Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 05:51 PM EDT

PDB ID	:	4YCZ
Title	:	Y-COMPLEX HUB (NUP85-NUP120-NUP145C-SEC13 COMPLEX) FROM M. THERMOPHILA (A.K.A. T. HETEROTHALLICA)
Authors	:	Kelley, K.; Knockenhauer, K.E.; Schwartz, T.U.
Deposited on	:	2015-02-20
Resolution	:	4.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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 (i)) were used in the production of this report:

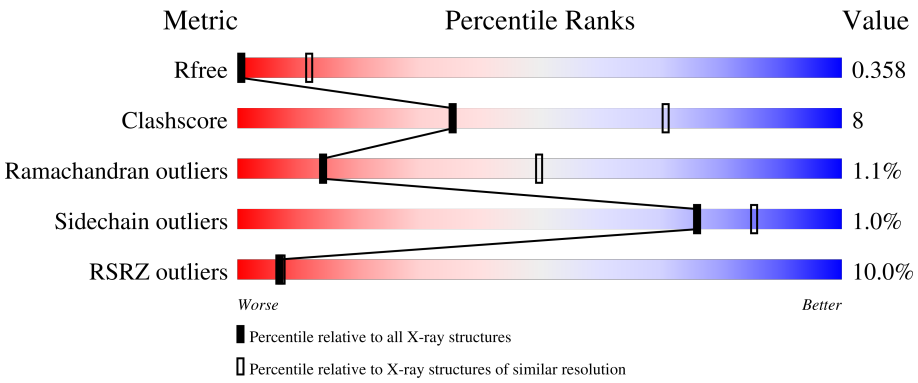
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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}	130704	1193 (4.50-3.70)
Clashscore	141614	1003 (4.44-3.76)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)
RSRZ outliers	127900	1034 (4.50-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	876	9% 67% 14% 19%
2	B	933	6% 53% 10% 37%
3	C	313	6% 48% 14% 38%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10051 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 Fusion Protein of Sec13 and Nup145C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	713	4777	3049	843	874	11	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP G2QES5
A	2	PRO	-	expression tag	UNP G2QES5
A	3	GLY	-	expression tag	UNP G2QES5
A	4	SER	-	expression tag	UNP G2QES5

- Molecule 2 is a protein called Nup85.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	B	590	3962	2596	644	705	5	12	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	249	GLY	-	expression tag	UNP G2Q7J4
B	250	PRO	-	expression tag	UNP G2Q7J4
B	251	GLY	-	expression tag	UNP G2Q7J4
B	252	SER	-	expression tag	UNP G2Q7J4
B	253	GLU	-	expression tag	UNP G2Q7J4
B	254	PHE	-	expression tag	UNP G2Q7J4
B	255	GLU	-	expression tag	UNP G2Q7J4
B	256	LEU	-	expression tag	UNP G2Q7J4

- Molecule 3 is a protein called Nup120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	195	1312	846	220	241	5	0	0	0

There are 23 discrepancies between the modelled and reference sequences:

