1.74	0.52
1:T:1216:ILE:HD11	1:T:1241:LEU:HD21	1.91	0.52
1:T:1805:ASN:O	1:T:1809:SER:OG	2.28	0.52
1:T:2349:LEU:HA	1:T:2352:ILE:HG12	1.91	0.52
1:T:3392:MET:HA	1:T:3402:SER:HA	1.90	0.52
1:T:608:PRO:O	1:T:612:THR:N	2.41	0.52
1:T:2584:ILE:HG23	1:T:2623:VAL:HG21	1.90	0.52
1:T:1837:LEU:HG	1:T:1840:LYS:HE3	1.92	0.52
1:T:2865:THR:HA	1:T:2867:VAL:HG23	1.91	0.52
1:T:2878:LYS:O	1:T:2882:GLN:HB2	2.10	0.52
1:T:3019:LYS:O	1:T:3022:PHE:HB2	2.09	0.52
1:T:3246:PHE:HB2	1:T:3321:LEU:HD12	1.91	0.52
1:T:2817:CYS:O	1:T:2820:GLY:N	2.42	0.52
1:T:118:CYS:O	1:T:122:LEU:CB	2.51	0.52
1:T:1520:ARG:HD2	1:T:1569:PHE:HZ	1.75	0.52
1:T:1635:GLU:HA	1:T:1638:GLU:HG2	1.92	0.52
1:T:1726:GLN:HE22	1:T:1758:ALA:HB3	1.75	0.52
1:T:1:MET:O	1:T:6:GLN:NE2	2.39	0.52
1:T:2588:SER:HB2	1:T:2623:VAL:HG13	1.92	0.52
1:T:1116:ASN:O	1:T:1120:LEU:CB	2.58	0.52
1:T:1044:LYS:NZ	1:T:2514:VAL:O	2.40	0.52
1:T:3371:ILE:HG22	1:T:3393:ILE:HG21	1.91	0.52
1:T:3614:PHE:HE2	1:T:3667:ILE:HG23	1.75	0.52
1:T:2090:LEU:HD23	1:T:2093:ARG:HH11	1.75	0.51
1:T:1641:GLU:OE2	1:T:1680:ASN:ND2	2.43	0.51
1:T:1879:ILE:HD12	1:T:1882:ILE:HG13	1.92	0.51
1:T:1995:LEU:O	1:T:2041:LYS:NZ	2.43	0.51
1:T:2280:LYS:O	1:T:2284:LYS:N	2.42	0.51
1:T:3473:GLU:O	1:T:3477:LYS:CB	2.57	0.51
1:T:3261:ASN:OD1	1:T:3267:ARG:NH1	2.43	0.51
1:T:3211:LEU:O	1:T:3215:LEU:CB	2.57	0.51
1:T:2996:MET:HG2	1:T:3032:LYS:HE3	1.91	0.51
1:T:611:TYR:OH	1:T:1585:ARG:NH2	2.36	0.51
1:T:920:VAL:HG12	1:T:923:ASP:HB2	1.93	0.51
1:T:2094:GLU:O	1:T:2098:ALA:CB	2.58	0.51
1:T:3309:THR:O	1:T:3313:ARG:CB	2.59	0.51
1:T:1437:ARG:HA	1:T:1440:ILE:HG12	1.93	0.51
1:T:3659:LEU:O	1:T:3663:LEU:HB2	2.11	0.50
1:T:695:ASN:HA	1:T:698:PHE:HB3	1.92	0.50
1:T:848:THR:OG1	1:T:849:ALA:N	2.37	0.50
1:T:1203:ASP:O	1:T:1209:LYS:NZ	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:3067:ARG:HH11	1:T:3077:PHE:HZ	1.59	0.50
1:T:1423:LEU:HD12	1:T:1440:ILE:HD11	1.93	0.50
1:T:1355:ASP:O	1:T:1358:THR:OG1	2.29	0.50
1:T:2240:THR:HG22	1:T:2256:GLY:HA2	1.94	0.50
1:T:2232:GLY:O	1:T:2235:PHE:HB3	2.11	0.50
1:T:793:LEU:HB3	1:T:831:ILE:HD11	1.94	0.50
1:T:1473:LEU:HD21	1:T:1477:LEU:HB3	1.94	0.50
1:T:2837:PRO:O	1:T:2840:LYS:HB3	2.12	0.50
