Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2022 – 06:25 pm GMT

PDB ID	:	7BII
Title	:	Crystal structure of Nematocida HUWE1
Authors	:	Grabarczyk, D.B.; Petrova, O.A.; Meinhart, A.; Kessler, D.; Clausen, T.
Deposited on	:	2021-01-12
Resolution	:	3.04 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 following versions of software and data (see references ⓘ) were used in the production of this report:

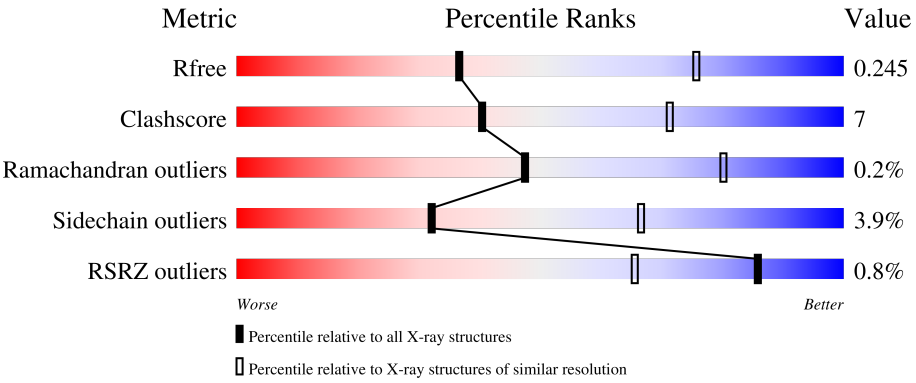
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.26
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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 3.04 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	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

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	2492	% 70% 15% · 14%
