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PDB ID	:	8X2H
EMDB ID	:	EMD-38010
Title	:	Cryo-EM structure of the TcsL at pH 5.0 in its closed conformation
Authors	:	Zhan, X.; Tao, L.
Deposited on	:	2023-11-09
Resolution	:	2.90 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 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 2.90 Å.

Sidechain outliers

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.



154315

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq=3, 2, 1$  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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

3826

Mol	Chain	Length	Quality of cha	in	
			9%		
1	А	2372	59%	36%	5%



# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 19088 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 Cytotoxin-L.

Mol	Chain	Residues	Atoms				AltConf	Trace	
1	А	2363	Total 19087	C 12219	N 3035	O 3786	S 47	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	2365	HIS	-	expression tag	UNP T0D3N5
А	2366	HIS	-	expression tag	UNP T0D3N5
А	2367	HIS	-	expression tag	UNP T0D3N5
А	2368	HIS	-	expression tag	UNP T0D3N5
А	2369	HIS	-	expression tag	UNP T0D3N5
А	2370	HIS	-	expression tag	UNP T0D3N5
А	2371	HIS	-	expression tag	UNP T0D3N5
А	2372	HIS	-	expression tag	UNP T0D3N5

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
2	А	1	Total Zn 1 1	0



# 3 Residue-property plots (i)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Cytotoxin-L



1892     1892       1893     1893       1893     1893       1894     1911       1911     1911       1911     1911       1911     1911       1912     1913       1913     1914       1914     1913       1915     1935       1935     1936       1936     1936       1936     1936       1936     1936       1936     1936       1936     1936       1936     1936       1936     1936       1936     1936       1936     1936       1936     1936       1936     1936       1936     1936       1936     1936       1936     1936       1937     1936       1936     1936       1937     1937       1936     1936       1937     1937       1938     1937       1937
V983       A984       A984       A984       K1005       E1009       L1011       S1012       F1013       L1025       L1026       L1026       L1025       L1026       L1026       L1026       L1026       L1026       L1026       L1026       L1057       L1058       L1056       L1057       L1058       A1068       A1068       A1077       L1078       L1078       L1078       L1078       L1078       L1078 <tr td=""></tr>
I.1     102       I.1     105       I.1     105       I.1     111       I.1     112       I.1     112       I.1     12       I.1     13       I.1     14       I.1     15       I.1     15       I.1     15       I.1     16       I.1     15
HI 186 F1 187 S11 192 S11 192 S11 192 L1 192 H1 202 H1 202 H1 202 H1 205 H1 205
RI281       R1282       F1284       F1284       F1284       F1284       F1284       F1284       F1284       R1285       R1285       R1286       R1286       R1306       R1311       L1306       R1332       R1342       R1342<
I1389       11389       11389       11389       11386       11396       11396       11396       11396       11396       11396       11396       11396       11396       1140       1140       1140       1140       1140       1140       11416       11416       11418       11418       11418       11418       11418       11418       11418       11418       11418       11418       11418       11418       11418       11418       11419       11418       11418       11419       11418       11447       11448       11448       11449       11447       11448       11448       11448
0.482       1.483       1.483       1.483       1.483       1.483       1.486       1.486       1.486       1.486       1.486       1.486       1.486       1.486       1.486       1.486       1.486       1.506       1.506       1.506       1.506       1.507       1.506       1.506       1.507       1.506       1.507       1.507       1.506       1.507       1.506       1.507       1.507       1.508       1.508       1.508       1.508       1.508       1.508       1.508       1.508       1.508       1.508       1.508       1.508       1.508       1.508       1.508       1.508<
q1564   N1565   N1565   N1577   N1575   N1577   N1592   N1502   N1502   N1502   N1502   N1502   N1502   N1503   N1503   N1503   N1505   N1555   N1555   N1555   N1555   N1555
Y1662 H1653 L1665 D1665 D1665 D1665 D1665 C1651 C1665 C1665 C1660 F1671 C1660 F1660 F1660 F1660 F1660 F1660 F1660 F1715 F1715 F1715 F1715 F1715 F1715 F1715 F1715 F1725
11751 11755 11755 11755 11755 11755 11755 11755 11755 11755 11755 11755 11755 11755 11755 11775 11777
P1 848 P1 848 P1 843 P1 843 P1 843 P1 853 P1 853 P1 855 P1 856 P1 856 P1 866 P1 86
Y1937     Y1937       F13938     F13938       F13945     A1344       A1345     A1345       V1345     V1345       V1345     F1395       V1345     F1395       V1345     F1395       V1345     F1395       P1395     P1395       P139
R2026 R2027 L2028 V2030 (22029 V2030 F2046 F2046 F2046 F2046 F2046 F2046 F2046 F2046 F2046 F2046 F2046 F2046 F2046 F2065 F206







# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	410049	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 $(6k \ge 4k)$	Depositor
Maximum map value	4.347	Depositor
Minimum map value	-2.594	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.22	Depositor
Map size (Å)	434.80002, 434.80002, 434.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor



# 5 Model quality (i)

# 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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).

Mal	Chain	Bond	lengths	Bond angles		
		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.30	0/19471	0.52	2/26343~(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	А	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	1683	TYR	CB-CA-C	-12.45	85.50	110.40
1	А	363	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	1068	ALA	Peptide
1	А	1774	SER	Peptide
1	А	841	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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	19087	0	18641	598	0
2	А	1	0	0	0	0
All	All	19088	0	18641	598	0

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.

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 16.

All (598) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:578:ILE:O	1:A:647:LYS:HB3	1.66	0.96
1:A:2028:LEU:HA	1:A:2040:PHE:O	1.73	0.89
1:A:2307:ASN:ND2	1:A:2312:ASN:O	2.05	0.88
1:A:1052:ASN:HD21	1:A:1057:ARG:HB3	1.40	0.86
1:A:1547:THR:O	1:A:1597:ASN:ND2	2.10	0.84
1:A:410:LEU:HD13	1:A:468:LEU:HD11	1.60	0.83
1:A:2058:ASN:ND2	1:A:2071:ASP:O	2.12	0.81
1:A:1760:ASN:HA	1:A:1849:PRO:HD3	1.62	0.81
1:A:12:MET:SD	1:A:975:LYS:NZ	2.55	0.80
1:A:5:ASN:OD1	1:A:5:ASN:N	2.15	0.79
1:A:84:LEU:O	1:A:88:ASN:ND2	2.16	0.77
1:A:1590:ASN:OD1	1:A:1593:ASN:ND2	2.19	0.76
1:A:2307:ASN:O	1:A:2309:LEU:N	2.12	0.76
1:A:124:ASP:OD1	1:A:124:ASP:N	2.17	0.76
1:A:1432:ASN:HB3	1:A:1435:LYS:HB2	1.67	0.76
1:A:2259:ASN:HB3	1:A:2288:LYS:HG2	1.67	0.76
1:A:339:ASP:OD1	1:A:339:ASP:N	2.16	0.75
1:A:1574:SER:HB2	1:A:1836:LEU:HG	1.67	0.75
1:A:109:ASP:O	1:A:113:ASN:ND2	2.21	0.74
1:A:1377:ILE:HD11	1:A:1420:LEU:HD23	1.70	0.74
1:A:119:LYS:HB3	1:A:127:VAL:HG21	1.68	0.73
1:A:1960:ASN:OD1	1:A:1960:ASN:N	2.22	0.73
1:A:2240:LYS:NZ	1:A:2269:MET:SD	2.59	0.73
1:A:1377:ILE:HD11	1:A:1420:LEU:HA	1.71	0.73
1:A:2264:ASN:HB3	1:A:2270:GLN:HE22	1.54	0.72
1:A:125:TYR:OH	1:A:363:LEU:O	2.04	0.72
1:A:2222:PHE:HA	1:A:2229:ALA:HA	1.71	0.72
1:A:366:ILE:HG12	1:A:507:LYS:HE2	1.71	0.72
1:A:95:GLU:OE1	1:A:95:GLU:N	2.18	0.71



