



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:06 AM UTC

PDB ID : 4YCZ / pdb_00004ycz
Title : Y-COMPLEX HUB (NUP85-NUP120-NUP145C-SEC13 COMPLEX) FROM
M. THERMOPHILA (A.K.A. T. HETEROTHALLICA)
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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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

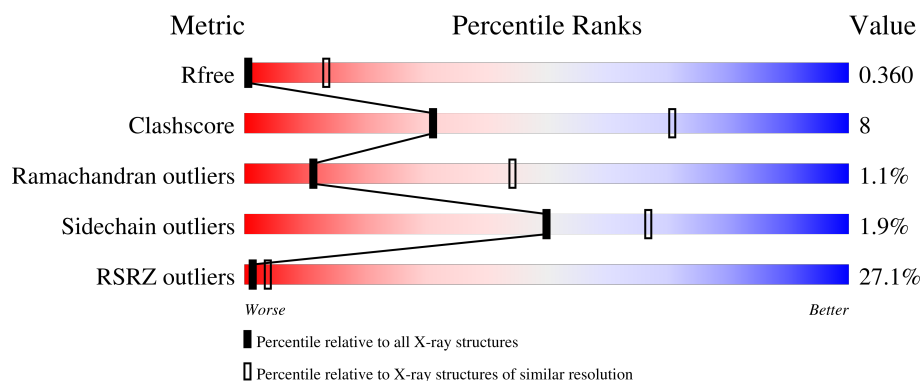
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1243 (4.40-3.80)
Clashscore	190562	1293 (4.40-3.80)
Ramachandran outliers	187476	1206 (4.40-3.80)
Sidechain outliers	187428	1193 (4.40-3.80)
RSRZ outliers	180081	1240 (4.40-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	876	
2	B	933	
3	C	313	

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
1	A	713	Total	C	N	O	S	0	0	0
			4777	3049	843	874	11			

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
2	B	590	Total	C	N	O	S	Se	0	0	0
			3962	2596	644	705	5	12			

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
3	C	195	Total	C	N	O	S	0	0	0
			1312	846	220	241	5			