1	B	2492	% 69% 17% · 14%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 34901 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 E3 ubiquitin-protein ligase HUWE1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2143	Total	C	N	O	S	0	0	0
			17453	11280	2862	3213	98			
1	B	2144	Total	C	N	O	S	0	0	0
			17448	11273	2861	3216	98			

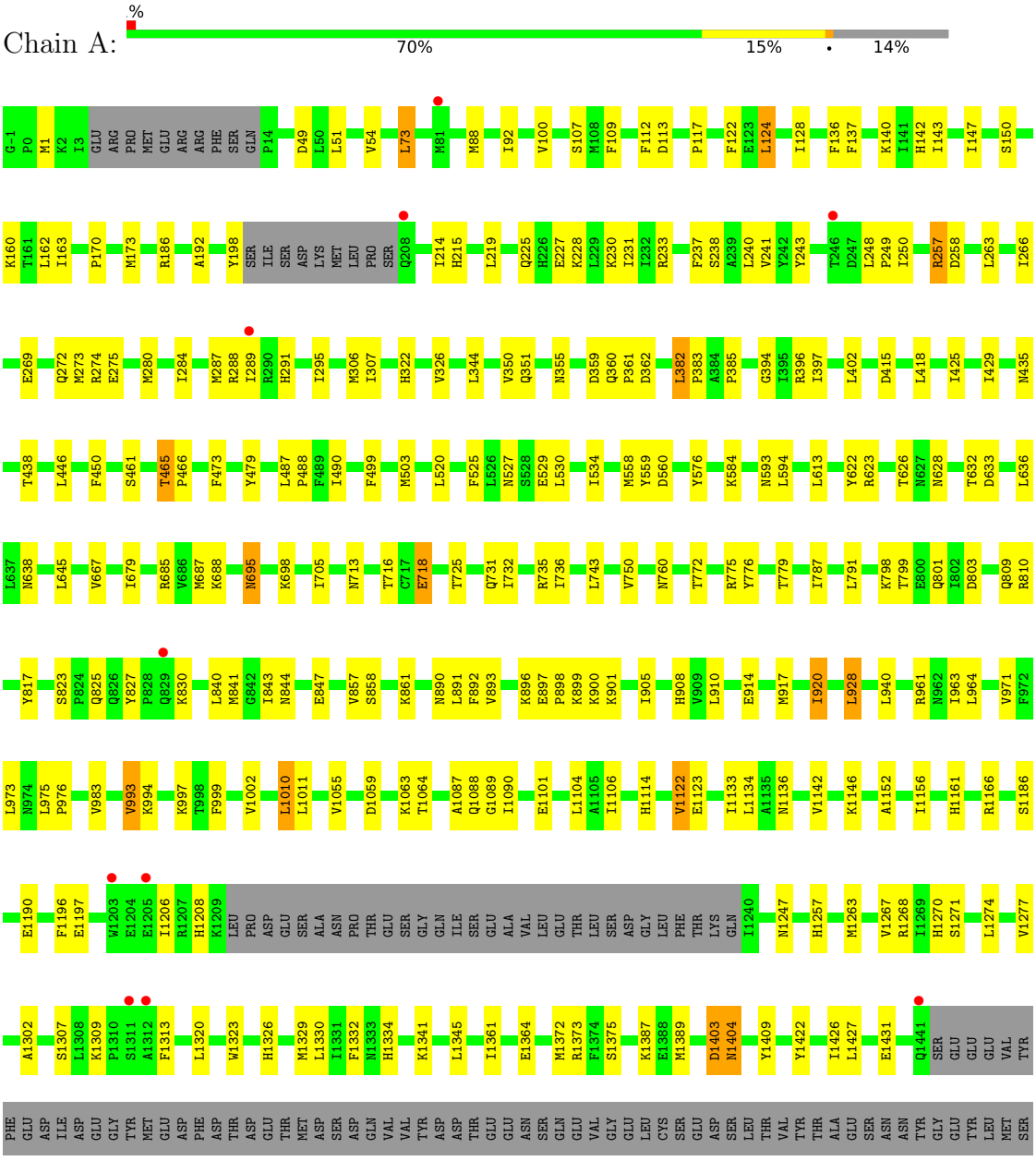
There are 6 discrepancies between the modelled and reference sequences:

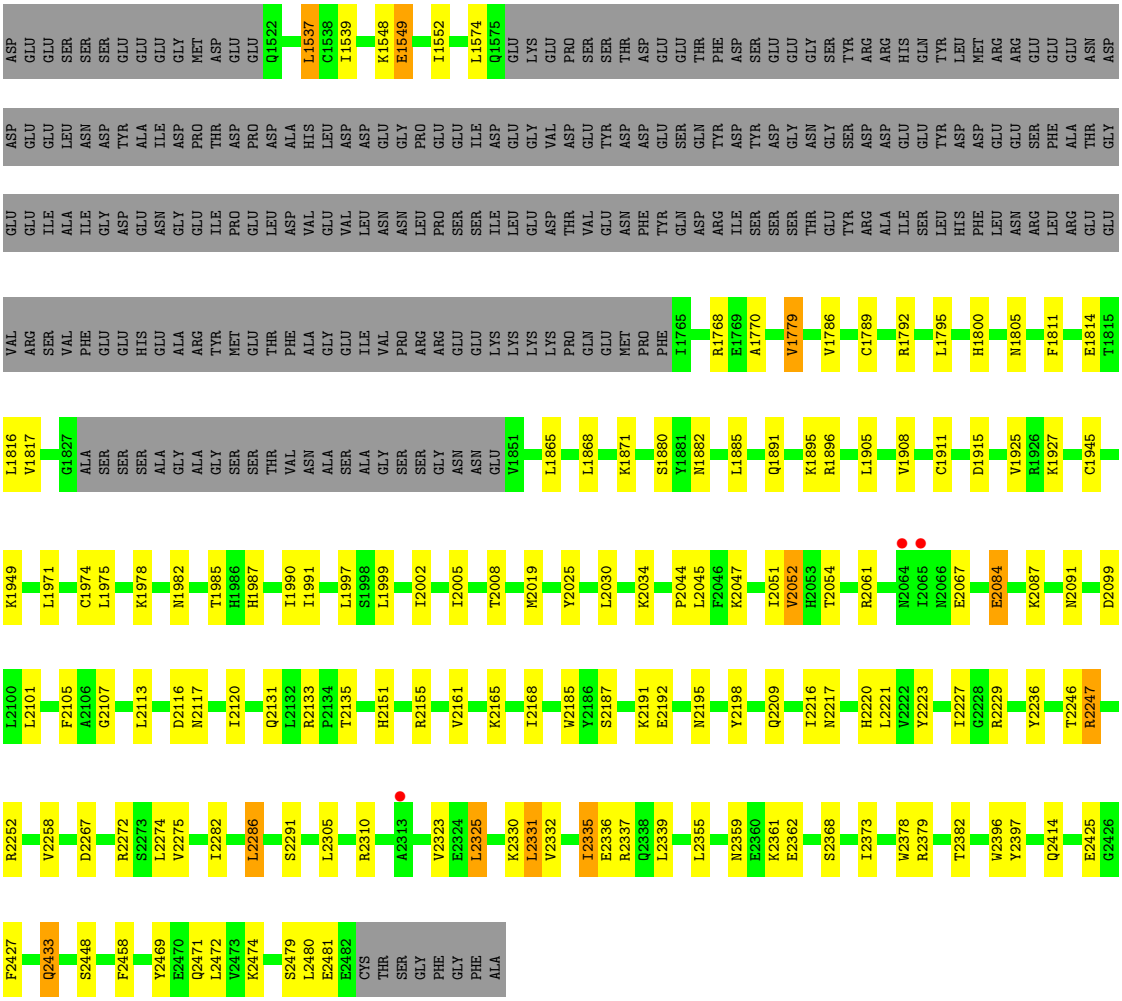
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A177ELV2
A	0	PRO	-	expression tag	UNP A0A177ELV2
A	2457	ALA	CYS	engineered mutation	UNP A0A177ELV2
B	-1	GLY	-	expression tag	UNP A0A177ELV2
B	0	PRO	-	expression tag	UNP A0A177ELV2
B	2457	ALA	CYS	engineered mutation	UNP A0A177ELV2

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.