	juo pugo	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:646:ILE:HG23	1:A:691:ILE:HA	1.71	0.71
1:A:58:ASN:O	1:A:62:THR:OG1	2.09	0.71
1:A:373:VAL:HG23	1:A:395:CYS:HB3	1.73	0.71
1:A:1863:ASN:HD22	1:A:1894:ILE:HD13	1.56	0.71
1:A:801:LEU:HD21	1:A:805:ARG:HH11	1.56	0.71
1:A:1758:GLU:HB2	1:A:1761:GLN:HG3	1.72	0.70
1:A:754:ILE:HD11	1:A:764:LYS:HB3	1.72	0.70
1:A:1115:ASP:O	1:A:1277:LYS:NZ	2.23	0.70
1:A:1121:ILE:HD13	1:A:1245:ASN:HD21	1.56	0.70
1:A:1680:LYS:O	1:A:1683:TYR:HD2	1.74	0.70
1:A:528:LYS:NZ	1:A:699:ASN:OD1	2.24	0.69
1:A:578:ILE:HB	1:A:646:ILE:HA	1.74	0.69
1:A:148:SER:OG	1:A:182:LYS:NZ	2.24	0.69
1:A:549:LEU:HD21	1:A:589:ILE:HD12	1.73	0.69
1:A:435:LEU:HD21	1:A:447:MET:HB3	1.75	0.68
1:A:2329:LYS:HG3	1:A:2359:GLU:HG3	1.74	0.68
1:A:283:VAL:HG11	1:A:363:LEU:HD21	1.73	0.68
1:A:976:GLU:OE1	1:A:982:SER:N	2.24	0.68
1:A:2300:PHE:HB2	1:A:2339:ALA:HB3	1.76	0.68
1:A:752:ARG:HD3	1:A:752:ARG:H	1.58	0.68
1:A:2296:THR:OG1	1:A:2298:ASP:OD2	2.11	0.68
1:A:1469:THR:HG22	1:A:1471:TYR:HE2	1.57	0.68
1:A:8:GLN:NE2	1:A:870:TYR:OH	2.27	0.67
1:A:1744:ASP:OD1	1:A:1745:ASN:N	2.24	0.67
1:A:690:TYR:HB2	1:A:734:SER:HB3	1.76	0.67
1:A:1124:PHE:HA	1:A:1127:ILE:HD12	1.77	0.67
1:A:1230:PHE:HB3	1:A:1278:LEU:HD11	1.75	0.67
1:A:1156:ASP:OD1	1:A:1159:ASN:N	2.27	0.66
1:A:90:SER:O	1:A:90:SER:OG	2.10	0.66
1:A:1326:SER:HA	1:A:1347:ASP:HB3	1.76	0.66
1:A:2103:THR:O	1:A:2109:LYS:HA	1.94	0.66
1:A:207:LYS:NZ	1:A:222:ASN:OD1	2.29	0.66
1:A:273:ARG:NH1	1:A:284:TYR:OH	2.29	0.66
1:A:1340:GLU:HA	1:A:1399:ASN:HD21	1.60	0.65
1:A:802:GLN:O	1:A:806:ASN:ND2	2.24	0.65
1:A:2148:ASN:OD1	1:A:2185:GLN:NE2	2.29	0.65
1:A:795:HIS:CE1	1:A:1802:LEU:HD12	2.31	0.65
1:A:364:ASP:OD1	1:A:365:ASP:N	2.29	0.65
1:A:2144:ASN:OD1	1:A:2144:ASN:N	2.29	0.65
1:A:1531:TYR:OH	1:A:1589:ILE:O	2.10	0.65
1:A:73:LYS:HE3	1:A:1726:ILE:HG12	1.77	0.65



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:11:LYS:NZ	1:A:977:SER:O	2.28	0.65
1:A:655:LYS:O	1:A:699:ASN:ND2	2.27	0.65
1:A:1116:LYS:HZ3	1:A:1118:THR:HG22	1.61	0.65
1:A:1956:THR:HB	1:A:1986:MET:HB3	1.78	0.65
1:A:2113:ASP:HB3	1:A:2119:GLN:HE21	1.62	0.65
1:A:1307:GLN:HA	1:A:1310:LYS:HB2	1.78	0.64
1:A:1935:LYS:NZ	1:A:1965:GLU:OE2	2.29	0.64
1:A:2257:GLU:O	1:A:2259:ASN:ND2	2.31	0.64
1:A:479:GLN:HE21	1:A:493:LEU:HG	1.62	0.64
1:A:1505:LEU:HD13	1:A:1507:ILE:HD11	1.79	0.64
1:A:1407:SER:OG	1:A:1413:ASN:OD1	2.13	0.64
1:A:374:LYS:HD3	1:A:503:PHE:HA	1.79	0.63
1:A:1899:VAL:HG23	1:A:1932:ILE:HD11	1.79	0.63
1:A:1992:THR:HG22	1:A:1997:VAL:HG22	1.81	0.63
1:A:463:ARG:O	1:A:465:THR:N	2.31	0.63
1:A:1116:LYS:NZ	1:A:1118:THR:HG22	2.13	0.63
1:A:1652:ASN:O	1:A:1655:ASN:ND2	2.30	0.63
1:A:650:PHE:HB2	1:A:695:LEU:HD23	1.80	0.62
1:A:937:PHE:HB3	1:A:945:VAL:HG23	1.80	0.62
1:A:651:ILE:HG23	1:A:696:LEU:HB3	1.82	0.62
1:A:2215:ASN:HD21	1:A:2218:ASP:HB2	1.65	0.62
1:A:340:GLU:OE1	1:A:344:ARG:NH1	2.33	0.62
1:A:1407:SER:HA	1:A:1413:ASN:HA	1.82	0.62
1:A:363:LEU:HA	1:A:507:LYS:HE3	1.80	0.62
1:A:16:LYS:H	1:A:16:LYS:HD2	1.65	0.62
1:A:1367:LEU:HD11	1:A:1408:ILE:HA	1.80	0.61
1:A:97:ASN:ND2	1:A:280:ASP:OD1	2.33	0.61
1:A:932:ILE:HD11	1:A:962:ALA:HA	1.81	0.61
1:A:2112:PHE:HA	1:A:2118:ARG:HA	1.82	0.61
1:A:93:PRO:HA	1:A:367:LYS:HA	1.82	0.61
1:A:883:PHE:HB2	1:A:984:ALA:HB2	1.81	0.61
1:A:1970:LEU:HD12	1:A:1993:ILE:HD12	1.81	0.61
1:A:2182:ILE:N	1:A:2185:GLN:OE1	2.30	0.61
1:A:2215:ASN:O	1:A:2217:THR:N	2.27	0.61
1:A:794:LEU:O	1:A:798:SER:OG	2.17	0.61
1:A:1793:VAL:O	1:A:1797:ILE:HG13	2.01	0.61
1:A:2282:TYR:HB2	1:A:2303:PHE:CZ	2.36	0.61
1:A:2114:ASP:OD2	1:A:2115:ASN:ND2	2.35	0.60
1:A:1948:GLU:HB3	1:A:1958:TYR:CZ	2.36	0.60
1:A:1029:LEU:HB2	1:A:1031:ILE:HG12	1.83	0.60
1:A:1927:ILE:HD12	1:A:1941:ASP:HA	1.83	0.60



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:870:TYR:HB2	1:A:979:SER:HB3	1.83	0.60
1:A:2239:ILE:HG12	1:A:2268:LYS:HE3	1.84	0.60
1:A:1352:VAL:HG21	1:A:1406:PHE:HB2	1.82	0.60
1:A:925:ILE:HD13	1:A:968:LEU:HD21	1.83	0.60
1:A:1827:ASN:OD1	1:A:1831:ASN:N	2.34	0.59
1:A:148:SER:OG	1:A:148:SER:O	2.17	0.59
1:A:1530:ASN:HD22	1:A:1537:LYS:HG3	1.67	0.59
1:A:113:ASN:HB3	1:A:328:PRO:HD2	1.84	0.59
1:A:526:ARG:HH11	1:A:526:ARG:HG3	1.67	0.59
1:A:1400:ARG:NH2	1:A:1419:ASP:OD2	2.35	0.59
1:A:479:GLN:HE22	1:A:492:HIS:H	1.51	0.58
1:A:1276:THR:HG22	1:A:1277:LYS:H	1.67	0.58
1:A:2210:THR:HA	1:A:2222:PHE:HB2	1.84	0.58
1:A:1686:ASP:OD2	1:A:1712:ASN:ND2	2.36	0.58
1:A:239:ASP:OD1	1:A:241:ARG:N	2.26	0.58
1:A:2078:VAL:HG11	1:A:2093:ASP:HA	1.85	0.58
1:A:336:ASP:HA	1:A:343:GLN:HE22	1.68	0.58
1:A:2171:TYR:HB3	1:A:2187:VAL:HG12	1.86	0.58
1:A:169:ASN:O	1:A:173:ARG:HG3	2.03	0.58
1:A:899:ARG:HH21	1:A:901:ILE:HD11	1.69	0.58
1:A:2113:ASP:OD1	1:A:2117:ILE:N	2.36	0.58
1:A:70:LYS:HG3	1:A:1698:LEU:HD11	1.84	0.58
1:A:1221:VAL:HG22	1:A:1299:ILE:HD13	1.86	0.58
1:A:1236:TRP:HB2	1:A:2254:ILE:HA	1.85	0.58
1:A:1902:THR:OG1	1:A:1903:SER:N	2.37	0.57
1:A:363:LEU:HG	1:A:366:ILE:HD11	1.86	0.57
1:A:2171:TYR:O	1:A:2187:VAL:N	2.33	0.57
1:A:2307:ASN:O	1:A:2312:ASN:ND2	2.38	0.57
1:A:1046:LYS:HG2	1:A:1066:ILE:HD13	1.85	0.57
1:A:1520:ASN:HD22	1:A:1525:LYS:HG3	1.70	0.57
1:A:1774:SER:O	1:A:1776:THR:HG22	2.05	0.57
1:A:1868:ASP:OD1	1:A:1870:THR:HG22	2.04	0.57
1:A:1948:GLU:O	1:A:1958:TYR:HA	2.04	0.57
1:A:10:GLN:HE21	1:A:20:GLN:HE22	1.53	0.57
1:A:2039:PHE:O	1:A:2055:THR:OG1	2.21	0.57
1:A:402:GLN:HB3	1:A:473:VAL:HG22	1.87	0.57
1:A:1680:LYS:O	1:A:1683:TYR:CD2	2.57	0.56
1:A:101:ILE:HD12	1:A:284:TYR:HE1	1.70	0.56
1:A:1397:GLU:OE1	1:A:1400:ARG:NH1	2.38	0.56
1:A:1577:ASN:O	1:A:1632:ILE:N	2.31	0.56
1:A:2195:VAL:HG22	1:A:2196:ASN:H	1.69	0.56