1:T:1804:LYS:HE2	1:T:1863:GLU:HB2	1.94	0.50
1:T:2022:SER:OG	1:T:2023:ASP:N	2.44	0.50
1:T:4:THR:HG22	1:T:7:ILE:HD12	1.94	0.50
1:T:1649:ASP:O	1:T:1653:SER:CB	2.60	0.49
1:T:2373:ALA:HA	1:T:2415:ARG:HH21	1.77	0.49
1:T:3289:ALA:HA	1:T:3293:ARG:HH21	1.77	0.49
1:T:1036:PRO:HG2	1:T:1039:TYR:HB2	1.94	0.49
1:T:2376:LEU:HD12	1:T:2379:MET:HG3	1.95	0.49
1:T:1340:LYS:NZ	1:T:1344:ALA:O	2.45	0.49
1:T:152:PRO:HA	1:T:155:ILE:HG12	1.94	0.49
1:T:1932:ARG:HE	1:T:1933:SER:H	1.59	0.49
1:T:24:ARG:HA	1:T:28:LEU:HD23	1.93	0.49
1:T:3620:VAL:HG11	1:T:3733:LEU:HD23	1.95	0.49
1:T:602:LYS:HB3	1:T:624:ARG:HH21	1.77	0.49
1:T:1237:LEU:HD13	1:T:1267:LEU:HD11	1.95	0.49
1:T:776:PHE:O	1:T:778:ASN:N	2.43	0.49
1:T:1757:LYS:HZ2	1:T:1805:ASN:HB3	1.77	0.49
1:T:1861:ARG:HH12	1:T:1896:LEU:HG	1.78	0.49
1:T:2877:ILE:O	1:T:2881:LEU:HB3	2.12	0.49
1:T:13:ARG:HH22	1:T:30:GLU:HA	1.78	0.49
1:T:1286:GLU:OE2	1:T:1328:HIS:NE2	2.46	0.49
1:T:485:ILE:HG23	1:T:579:PRO:HB2	1.94	0.48
1:T:944:ASN:OD1	1:T:947:ARG:NH2	2.42	0.48
1:T:2244:THR:HA	1:T:2253:VAL:HG23	1.94	0.48
1:T:3082:ILE:O	1:T:3086:LEU:HB2	2.13	0.48
1:T:407:GLN:N	1:T:410:GLU:OE2	2.45	0.48
1:T:1914:SER:HA	1:T:1952:VAL:HG21	1.95	0.48
1:T:2303:GLU:O	1:T:2307:THR:OG1	2.21	0.48
1:T:983:ASN:ND2	1:T:2480:PHE:O	2.45	0.48
1:T:1062:ASP:O	1:T:3320:ARG:NH1	2.46	0.48
1:T:2240:THR:HA	1:T:2243:ILE:HG22	1.94	0.48
1:T:3234:ASN:OD1	1:T:3452:SER:OG	2.30	0.48
1:T:732:THR:HB	1:T:735:ASN:HD22	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:952:LEU:HB2	1:T:955:ARG:HB2	1.95	0.48
1:T:1702:THR:HA	1:T:1705:THR:HG22	1.96	0.48
1:T:1767:PHE:HA	1:T:1770:ILE:HD12	1.94	0.48
1:T:2862:LEU:HD13	1:T:2865:THR:HB	1.96	0.48
1:T:13:ARG:HH12	1:T:30:GLU:HB2	1.77	0.48
1:T:1779:GLN:HA	1:T:1782:PHE:HD2	1.79	0.48
1:T:1246:LYS:HA	1:T:1303:VAL:HG21	1.96	0.48
1:T:1796:LEU:HB3	1:T:1799:ARG:HB2	1.96	0.48
1:T:2175:LYS:HG2	1:T:2179:TRP:HB3	1.96	0.48
1:T:1128:THR:HG21	1:T:3291:TYR:HB2	1.95	0.48
1:T:1519:GLY:O	1:T:1523:LEU:HB2	2.14	0.48
1:T:1670:VAL:O	1:T:1674:ASN:HB2	2.14	0.48
1:T:2184:LEU:HA	1:T:2187:ILE:HG22	1.95	0.48
1:T:770:PHE:HE1	1:T:784:LEU:HD21	1.77	0.48
1:T:1837:LEU:HD21	1:T:1886:ILE:HD11	1.95	0.47