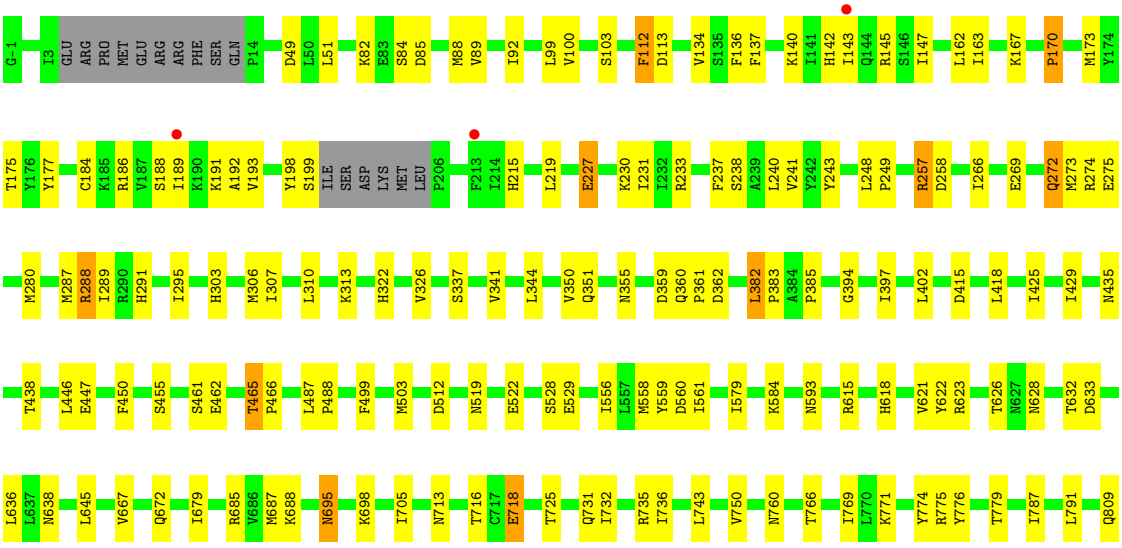
- Molecule 1: E3 ubiquitin-protein ligase HUWE1

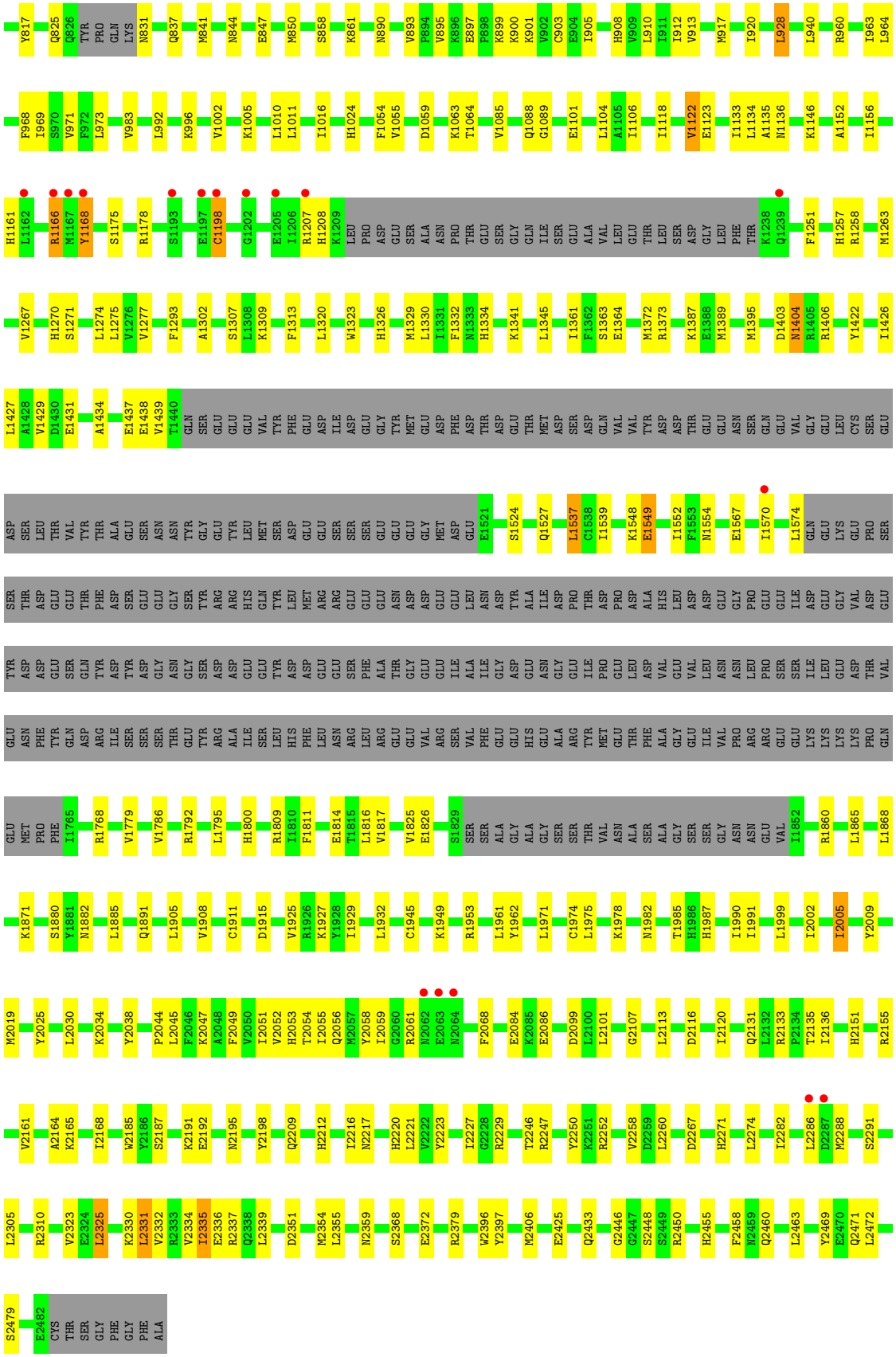




• Molecule 1: E3 ubiquitin-protein ligase HUWE1

Chain B:




Y817 Q825 Q826 TYR PRO GLN LYS N831 Q837 M841 N844 E847 M850 S858 K861 N890 V893 P894 V895 K896 E897 P898 K899 K900 K901 V902 C903 E904 I905 H908 V909 L910 I911 I912 V913 M917 I920 L928 L940 R960 I963 L964
F968 I969 S970 V971 F972 L973 V983 L992 K996 V1002 K1005 L1010 L1011 I1016 H1024 F1054 V1055 D1059 K1063 T1064 V1085 Q1088 G1089 E1101 L1104 A1105 I1106 I1118 V1122 E1123 I1133 L1134 A1135 N1136 K1146 A1152 I1156
H1161 L1162 R1166 M1167 Y1168 S1175 R1178 S1193 E1197 C1198 G1202 E1205 I1206 R1207 H1208 K1209 LEU PRO ASP GLU SER ALA ASN PRO THR GLU SER GLY GLN ILE SER GLU ALA VAL LEU GLU THR LEU SER ASP GLY LEU PHE THR K1238 Q1239 F1251 H1257 R1258 M1263
V1267 H1270 S1271 L1274 L1275 V1276 V1277 F1293 A1302 S1307 L1308 K1309 F1313 L1320 W1323 H1326 M1329 L1330 I1331 F1332 N1333 H1334 K1341 L1345 I1361 F1362 S1363 E1364 M1372 R1373 K1387 E1388 M1389 M1395 D1403 N1404 R1405 R1406 Y1422 I1426
L1427 A1428 V1429 D1430 E1431 A1434 E1437 E1438 V1439 T1440 GLN SER GLU GLU GLU VAL TYR PHE GLU ASP ILE ASP GLU GLY TYR MET GLU ASP PHE ASP THR ASP GLU THR MET ASP SER ASP GLN VAL VAL TYR ASP ASP THR GLU GLU ASN SER GLN GLU VAL GLY GLU LEU GLU CYS SER GLU
ASP SER LEU THR VAL TYR THR ALA GLU SER ASN ASN TYR GLY GLU TYR LEU MET SER ASP GLU GLU SER SER GLU GLU GLY MET ASP GLU E1521 S1524 Q1527 L1537 C1538 I1539 K1548 E1549 I1552 F1553 N1554 E1567 I1570 L1574 GLN GLU LYS GLU PRO SER