	ab page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:801:LEU:HG	1:A:805:ARG:HE	1.70	0.56
1:A:865:ILE:HG12	1:A:921:TYR:CZ	2.40	0.56
1:A:1822:ASP:OD2	1:A:1850:LYS:NZ	2.29	0.56
1:A:2120:LEU:HD21	1:A:2133:SER:O	2.05	0.56
1:A:134:ASN:O	1:A:202:ILE:HB	2.06	0.56
1:A:756:ASP:OD1	1:A:757:HIS:N	2.39	0.56
1:A:1405:THR:O	1:A:1405:THR:OG1	2.22	0.56
1:A:573:ARG:HH21	1:A:1805:TYR:HB3	1.70	0.56
1:A:672:SER:HA	1:A:675:ILE:HD12	1.88	0.56
1:A:764:LYS:O	1:A:768:ILE:HG13	2.05	0.56
1:A:1926:PHE:HB3	1:A:1939:PHE:CD1	2.41	0.56
1:A:103:ILE:HD12	1:A:265:LEU:HD22	1.88	0.56
1:A:23:GLU:N	1:A:23:GLU:OE1	2.39	0.56
1:A:648:LEU:HG	1:A:678:ILE:HD13	1.88	0.56
1:A:1625:ILE:HD12	1:A:1633:GLN:HG3	1.89	0.55
1:A:2305:HIS:CG	1:A:2306:GLN:H	2.24	0.55
1:A:1144:ILE:HB	1:A:1220:MET:HG3	1.88	0.55
1:A:1754:ALA:HB3	1:A:1764:VAL:HB	1.89	0.55
1:A:2181:ASN:ND2	1:A:2182:ILE:O	2.40	0.55
1:A:126:THR:O	1:A:126:THR:OG1	2.25	0.55
1:A:95:GLU:OE2	1:A:391:LYS:HB2	2.06	0.55
1:A:1202:ILE:O	1:A:1205:VAL:HG22	2.07	0.55
1:A:52:ILE:HG22	1:A:79:LEU:HD11	1.87	0.54
1:A:60:LEU:HD13	1:A:73:LYS:HE2	1.89	0.54
1:A:800:LEU:O	1:A:804:ILE:HG13	2.07	0.54
1:A:1841:ASP:O	1:A:1842:SER:OG	2.23	0.54
1:A:1078:ILE:HG21	1:A:1415:ILE:HD11	1.89	0.54
1:A:2019:TYR:O	1:A:2027:GLN:NE2	2.31	0.54
1:A:1722:ASP:OD1	1:A:1722:ASP:N	2.40	0.54
1:A:2228:LYS:HZ2	1:A:2231:LYS:HE3	1.73	0.54
1:A:549:LEU:HD22	1:A:587:ASP:HB2	1.90	0.54
1:A:1111:LEU:HD13	1:A:1282:TYR:CE2	2.42	0.54
1:A:735:ILE:O	1:A:779:SER:OG	2.17	0.54
1:A:1111:LEU:HD13	1:A:1282:TYR:HE2	1.73	0.54
1:A:393:SER:OG	1:A:394:TYR:N	2.41	0.54
1:A:790:LYS:HG3	1:A:791:SER:H	1.73	0.54
1:A:1400:ARG:HA	1:A:1420:LEU:HD12	1.90	0.54
1:A:246:PHE:CD2	1:A:252:VAL:HG12	2.43	0.53
1:A:846:ASN:HD21	1:A:1767:ARG:HH22	1.56	0.53
1:A:2190:SER:HA	1:A:2202:PHE:HB2	1.90	0.53
1:A:1152:LEU:HD22	1:A:1164:LEU:HA	1.89	0.53



	h i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1881:THR:O	1:A:1881:THR:OG1	2.24	0.53
1:A:31:LEU:O	1:A:35:HIS:HD2	1.92	0.53
1:A:148:SER:HG	1:A:182:LYS:NZ	2.06	0.53
1:A:1327:LEU:HD11	1:A:1389:ILE:HD11	1.91	0.53
1:A:1594:ILE:HG13	1:A:1595:PHE:H	1.73	0.53
1:A:932:ILE:HG21	1:A:1021:LEU:HD22	1.91	0.53
1:A:1224:ASN:N	1:A:1224:ASN:OD1	2.41	0.53
1:A:485:LYS:HG2	1:A:486:ASP:H	1.74	0.53
1:A:1955:GLU:HB3	1:A:1985:ILE:HG23	1.90	0.53
1:A:2177:THR:OG1	1:A:2181:ASN:OD1	2.22	0.53
1:A:136:PHE:H	1:A:203:ASP:CG	2.11	0.53
1:A:1613:ILE:HG13	1:A:1614:SER:N	2.23	0.53
1:A:100:PHE:O	1:A:101:ILE:HG13	2.09	0.53
1:A:1429:LEU:HD11	1:A:1447:ILE:HD11	1.91	0.53
1:A:1677:PHE:CZ	1:A:1692:VAL:HG11	2.43	0.53
1:A:332:SER:O	1:A:332:SER:OG	2.25	0.52
1:A:566:ILE:HG12	1:A:599:SER:HA	1.91	0.52
1:A:596:ASN:ND2	1:A:743:GLU:OE2	2.42	0.52
1:A:1113:LEU:HD23	1:A:1114:GLN:HG2	1.91	0.52
1:A:1160:ASN:O	1:A:1212:LYS:N	2.41	0.52
1:A:373:VAL:O	1:A:478:TYR:OH	2.16	0.52
1:A:975:LYS:O	1:A:979:SER:OG	2.17	0.52
1:A:1432:ASN:O	1:A:1436:LEU:N	2.36	0.52
1:A:1469:THR:HG22	1:A:1471:TYR:CE2	2.43	0.52
1:A:1988:THR:HG21	1:A:2002:ASN:HA	1.91	0.52
1:A:108:ASN:O	1:A:112:ILE:HD12	2.10	0.52
1:A:696:LEU:HD11	1:A:742:TYR:O	2.09	0.52
1:A:869:LEU:HD11	1:A:979:SER:HB2	1.91	0.52
1:A:421:GLY:HA3	1:A:427:THR:HB	1.92	0.52
1:A:744:VAL:HG22	1:A:754:ILE:HG22	1.92	0.52
1:A:1377:ILE:HG23	1:A:1423:LYS:HA	1.91	0.52
1:A:2302:TYR:HB2	1:A:2333:PHE:CZ	2.45	0.52
1:A:1730:ILE:HG12	1:A:1780:LYS:HB3	1.90	0.52
1:A:573:ARG:HG3	1:A:574:ASN:N	2.24	0.51
1:A:1284:ASP:HA	1:A:1311:ASN:HB3	1.92	0.51
1:A:1531:TYR:HD2	1:A:1532:PHE:N	2.08	0.51
1:A:1264:TRP:HB2	1:A:1275:ILE:HB	1.92	0.51
1:A:1625:ILE:HD11	1:A:1635:TYR:HD2	1.76	0.51
1:A:239:ASP:OD1	1:A:240:ILE:N	2.42	0.51
1:A:655:LYS:HB2	1:A:660:THR:HB	1.92	0.51
1:A:479:GLN:NE2	1:A:493:LEU:HG	2.26	0.51