1:T:2273:PRO:HB2	1:T:2274:LEU:HD12	1.95	0.47
1:T:3491:ASP:O	1:T:3495:ALA:CB	2.62	0.47
1:T:1482:LEU:HB2	1:T:1486:LEU:HD13	1.96	0.47
1:T:2621:HIS:CE1	1:T:2661:ALA:HB3	2.49	0.47
1:T:1116:ASN:O	1:T:1120:LEU:HB3	2.14	0.47
1:T:1056:GLY:N	1:T:2506:GLU:OE1	2.47	0.47
1:T:1120:LEU:HD22	1:T:2500:LEU:HD11	1.97	0.47
1:T:2877:ILE:O	1:T:2881:LEU:CB	2.62	0.47
1:T:776:PHE:HB3	1:T:779:ILE:HG12	1.96	0.47
1:T:1649:ASP:O	1:T:1653:SER:HB3	2.14	0.47
1:T:2998:GLU:O	1:T:3002:GLY:N	2.48	0.47
1:T:327:ASP:O	1:T:331:ARG:CB	2.63	0.47
1:T:2962:VAL:O	1:T:2966:GLN:N	2.47	0.47
1:T:132:ILE:HD13	1:T:134:GLN:HG2	1.96	0.47
1:T:2276:THR:O	1:T:2279:MET:HB3	2.14	0.47
1:T:3003:LEU:HD12	1:T:3026:LYS:HB2	1.97	0.47
1:T:345:LYS:HG2	1:T:387:LEU:HD11	1.96	0.47
1:T:740:LEU:HD12	1:T:769:SER:HB3	1.96	0.47
1:T:1355:ASP:HA	1:T:1358:THR:HG23	1.97	0.47
1:T:110:GLU:HG2	1:T:154:LEU:HD21	1.96	0.47
1:T:2950:PHE:HA	1:T:2953:VAL:HG12	1.96	0.47
1:T:2980:GLU:O	1:T:2984:LYS:CB	2.63	0.47
1:T:3587:LEU:HA	1:T:3588:PRO:HD3	1.75	0.47
1:T:3623:ARG:NH2	1:T:3744:PHE:O	2.47	0.47
1:T:1079:PHE:HD2	1:T:1144:LEU:HD11	1.80	0.46
1:T:48:LEU:HA	1:T:51:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:3241:THR:HB	1:T:3288:LEU:HD22	1.97	0.46
1:T:1535:LEU:HA	1:T:1538:LEU:HD23	1.96	0.46
1:T:1884:LYS:HA	1:T:1887:ILE:HD12	1.98	0.46
1:T:2481:ASN:O	1:T:2538:SER:OG	2.32	0.46
1:T:1342:LEU:HB3	1:T:1377:LEU:HD12	1.96	0.46
1:T:24:ARG:NH2	1:T:69:HIS:O	2.36	0.46
1:T:742:ARG:HH21	1:T:1545:GLU:H	1.61	0.46
1:T:1535:LEU:HD12	1:T:1584:LEU:HD21	1.97	0.46
1:T:2851:GLU:OE1	1:T:2884:TRP:NE1	2.49	0.46
1:T:790:ASP:O	1:T:794:ASN:CB	2.64	0.46
1:T:1519:GLY:O	1:T:1523:LEU:HB3	2.16	0.46
1:T:1902:LYS:O	1:T:1906:TYR:CB	2.55	0.46
1:T:2676:TYR:HB3	1:T:2680:ARG:HH21	1.81	0.46
1:T:2979:GLN:HG3	1:T:2982:PHE:HD2	1.79	0.46
1:T:3106:TRP:HE3	1:T:3107:LEU:HD22	1.80	0.46
1:T:791:LEU:O	1:T:795:SER:CB	2.64	0.45
1:T:122:LEU:O	1:T:126:PHE:CB	2.64	0.45
1:T:232:VAL:O	1:T:236:SER:CB	2.64	0.45
1:T:2373:ALA:O	1:T:2415:ARG:NH2	2.48	0.45
1:T:3354:ILE:HD13	1:T:3401:HIS:CE1	2.51	0.45
1:T:1789:PHE:O	1:T:1792:SER:OG	2.34	0.45
1:T:1941:LEU:HD13	1:T:1944:GLN:HE21	1.81	0.45