SER THR ASP GLU GLU THR PHE ASP SER GLU GLU GLY SER TYR ARG ARG HIS GLN TYR LEU MET ARG ARG GLU GLU SER PRO THR ASP PRO ASP ALA HIS LEU ASP ASP GLU GLY PRO GLU GLU ILE ASP GLU GLY ASP GLU GLU LEU ASN ASP TYR ALA ILE ASP PRO ASP ALA HIS LEU ASP GLU GLY PRO GLU GLU ILE ASP GLU GLY ASP GLU GLU ILE ALA ILE ASP PRO ASP ALA VAL GLU VAL LEU ASN ASN LEU PRO SER SER ILE LEU LEU GLU ASP THR VAL
TYR ASP ASP GLU SER GLN ASP TYR ASP TYR ASP ASP GLY ASN GLY SER ASP TYR ASP GLU GLU SER PHE ALA THR GLY GLU GLU ILE ALA ILE ASP GLY ASP GLU ASN GLY GLU ILE PRO GLU GLU SER ASP GLU LEU ASP VAL GLU VAL LEU ASN ASN LEU PRO SER SER ILE LEU GLU GLU LYS LYS LYS LYS PRO GLN
GLU ASN PHE TYR GLN ASP ARG ILE SER SER SER THR GLU TYR ARG ALA ILE SER LEU HIS PHE LEU GLU ASN ARG LEU ARG GLU GLU VAL ARG SER VAL PHE GLU GLU VAL LEU ILE ALA THR PHE ALA GLY GLU ILE VAL PRO ARG ARG GLU GLU GLU LYS LYS LYS LYS PRO GLN
GLU MET PRO PHE I1765 R1768 V1779 V1786 R1792 L1795 H1800 R1809 I1810 F1811 E1814 T1815 L1816 V1817 V1825 E1826 S1829 SER SER ALA GLY ALA GLY SER SER THR VAL ASN ALA SER ALA GLY SER SER GLY ASN ASN SER ALA GLY GLU ILE VAL PRO ARG ARG GLU GLU VAL I1852 R1860 L1865 L1868
K1871 S1880 Y1881 N1882 L1885 Q1891 L1905 V1908 C1911 D1915 V1925 R1926 K1927 Y1928 I1929 L1932 C1945 K1949 R1953 L1961 Y1962 L1971 C1974 L1975 K1978 N1982 T1985 H1986 H1987 I1990 I1991 L1999 I2002 I2005 Y2009
M2019 Y2025 L2030 K2034 Y2038 P2044 L2045 F2046 K2047 A2048 F2049 V2050 I2051 V2052 H2053 T2054 I2055 Q2056 M2057 Y2058 I2059 G2060 R2061 N2062 E2063 N2064 F2068 E2084 K2085 E2086 D2099 L2100 L2101 G2107 L2113 D2116 I2120 Q2131 L2132 R2133 P2134 T2135 I2136 H2151 R2155