	h h a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1384:LEU:HD22	1:A:1404:LEU:HD13	1.92	0.51
1:A:2083:LEU:HG	1:A:2085:ASP:H	1.76	0.51
1:A:2306:GLN:NE2	1:A:2307:ASN:OD1	2.44	0.51
1:A:1136:PHE:HE2	1:A:1162:ILE:HG21	1.75	0.51
1:A:1728:GLU:OE1	1:A:1728:GLU:N	2.36	0.51
1:A:2219:LYS:HB3	1:A:2219:LYS:HZ2	1.76	0.51
1:A:695:LEU:H	1:A:739:ALA:HA	1.75	0.51
1:A:2327:ASP:C	1:A:2329:LYS:H	2.14	0.51
1:A:161:LEU:HD23	1:A:162:ASN:H	1.75	0.51
1:A:504:PRO:HB2	1:A:507:LYS:HB2	1.93	0.51
1:A:246:PHE:HE1	1:A:272:LEU:HD12	1.76	0.51
1:A:606:ILE:HG12	1:A:620:TYR:HB2	1.93	0.51
1:A:1836:LEU:HD22	1:A:1843:LEU:HD11	1.92	0.51
1:A:270:ASP:HA	1:A:273:ARG:HE	1.75	0.50
1:A:1970:LEU:HD22	1:A:1977:LYS:HD3	1.93	0.50
1:A:1058:GLN:HA	1:A:1061:GLU:HG2	1.93	0.50
1:A:959:LEU:HD13	1:A:1023:PRO:HD2	1.91	0.50
1:A:1152:LEU:HD11	1:A:1162:ILE:HD12	1.93	0.50
1:A:148:SER:O	1:A:182:LYS:NZ	2.44	0.50
1:A:421:GLY:HA2	1:A:426:THR:HG22	1.94	0.50
1:A:1379:ASP:OD1	1:A:1380:ASN:N	2.45	0.50
1:A:2240:LYS:HZ2	1:A:2263:PHE:HZ	1.60	0.50
1:A:885:SER:OG	1:A:885:SER:O	2.30	0.50
1:A:2163:PHE:HB2	1:A:2172:PHE:HE2	1.77	0.50
1:A:42:VAL:HG11	1:A:90:SER:OG	2.11	0.50
1:A:587:ASP:OD1	1:A:587:ASP:N	2.44	0.50
1:A:852:ILE:HD13	1:A:1721:LEU:HD21	1.92	0.50
1:A:1569:MET:HG2	1:A:1576:LEU:HD13	1.92	0.50
1:A:765:GLU:HG2	1:A:766:GLU:H	1.77	0.50
1:A:1880:ILE:HG22	1:A:1882:ILE:HG13	1.93	0.50
1:A:103:ILE:HD11	1:A:269:SER:HB2	1.93	0.49
1:A:493:LEU:HD22	1:A:497:GLU:HG2	1.93	0.49
1:A:973:THR:HG22	1:A:975:LYS:H	1.77	0.49
1:A:1116:LYS:O	1:A:1120:VAL:HG23	2.11	0.49
1:A:1237:THR:HB	1:A:1240:PHE:HE1	1.76	0.49
1:A:1382:ILE:HD13	1:A:1418:ILE:HD12	1.94	0.49
1:A:2218:ASP:HB3	1:A:2248:ILE:HG23	1.94	0.49
1:A:2275:ASN:HB3	1:A:2280:MET:HE1	1.94	0.49
1:A:1777:ALA:HB1	1:A:1780:LYS:HD3	1.94	0.49
1:A:1481:GLU:OE1	1:A:1496:ASN:ND2	2.46	0.49
1:A:57:ASP:OD1	1:A:76:LYS:NZ	2.29	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:277:LEU:HD13	1:A:389:SER:HB3	1.94	0.49
1:A:829:ALA:O	1:A:832:ILE:HG13	2.13	0.49
1:A:96:LYS:HD2	1:A:124:ASP:HB2	1.95	0.49
1:A:892:THR:OG1	1:A:893:GLU:N	2.45	0.49
1:A:1046:LYS:HD3	1:A:1519:ILE:HG21	1.93	0.49
1:A:1036:ILE:HG21	1:A:1521:LYS:HG2	1.93	0.49
1:A:1164:LEU:HD12	1:A:1164:LEU:H	1.78	0.49
1:A:402:GLN:HE21	1:A:402:GLN:HA	1.77	0.49
1:A:552:ALA:N	1:A:586:GLY:O	2.46	0.49
1:A:1292:ASP:O	1:A:1323:TYR:OH	2.20	0.49
1:A:1418:ILE:HG23	1:A:1425:TYR:HB3	1.95	0.49
1:A:1723:ALA:HB3	1:A:1725:TYR:CZ	2.48	0.49
1:A:1035:ILE:HD12	1:A:1612:ILE:HD11	1.94	0.49
1:A:1138:LEU:HG	1:A:1141:ASP:HA	1.95	0.49
1:A:1314:TYR:HE2	1:A:1332:MET:HG2	1.77	0.49
1:A:283:VAL:HG22	1:A:388:ILE:HG23	1.94	0.49
1:A:936:ILE:HD13	1:A:944:LEU:HD22	1.94	0.49
1:A:1284:ASP:OD1	1:A:1311:ASN:ND2	2.45	0.49
1:A:2030:VAL:HG12	1:A:2037:PHE:HB3	1.95	0.49
1:A:2273:TYR:CE2	1:A:2280:MET:HG3	2.48	0.49
1:A:309:ASN:OD1	1:A:310:THR:N	2.46	0.48
1:A:386:ALA:O	1:A:387:LEU:HD23	2.13	0.48
1:A:631:ILE:HG22	1:A:632:ASP:N	2.28	0.48
1:A:765:GLU:HG2	1:A:766:GLU:N	2.27	0.48
1:A:915:LYS:HB3	1:A:917:ILE:HG22	1.94	0.48
1:A:1048:LEU:C	1:A:1050:GLU:H	2.16	0.48
1:A:550:ASP:O	1:A:553:GLN:HG2	2.12	0.48
1:A:1377:ILE:HD12	1:A:1382:ILE:HG12	1.95	0.48
1:A:2212:TRP:CE2	1:A:2221:TYR:HD2	2.31	0.48
1:A:5:ASN:O	1:A:8:GLN:N	2.45	0.48
1:A:860:LYS:HB3	1:A:860:LYS:HE2	1.50	0.48
1:A:1082:ALA:HB1	1:A:1085:ILE:HG12	1.94	0.48
1:A:2173:ALA:HB1	1:A:2177:THR:HG21	1.94	0.48
1:A:691:ILE:HG12	1:A:693:ILE:HG13	1.96	0.48
1:A:1592:LYS:HE2	1:A:1605:PHE:CD2	2.49	0.48
1:A:1612:ILE:HG12	1:A:1625:ILE:HG22	1.96	0.48
1:A:1857:PHE:CE1	1:A:1866:TYR:HB2	2.49	0.48
1:A:119:LYS:HG3	1:A:120:ASP:OD1	2.14	0.48
1:A:217:ASP:OD2	1:A:217:ASP:N	2.36	0.48
1:A:1245:ASN:OD1	1:A:1247:GLY:N	2.45	0.48
1:A:1533:LYS:HD3	1:A:1590:ASN:HD22	1.79	0.48