1:T:628:TYR:CG	1:T:1622:LEU:HD21	2.51	0.45
1:T:685:TYR:O	1:T:689:MET:CB	2.62	0.45
1:T:585:TYR:O	1:T:589:THR:OG1	2.28	0.45
1:T:588:ARG:O	1:T:592:SER:HB2	2.17	0.45
1:T:2989:ALA:HB2	1:T:3006:ILE:HG21	1.99	0.45
1:T:1667:THR:HG21	1:T:1717:GLN:HB2	1.99	0.45
1:T:1787:THR:HG21	1:T:1833:TRP:HB2	1.99	0.45
1:T:2399:LEU:HD12	1:T:2438:ILE:HD11	1.98	0.45
1:T:3288:LEU:HD11	1:T:3292:ILE:HG12	1.99	0.45
1:T:3467:LEU:HD22	1:T:3527:LEU:HD11	1.99	0.45
1:T:2377:THR:HG23	1:T:2415:ARG:HH22	1.82	0.45
1:T:3054:ALA:O	1:T:3058:ALA:N	2.49	0.45
1:T:3294:PRO:O	1:T:3298:ALA:HB2	2.16	0.45
1:T:1770:ILE:HG23	1:T:1810:THR:HA	1.99	0.45
1:T:1087:PHE:CG	1:T:1153:LEU:HD11	2.52	0.45
1:T:1840:LYS:HE2	1:T:1864:LEU:HD12	1.99	0.45
1:T:1905:ALA:HA	1:T:1908:VAL:HG22	1.98	0.45
1:T:3551:GLN:O	1:T:3555:PHE:N	2.50	0.44
1:T:154:LEU:HD22	1:T:214:LEU:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:1946:LEU:HD23	1:T:1989:LEU:HD22	1.99	0.44
1:T:2257:VAL:O	1:T:2261:TRP:CB	2.64	0.44
1:T:2278:LEU:O	1:T:2281:THR:HB	2.17	0.44
1:T:3103:ARG:HG3	1:T:3107:LEU:HD23	1.99	0.44
1:T:3019:LYS:HB2	1:T:3049:ILE:HG21	1.98	0.44
1:T:1800:ILE:HA	1:T:1803:LEU:HB2	2.00	0.44
1:T:2347:ASN:O	1:T:2351:LYS:NZ	2.47	0.44
1:T:2858:ILE:HD11	1:T:2877:ILE:HD13	1.98	0.44
1:T:3416:GLU:HG2	1:T:3586:MET:H	1.81	0.44
1:T:1241:LEU:HD23	1:T:1241:LEU:HA	1.84	0.44
1:T:1378:LEU:HD12	1:T:1415:CYS:SG	2.57	0.44
1:T:1379:GLN:NE2	1:T:1439:ARG:HD3	2.33	0.44
1:T:730:GLU:OE1	1:T:732:THR:OG1	2.31	0.44
1:T:2643:ILE:O	1:T:2647:THR:N	2.44	0.44
1:T:3112:ASP:HA	1:T:3113:ALA:HA	1.59	0.44
1:T:3522:VAL:HG11	1:T:3743:TRP:HD1	1.83	0.44
1:T:413:LYS:HA	1:T:416:LYS:HG2	1.99	0.44
1:T:1129:PHE:HB3	1:T:1131:ILE:HG12	1.99	0.44
1:T:2351:LYS:O	1:T:2355:MET:HB2	2.17	0.44
1:T:2985:LEU:HD12	1:T:3006:ILE:HG23	2.00	0.44
1:T:3054:ALA:HB3	1:T:3092:TYR:HB2	2.00	0.44
1:T:901:LEU:HD12	1:T:948:ILE:HD13	1.99	0.44
1:T:2334:SER:O	1:T:2338:LEU:HB2	2.18	0.44
1:T:2869:ASN:ND2	1:T:2872:SER:OG	2.51	0.44
1:T:307:TYR:HE1	1:T:346:GLU:HB2	1.82	0.44
1:T:3280:LEU:HA	1:T:3283:PHE:HB2	1.99	0.44
1:T:749:LYS:HA	1:T:798:TYR:CE2	2.53	0.44
1:T:1275:VAL:HG23	1:T:1280:LEU:HB2	2.00	0.43
1:T:1726:GLN:NE2	1:T:1758:ALA:O	2.51	0.43