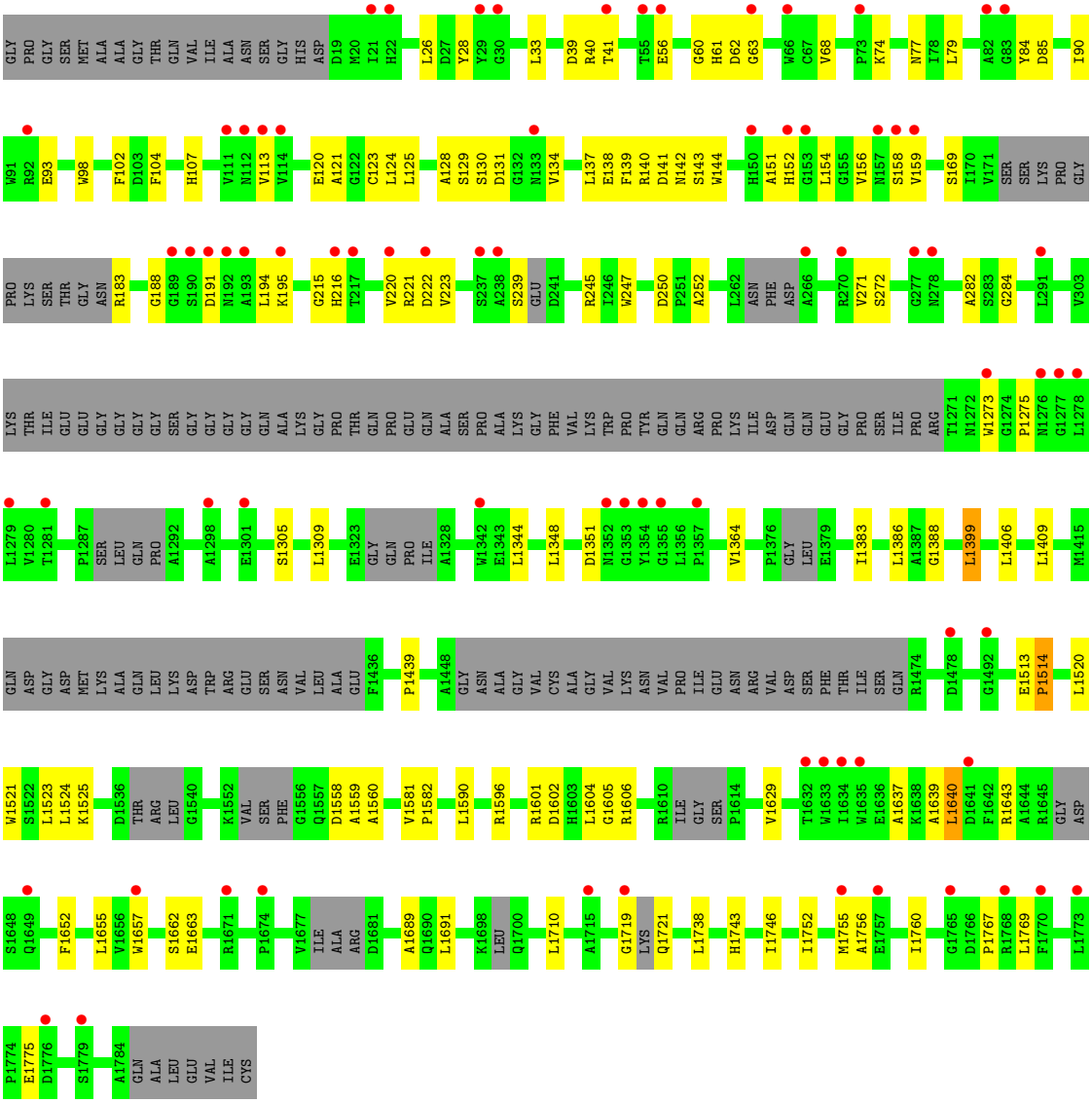
Chain	Residue	Modelled	Actual	Comment	Reference
C	943	GLY	-	expression tag	UNP G2Q2S2
C	944	PRO	-	expression tag	UNP G2Q2S2
C	945	GLY	-	expression tag	UNP G2Q2S2
C	946	SER	-	expression tag	UNP G2Q2S2
C	947	GLU	-	expression tag	UNP G2Q2S2
C	948	PHE	-	expression tag	UNP G2Q2S2
C	949	GLU	-	expression tag	UNP G2Q2S2
C	950	LEU	-	expression tag	UNP G2Q2S2
C	951	MET	-	expression tag	UNP G2Q2S2
C	1242	GLY	-	expression tag	UNP G2Q2S2
C	1243	GLY	-	expression tag	UNP G2Q2S2
C	1244	SER	-	expression tag	UNP G2Q2S2
C	1245	GLY	-	expression tag	UNP G2Q2S2
C	1246	HIS	-	expression tag	UNP G2Q2S2
C	1247	HIS	-	expression tag	UNP G2Q2S2
C	1248	HIS	-	expression tag	UNP G2Q2S2
C	1249	HIS	-	expression tag	UNP G2Q2S2
C	1250	HIS	-	expression tag	UNP G2Q2S2
C	1251	HIS	-	expression tag	UNP G2Q2S2
C	1252	HIS	-	expression tag	UNP G2Q2S2
C	1253	HIS	-	expression tag	UNP G2Q2S2
C	1254	HIS	-	expression tag	UNP G2Q2S2
C	1255	HIS	-	expression tag	UNP G2Q2S2

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 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.

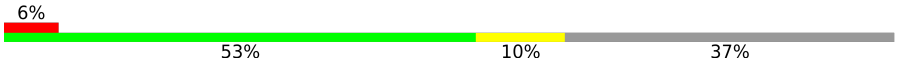
- Molecule 1: Fusion Protein of Sec13 and Nup145C