V2161 A2164 K2165 I2168 W2185 Y2186 S2187 K2191 E2192 N2195 Y2198 Q2209 H2212 I2216 N2217 H2220 L2221 V2222 Y2223 I2227 G2228 R2229 T2246 R2247 Y2250 K2251 R2252 V2258 D2259 L2260 D2267 H2271 L2274 I2282 L2286 D2287 M2288 S2291
L2305 R2310 V2323 E2324 L2325 K2330 L2331 V2332 R2333 V2334 I2335 E2336 R2337 Q2338 L2339 D2351 M2364 L2355 N2369 S2368 E2372 R2379 W2396 Y2397 M2406 E2425 Q2433 G2446 G2447 S2448 S2449 R2450 H2455 F2458 N2459 Q2460 L2463 Y2469 E2470 Q2471 L2472
S2479 E2482 CYS THR SER GLY PHE GLY PHE ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	95.52Å 96.22Å 199.66Å 92.22° 100.45° 95.33°	Depositor
Resolution (Å)	196.03 – 3.04 196.03 – 3.04	Depositor EDS
% Data completeness (in resolution range)	56.3 (196.03-3.04) 56.3 (196.03-3.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.10.3 (6-FEB-2020)	Depositor
R, R_{free}	0.202 , 0.233 0.217 , 0.245	Depositor DCC
R_{free} test set	3733 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	75.9	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	34901	wwPDB-VP
Average B, all atoms (Å^2)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.33	0/17792	0.52	0/24002
1	B	0.32	0/17785	0.52	0/23989
All	All	0.32	0/35577	0.52	0/47991

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

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	17453	0	17745	251	0
1	B	17448	0	17737	252	0
All	All	34901	0	35482	503	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 7.