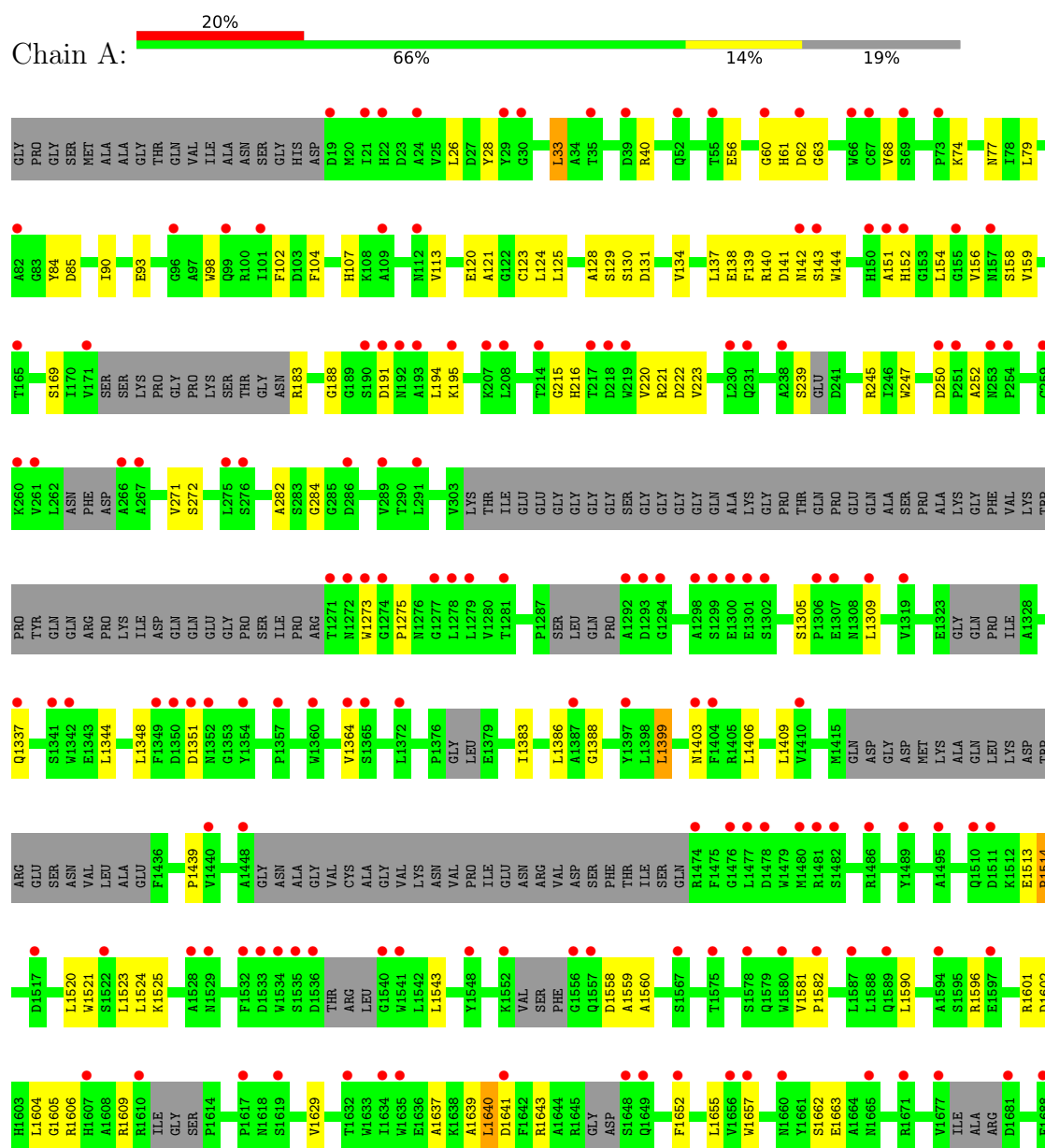
There are 23 discrepancies between the modelled and reference sequences:

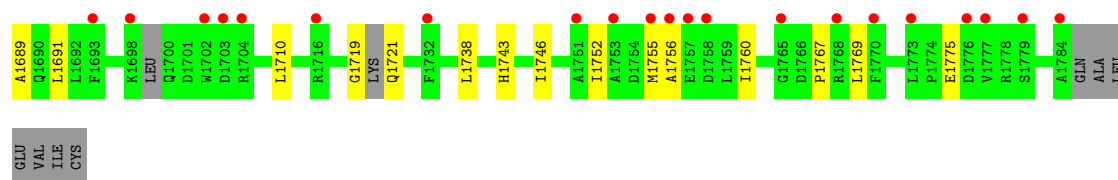
Chain	Residue	Modelled	Actual	Comment	Reference
C	943	GLY	-	expression tag	UNP G2Q2S2
C	944	PRO	-	expression tag	UNP G2Q2S2
C	945	GLY	-	expression tag	UNP G2Q2S2
C	946	SER	-	expression tag	UNP G2Q2S2
C	947	GLU	-	expression tag	UNP G2Q2S2
C	948	PHE	-	expression tag	UNP G2Q2S2
C	949	GLU	-	expression tag	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](#)