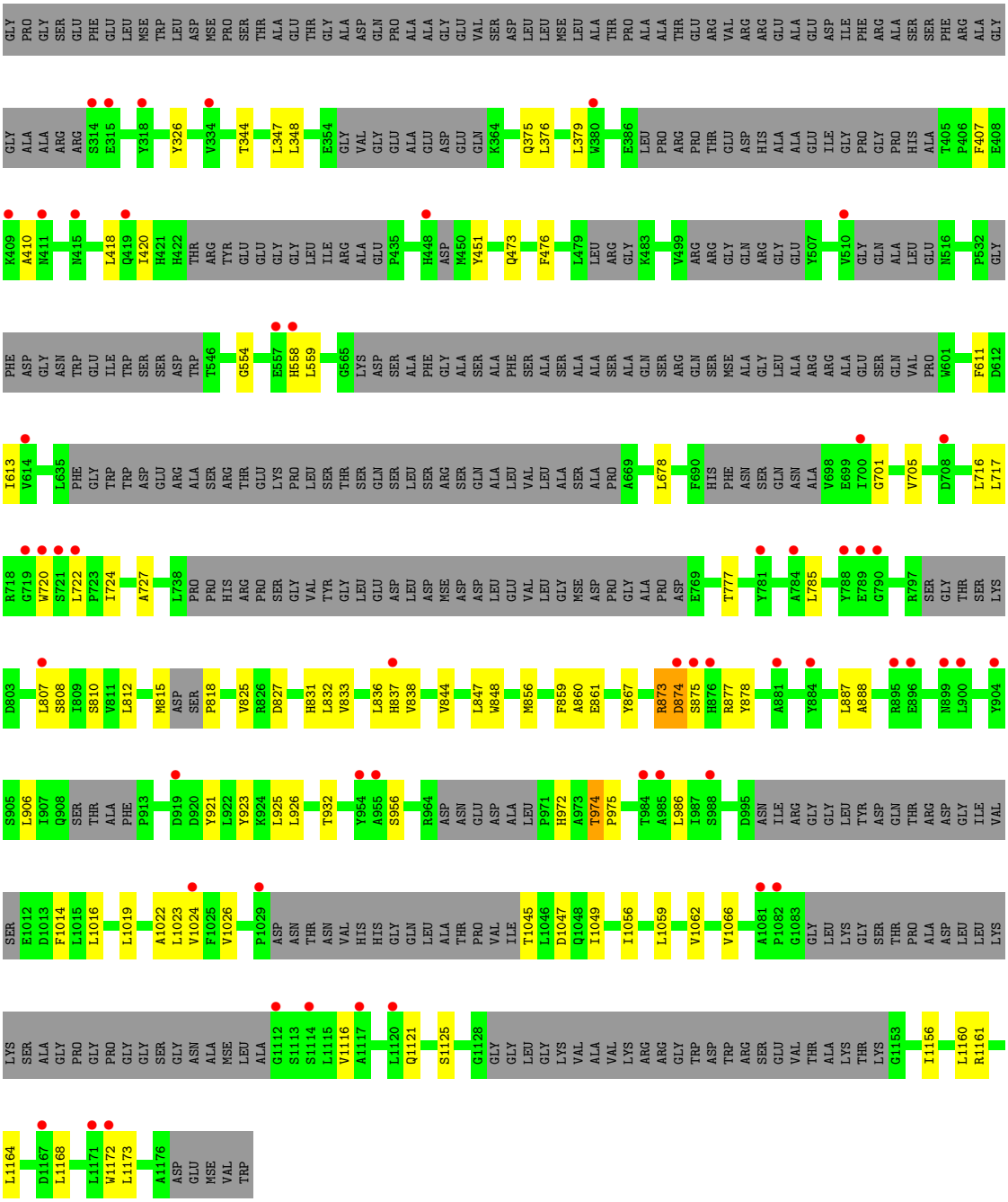
Chain A: 9% 67% 14% 19%



- Molecule 2: Nup85

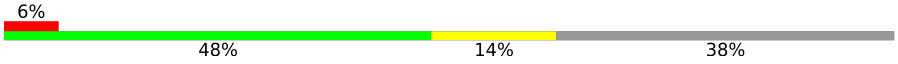
Chain B:

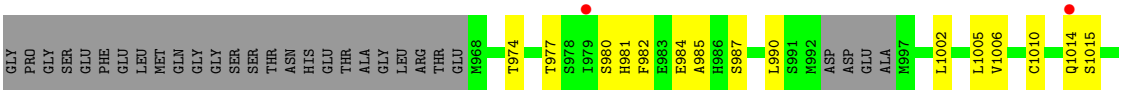


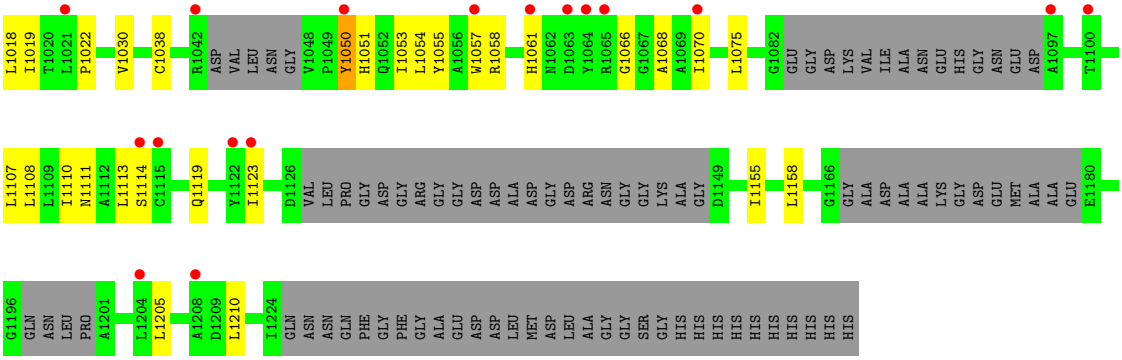


- Molecule 3: Nup120

Chain C:






L1018 I1019 T1020 L1021 P1022 V1030 C1038 R1042 ASP VAL LEU ASN GLY V1048 P1049 Y1050 H1051 Q1052 I1053 L1054 Y1055 A1056 W1057 R1058 H1061 N1062 D1063 Y1064 R1065 G1066 G1067 A1068 A1069 I1070 L1075 G1082 GLU GLY ASP LYS VAL ILE ALA ASN GLU HIS GLY ASN GLU ASP A1097 T1100
L1107 L1108 L1109 I1110 N1111 A1112 L1113 S1114 C1115 Q1119 Y1122 I1123 D1126 VAL LEU PRO GLY ASP GLY ARG GLY GLY ASP ASP ALA ASP GLY ASP ARG ASN GLY GLY LYS ALA GLY D1149 I1155 L1158 G1166 GLY ALA ASP ALA ALA LYS GLY ASP GLU MET ALA ALA GLU E1180
G1196 GLN ASN LEU PRO A1201 L1204 L1205 A1208 D1209 L1210 I1224 GLN ASN ASN GLN PHE GLY PHE GLY ALA GLU ASP ASP LEU MET ASP LEU ALA GLY GLY SER GLY HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	104.98Å 212.02Å 170.64Å 90.00° 107.21° 90.00°	Depositor
Resolution (Å)	163.00 – 4.10 163.00 – 4.10	Depositor EDS
% Data completeness (in resolution range)	97.4 (163.00-4.10) 97.5 (163.00-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.19	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 4.15Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1951)	Depositor
R, R_{free}	0.319 , 0.358 0.319 , 0.358	Depositor DCC
R_{free} test set	1975 reflections (7.25%)	wwPDB-VP
Wilson B-factor (Å^2)	160.4	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 350.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.079 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	10051	wwPDB-VP
Average B, all atoms (Å^2)	158.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.20	0/4879	0.36	0/6697
2	B	0.20	0/4014	0.35	0/5488
3	C	0.23	0/1322	0.39	0/1805
All	All	0.20	0/10215	0.36	0/13990