All (503) 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:1059:ASP:HA	1:A:1063:LYS:HB3	1.29	1.15
1:B:1059:ASP:HA	1:B:1063:LYS:HB3	1.28	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2282:ILE:HG12	1:A:2286:LEU:HG	1.33	1.05
1:A:225:GLN:HE21	1:A:228:LYS:NZ	1.55	1.03
1:A:1987:HIS:CE1	1:A:1991:ILE:HD11	1.97	0.99
1:B:1987:HIS:CE1	1:B:1991:ILE:HD11	1.97	0.99
1:A:731:GLN:HE21	1:A:735:ARG:HH21	1.10	0.96
1:B:825:GLN:HE21	1:B:831:ASN:HD21	1.09	0.93
1:B:731:GLN:HE21	1:B:735:ARG:HH21	1.11	0.92
1:B:858:SER:HA	1:B:861:LYS:HD2	1.56	0.88
1:B:1882:ASN:HB3	1:B:1885:LEU:HG	1.56	0.88
1:A:798:LYS:HE2	1:A:810:ARG:HE	1.39	0.87
1:A:225:GLN:HE21	1:A:228:LYS:HZ3	1.22	0.86
1:A:1882:ASN:HB3	1:A:1885:LEU:HG	1.58	0.86
1:B:825:GLN:HE21	1:B:831:ASN:ND2	1.73	0.85
1:A:858:SER:HA	1:A:861:LYS:HD2	1.56	0.85
1:A:1987:HIS:ND1	1:A:1991:ILE:HD11	1.92	0.85
1:A:248:LEU:HG	1:A:249:PRO:HD2	1.59	0.84
1:B:1987:HIS:ND1	1:B:1991:ILE:HD11	1.94	0.83
1:B:248:LEU:HG	1:B:249:PRO:HD2	1.59	0.82
1:A:2192:GLU:O	1:A:2195:ASN:HB2	1.79	0.81
1:A:2091:ASN:HD22	1:A:2117:ASN:HD22	1.27	0.81
1:B:731:GLN:NE2	1:B:735:ARG:HH21	1.78	0.81
1:A:731:GLN:NE2	1:A:735:ARG:HH21	1.79	0.80
1:A:695:ASN:HA	1:A:698:LYS:HD2	1.63	0.79
1:A:731:GLN:HE21	1:A:735:ARG:NH2	1.81	0.79
1:B:731:GLN:HE21	1:B:735:ARG:NH2	1.81	0.79
1:B:215:HIS:NE2	1:B:219:LEU:HD21	1.98	0.78
1:B:725:THR:HG22	1:B:787:ILE:HD11	1.66	0.78
1:A:215:HIS:NE2	1:A:219:LEU:HD21	1.98	0.78
1:B:695:ASN:HA	1:B:698:LYS:HD2	1.64	0.77
1:A:725:THR:HG22	1:A:787:ILE:HD11	1.67	0.77
1:A:1880:SER:HB3	1:A:1911:CYS:HB2	1.68	0.75
1:B:1880:SER:HB3	1:B:1911:CYS:HB2	1.67	0.74
1:A:2133:ARG:HH12	1:A:2236:TYR:HE2	1.37	0.73
1:B:973:LEU:HD21	1:B:1002:VAL:HG12	1.72	0.72
1:A:890:ASN:HB2	1:A:893:VAL:HB	1.70	0.72
1:B:269:GLU:O	1:B:274:ARG:HD2	1.89	0.71
1:A:973:LEU:HD21	1:A:1002:VAL:HG12	1.72	0.71
1:B:890:ASN:HB2	1:B:893:VAL:HB	1.72	0.71
1:A:225:GLN:NE2	1:A:228:LYS:HZ3	1.88	0.71
1:B:82:LYS:NZ	1:B:84:SER:HB3	2.06	0.70
1:A:743:LEU:HB3	1:A:750:VAL:HG21	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2030:LEU:HG	1:A:2034:LYS:HE3	1.73	0.70
1:A:1257:HIS:ND1	1:A:1268:ARG:NH2	2.40	0.69
1:B:2030:LEU:HG	1:B:2034:LYS:HE3	1.73	0.69
1:A:825:GLN:HE22	1:A:830:LYS:H	1.41	0.68
1:B:743:LEU:HB3	1:B:750:VAL:HG21	1.75	0.68
1:A:847:GLU:HA	1:A:908:HIS:CE1	2.29	0.67
1:B:175:THR:HG22	1:B:186:ARG:HG2	1.76	0.67
1:A:1982:ASN:HB3	1:A:1985:THR:HB	1.75	0.67
1:B:1982:ASN:HB3	1:B:1985:THR:HB	1.76	0.66
1:B:303:HIS:HD1	1:B:2038:TYR:HD2	1.43	0.66
1:B:685:ARG:HA	1:B:688:LYS:HE3	1.78	0.65
1:B:2192:GLU:O	1:B:2195:ASN:HB2	1.95	0.65
1:B:1990:ILE:HD12	1:B:2044:PRO:HB2	1.79	0.65
1:B:996:LYS:NZ	1:B:1024:HIS:HD2	1.95	0.65
1:A:1990:ILE:HD12	1:A:2044:PRO:HB2	1.77	0.65
1:B:2212:HIS:NE2	1:B:2334:VAL:HG11	2.11	0.64