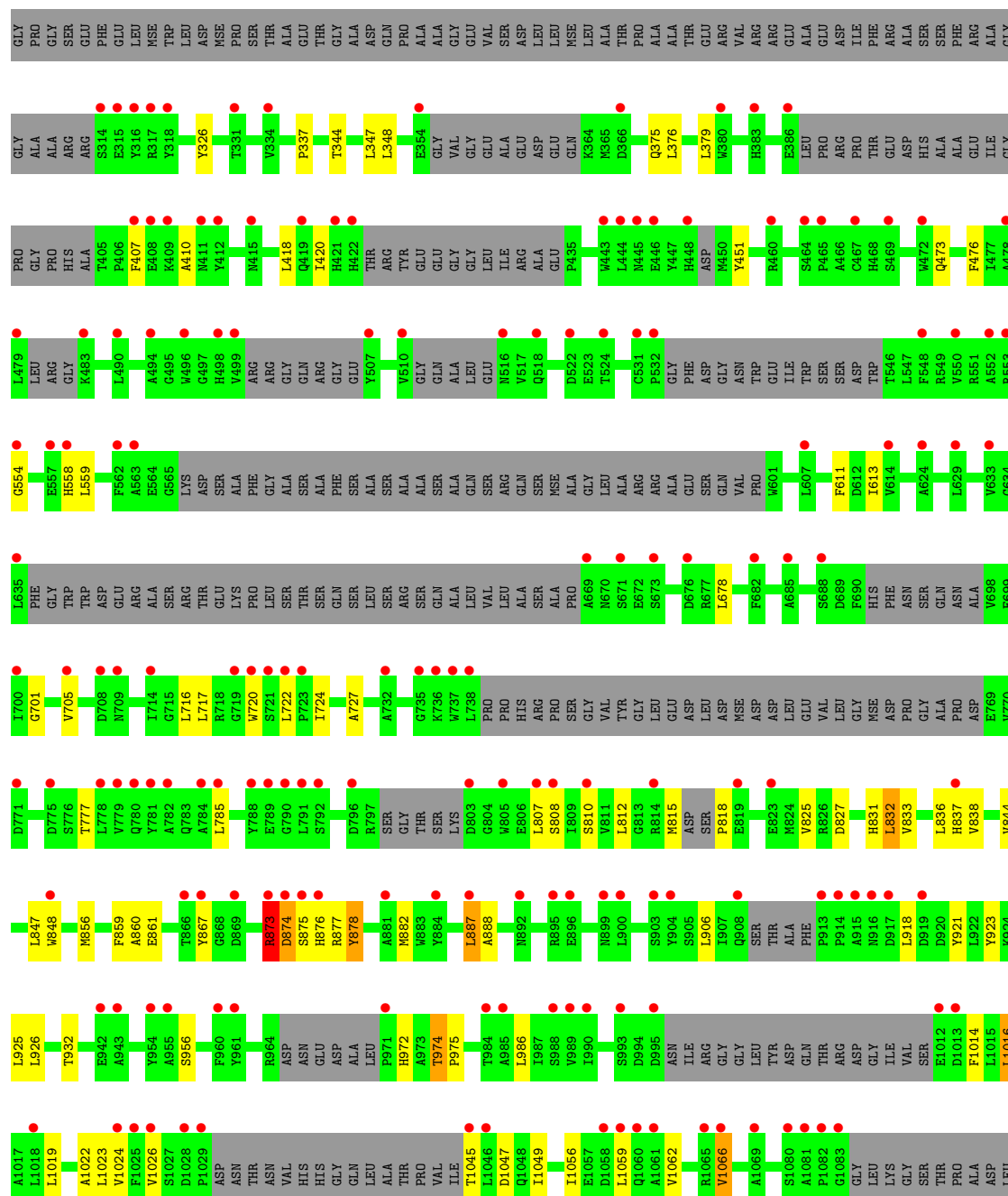
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