1:T:2772:ASP:HB2	1:T:2775:ALA:HB3	1.99	0.43
1:T:3322:GLU:OE2	1:T:3382:ARG:NH2	2.51	0.43
1:T:2644:GLN:NE2	1:T:3634:ASP:OD2	2.51	0.43
1:T:984:GLY:HA3	1:T:2447:ILE:HG22	2.00	0.43
1:T:988:ASP:N	1:T:988:ASP:OD1	2.49	0.43
1:T:977:ILE:HA	1:T:992:SER:HA	2.00	0.43
1:T:1173:GLU:O	1:T:1177:LEU:CB	2.60	0.43
1:T:2748:GLU:O	1:T:2752:HIS:ND1	2.50	0.43
1:T:3240:THR:HG23	1:T:3242:ASP:H	1.81	0.43
1:T:1302:LYS:O	1:T:1306:ALA:HB2	2.19	0.43
1:T:1841:ILE:HD11	1:T:1886:ILE:HD13	2.01	0.43
1:T:2661:ALA:HA	1:T:2664:GLU:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:2684:LYS:HB3	1:T:2719:LEU:HD13	2.00	0.43
1:T:964:THR:HA	1:T:3578:SER:HB3	2.00	0.43
1:T:1885:ASP:HA	1:T:1888:LYS:HG2	1.99	0.43
1:T:2460:TRP:HE1	1:T:2462:PHE:HD1	1.67	0.43
1:T:2680:ARG:HH12	1:T:2693:SER:HB3	1.83	0.43
1:T:3025:LEU:HA	1:T:3028:MET:HG2	2.01	0.43
1:T:1090:THR:HG21	1:T:1163:VAL:HG11	2.00	0.43
1:T:217:SER:HA	1:T:304:PHE:HD2	1.83	0.43
1:T:3111:ASP:HA	1:T:3117:LEU:HD22	2.01	0.43
1:T:445:ARG:O	1:T:449:LEU:CB	2.67	0.43
1:T:2673:ASP:HB3	1:T:3640:ILE:HG12	2.01	0.43
1:T:2855:ALA:HA	1:T:2858:ILE:HG22	1.99	0.43
1:T:613:VAL:HG12	1:T:615:ASN:H	1.83	0.43
1:T:2621:HIS:CE1	1:T:2658:ASN:HA	2.54	0.43
1:T:3018:GLN:HG3	1:T:3021:GLU:HB3	2.01	0.43
1:T:3144:LEU:HD11	1:T:3207:TYR:HB2	2.01	0.43
1:T:3448:ALA:HA	1:T:3458:MET:HB3	2.01	0.43
1:T:897:GLY:O	1:T:901:LEU:HB2	2.18	0.43
1:T:3099:GLU:HG3	1:T:3661:THR:HG21	2.01	0.42
1:T:3466:THR:HG22	1:T:3573:HIS:CD2	2.54	0.42
1:T:695:ASN:HB3	1:T:732:THR:HG21	2.01	0.42
1:T:1116:ASN:HD22	1:T:2500:LEU:HD12	1.84	0.42
1:T:1685:LEU:HD22	1:T:1685:LEU:HA	1.84	0.42
1:T:1722:ILE:HD13	1:T:1754:ASN:HD22	1.84	0.42
1:T:2037:TYR:O	1:T:2041:LYS:N	2.53	0.42
1:T:2372:LYS:O	1:T:2376:LEU:CB	2.61	0.42
1:T:1026:LEU:HD21	1:T:1102:LEU:HD21	2.00	0.42
1:T:1584:LEU:HB2	1:T:1586:LEU:HD23	2.00	0.42
1:T:2610:ILE:HD12	1:T:2616:LEU:HD11	2.01	0.42
1:T:79:MET:HA	1:T:82:ILE:HD12	2.00	0.42
1:T:1864:LEU:HA	1:T:1864:LEU:HD13	1.84	0.42
1:T:2222:VAL:HG11	1:T:2229:GLU:HB3	2.01	0.42
1:T:2658:ASN:O	1:T:2662:LEU:HB2	2.20	0.42
1:T:327:ASP:O	1:T:331:ARG:HB2	2.19	0.42
1:T:396:ALA:HB1	1:T:438:LEU:HG	2.00	0.42