1:A:685:ARG:HA	1:A:688:LYS:HE3	1.78	0.64
1:B:163:ILE:HD11	1:B:240:LEU:HD12	1.79	0.64
1:A:827:TYR:HD2	1:A:830:LYS:HB2	1.63	0.63
1:B:1258:ARG:HH22	1:B:1293:PHE:HD1	1.46	0.63
1:B:173:MET:HG3	1:B:188:SER:HA	1.80	0.63
1:B:303:HIS:ND1	1:B:2038:TYR:HD2	1.97	0.63
1:A:128:ILE:HD11	1:A:231:ILE:HG13	1.80	0.62
1:A:2161:VAL:HG11	1:A:2229:ARG:HD3	1.81	0.62
1:A:1257:HIS:CE1	1:A:1268:ARG:HH22	2.17	0.62
1:B:82:LYS:HZ2	1:B:84:SER:HB3	1.63	0.62
1:A:891:LEU:HG	1:A:892:PHE:HD1	1.65	0.62
1:B:844:ASN:HB3	1:B:847:GLU:HB3	1.82	0.62
1:A:163:ILE:HD11	1:A:240:LEU:HD12	1.81	0.61
1:B:429:ILE:HG13	1:B:450:PHE:CZ	2.35	0.61
1:B:1945:CYS:O	1:B:1949:LYS:HG3	2.00	0.61
1:A:920:ILE:HD11	1:A:975:LEU:HD11	1.82	0.61
1:A:2274:LEU:HD22	1:A:2323:VAL:HG22	1.83	0.61
1:B:2161:VAL:HG11	1:B:2229:ARG:HD3	1.81	0.61
1:B:1152:ALA:O	1:B:1156:ILE:HG12	2.01	0.61
1:A:275:GLU:CD	1:A:322:HIS:HD2	2.04	0.61
1:A:1186:SER:O	1:A:1190:GLU:HG2	2.01	0.61
1:B:1786:VAL:HG12	1:B:1795:LEU:HD22	1.83	0.61
1:A:844:ASN:HB3	1:A:847:GLU:HB3	1.83	0.60
1:A:1152:ALA:O	1:A:1156:ILE:HG12	2.01	0.60
1:A:1403:ASP:HA	1:A:1409:TYR:CE2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1101:GLU:HG2	1:A:1146:LYS:HG3	1.83	0.60
1:A:1786:VAL:HG12	1:A:1795:LEU:HD22	1.83	0.60
1:B:227:GLU:OE1	1:B:272:GLN:NE2	2.33	0.60
1:B:1101:GLU:HG2	1:B:1146:LYS:HG3	1.83	0.60
1:A:1789:CYS:O	1:A:1792:ARG:HD3	2.02	0.60
1:A:88:MET:O	1:A:92:ILE:HG12	2.02	0.59
1:B:771:LYS:O	1:B:775:ARG:HG2	2.02	0.59
1:B:858:SER:HA	1:B:861:LYS:CD	2.30	0.59
1:A:429:ILE:HG13	1:A:450:PHE:CZ	2.37	0.59
1:A:231:ILE:HG21	1:A:273:MET:HA	1.84	0.59
1:B:88:MET:O	1:B:92:ILE:HG12	2.02	0.59
1:B:100:VAL:HG23	1:B:136:PHE:HE2	1.68	0.58
1:B:2274:LEU:HD22	1:B:2323:VAL:HG22	1.84	0.58
1:A:993:VAL:HG22	1:A:999:PHE:HA	1.84	0.58
1:A:2223:TYR:O	1:A:2227:ILE:HG12	2.02	0.58
1:B:177:TYR:HB3	1:B:1406:ARG:HD3	1.84	0.58
1:A:269:GLU:O	1:A:274:ARG:HD2	2.03	0.58
1:A:858:SER:HA	1:A:861:LYS:CD	2.30	0.58
1:B:2252:ARG:HG2	1:B:2339:LEU:HG	1.86	0.57
1:A:288:ARG:HA	1:A:291:HIS:HD2	1.70	0.57
1:B:633:ASP:HB3	1:B:636:LEU:HB2	1.87	0.57
1:B:584:LYS:NZ	1:B:633:ASP:HB2	2.19	0.57
1:B:2221:LEU:HD21	1:B:2337:ARG:HB3	1.87	0.57
1:B:394:GLY:HA2	1:B:397:ILE:HD12	1.87	0.57
1:B:2168:ILE:HG21	1:B:2185:TRP:HB2	1.86	0.57
1:A:633:ASP:HB3	1:A:636:LEU:HB2	1.87	0.57
1:A:2221:LEU:HD21	1:A:2337:ARG:HB3	1.86	0.57
1:A:584:LYS:NZ	1:A:633:ASP:HB2	2.20	0.56
1:A:1332:PHE:HA	1:A:1341:LYS:HE2	1.86	0.56
1:A:2054:THR:HG23	1:A:2107:GLY:HA3	1.87	0.56
1:B:266:ILE:HA	1:B:274:ARG:HB2	1.86	0.56
1:A:394:GLY:HA2	1:A:397:ILE:HD12	1.88	0.56
1:A:2373:ILE:HD11	1:A:2427:PHE:HZ	1.70	0.56
1:A:225:GLN:HE21	1:A:228:LYS:HZ1	1.51	0.56
1:A:225:GLN:HG3	1:A:228:LYS:HZ3	1.69	0.56
1:A:1997:LEU:HD22	1:A:2052:VAL:HG13	1.86	0.56