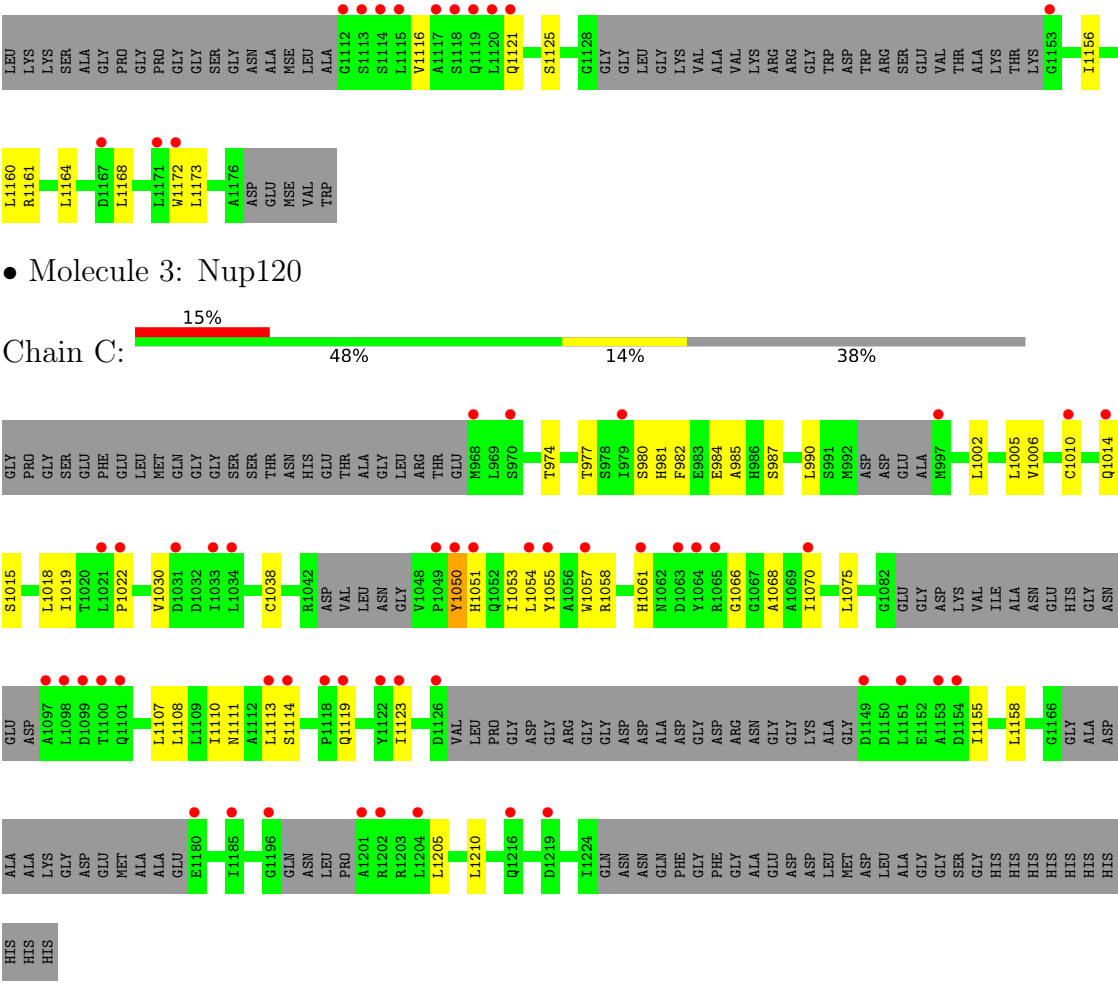
- Molecule 1: Fusion Protein of Sec13 and Nup145C





• Molecule 2: Nup85





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 4.15Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1951)	Depositor
R, R_{free}	0.319 , 0.358 0.320 , 0.360	Depositor DCC
R_{free} test set	1975 reflections (7.07%)	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)	0.38 , 704.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.079 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.87	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/4879	0.72	2/6697 (0.0%)
2	B	0.27	0/4014	0.71	3/5488 (0.1%)
3	C	0.28	0/1322	0.73	0/1805
All	All	0.28	0/10215	0.72	5/13990 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	873	ARG	CB-CA-C	-5.69	110.00	116.54
1	A	1403	ASN	CB-CA-C	-5.50	109.75	117.23
1	A	1337	GLN	CB-CA-C	-5.43	109.84	117.23
2	B	337	PRO	N-CA-C	5.26	117.12	110.70
2	B	918	LEU	CB-CA-C	-5.08	110.32	117.23