	h h	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:818:LYS:O	1:A:822:THR:OG1	2.24	0.48
1:A:1118:THR:O	1:A:1121:ILE:HG13	2.14	0.48
1:A:2230:TYR:HB3	1:A:2234:ASN:ND2	2.29	0.48
1:A:397:ASP:OD1	1:A:398:LEU:N	2.47	0.48
1:A:449:LYS:O	1:A:464:SER:HA	2.14	0.48
1:A:584:LEU:HB2	1:A:651:ILE:O	2.14	0.48
1:A:1380:ASN:HB2	1:A:1391:PHE:O	2.13	0.48
1:A:2100:ILE:HA	1:A:2112:PHE:HB2	1.95	0.48
1:A:151:ASN:O	1:A:155:GLU:N	2.46	0.48
1:A:578:ILE:O	1:A:647:LYS:CB	2.53	0.48
1:A:675:ILE:O	1:A:679:LEU:HG	2.14	0.48
1:A:954:HIS:O	1:A:958:THR:HG23	2.14	0.47
1:A:1177:GLY:HA3	1:A:1188:PHE:CD2	2.49	0.47
1:A:1514:LYS:HB3	1:A:1515:ASP:OD1	2.14	0.47
1:A:1787:ASP:OD1	1:A:1787:ASP:N	2.40	0.47
1:A:15:VAL:HG12	1:A:18:ARG:HB2	1.97	0.47
1:A:1169:ILE:HB	1:A:1202:ILE:HD11	1.96	0.47
1:A:1340:GLU:HA	1:A:1399:ASN:ND2	2.28	0.47
1:A:1682:LEU:HD12	1:A:1689:VAL:HG21	1.96	0.47
1:A:1498:TYR:CE1	1:A:1500:PRO:HD2	2.49	0.47
1:A:1908:TYR:CE1	1:A:1910:ALA:HB2	2.48	0.47
1:A:963:PHE:O	1:A:967:SER:OG	2.28	0.47
1:A:1269:PHE:CZ	1:A:2277:LYS:HG2	2.49	0.47
1:A:1291:LEU:HD21	1:A:1316:PHE:HD1	1.79	0.47
1:A:1948:GLU:H	1:A:1948:GLU:HG3	1.26	0.47
1:A:2342:GLY:HA2	1:A:2353:PHE:O	2.14	0.47
1:A:861:LEU:O	1:A:865:ILE:HG13	2.14	0.47
1:A:1229:VAL:HG13	1:A:1281:ARG:HD3	1.97	0.47
1:A:2049:THR:HG21	1:A:2055:THR:HG22	1.96	0.47
1:A:2112:PHE:CE1	1:A:2118:ARG:HB2	2.50	0.47
1:A:34:TYR:HB2	1:A:48:LYS:HG2	1.97	0.47
1:A:834:ARG:O	1:A:838:GLU:HG2	2.14	0.47
1:A:1382:ILE:HG13	1:A:1391:PHE:HE2	1.79	0.47
1:A:2037:PHE:HB2	1:A:2076:ALA:HB3	1.96	0.47
1:A:791:SER:HB3	1:A:840:ARG:O	2.14	0.47
1:A:1698:LEU:HB3	1:A:1724:ASN:O	2.15	0.47
1:A:2308:THR:HB	1:A:2312:ASN:HD21	1.79	0.47
1:A:747:ASN:OD1	1:A:750:GLY:N	2.48	0.47
1:A:1132:THR:OG1	1:A:1133:GLU:OE2	2.32	0.47
1:A:313:GLU:HB2	1:A:511:LEU:HD12	1.96	0.46
1:A:1025:LEU:HB2	1:A:1623:GLU:OE2	2.15	0.46