1:T:459:ARG:O	1:T:463:LEU:HB2	2.18	0.42
1:T:588:ARG:O	1:T:592:SER:CB	2.67	0.42
1:T:1379:GLN:NE2	1:T:1439:ARG:O	2.53	0.42
1:T:2242:VAL:O	1:T:2245:GLN:HB2	2.20	0.42
1:T:2870:LEU:HD12	1:T:2938:ARG:HG3	2.02	0.42
1:T:491:ARG:O	1:T:495:HIS:ND1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:1927:PHE:HZ	1:T:1966:TRP:HB2	1.84	0.42
1:T:2191:LEU:HD22	1:T:2194:CYS:HB2	2.01	0.42
1:T:3244:ASP:O	1:T:3248:LEU:HB2	2.20	0.42
1:T:2877:ILE:HG21	1:T:2940:TYR:HE1	1.85	0.42
1:T:3240:THR:HG23	1:T:3243:GLU:H	1.85	0.42
1:T:1727:ALA:O	1:T:1731:ARG:HB2	2.20	0.41
1:T:2308:THR:HA	1:T:2311:LEU:HD23	2.01	0.41
1:T:2906:GLN:HG2	1:T:2943:ILE:HG23	2.02	0.41
1:T:3013:TYR:HB2	1:T:3019:LYS:HZ1	1.85	0.41
1:T:3549:ALA:HA	1:T:3632:ILE:HD11	2.01	0.41
1:T:3613:ILE:HG13	1:T:3613:ILE:H	1.64	0.41
1:T:408:LEU:HD23	1:T:459:ARG:HH21	1.83	0.41
1:T:727:LEU:HB3	1:T:736:PHE:HD2	1.85	0.41
1:T:1803:LEU:HA	1:T:1806:VAL:HG12	2.02	0.41
1:T:232:VAL:O	1:T:236:SER:OG	2.29	0.41
1:T:2727:ALA:HA	1:T:2730:GLU:HG2	2.02	0.41
1:T:2946:VAL:O	1:T:2950:PHE:CB	2.68	0.41
1:T:3321:LEU:HD22	1:T:3321:LEU:HA	1.92	0.41
1:T:63:PRO:HB2	1:T:64:ILE:HG13	2.00	0.41
1:T:1392:LEU:HD22	1:T:1396:ILE:HA	2.02	0.41
1:T:1649:ASP:O	1:T:1653:SER:OG	2.36	0.41
1:T:2519:LEU:HA	1:T:2522:PHE:HB3	2.02	0.41
1:T:3165:GLN:HE22	1:T:3353:GLU:N	2.18	0.41
1:T:1608:THR:HG22	1:T:1640:PHE:HE1	1.85	0.41
1:T:977:ILE:HG22	1:T:2490:ASN:HD22	1.85	0.41
1:T:3484:ASP:O	1:T:3488:PHE:HB2	2.20	0.41
1:T:3489:MET:O	1:T:3493:LEU:HB2	2.19	0.41
1:T:1290:THR:O	1:T:1294:CYS:HB2	2.21	0.41
1:T:95:TYR:O	1:T:99:VAL:HB	2.20	0.41
1:T:1276:LYS:HG2	1:T:1318:THR:HG21	2.02	0.41
1:T:2803:PHE:HE2	1:T:2860:ALA:HB2	1.85	0.41
1:T:3121:PHE:HZ	1:T:3155:ILE:HD11	1.86	0.41
1:T:2100:LEU:HD22	1:T:2124:LEU:HB2	2.02	0.41
1:T:2234:THR:HG22	1:T:2237:GLN:HE21	1.86	0.41
1:T:2333:LEU:HD22	1:T:2375:ILE:HG21	2.02	0.41
1:T:2447:ILE:HD13	1:T:2479:SER:HB3	2.02	0.41
1:T:2719:LEU:HA	1:T:2720:PRO:HD3	1.91	0.41
1:T:2777:GLU:HA	1:T:2780:VAL:HB	2.03	0.41
1:T:3644:ASN:O	1:T:3648:ILE:HD12	2.21	0.41
1:T:1402:TYR:HA	1:T:1405:SER:HB3	2.02	0.41
1:T:1861:ARG:HH11	1:T:1893:PHE:HD1	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:1864:LEU:O	1:T:1868:SER:CB	2.69	0.41