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	74	0
2	B	3962	0	3566	58	0
3	C	1312	0	1190	32	0
All	All	10051	0	8766	155	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 (155) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:C:984:GLU:O	3:C:987:SER:OG	2.22	0.47
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:107:HIS:CG	1:A:129:SER:HG	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:1752:ILE:HG22	1:A:1755:MET:HE2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:1006:VAL:HG21	3:C:1030:VAL:HG23	2.01	0.42
2:B:876:HIS:C	2:B:878:TYR:H	2.28	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: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
1:A:1609:ARG:HA	1:A:1641:ASP:CG	2.47	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%)	12	46
2	B	548/933 (59%)	507 (92%)	36 (7%)	5 (1%)	14	49
3	C	181/313 (58%)	164 (91%)	14 (8%)	3 (2%)	7	36
All	All	1408/2122 (66%)	1282 (91%)	111 (8%)	15 (1%)	11	44

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%)	352 (99%)	4 (1%)	65	74
2	B	320/725 (44%)	310 (97%)	10 (3%)	35	56
3	C	108/253 (43%)	107 (99%)	1 (1%)	70	76
All	All	784/1678 (47%)	769 (98%)	15 (2%)	50	67

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	1399	LEU
1	A	1543	LEU
1	A	1640	LEU
2	B	678	LEU
2	B	777	THR
2	B	832	LEU
2	B	873	ARG
2	B	874	ASP
2	B	882	MSE
2	B	887	LEU
2	B	974	THR
2	B	1016	LEU
2	B	1066	VAL
3	C	1050	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1718	GLN
3	C	1014	GLN
3	C	1027	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	713/876 (81%)	1.35	175 (24%) 2 4	60, 142, 204, 287	0
2	B	578/933 (61%)	1.63	182 (31%) 1 3	82, 166, 228, 311	0
3	C	195/313 (62%)	1.30	46 (23%) 2 4	85, 178, 243, 270	0
All	All	1486/2122 (70%)	1.45	403 (27%) 1 4	60, 156, 226, 311	0

All (403) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	988	SER	8.7
3	C	1050	TYR	7.9
2	B	899	ASN	7.2
2	B	516	ASN	7.1
2	B	805	TRP	6.6
2	B	737	TRP	6.4
2	B	955	ALA	6.3
3	C	1063	ASP	6.1
2	B	895	ARG	6.0
2	B	1117	ALA	6.0
2	B	1120	LEU	6.0
2	B	896	GLU	5.9
2	B	781	TYR	5.9
1	A	1681	ASP	5.7
2	B	558	HIS	5.7
2	B	1045	THR	5.7
2	B	984	THR	5.6
2	B	985	ALA	5.5
1	A	1779	SER	5.5
2	B	331	THR	5.5
1	A	1281	THR	5.3
2	B	448	HIS	5.3
3	C	1122	TYR	5.2