	jae page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1600:ASP:HB2	1:A:1602:ASN:OD1	2.15	0.46
1:A:1679:GLN:HA	1:A:1682:LEU:HD23	1.96	0.46
1:A:917:ILE:HD11	1:A:921:TYR:OH	2.15	0.46
1:A:1532:PHE:HB3	1:A:1534:ASP:H	1.80	0.46
1:A:288:ASP:N	1:A:288:ASP:OD2	2.48	0.46
1:A:932:ILE:HD13	1:A:1021:LEU:HD22	1.97	0.46
1:A:1352:VAL:HG21	1:A:1406:PHE:CB	2.46	0.46
1:A:294:GLN:HE21	1:A:361:LEU:HB2	1.80	0.46
1:A:870:TYR:CD2	1:A:978:LEU:HB3	2.51	0.46
1:A:1186:HIS:CD2	1:A:1267:PHE:HB3	2.50	0.46
1:A:1251:LEU:O	1:A:1254:ILE:HG22	2.15	0.46
1:A:1746:ASP:HB2	1:A:1751:ILE:HD11	1.96	0.46
1:A:1937:TYR:CE1	1:A:1964:GLY:HA3	2.49	0.46
1:A:269:SER:O	1:A:269:SER:OG	2.31	0.46
1:A:1575:ALA:HB3	1:A:1577:ASN:OD1	2.16	0.46
1:A:1959:PHE:HA	1:A:1965:GLU:O	2.16	0.46
1:A:23:GLU:O	1:A:27:ILE:HG13	2.15	0.46
1:A:114:TYR:HE1	1:A:327:ILE:HG21	1.81	0.46
1:A:631:ILE:HG22	1:A:632:ASP:H	1.81	0.46
1:A:1077:ALA:O	1:A:1082:ALA:N	2.49	0.46
1:A:213:GLU:HB3	1:A:214:TYR:HD2	1.81	0.46
1:A:577:TYR:O	1:A:643:LYS:HG3	2.16	0.46
1:A:676:GLU:OE2	1:A:722:ARG:NE	2.49	0.46
1:A:865:ILE:HG12	1:A:921:TYR:CE2	2.51	0.46
1:A:1560:ASN:O	1:A:1564:GLN:HG2	2.15	0.46
1:A:1926:PHE:O	1:A:1927:ILE:HD13	2.15	0.46
1:A:2181:ASN:HD22	1:A:2185:GLN:HG2	1.81	0.46
1:A:2274:LEU:HD21	1:A:2283:PHE:HD2	1.81	0.46
1:A:512:THR:O	1:A:515:GLU:HB3	2.16	0.46
1:A:1226:PRO:HD3	1:A:1308:ILE:HG23	1.97	0.46
1:A:312:TRP:NE1	1:A:316:LYS:HE3	2.32	0.45
1:A:554:ASN:HB3	1:A:612:ILE:HG12	1.97	0.45
1:A:1433:CYS:HA	1:A:1436:LEU:HB2	1.98	0.45
1:A:2007:GLN:HB3	1:A:2011:ILE:HD13	1.96	0.45
1:A:335:PHE:HE1	1:A:346:PHE:HD1	1.65	0.45
1:A:478:TYR:N	1:A:478:TYR:CD1	2.84	0.45
1:A:1237:THR:HB	1:A:1240:PHE:CE1	2.51	0.45
1:A:2223:ASP:N	1:A:2228:LYS:O	2.46	0.45
1:A:1496:ASN:HB3	1:A:1506:PHE:CD2	2.51	0.45
1:A:1085:ILE:H	1:A:1085:ILE:HG13	1.39	0.45
1:A:1548:ASN:ND2	1:A:1600:ASP:OD1	2.37	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:221:LEU:O	1:A:225:ILE:HG13	2.17	0.45
1:A:882:HIS:HD2	1:A:900:PHE:HB3	1.81	0.45
1:A:115:ILE:O	1:A:118:TRP:N	2.50	0.45
1:A:769:ILE:HG12	1:A:804:ILE:HD11	1.97	0.45
1:A:865:ILE:HA	1:A:921:TYR:CE1	2.51	0.45
1:A:1441:SER:OG	1:A:1500:PRO:O	2.35	0.45
1:A:1525:LYS:O	1:A:1543:THR:HG23	2.17	0.45
1:A:775:LYS:O	1:A:792:LYS:HE2	2.17	0.45
1:A:976:GLU:OE1	1:A:981:LEU:N	2.50	0.45
1:A:1968:LYS:HD3	1:A:1982:ASP:HA	1.98	0.45
1:A:466:ILE:HA	1:A:470:GLY:HA3	1.99	0.45
1:A:1189:SER:HB3	1:A:2311:GLU:OE2	2.16	0.45
1:A:283:VAL:HG21	1:A:366:ILE:HD12	1.98	0.45
1:A:309:ASN:HD21	1:A:786:LYS:HE2	1.81	0.45
1:A:378:ALA:O	1:A:380:ASN:N	2.50	0.45
1:A:1442:ASP:OD1	1:A:1442:ASP:N	2.48	0.45
1:A:1877:ILE:HA	1:A:1889:PHE:HB2	1.99	0.45
1:A:382:VAL:HG23	1:A:471:PRO:HB3	1.99	0.44
1:A:402:GLN:HE21	1:A:402:GLN:CA	2.30	0.44
1:A:526:ARG:HG3	1:A:526:ARG:NH1	2.32	0.44
1:A:1370:ASN:HB3	1:A:1373:SER:OG	2.17	0.44
1:A:1863:ASN:ND2	1:A:1894:ILE:HD13	2.27	0.44
1:A:2341:THR:O	1:A:2353:PHE:HB2	2.17	0.44
1:A:130:PHE:CE2	1:A:276:MET:HG2	2.51	0.44
1:A:549:LEU:HD23	1:A:549:LEU:HA	1.81	0.44
1:A:583:GLN:NE2	1:A:585:GLN:O	2.50	0.44
1:A:1058:GLN:HA	1:A:1061:GLU:CG	2.46	0.44
1:A:1394:ASP:HB3	1:A:1396:ASN:HD22	1.82	0.44
1:A:48:LYS:HE2	1:A:48:LYS:HA	2.00	0.44
1:A:555:THR:O	1:A:609:GLN:NE2	2.43	0.44
1:A:1442:ASP:HA	1:A:1445:GLN:HG3	2.00	0.44
1:A:1583:MET:O	1:A:1587:GLU:HG3	2.16	0.44
1:A:377:PHE:CE1	1:A:382:VAL:HG12	2.52	0.44
1:A:396:SER:O	1:A:400:ILE:HD12	2.17	0.44
1:A:2302:TYR:O	1:A:2317:SER:HA	2.17	0.44
1:A:244:GLU:CD	1:A:244:GLU:H	2.21	0.44
1:A:549:LEU:HD11	1:A:653:HIS:CE1	2.53	0.44
1:A:673:SER:O	1:A:677:THR:HG23	2.18	0.44
1:A:795:HIS:HE1	1:A:1802:LEU:HD12	1.80	0.44
1:A:862:ILE:HG21	1:A:971:TYR:HD2	1.83	0.44
1:A:973:THR:HG22	1:A:974:THR:N	2.32	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:1140:ASP:O	1:A:1142:LYS:HG3	2.17	0.44
1:A:2111:TYR:O	1:A:2119:GLN:N	2.49	0.44
1:A:2285:LYS:HB2	1:A:2285:LYS:HE2	1.72	0.44
1:A:1888:TYR:O	1:A:1896:GLN:HB2	2.18	0.44
1:A:2172:PHE:HA	1:A:2186:ALA:HA	2.00	0.44
1:A:102:TRP:CE3	1:A:107:ILE:HG13	2.53	0.44
1:A:161:LEU:HD23	1:A:162:ASN:N	2.32	0.44
1:A:835:GLN:NE2	1:A:840:ARG:HD2	2.32	0.44
1:A:2029:GLY:O	1:A:2039:PHE:HA	2.18	0.44
1:A:539:PHE:HB2	1:A:540:GLU:HG2	1.99	0.44
1:A:869:LEU:HA	1:A:918:PHE:HZ	1.83	0.44
1:A:1075:SER:HA	1:A:1078:ILE:HD12	2.00	0.44
1:A:1444:GLN:HG3	1:A:1499:MET:HB3	1.99	0.44
1:A:1918:ASN:HB2	1:A:1922:GLU:HB2	2.00	0.44
1:A:2190:SER:OG	1:A:2191:GLY:N	2.50	0.44
1:A:118:TRP:CE3	1:A:291:PRO:HG3	2.53	0.43
1:A:366:ILE:HD13	1:A:388:ILE:HD13	1.98	0.43
1:A:246:PHE:HD2	1:A:252:VAL:HG12	1.82	0.43
1:A:580:TYR:OH	1:A:633:LYS:O	2.35	0.43
1:A:765:GLU:HA	1:A:768:ILE:HD12	2.00	0.43
1:A:1545:GLU:OE2	1:A:1546:ASP:HB2	2.18	0.43
1:A:2066:LYS:HB3	1:A:2068:TYR:CE2	2.53	0.43
1:A:1370:ASN:HD22	1:A:1370:ASN:HA	1.65	0.43
1:A:2053:GLU:HG2	1:A:2054:LEU:N	2.33	0.43
1:A:259:LEU:HD12	1:A:259:LEU:HA	1.81	0.43
1:A:2163:PHE:O	1:A:2169:TYR:HA	2.18	0.43
1:A:42:VAL:HG21	1:A:370:PRO:HG2	2.00	0.43
1:A:622:SER:HA	1:A:639:GLN:HE22	1.84	0.43
1:A:716:LEU:HB2	1:A:737:VAL:HG21	2.00	0.43
1:A:1181:THR:HB	1:A:1186:HIS:CE1	2.52	0.43
1:A:1210:LYS:HE3	1:A:1210:LYS:HB2	1.83	0.43
1:A:2100:ILE:HG22	1:A:2116:GLY:HA2	2.01	0.43
1:A:2341:THR:HG22	1:A:2342:GLY:H	1.83	0.43
1:A:466:ILE:HG23	1:A:471:PRO:HD2	1.99	0.43
1:A:579:HIS:HB3	1:A:605:SER:HA	2.00	0.43
1:A:702:SER:CB	1:A:776:GLU:H	2.31	0.43
1:A:869:LEU:CD1	1:A:979:SER:HB2	2.48	0.43
1:A:1918:ASN:HD22	1:A:1924:VAL:HG12	1.83	0.43
1:A:2102:LEU:HD21	1:A:2109:LYS:HB2	2.00	0.43
1:A:2215:ASN:ND2	1:A:2218:ASP:HB2	2.30	0.43
1:A:573:ARG:NH2	1:A:1805:TYR:HB3	2.32	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:102:TRP:HZ3	1:A:111:ALA:HB2	1.83	0.43
1:A:1513:LEU:HD12	1:A:1530:ASN:O	2.18	0.43
1:A:766:GLU:HG3	1:A:820:MET:SD	2.59	0.43
1:A:897:ARG:HE	1:A:910:PHE:HE1	1.66	0.43
1:A:1352:VAL:HG12	1:A:1371:ILE:HG12	2.01	0.43
1:A:339:ASP:O	1:A:342:VAL:HG12	2.19	0.43
1:A:1352:VAL:HG23	1:A:1353:LYS:HG3	2.00	0.43
1:A:317:LEU:HA	1:A:317:LEU:HD23	1.87	0.42
1:A:553:GLN:HE21	1:A:587:ASP:HA	1.83	0.42
1:A:2307:ASN:HA	1:A:2312:ASN:O	2.19	0.42
1:A:6:LYS:HD2	1:A:28:LEU:HB3	2.02	0.42
1:A:49:LEU:HD11	1:A:82:GLU:HG3	2.01	0.42
1:A:525:ALA:HB2	1:A:701:PHE:CG	2.55	0.42
1:A:1594:ILE:HG13	1:A:1595:PHE:N	2.34	0.42
1:A:1625:ILE:H	1:A:1625:ILE:HG13	1.77	0.42
1:A:2120:LEU:HD13	1:A:2121:GLY:N	2.33	0.42
1:A:213:GLU:HB3	1:A:214:TYR:CD2	2.54	0.42
1:A:447:MET:HA	1:A:450:ILE:HG12	2.01	0.42
1:A:732:GLN:HB2	1:A:782:PRO:HG3	2.01	0.42
1:A:876:ASN:ND2	1:A:911:ILE:HG23	2.35	0.42
1:A:1622:PHE:HD1	1:A:1637:ILE:HG23	1.84	0.42
1:A:324:LYS:HA	1:A:324:LYS:HD3	1.83	0.42
1:A:643:LYS:O	1:A:686:ILE:HD11	2.20	0.42
1:A:817:LYS:HB3	1:A:817:LYS:HE3	1.78	0.42
1:A:2301:LYS:HG3	1:A:2317:SER:OG	2.20	0.42
1:A:131:TYR:HE2	1:A:133:SER:HB3	1.85	0.42
1:A:1009:GLU:O	1:A:1013:THR:HG22	2.20	0.42
1:A:1055:LEU:HD22	1:A:1401:PHE:CZ	2.54	0.42
1:A:2151:TYR:HB3	1:A:2159:LEU:HB2	2.00	0.42
1:A:2330:ARG:HD3	1:A:2330:ARG:N	2.35	0.42
1:A:154:LEU:HD23	1:A:154:LEU:HA	1.90	0.42
1:A:188:ASP:O	1:A:192:SER:OG	2.31	0.42
1:A:476:GLY:HA2	1:A:491:ILE:HD11	2.01	0.42
1:A:764:LYS:HE2	1:A:764:LYS:HA	2.00	0.42
1:A:1142:LYS:HE3	1:A:1142:LYS:HB2	1.67	0.42
1:A:1948:GLU:HB3	1:A:1958:TYR:CE2	2.55	0.42
1:A:634:TYR:CD2	1:A:678:ILE:HG13	2.54	0.42
1:A:653:HIS:O	1:A:664:ALA:N	2.51	0.42
1:A:864:SER:OG	1:A:921:TYR:OH	2.37	0.42
1:A:1919:LEU:H	1:A:1922:GLU:CD	2.23	0.42
1:A:2275:ASN:OD1	1:A:2275:ASN:N	2.53	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:2301:LYS:NZ	1:A:2337:TYR:HB3	2.34	0.42
1:A:2304:ALA:HB1	1:A:2308:THR:HG21	2.01	0.42
1:A:1232:TYR:HB3	1:A:1278:LEU:HD13	2.02	0.42
1:A:1915:LEU:HD22	1:A:1924:VAL:HB	2.02	0.42
1:A:1371:ILE:HD12	1:A:1371:ILE:HA	1.91	0.42
1:A:1515:ASP:OD1	1:A:1515:ASP:N	2.53	0.42
1:A:1516:ILE:HA	1:A:1528:ILE:O	2.20	0.42
1:A:1544:ILE:HG12	1:A:1550:ILE:HG12	2.01	0.42
1:A:1567:LYS:NZ	1:A:1567:LYS:HB3	2.34	0.42
1:A:1840:ASN:C	1:A:1840:ASN:HD22	2.22	0.42
1:A:34:TYR:HD1	1:A:48:LYS:HG2	1.85	0.42
1:A:247:ALA:HA	1:A:275:SER:HB3	2.02	0.42
1:A:324:LYS:NZ	1:A:350:LEU:O	2.37	0.42
1:A:1679:GLN:HE22	1:A:1716:PRO:HD2	1.85	0.42
1:A:2182:ILE:HG22	1:A:2183:TYR:H	1.84	0.42
1:A:2198:ASP:HA	1:A:2228:LYS:HZ3	1.85	0.42
1:A:2208:ILE:HG23	1:A:2227:LYS:HE3	2.02	0.42
1:A:122:ASN:HB3	1:A:125:TYR:CD1	2.55	0.41
1:A:1552:LEU:HD22	1:A:1552:LEU:HA	1.85	0.41
1:A:452:ASN:HB3	1:A:462:VAL:HG13	2.03	0.41
1:A:505:LYS:HB3	1:A:505:LYS:HE3	1.74	0.41
1:A:616:GLU:HG3	1:A:633:LYS:HB2	2.02	0.41
1:A:652:GLY:O	1:A:697:GLY:HA3	2.19	0.41
1:A:2198:ASP:HA	1:A:2228:LYS:NZ	2.35	0.41
1:A:1557:LEU:HB3	1:A:1561:GLY:HA3	2.03	0.41
1:A:1568:PHE:CE1	1:A:1576:LEU:HD12	2.55	0.41
1:A:76:LYS:HB3	1:A:76:LYS:HE3	1.68	0.41
1:A:413:ASN:O	1:A:416:PRO:HD2	2.21	0.41
1:A:1543:THR:HG22	1:A:1544:ILE:H	1.85	0.41
1:A:10:GLN:HE21	1:A:20:GLN:NE2	2.19	0.41
1:A:1034:THR:O	1:A:1035:ILE:HG13	2.20	0.41
1:A:1520:ASN:ND2	1:A:1525:LYS:HG3	2.34	0.41
1:A:96:LYS:HA	1:A:125:TYR:CE2	2.56	0.41
1:A:246:PHE:HE1	1:A:272:LEU:CD1	2.33	0.41
1:A:1904:ASP:O	1:A:1944:ARG:NH1	2.54	0.41
1:A:1996:LYS:HA	1:A:1996:LYS:HE3	2.01	0.41
1:A:346:PHE:HD2	1:A:346:PHE:HA	1.79	0.41
1:A:714:LYS:HB2	1:A:714:LYS:HE2	1.75	0.41
1:A:793:TYR:HD1	1:A:793:TYR:HA	1.69	0.41
1:A:899:ARG:HE	1:A:901:ILE:HD11	1.85	0.41
1:A:917:ILE:O	1:A:920:GLU:HB2	2.20	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1172:ALA:N	1:A:1261:GLN:O	2.49	0.41
1:A:1299:ILE:HD12	1:A:1299:ILE:H	1.86	0.41
1:A:1308:ILE:O	1:A:1312:LEU:HB2	2.21	0.41
1:A:1682:LEU:CD1	1:A:1689:VAL:HG21	2.51	0.41
1:A:1757:GLU:HB2	1:A:1758:GLU:OE1	2.19	0.41
1:A:567:LEU:HD12	1:A:568:SER:N	2.35	0.41
1:A:835:GLN:HE22	1:A:840:ARG:NH1	2.18	0.41
1:A:1276:THR:HG22	1:A:1277:LYS:HD2	2.02	0.41
1:A:1469:THR:CG2	1:A:1471:TYR:HE2	2.31	0.41
1:A:1832:MET:HB3	1:A:1832:MET:HE2	1.92	0.41
1:A:1899:VAL:CG2	1:A:1932:ILE:HD11	2.49	0.41
1:A:2153:ASP:HB3	1:A:2159:LEU:HD21	2.03	0.41
1:A:2060:ILE:O	1:A:2061:LEU:HD22	2.21	0.41
1:A:2280:MET:HB3	1:A:2317:SER:HB2	2.02	0.41
1:A:323:TYR:HD2	1:A:350:LEU:HG	1.86	0.40
1:A:1899:VAL:HG23	1:A:1932:ILE:CD1	2.48	0.40
1:A:2062:ASN:HA	1:A:2066:LYS:O	2.21	0.40
1:A:363:LEU:HD12	1:A:507:LYS:HD3	2.03	0.40
1:A:563:SER:O	1:A:566:ILE:HB	2.22	0.40
1:A:1003:ASP:HB3	1:A:1006:LYS:HD2	2.04	0.40
1:A:1116:LYS:HG2	1:A:1117:ALA:H	1.86	0.40
1:A:1152:LEU:HD22	1:A:1152:LEU:HA	1.95	0.40
1:A:1706:THR:HA	1:A:1707:PRO:HD3	1.88	0.40
1:A:1825:TYR:CZ	1:A:1839:ILE:HG12	2.56	0.40
1:A:1906:LEU:HB3	1:A:1945:ALA:HB3	2.03	0.40
1:A:271:ILE:H	1:A:271:ILE:HG13	1.67	0.40
1:A:760:LYS:HE3	1:A:760:LYS:HB3	1.81	0.40
1:A:1041:LEU:O	1:A:1045:ILE:HG12	2.21	0.40
1:A:142:LYS:HG3	1:A:263:TRP:HE3	1.85	0.40
1:A:1114:GLN:HB2	1:A:1120:VAL:HG22	2.03	0.40
1:A:760:LYS:HG2	1:A:761:TRP:N	2.37	0.40
1:A:1426:LYS:HB3	1:A:1426:LYS:HE3	1.72	0.40
1:A:1443:ILE:O	1:A:1447:ILE:HG13	2.22	0.40
1:A:1634:PRO:HG3	1:A:1688:TYR:CD1	2.56	0.40
1:A:1755:ASN:ND2	1:A:1763:GLN:HE21	2.20	0.40
1:A:2120:LEU:HD22	1:A:2120:LEU:HA	1.91	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 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	А	2361/2372~(100%)	2151 (91%)	206 (9%)	4 (0%)	47 78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	464	SER
1	А	1775	ASP
1	А	2308	THR
1	А	2216	GLU