1:T:2658:ASN:O	1:T:2662:LEU:CB	2.69	0.41
1:T:3583:THR:OG1	1:T:3586:MET:SD	2.73	0.41
1:T:3614:PHE:CE2	1:T:3667:ILE:HD12	2.56	0.41
1:T:1155:TYR:HD2	1:T:1157:ILE:HG12	1.86	0.41
1:T:1931:LEU:HD22	1:T:1970:VAL:HG22	2.02	0.41
1:T:2628:ILE:HA	1:T:2628:ILE:HD12	1.83	0.41
1:T:346:GLU:HA	1:T:349:HIS:HB2	2.03	0.41
1:T:1781:ASN:HA	1:T:1784:ASN:HD22	1.86	0.41
1:T:1931:LEU:HD11	1:T:1969:TRP:HB3	2.03	0.41
1:T:1935:HIS:ND1	1:T:1937:GLU:OE1	2.54	0.41
1:T:2102:ARG:O	1:T:2106:ALA:CB	2.68	0.41
1:T:2911:VAL:O	1:T:2915:ALA:HB3	2.20	0.41
1:T:1223:VAL:HG12	1:T:1227:SER:HB2	2.03	0.40
1:T:1787:THR:HA	1:T:1790:VAL:HG12	2.03	0.40
1:T:1903:GLN:HA	1:T:1906:TYR:HB3	2.02	0.40
1:T:2365:ILE:HG22	1:T:2367:PRO:HA	2.03	0.40
1:T:3087:GLN:HE21	1:T:3124:PHE:HD1	1.70	0.40
1:T:1543:LEU:O	1:T:1545:GLU:N	2.54	0.40
1:T:302:THR:O	1:T:305:LEU:HB3	2.21	0.40
1:T:3202:ARG:HB3	1:T:3203:GLN:H	1.59	0.40
1:T:587:TYR:O	1:T:591:MET:HB2	2.22	0.40
1:T:1382:ILE:HG22	1:T:1412:ARG:HG3	2.02	0.40
1:T:2672:GLU:OE2	1:T:3438:ARG:NH1	2.54	0.40
1:T:2298:ALA:HB1	1:T:2302:GLU:HG3	2.03	0.40
1:T:2847:GLN:HE21	1:T:2887:ARG:HD3	1.87	0.40
1:T:3708:HIS:CE1	1:T:3710:ASN:HB3	2.56	0.40
1:T:900:THR:HA	1:T:903:LEU:HD22	2.04	0.40
1:T:1197:PHE:HB3	1:T:1216:ILE:HG23	2.03	0.40
1:T:1416:ILE:HG21	1:T:1459:THR:HG22	2.03	0.40
1:T:2462:PHE:CE2	1:T:2466:TYR:HB3	2.56	0.40
1:T:743:PHE:HD2	1:T:744:LEU:HD12	1.86	0.40
1:T:997:ILE:HD13	1:T:1078:LEU:HD21	2.03	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 PDB entries followed by that with respect to all EM entries.

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	T	3443/3767 (91%)	2913 (85%)	508 (15%)	22 (1%)	27 68

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	T	1544	ALA
1	T	2889	PRO
1	T	1158	PRO
1	T	1157	ILE
1	T	3655	PRO
1	T	777	PRO
1	T	849	ALA
1	T	852	PRO
1	T	2223	SER
1	T	228	PRO
1	T	247	PRO
1	T	510	ASN
1	T	1206	TYR
1	T	1341	PRO
1	T	3657	ASN
1	T	695	ASN
1	T	1543	LEU
1	T	2620	PRO
1	T	2621	HIS
1	T	63	PRO
1	T	2619	PRO
1	T	2226	ILE

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 PDB entries followed by that with respect to all EM entries.