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Mol	Chain	Res	Type	RSRZ
2	B	315	GLU	5.2
2	B	721	SER	5.2
1	A	1540	GLY	5.1
1	A	1765	GLY	5.1
2	B	919	ASP	5.1
1	A	1354	TYR	5.0
2	B	989	VAL	5.0
2	B	779	VAL	5.0
1	A	1298	ALA	4.9
1	A	1757	GLU	4.9
1	A	1277	GLY	4.9
3	C	1100	THR	4.9
1	A	1776	ASP	4.9
2	B	900	LEU	4.8
2	B	995	ASP	4.8
2	B	1113	SER	4.8
1	A	29	TYR	4.6
2	B	993	SER	4.6
1	A	1535	SER	4.5
1	A	157	ASN	4.4
2	B	784	ALA	4.4
2	B	314	SER	4.3
2	B	881	ALA	4.2
1	A	1365	SER	4.1
1	A	171	VAL	4.1
3	C	1014	GLN	4.1
2	B	914	PRO	4.1
1	A	1660	ASN	4.1
2	B	954	TYR	4.1
1	A	112	ASN	4.1
2	B	557	GLU	4.0
1	A	193	ALA	4.0
1	A	1677	VAL	4.0
1	A	259	CYS	4.0
2	B	1172	TRP	4.0
2	B	1060	GLN	3.9
2	B	1119	GLN	3.9
2	B	775	ASP	3.9
1	A	1607	HIS	3.9
2	B	904	TYR	3.9
1	A	1649	GLN	3.8
3	C	1119	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	1610	ARG	3.8
3	C	1055	TYR	3.8
2	B	422	HIS	3.8
1	A	66	TRP	3.8
1	A	1556	GLY	3.8
1	A	67	CYS	3.7
1	A	1403	ASN	3.7
1	A	1279	LEU	3.7
2	B	316	TYR	3.7
1	A	1784	ALA	3.7
2	B	469	SER	3.6
1	A	1657	TRP	3.6
1	A	24	ALA	3.6
1	A	1693	PHE	3.6
1	A	150	HIS	3.6
2	B	1046	LEU	3.6
1	A	1357	PRO	3.5
1	A	1337	GLN	3.5
1	A	1480	MET	3.5
2	B	499	VAL	3.5
1	A	1301	GLU	3.5
1	A	1352	ASN	3.5
2	B	709	ASN	3.5
2	B	1171	LEU	3.5
2	B	409	LYS	3.5
2	B	1081	ALA	3.5
2	B	635	LEU	3.5
3	C	1054	LEU	3.5
1	A	1703	ASP	3.5
2	B	548	PHE	3.5
1	A	1529	ASN	3.5
2	B	700	ILE	3.5
2	B	908	GLN	3.4
3	C	1064	TYR	3.4
1	A	1528	ALA	3.4
2	B	354	GLU	3.4
2	B	682	PHE	3.4
2	B	1080	SER	3.4
1	A	1580	TRP	3.3
1	A	1597	GLU	3.3
2	B	942	GLU	3.3
2	B	785	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	837	HIS	3.3
2	B	380	TRP	3.3
1	A	1770	PHE	3.3
2	B	943	ALA	3.3
2	B	1025	PHE	3.3
2	B	1114	SER	3.3
1	A	190	SER	3.3
2	B	719	GLY	3.2
2	B	1024	VAL	3.2
2	B	714	ILE	3.2
1	A	219	TRP	3.2
2	B	790	GLY	3.2
1	A	1278	LEU	3.2
2	B	778	LEU	3.2
2	B	421	HIS	3.2
2	B	771	ASP	3.2
2	B	445	ASN	3.2
1	A	238	ALA	3.2
2	B	386	GLU	3.2
2	B	735	GLY	3.2
3	C	1196	GLY	3.2
2	B	553	ARG	3.2
1	A	291	LEU	3.1
1	A	1360	TRP	3.1
3	C	1114	SER	3.1
2	B	507	TYR	3.1
3	C	1201	ALA	3.1
1	A	1350	ASP	3.1
2	B	1013	ASP	3.1
1	A	267	ALA	3.1
2	B	318	TYR	3.1
1	A	1293	ASP	3.1
1	A	1342	TRP	3.1
2	B	562	PHE	3.1
2	B	317	ARG	3.1
1	A	60	GLY	3.0
2	B	1153	GLY	3.0
2	B	688	SER	3.0
2	B	411	ASN	3.0
2	B	334	VAL	3.0
3	C	1051	HIS	3.0