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4777	0	4010	73	0
2	B	3962	0	3566	57	0
3	C	1312	0	1190	32	0
All	All	10051	0	8766	153	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 (153) 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:62:ASP:HB2	1:A:85:ASP:HB3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1605:GLY:HA2	1:A:1637:ALA:HB1	1.76	0.68
2:B:722:LEU:HD13	2:B:724:ILE:HD12	1.76	0.67
2:B:1023:LEU:HG	2:B:1160:LEU:HD23	1.80	0.64
2:B:815:MSE:HB3	2:B:818:PRO:HG2	1.79	0.64
2:B:1161:ARG:NH1	3:C:1114:SER:OG	2.31	0.64
1:A:169:SER:HB2	1:A:1640:LEU:HD12	1.80	0.63
2:B:1023:LEU:HD13	2:B:1156:ILE:HG22	1.81	0.62
2:B:1172:TRP:HE1	3:C:1054:LEU:HD22	1.64	0.62
3:C:1050:TYR:HE2	3:C:1054:LEU:HD21	1.64	0.62
3:C:1050:TYR:CE2	3:C:1054:LEU:HD21	2.35	0.61
2:B:827:ASP:O	2:B:831:HIS:ND1	2.34	0.60
1:A:188:GLY:HA2	1:A:194:LEU:HD22	1.82	0.60
1:A:216:HIS:CE1	1:A:245:ARG:HG2	2.38	0.59
1:A:1769:LEU:HD13	1:A:1775:GLU:HG3	1.84	0.59
2:B:554:GLY:O	2:B:558:HIS:ND1	2.34	0.59
1:A:77:ASN:ND2	1:A:93:GLU:OE1	2.34	0.58
1:A:63:GLY:HA3	1:A:84:TYR:HB3	1.86	0.58
1:A:130:SER:HA	1:A:156:VAL:H	1.69	0.57
1:A:1305:SER:O	1:A:1309:LEU:N	2.36	0.57
2:B:1056:ILE:HG22	2:B:1161:ARG:HH21	1.70	0.57
1:A:134:VAL:HG22	1:A:151:ALA:HB2	1.85	0.57
1:A:40:ARG:NE	1:A:61:HIS:O	2.37	0.57
2:B:1168:LEU:HD13	3:C:1108:LEU:HD13	1.88	0.56
3:C:1010:CYS:SG	3:C:1014:GLN:NE2	2.79	0.56
3:C:1010:CYS:O	3:C:1014:GLN:NE2	2.31	0.56
1:A:1691:LEU:HD11	3:C:1155:ILE:HG23	1.87	0.55
2:B:326:TYR:HB3	2:B:716:LEU:HD23	1.87	0.55
2:B:1173:LEU:HD21	3:C:1055:TYR:HA	1.87	0.55
2:B:856:MSE:HB3	2:B:859:PHE:HD2	1.71	0.55
1:A:152:HIS:CD2	1:A:195:LYS:HE2	2.41	0.55
2:B:1023:LEU:HD11	2:B:1160:LEU:HB2	1.89	0.55
1:A:1689:ALA:HB1	1:A:1710:LEU:HB2	1.88	0.55
1:A:1719:GLY:O	1:A:1721:GLN:N	2.40	0.55
1:A:1657:TRP:HB2	3:C:1158:LEU:HD13	1.89	0.54
2:B:473:GLN:HA	2:B:476:PHE:HD2	1.71	0.54
1:A:121:ALA:HB1	1:A:183:ARG:HD3	1.89	0.54
1:A:120:GLU:OE2	1:A:1601:ARG:NH2	2.41	0.54
1:A:74:LYS:O	1:A:1643:ARG:NH1	2.41	0.53
1:A:1364:VAL:HG11	1:A:1388:GLY:HA2	1.90	0.53
2:B:1019:LEU:O	2:B:1023:LEU:HB2	2.10	0.52
1:A:272:SER:OG	1:A:1275:PRO:O	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:410:ALA:HB3	2:B:722:LEU:HD12	1.91	0.52
1:A:1752:ILE:HA	1:A:1755:MET:HG2	1.91	0.52
2:B:1024:VAL:HG11	2:B:1116:VAL:HA	1.92	0.52
1:A:1643:ARG:HE	1:A:1652:PHE:HE1	1.56	0.52
2:B:836:LEU:HD11	2:B:844:VAL:HG22	1.92	0.51
2:B:407:PHE:HD1	2:B:722:LEU:HD11	1.74	0.51