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	T	3200/3474 (92%)	3107 (97%)	93 (3%)	45 75

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	T	13	ARG
1	T	15	ARG
1	T	37	LEU
1	T	38	LEU
1	T	88	MET
1	T	114	ASN
1	T	231	MET
1	T	246	LEU
1	T	331	ARG
1	T	340	LEU
1	T	399	ILE
1	T	440	LEU
1	T	447	LEU
1	T	463	LEU
1	T	499	LYS
1	T	594	LEU
1	T	617	LYS
1	T	677	LYS
1	T	691	MET
1	T	783	VAL
1	T	788	LEU
1	T	794	ASN
1	T	829	ARG
1	T	876	LEU
1	T	880	MET
1	T	920	VAL
1	T	930	ASN
1	T	957	ARG
1	T	961	LYS
1	T	994	THR
1	T	1002	ASN
1	T	1082	LEU
1	T	1119	LEU
1	T	1130	ASN
1	T	1137	ASN

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Mol	Chain	Res	Type
1	T	1340	LYS
1	T	1345	LEU
1	T	1365	ASN
1	T	1366	THR
1	T	1368	LEU
1	T	1377	LEU
1	T	1475	LYS
1	T	1488	ASN
1	T	1515	LYS
1	T	1574	LEU
1	T	1618	ARG
1	T	1626	ASN
1	T	1654	ASN
1	T	1685	LEU
1	T	1690	ASN
1	T	1718	LEU
1	T	1775	ASN
1	T	1808	ASN
1	T	1825	LEU
1	T	1865	LEU
1	T	2122	ASN
1	T	2168	LEU
1	T	2177	LYS
1	T	2191	LEU
1	T	2278	LEU
1	T	2311	LEU
1	T	2315	LEU
1	T	2318	LEU
1	T	2324	LEU
1	T	2330	ARG
1	T	2350	ARG
1	T	2477	TYR
1	T	2481	ASN
1	T	2494	LEU
1	T	2500	LEU
1	T	2573	LYS
1	T	2646	ASN
1	T	2678	LEU
1	T	2682	ARG
1	T	2808	LYS
1	T	2815	LYS
1	T	2861	ASN

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Mol	Chain	Res	Type
1	T	2869	ASN
1	T	2896	ASN
1	T	2899	ASN
1	T	2959	MET
1	T	3026	LYS
1	T	3053	LEU
1	T	3080	ASN
1	T	3151	MET
1	T	3212	ASN
1	T	3267	ARG
1	T	3280	LEU
1	T	3321	LEU
1	T	3390	ARG
1	T	3445	LEU
1	T	3458	MET
1	T	3706	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	T	49	GLN
1	T	298	GLN
1	T	510	ASN
1	T	565	ASN
1	T	639	HIS
1	T	794	ASN
1	T	840	GLN
1	T	930	ASN
1	T	956	ASN
1	T	1002	ASN
1	T	1114	GLN
1	T	1130	ASN
1	T	1137	ASN
1	T	1365	ASN
1	T	1379	GLN
1	T	1397	GLN
1	T	1488	ASN
1	T	1601	ASN
1	T	1654	ASN
1	T	1690	ASN
1	T	1726	GLN
1	T	1775	ASN

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Mol	Chain	Res	Type
1	T	1779	GLN
1	T	1784	ASN
1	T	1805	ASN
1	T	1808	ASN
1	T	1839	ASN
1	T	1983	ASN
1	T	2122	ASN
1	T	2183	ASN
1	T	2207	GLN
1	T	2237	GLN
1	T	2289	HIS
1	T	2294	GLN
1	T	2481	ASN
1	T	2595	GLN
1	T	2658	ASN
1	T	2670	GLN
1	T	2822	GLN
1	T	2839	HIS
1	T	2861	ASN
1	T	2863	HIS
1	T	2869	ASN
1	T	2896	ASN
1	T	2899	ASN
1	T	2907	HIS
1	T	2975	ASN
1	T	3080	ASN
1	T	3087	GLN
1	T	3154	HIS
1	T	3165	GLN
1	T	3250	ASN
1	T	3361	ASN
1	T	3385	HIS
1	T	3537	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.