3	C	997	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	1517	ASP	3.0
2	B	1066	VAL	3.0
1	A	22	HIS	3.0
1	A	251	PRO	3.0
1	A	21	ILE	3.0
2	B	788	TYR	3.0
2	B	780	GLN	3.0
1	A	1533	ASP	3.0
2	B	483	LYS	3.0
2	B	460	ARG	3.0
2	B	510	VAL	3.0
3	C	1202	ARG	3.0
1	A	1532	PHE	3.0
1	A	1552	LYS	3.0
1	A	1541	TRP	3.0
1	A	1578	SER	3.0
3	C	1098	LEU	3.0
2	B	1058	ASP	3.0
1	A	207	LYS	3.0
1	A	1474	ARG	3.0
1	A	1557	GLN	3.0
2	B	705	VAL	3.0
1	A	35	THR	2.9
1	A	143	SER	2.9
2	B	522	ASP	2.9
1	A	1617	PRO	2.9
1	A	73	PRO	2.9
1	A	101	ILE	2.9
3	C	1151	LEU	2.9
3	C	1180	GLU	2.9
3	C	1118	PRO	2.9
1	A	1755	MET	2.9
1	A	1773	LEU	2.9
1	A	1536	ASP	2.9
2	B	874	ASP	2.9
2	B	532	PRO	2.9
1	A	1387	ALA	2.9
2	B	444	LEU	2.8
2	B	819	GLU	2.8
1	A	250	ASP	2.8
1	A	195	LYS	2.8
1	A	217	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1299	SER	2.8
2	B	563	ALA	2.8
2	B	1018	LEU	2.8
1	A	1300	GLU	2.8
3	C	1061	HIS	2.8
1	A	1292	ALA	2.8
2	B	803	ASP	2.8
1	A	231	GLN	2.8
2	B	875	SER	2.8
1	A	1486	ARG	2.7
1	A	266	ALA	2.7
1	A	1567	SER	2.7
2	B	708	ASP	2.7
1	A	1671	ARG	2.7
2	B	419	GLN	2.7
3	C	1101	GLN	2.7
2	B	524	THR	2.7
1	A	62	ASP	2.7
2	B	415	ASN	2.7
1	A	1702	TRP	2.7
1	A	1641	ASP	2.7
2	B	884	TYR	2.7
2	B	1121	GLN	2.7
2	B	867	TYR	2.7
2	B	990	ILE	2.7
1	A	1478	ASP	2.7
2	B	971	PRO	2.7
2	B	1026	VAL	2.7
2	B	738	LEU	2.7
2	B	866	THR	2.7
2	B	412	TYR	2.6
1	A	152	HIS	2.6
2	B	676	ASP	2.6
1	A	230	LEU	2.6
1	A	275	LEU	2.6
1	A	1341	SER	2.6
2	B	808	SER	2.6
3	C	1033	ILE	2.6
1	A	214	THR	2.6
1	A	1272	ASN	2.6
2	B	446	GLU	2.6
1	A	1294	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
3	C	1070	ILE	2.6
1	A	1704	ARG	2.6
2	B	961	TYR	2.6
2	B	823	GLU	2.6
2	B	1012	GLU	2.6
1	A	1440	VAL	2.6
1	A	165	THR	2.6
2	B	443	TRP	2.5
3	C	979	ILE	2.5
2	B	614	VAL	2.5
2	B	916	ASN	2.5
3	C	1123	ILE	2.5
1	A	52	GLN	2.5
3	C	1010	CYS	2.5
2	B	736	LYS	2.5
2	B	629	LEU	2.5
1	A	1698	LYS	2.5
2	B	723	PRO	2.5
3	C	1022	PRO	2.5
1	A	30	GLY	2.5
1	A	1306	PRO	2.5
2	B	720	TRP	2.5
2	B	518	GLN	2.5
2	B	789	GLU	2.5
1	A	1652	PHE	2.5
2	B	1028	ASP	2.5
2	B	550	VAL	2.5
2	B	792	SER	2.5
1	A	1589	GLN	2.5
1	A	191	ASP	2.5
1	A	1495	ALA	2.5
2	B	479	LEU	2.4
2	B	807	LEU	2.4
1	A	1510	GLN	2.4
2	B	796	ASP	2.4
1	A	1751	ALA	2.4
2	B	782	ALA	2.4
1	A	208	LEU	2.4
1	A	1372	LEU	2.4
1	A	55	THR	2.4
1	A	1548	TYR	2.4
3	C	1065	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	607	LEU	2.4
1	A	1271	THR	2.4