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	2137/2146~(100%)	1861 (87%)	276 (13%)	4 13

All (276) residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	4	VAL
1	А	5	ASN
1	А	17	PHE
1	А	18	ARG
1	А	48	LYS
1	А	62	THR
1	А	68	ARG



Mol	Chain	Res	Type
1	А	81	MET
1	А	90	SER
1	А	92	THR
1	А	99	HIS
1	А	103	ILE
1	А	121	VAL
1	А	124	ASP
1	А	126	THR
1	А	128	LYS
1	А	136	PHE
1	А	141	LEU
1	А	148	SER
1	А	150	THR
1	A	159	GLU
1	А	186	PHE
1	А	190	TYR
1	А	197	ASN
1	А	200	PHE
1	А	213	GLU
1	А	233	THR
1	А	246	PHE
1	А	253	ARG
1	А	260	VAL
1	А	262	ARG
1	А	276	MET
1	А	278	LYS
1	А	288	ASP
1	А	317	LEU
1	А	318	GLU
1	А	321	MET
1	А	332	SER
1	A	339	ASP
1	A	345	SER
1	A	346	PHE
1	A	350	LEU
1	A	351	SER
1	А	352	SER
1	А	361	LEU
1	A	365	ASP
1	A	370	PRO
1	A	374	LYS
1	А	377	PHE



Mol	Chain	Res	Type
1	А	379	ASN
1	А	384	ASN
1	А	402	GLN
1	А	404	LYS
1	А	405	ASN
1	А	410	LEU
1	А	417	SER
1	А	449	LYS
1	А	451	THR
1	А	454	LEU
1	А	465	THR
1	А	473	VAL
1	А	492	HIS
1	A	494	LEU
1	A	495	GLU
1	A	505	LYS
1	А	509	SER
1	А	522	PHE
1	А	529	SER
1	А	530	GLN
1	А	549	LEU
1	А	565	LYS
1	А	568	SER
1	А	572	THR
1	А	573	ARG
1	А	575	LYS
1	А	576	GLU
1	А	580	TYR
1	А	599	SER
1	А	608	TYR
1	A	612	ILE
1	A	613	GLU
1	A	616	GLU
1	A	617	THR
1	A	619	TYR
1	A	632	ASP
1	А	636	ILE
1	A	638	TYR
1	A	640	ILE
1	А	642	ASN
1	A	648	LEU
1	А	660	THR