1:A:250:ASP:O	1:A:252:ALA:N	2.40	0.51
3:C:982:PHE:HD2	3:C:985:ALA:H	1.57	0.51
1:A:1746:ILE:HG23	3:C:1119:GLN:HA	1.92	0.50
2:B:717:LEU:HA	2:B:720:TRP:HD1	1.76	0.50
2:B:1161:ARG:HH11	3:C:1111:ASN:HA	1.75	0.50
3:C:1123:ILE:HB	3:C:1205:LEU:HB2	1.93	0.50
1:A:1513:GLU:N	1:A:1514:PRO:HD3	2.28	0.49
2:B:1121:GLN:O	2:B:1125:SER:OG	2.29	0.49
3:C:1070:ILE:HG12	3:C:1123:ILE:HG23	1.93	0.49
2:B:861:GLU:HA	2:B:888:ALA:HB1	1.94	0.48
1:A:93:GLU:HA	1:A:98:TRP:HA	1.95	0.48
2:B:956:SER:HB2	2:B:986:LEU:HD21	1.95	0.48
2:B:1045:THR:O	2:B:1047:ASP:N	2.44	0.48
2:B:833:VAL:HA	2:B:836:LEU:HB2	1.95	0.48
2:B:921:TYR:O	2:B:925:LEU:N	2.47	0.48
1:A:68:VAL:HB	1:A:79:LEU:HD11	1.96	0.48
2:B:347:LEU:HD21	2:B:727:ALA:HA	1.96	0.48
1:A:26:LEU:HD13	1:A:33:LEU:HD23	1.95	0.48
1:A:1558:ASP:O	1:A:1560:ALA:N	2.42	0.48
1:A:158:SER:OG	1:A:223:VAL:N	2.42	0.48
1:A:271:VAL:HG22	1:A:282:ALA:HA	1.95	0.48
1:A:124:LEU:HD22	1:A:138:GLU:HG2	1.96	0.47
1:A:1602:ASP:OD2	1:A:1606:ARG:NH2	2.48	0.47
1:A:56:GLU:HG3	1:A:98:TRP:CD1	2.50	0.47
2:B:906:LEU:HD12	2:B:1014:PHE:HB2	1.96	0.47
2:B:926:LEU:HB3	2:B:932:THR:HG21	1.96	0.47
3:C:974:THR:O	3:C:977:THR:OG1	2.26	0.47
2:B:1016:LEU:HG	2:B:1059:LEU:HD21	1.97	0.47
1:A:125:LEU:HB3	1:A:137:LEU:HB2	1.97	0.46
2:B:785:LEU:HD23	2:B:808:SER:HB2	1.98	0.46
3:C:982:PHE:HD2	3:C:984:GLU:H	1.63	0.46
1:A:102:PHE:CE2	1:A:104:PHE:HB2	2.50	0.46
3:C:984:GLU:O	3:C:987:SER:OG	2.22	0.46
1:A:140:ARG:HB3	1:A:143:SER:O	2.16	0.46
2:B:1173:LEU:HD22	3:C:1018:LEU:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:TYR:OH	1:A:1602:ASP:OD1	2.25	0.46
1:A:194:LEU:HD21	1:A:220:VAL:HG11	1.96	0.46
1:A:215:GLY:O	1:A:245:ARG:NH1	2.49	0.46
1:A:1604:LEU:HD11	1:A:1629:VAL:HG11	1.97	0.46
1:A:129:SER:OG	1:A:131:ASP:OD1	2.33	0.46
2:B:836:LEU:O	2:B:838:VAL:N	2.49	0.45
2:B:376:LEU:HD11	2:B:418:LEU:HD12	1.98	0.45
1:A:1383:ILE:HD11	1:A:1439:PRO:HB3	1.98	0.45
1:A:1639:ALA:HB1	1:A:1655:LEU:HD23	1.98	0.45
3:C:1113:LEU:HD22	3:C:1210:LEU:HD11	1.98	0.45
2:B:832:LEU:HD12	2:B:847:LEU:HD22	1.99	0.45
3:C:1107:LEU:O	3:C:1110:ILE:HG12	2.17	0.45
2:B:825:VAL:HG11	2:B:856:MSE:SE	2.66	0.45
1:A:113:VAL:HG13	1:A:159:VAL:HG12	1.99	0.45
1:A:141:ASP:OD1	1:A:142:ASN:N	2.50	0.44
2:B:344:THR:HG21	2:B:807:LEU:HD13	1.98	0.44
2:B:348:LEU:HD21	2:B:810:SER:HB2	1.99	0.44
1:A:221:ARG:H	1:A:239:SER:HA	1.81	0.44
2:B:877:ARG:O	2:B:923:TYR:HB3	2.17	0.44
1:A:128:ALA:HA	1:A:134:VAL:HG12	2.00	0.44
1:A:194:LEU:HD12	1:A:247:TRP:CZ3	2.52	0.44