2	B	1059	LEU	2.4
3	C	1113	LEU	2.4
2	B	490	LEU	2.4
2	B	722	LEU	2.4
1	A	1758	ASP	2.4
1	A	1309	LEU	2.4
1	A	82	ALA	2.4
1	A	1482	SER	2.4
2	B	478	ALA	2.4
2	B	1118	SER	2.4
1	A	1397	TYR	2.4
3	C	1034	LEU	2.4
1	A	99	GLN	2.3
1	A	1404	PHE	2.3
1	A	286	ASP	2.3
2	B	869	ASP	2.3
2	B	465	PRO	2.3
1	A	1656	VAL	2.3
2	B	1029	PRO	2.3
1	A	1716	ARG	2.3
1	A	1273	TRP	2.3
1	A	1635	TRP	2.3
3	C	1049	PRO	2.3
2	B	554	GLY	2.3
2	B	1083	GLY	2.3
1	A	151	ALA	2.3
2	B	810	SER	2.3
1	A	1732	PHE	2.3
1	A	1448	ALA	2.3
3	C	1021	LEU	2.3
1	A	1648	SER	2.3
3	C	970	SER	2.3
2	B	1082	PRO	2.3
1	A	1511	ASP	2.3
2	B	494	ALA	2.3
3	C	1219	ASP	2.3
2	B	1115	LEU	2.3
2	B	848	TRP	2.3
1	A	1688	PHE	2.3
1	A	1634	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	109	ALA	2.3
1	A	1477	LEU	2.3
1	A	1777	VAL	2.3
2	B	498	HIS	2.3
2	B	407	PHE	2.2
3	C	1154	ASP	2.2
1	A	260	LYS	2.2
1	A	289	VAL	2.2
1	A	1522	SER	2.2
2	B	472	TRP	2.2
2	B	887	LEU	2.2
1	A	1364	VAL	2.2
1	A	1768	ARG	2.2
1	A	1619	SER	2.2
2	B	383	HIS	2.2
1	A	1307	GLU	2.2
2	B	366	ASP	2.2
3	C	1126	ASP	2.2
1	A	254	PRO	2.2
2	B	1069	ALA	2.2
2	B	1167	ASP	2.2
1	A	253	ASN	2.2
1	A	1632	THR	2.2
2	B	873	ARG	2.2
2	B	1061	ALA	2.2
2	B	1112	GLY	2.2
1	A	142	ASN	2.2
1	A	261	VAL	2.2
2	B	685	ALA	2.1
3	C	1097	ALA	2.1
3	C	1099	ASP	2.1
1	A	1349	PHE	2.1
1	A	1587	LEU	2.1
1	A	1319	VAL	2.1
2	B	903	SER	2.1
2	B	1065	ARG	2.1
2	B	915	ALA	2.1
3	C	1153	ALA	2.1
1	A	39	ASP	2.1
2	B	892	ASN	2.1
1	A	69	SER	2.1
1	A	1302	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1274	GLY	2.1
2	B	496	TRP	2.1
2	B	791	LEU	2.1
3	C	1204	LEU	2.1
2	B	673	SER	2.1
3	C	1057	TRP	2.1
2	B	467	CYS	2.1
3	C	1149	ASP	2.1
1	A	1665	ASN	2.1
1	A	96	GLY	2.1
2	B	624	ALA	2.1
2	B	732	ALA	2.1
3	C	1216	GLN	2.1
1	A	1582	PRO	2.1
1	A	1481	ARG	2.1
2	B	917	ASP	2.1
2	B	531	CYS	2.1
1	A	1489	TYR	2.1
1	A	1476	GLY	2.1
1	A	1753	ALA	2.1
3	C	1185	ILE	2.1
1	A	1410	VAL	2.1
1	A	1351	ASP	2.1
1	A	192	ASN	2.1
1	A	1594	ALA	2.1
2	B	814	ARG	2.0
1	A	218	ASP	2.0
2	B	552	ALA	2.0
2	B	669	ALA	2.0
2	B	960	PHE	2.0
1	A	1534	TRP	2.0
2	B	408	GLU	2.0
2	B	464	SER	2.0
3	C	968	MET	2.0
1	A	19	ASP	2.0
1	A	155	GLY	2.0
1	A	1756	ALA	2.0
3	C	1031	ASP	2.0
2	B	876	HIS	2.0
2	B	913	PRO	2.0
1	A	1575	THR	2.0
2	B	633	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	276	SER	2.0
2	B	671	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.