Mol	Chain	Res	Type
1	А	690	TYR
1	А	696	LEU
1	А	704	SER
1	А	717	LEU
1	А	720	LYS
1	А	741	GLN
1	А	745	ARG
1	А	746	ILE
1	А	752	ARG
1	А	757	HIS
1	А	762	ILE
1	А	780	PHE
1	А	785	ASN
1	А	790	LYS
1	А	791	SER
1	А	797	LEU
1	А	799	THR
1	А	802	GLN
1	А	811	SER
1	А	848	THR
1	А	849	SER
1	А	864	SER
1	А	869	LEU
1	А	874	HIS
1	А	875	GLN
1	А	885	SER
1	А	892	THR
1	А	919	SER
1	А	926	SER
1	А	935	THR
1	A	938	ASP
1	А	939	ASN
1	A	949	ASN
1	A	961	SER
1	A	974	THR
1	A	1009	GLU
1	А	1010	LEU
1	А	1012	SER
1	A	1017	GLU
1	А	1025	LEU
1	А	1031	ILE
1	А	1045	ILE



Mol	Chain	Res	Type
1	А	1047	GLU
1	А	1050	GLU
1	А	1055	LEU
1	А	1085	ILE
1	А	1092	LEU
1	А	1126	HIS
1	А	1149	ASP
1	А	1152	LEU
1	А	1155	ILE
1	А	1161	SER
1	А	1164	LEU
1	А	1167	CYS
1	А	1173	GLU
1	А	1192	SER
1	А	1274	LEU
1	А	1281	ARG
1	А	1282	TYR
1	А	1294	ASN
1	А	1312	LEU
1	А	1314	TYR
1	А	1340	GLU
1	А	1342	ASP
1	А	1358	GLU
1	А	1360	ASP
1	А	1366	GLU
1	A	1383	ILE
1	A	1394	ASP
1	A	1405	THR
1	А	1410	GLU
1	A	1418	ILE
1	A	1436	LEU
1	A	1459	TYR
1	A	1467	ASN
1	A	1472	ASN
1	A	1483	LEU
1	A	1485	THR
1	A	1506	PHE
1	A	1510	SER
1	A	1515	ASP
1	A	1526	LEU
1	A	1530	ASN
1	A	1531	TYR



Mol	Chain	Res	Type
1	А	1533	LYS
1	А	1536	MET
1	А	1540	LEU
1	А	1549	THR
1	А	1552	LEU
1	А	1613	ILE
1	А	1622	PHE
1	А	1624	LEU
1	А	1625	ILE
1	А	1628	LYS
1	А	1641	ILE
1	А	1645	SER
1	А	1650	VAL
1	А	1657	ILE
1	А	1662	TYR
1	А	1663	HIS
1	А	1665	ASP
1	А	1670	ILE
1	А	1671	SER
1	А	1698	LEU
1	А	1701	ASP
1	А	1702	GLU
1	А	1706	THR
1	А	1715	CYS
1	А	1722	ASP
1	А	1735	ASN
1	А	1736	ASP
1	А	1739	ILE
1	А	1748	SER
1	А	1774	SER
1	А	1788	LYS
1	A	1792	SER
1	А	1810	PHE
1	A	1818	SER
1	А	1819	LEU
1	А	1821	ASN
1	А	1828	SER
1	А	1837	ILE
1	A	1840	ASN
1	А	1848	PRO
1	A	1853	LEU
1	А	1857	PHE



Mol	Chain	Res	Type
1	А	1858	THR
1	А	1859	THR
1	А	1881	THR
1	А	1902	THR
1	А	1906	LEU
1	А	1931	ASN
1	А	1932	ILE
1	А	1935	LYS
1	А	1941	ASP
1	А	1947	VAL
1	А	1948	GLU
1	А	1959	PHE
1	А	1960	ASN
1	А	1970	LEU
1	А	1985	ILE
1	А	2017	TYR
1	А	2026	ARG
1	А	2027	GLN
1	А	2028	LEU
1	А	2035	ASP
1	А	2066	LYS
1	А	2085	ASP
1	А	2087	SER
1	А	2088	THR
1	А	2104	VAL
1	А	2114	ASP
1	А	2127	ASP
1	А	2140	LEU
1	А	2142	TYR
1	А	2144	ASN
1	А	2165	THR
1	A	2171	TYR
1	А	2178	VAL
1	A	2187	VAL
1	А	2194	ARG
1	A	2207	LYS
1	A	2216	GLU
1	A	2230	TYR
1	A	2231	LYS
1	А	2249	MET
1	A	2251	THR
1	А	2258	ASN



Mol	Chain	Res	Type
1	А	2268	LYS
1	А	2273	TYR
1	А	2274	LEU
1	А	2280	MET
1	А	2285	LYS
1	А	2298	ASP
1	А	2309	LEU
1	А	2313	PHE
1	А	2317	SER
1	А	2321	THR
1	А	2329	LYS
1	А	2330	ARG
1	А	2336	GLU
1	А	2341	THR
1	А	2345	THR
1	A	2349	TYR
1	А	2363	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	8	GLN
1	А	10	GLN
1	А	20	GLN
1	А	35	HIS
1	А	36	ASN
1	А	113	ASN
1	А	212	ASN
1	А	236	ASN
1	А	294	GLN
1	А	343	GLN
1	А	379	ASN
1	А	402	GLN
1	А	405	ASN
1	А	479	GLN
1	А	510	GLN
1	А	553	GLN
1	A	596	ASN
1	A	639	GLN
1	A	653	HIS
1	A	659	ASN
1	А	835	GLN



Mol	Chain	Res	Type
1	А	853	ASN
1	А	1052	ASN
1	А	1186	HIS
1	А	1257	HIS
1	А	1294	ASN
1	А	1307	GLN
1	А	1350	ASN
1	А	1370	ASN
1	А	1456	HIS
1	А	1503	ASN
1	А	1504	ASN
1	А	1520	ASN
1	А	1530	ASN
1	А	1553	ASN
1	А	1727	ASN
1	А	1735	ASN
1	А	1763	GLN
1	А	1784	ASN
1	А	1840	ASN
1	А	1851	ASN
1	А	1925	ASN
1	А	1976	ASN
1	A	2007	GLN
1	А	2115	ASN
1	А	2119	GLN
1	А	2176	ASN
1	А	2196	ASN
1	A	2234	ASN
1	A	2312	ASN

#### 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 monosaccharides in this entry.



## 5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-38010. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

# 6.1 Orthogonal projections (i)

#### 6.1.1 Primary map



6.1.2 Raw map



The images above show the map projected in three orthogonal directions.



### 6.2 Central slices (i)

#### 6.2.1 Primary map



X Index: 200



Y Index: 200



Z Index: 200

#### 6.2.2 Raw map



X Index: 200

Y Index: 200



The images above show central slices of the map in three orthogonal directions.



### 6.3 Largest variance slices (i)

## 6.3.1 Primary map



X Index: 202



Y Index: 187



Z Index: 201

#### 6.3.2 Raw map



X Index: 202

Y Index: 187



The images above show the largest variance slices of the map in three orthogonal directions.



## 6.4 Orthogonal standard-deviation projections (False-color) (i)

#### 6.4.1 Primary map



6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



## 6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.22. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

#### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

#### 6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.



# 7 Map analysis (i)

This section contains the results of statistical analysis of the map.

# 7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



## 7.2 Volume estimate (i)



The volume at the recommended contour level is 260  $\rm nm^3;$  this corresponds to an approximate mass of 235 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



### 7.3 Rotationally averaged power spectrum (i)



\*Reported resolution corresponds to spatial frequency of 0.345  ${\rm \AA}^{-1}$ 



# 8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

#### 8.1 FSC (i)



\*Reported resolution corresponds to spatial frequency of 0.345  $\mathrm{\AA^{-1}}$ 



#### 8.2 Resolution estimates (i)

$\begin{bmatrix} Bosolution ostimato (Å) \end{bmatrix}$	Estimation criterion (FSC cut-off)		
Resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.56	2.96
Unmasked-calculated*	3.74	8.30	3.81

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.74 differs from the reported value 2.9 by more than 10 %



# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-38010 and PDB model 8X2H. Per-residue inclusion information can be found in section 3 on page 4.

# 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.22 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



#### 9.2 Q-score mapped to coordinate model (i)



The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

#### 9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.22).



#### 9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.



## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8310	0.3930
А	0.8310	0.3930