3:C:1057:TRP:CD1	3:C:1068:ALA:HB1	2.52	0.44
1:A:1662:SER:OG	1:A:1663:GLU:N	2.49	0.44
2:B:1049:ILE:HG23	2:B:1164:LEU:HD13	1.99	0.44
3:C:1070:ILE:HG12	3:C:1123:ILE:HG12	2.00	0.44
2:B:376:LEU:HD21	2:B:418:LEU:HD12	2.00	0.44
2:B:873:ARG:HB3	2:B:874:ASP:H	1.60	0.44
2:B:887:LEU:HD22	2:B:888:ALA:H	1.82	0.43
1:A:1581:VAL:HB	1:A:1582:PRO:HD3	2.01	0.43
3:C:1015:SER:O	3:C:1019:ILE:HG13	2.18	0.43
1:A:1756:ALA:O	1:A:1760:ILE:HG13	2.18	0.43
2:B:848:TRP:CD1	2:B:860:ALA:HB1	2.54	0.43
1:A:1344:LEU:HD12	1:A:1523:LEU:HD23	2.01	0.43
1:A:90:ILE:HD12	1:A:102:PHE:HD2	1.84	0.43
1:A:1590:LEU:HD12	1:A:1596:ARG:HA	2.00	0.43
2:B:844:VAL:HG21	2:B:867:TYR:CD1	2.54	0.42
3:C:1002:LEU:O	3:C:1005:LEU:HG	2.19	0.42
2:B:559:LEU:HB2	2:B:611:PHE:CE2	2.55	0.42
3:C:980:SER:O	3:C:982:PHE:HD1	2.02	0.42
1:A:1348:LEU:HD21	1:A:1524:LEU:HA	2.01	0.42
1:A:107:HIS:CG	1:A:129:SER:HG	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1006:VAL:HG21	3:C:1030:VAL:HG23	2.01	0.42
1:A:158:SER:HB2	1:A:222:ASP:HA	2.01	0.42
2:B:476:PHE:HD1	2:B:613:ILE:HD12	1.85	0.42
2:B:1062:VAL:HG11	2:B:1066:VAL:HB	2.01	0.42
1:A:154:LEU:HD12	1:A:191:ASP:HA	2.02	0.42
1:A:1520:LEU:HA	1:A:1523:LEU:HB2	2.02	0.42
3:C:1050:TYR:CD2	3:C:1075:LEU:HD11	2.55	0.42
1:A:113:VAL:HG11	1:A:158:SER:HA	2.02	0.41
3:C:1058:ARG:O	3:C:1061:HIS:HB3	2.19	0.41
2:B:701:GLY:O	2:B:705:VAL:HG23	2.18	0.41
1:A:39:ASP:OD1	1:A:41:THR:OG1	2.34	0.41
1:A:158:SER:HB3	1:A:188:GLY:HA3	2.02	0.41
1:A:1386:LEU:HD13	1:A:1409:LEU:HD11	2.02	0.41
1:A:1399:LEU:HB2	1:A:1406:LEU:HD22	2.02	0.41
3:C:987:SER:HA	3:C:990:LEU:HG	2.02	0.41
3:C:1066:GLY:O	3:C:1070:ILE:HG13	2.20	0.41
1:A:284:GLY:O	1:A:1273:TRP:NE1	2.52	0.41
2:B:974:THR:N	2:B:975:PRO:HD2	2.36	0.41
2:B:1022:ALA:O	2:B:1026:VAL:HG23	2.20	0.41
1:A:123:CYS:HB3	1:A:139:PHE:HB3	2.01	0.41
2:B:1049:ILE:HG23	2:B:1164:LEU:HD22	2.02	0.41
1:A:1738:LEU:HD12	1:A:1752:ILE:HG21	2.03	0.41
1:A:151:ALA:HB1	1:A:156:VAL:HG21	2.03	0.41
1:A:1652:PHE:O	1:A:1655:LEU:HG	2.21	0.40
2:B:812:LEU:HD21	2:B:825:VAL:HA	2.03	0.40
1:A:1521:TRP:O	1:A:1525:LYS:HB2	2.22	0.40
2:B:375:GLN:O	2:B:379:LEU:HG	2.21	0.40
2:B:420:ILE:HD12	2:B:705:VAL:HG12	2.03	0.40
3:C:1038:CYS:SG	3:C:1053:ILE:HG12	2.61	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	679/876 (78%)	611 (90%)	61 (9%)	7 (1%)	15	52
2	B	548/933 (59%)	507 (92%)	36 (7%)	5 (1%)	17	54
3	C	181/313 (58%)	164 (91%)	14 (8%)	3 (2%)	9	42
All	All	1408/2122 (66%)	1282 (91%)	111 (8%)	15 (1%)	14	50

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	TRP
2	B	878	TYR
1	A	1514	PRO
2	B	837	HIS
2	B	875	SER
3	C	981	HIS
1	A	60	GLY
2	B	972	HIS
3	C	1051	HIS
1	A	1351	ASP
1	A	1743	HIS
2	B	451	TYR
1	A	1559	ALA
3	C	1022	PRO
1	A	1767	PRO

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	356/700 (51%)	354 (99%)	2 (1%)	86	92
2	B	320/725 (44%)	315 (98%)	5 (2%)	62	78
3	C	108/253 (43%)	107 (99%)	1 (1%)	78	87
All	All	784/1678 (47%)	776 (99%)	8 (1%)	76	85

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1399	LEU
1	A	1640	LEU
2	B	678	LEU
2	B	777	THR
2	B	873	ARG
2	B	874	ASP
2	B	974	THR
3	C	1050	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	1014	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	713/876 (81%)	0.61	76 (10%)	6	6	60, 142, 204, 287	0
2	B	578/933 (61%)	0.44	54 (9%)	8	8	82, 166, 228, 311	0
3	C	195/313 (62%)	0.31	19 (9%)	7	8	85, 178, 243, 270	0
All	All	1486/2122 (70%)	0.50	149 (10%)	7	7	60, 156, 226, 311	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	874	ASP	6.3
2	B	1120	LEU	5.7
2	B	721	SER	5.6
3	C	1050	TYR	5.3
1	A	1281	THR	5.2
1	A	1354	TYR	5.2
1	A	1279	LEU	5.1
2	B	875	SER	5.1
1	A	29	TYR	5.1
2	B	314	SER	5.1
2	B	315	GLU	4.8
1	A	1278	LEU	4.3
3	C	1063	ASP	4.3
1	A	157	ASN	4.3
3	C	1064	TYR	4.2
1	A	83	GLY	4.2
1	A	1301	GLU	4.1
1	A	112	ASN	4.1
1	A	1298	ALA	4.0
2	B	720	TRP	4.0
1	A	238	ALA	4.0
2	B	1024	VAL	3.8
1	A	1757	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	1492	GLY	3.6
2	B	896	GLU	3.6
1	A	114	VAL	3.6
2	B	881	ALA	3.6
2	B	415	ASN	3.6
1	A	66	TRP	3.6
1	A	152	HIS	3.6
3	C	1014	GLN	3.6
2	B	955	ALA	3.5
1	A	1657	TRP	3.5
2	B	448	HIS	3.5
3	C	1100	THR	3.5
1	A	82	ALA	3.5
2	B	788	TYR	3.4
2	B	984	THR	3.3
1	A	193	ALA	3.3
2	B	876	HIS	3.3
2	B	988	SER	3.3
1	A	1273	TRP	3.3
1	A	278	ASN	3.2
2	B	899	ASN	3.2
1	A	1355	GLY	3.1
1	A	195	LYS	3.1
2	B	781	TYR	3.1
1	A	1277	GLY	3.1
2	B	784	ALA	3.1
2	B	722	LEU	3.0
1	A	111	VAL	3.0
3	C	1122	TYR	3.0
1	A	189	GLY	3.0
1	A	192	ASN	3.0
2	B	1172	TRP	2.9
1	A	1632	THR	2.9
1	A	73	PRO	2.9
2	B	719	GLY	2.9
1	A	1353	GLY	2.9
1	A	190	SER	2.8
2	B	919	ASP	2.8
3	C	1021	LEU	2.8
3	C	1042	ARG	2.8
1	A	1478	ASP	2.8
2	B	1082	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	266	ALA	2.8
2	B	837	HIS	2.8
1	A	191	ASP	2.8
1	A	1770	PHE	2.8
1	A	1768	ARG	2.7
1	A	41	THR	2.7
1	A	1674	PRO	2.7
3	C	1061	HIS	2.7
2	B	904	TYR	2.7
1	A	1635	TRP	2.7
3	C	1057	TRP	2.7
1	A	92	ARG	2.7
1	A	1634	ILE	2.7
3	C	1065	ARG	2.7
1	A	21	ILE	2.6
1	A	277	GLY	2.6
3	C	1114	SER	2.5
1	A	291	LEU	2.5
1	A	1773	LEU	2.5
2	B	954	TYR	2.5
2	B	708	ASP	2.5
2	B	1114	SER	2.5
2	B	895	ARG	2.5
1	A	1715	ALA	2.5
1	A	113	VAL	2.4
2	B	1112	GLY	2.4
1	A	55	THR	2.4
1	A	1641	ASP	2.4
2	B	558	HIS	2.4
2	B	318	TYR	2.4
1	A	1719	GLY	2.4
3	C	1070	ILE	2.4
2	B	1081	ALA	2.4
2	B	334	VAL	2.3
2	B	557	GLU	2.3
1	A	22	HIS	2.3
1	A	270	ARG	2.3
1	A	1779	SER	2.3
2	B	411	ASN	2.3
3	C	1097	ALA	2.3
2	B	789	GLU	2.3
3	C	979	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1755	MET	2.3
1	A	63	GLY	2.3
1	A	1357	PRO	2.2
1	A	56	GLU	2.2
1	A	30	GLY	2.2
2	B	1117	ALA	2.2
1	A	217	THR	2.2
3	C	1115	CYS	2.2
1	A	1649	GLN	2.2
2	B	900	LEU	2.2
3	C	1208	ALA	2.2
1	A	1633	TRP	2.2
1	A	133	ASN	2.2
1	A	237	SER	2.2
1	A	1352	ASN	2.1
2	B	700	ILE	2.1
1	A	159	VAL	2.1
2	B	790	GLY	2.1
1	A	153	GLY	2.1
1	A	216	HIS	2.1
1	A	150	HIS	2.1
1	A	1765	GLY	2.1
2	B	1171	LEU	2.1
1	A	1342	TRP	2.1
2	B	1167	ASP	2.1
2	B	884	TYR	2.1
2	B	807	LEU	2.1
1	A	1276	ASN	2.1
1	A	1671	ARG	2.1
2	B	419	GLN	2.1
3	C	1204	LEU	2.1
1	A	1776	ASP	2.1
2	B	510	VAL	2.1
1	A	220	VAL	2.0
2	B	380	TRP	2.0
1	A	222	ASP	2.0
1	A	158	SER	2.0
2	B	614	VAL	2.0
2	B	985	ALA	2.0
2	B	1029	PRO	2.0
2	B	409	LYS	2.0
3	C	1123	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.