1:A:2168:ILE:HG21	1:A:2185:TRP:HB2	1.86	0.56
1:A:892:PHE:HD2	1:A:961:ARG:HB3	1.70	0.56
1:B:1768:ARG:HH22	1:B:1800:HIS:CD2	2.24	0.56
1:A:898:PRO:HA	1:A:900:LYS:NZ	2.21	0.56
1:B:996:LYS:HZ1	1:B:1024:HIS:HD2	1.51	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2151:HIS:CE1	1:B:2155:ARG:HH21	2.24	0.56
1:B:2223:TYR:O	1:B:2227:ILE:HG12	2.05	0.56
1:A:225:GLN:CG	1:A:228:LYS:HZ3	2.19	0.56
1:A:1971:LEU:HD13	1:A:2019:MET:HG3	1.88	0.56
1:A:827:TYR:HB3	1:A:830:LYS:HD3	1.88	0.55
1:A:798:LYS:HE2	1:A:810:ARG:NE	2.18	0.55
1:A:1768:ARG:HH22	1:A:1800:HIS:CD2	2.24	0.55
1:B:1178:ARG:NH1	1:B:1554:ASN:ND2	2.54	0.55
1:B:1868:LEU:O	1:B:1871:LYS:O	2.24	0.55
1:B:1932:LEU:HD12	1:B:1962:TYR:HE2	1.71	0.55
1:A:2187:SER:O	1:A:2191:LYS:HG3	2.05	0.55
1:A:1868:LEU:O	1:A:1871:LYS:O	2.24	0.55
1:B:1971:LEU:HD13	1:B:2019:MET:HG3	1.89	0.55
1:B:2133:ARG:HH11	1:B:2165:LYS:HZ3	1.55	0.55
1:A:1895:LYS:NZ	1:A:1896:ARG:NH2	2.53	0.55
1:A:2151:HIS:CE1	1:A:2155:ARG:HH21	2.25	0.55
1:A:2291:SER:HB3	1:A:2310:ARG:HA	1.89	0.55
1:B:1326:HIS:NE2	1:B:1330:LEU:HD21	2.22	0.55
1:B:2291:SER:HB3	1:B:2310:ARG:HA	1.89	0.55
1:A:288:ARG:HA	1:A:291:HIS:CD2	2.42	0.54
1:B:920:ILE:HG21	1:B:928:LEU:HD12	1.89	0.54
1:B:2195:ASN:HB3	1:B:2198:TYR:HB2	1.90	0.54
1:B:1326:HIS:CD2	1:B:1330:LEU:HD23	2.42	0.54
1:A:1895:LYS:HZ1	1:A:1896:ARG:NH2	2.06	0.54
1:A:2195:ASN:HB3	1:A:2198:TYR:HB2	1.90	0.54
1:B:415:ASP:HB3	1:B:418:LEU:HB3	1.90	0.54
1:B:2187:SER:O	1:B:2191:LYS:HG2	2.08	0.54
1:A:718:GLU:CD	1:A:718:GLU:H	2.11	0.54
1:A:898:PRO:HA	1:A:900:LYS:HZ3	1.73	0.54
1:B:275:GLU:CD	1:B:322:HIS:HD2	2.11	0.54
1:A:382:LEU:O	1:A:385:PRO:HD2	2.08	0.53
1:B:382:LEU:O	1:B:385:PRO:HD2	2.08	0.53
1:B:556:ILE:O	1:B:559:TYR:O	2.26	0.53
1:B:2209:GLN:HB3	1:B:2246:THR:CG2	2.38	0.53
1:A:638:ASN:HB2	1:A:667:VAL:HG11	1.90	0.53
1:A:1161:HIS:CD2	1:A:1208:HIS:NE2	2.77	0.53
1:B:731:GLN:NE2	1:B:735:ARG:NH2	2.49	0.53
1:B:1161:HIS:NE2	1:B:1208:HIS:CE1	2.76	0.53
1:A:122:PHE:HE1	1:A:214:ILE:HG23	1.72	0.53
1:B:1002:VAL:HG23	1:B:1011:LEU:HD11	1.90	0.53
1:A:1330:LEU:HD22	1:A:1334:HIS:CD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:LYS:HG2	1:B:193:VAL:HG22	1.90	0.53
1:B:718:GLU:HB3	1:B:776:TYR:OH	2.09	0.53
1:A:2209:GLN:HB3	1:A:2246:THR:CG2	2.39	0.53
1:B:2005:ILE:HG13	1:B:2009:TYR:HB2	1.91	0.52
1:A:731:GLN:NE2	1:A:735:ARG:NH2	2.50	0.52
1:B:1345:LEU:HD13	1:B:1389:MET:HG3	1.91	0.52
1:A:983:VAL:HG12	1:A:983:VAL:O	2.10	0.52
1:A:1197:GLU:HA	1:A:1208:HIS:CD2	2.44	0.52
1:B:435:ASN:HD22	1:B:438:THR:H	1.58	0.52
1:A:415:ASP:HB3	1:A:418:LEU:HB3	1.90	0.52
1:B:303:HIS:ND1	1:B:2038:TYR:CD2	2.72	0.52
1:A:1891:GLN:HG2	1:A:1927:LYS:NZ	2.25	0.52
1:B:718:GLU:H	1:B:718:GLU:CD	2.12	0.52
1:B:1270:HIS:NE2	1:B:1274:LEU:HD11	2.25	0.51
1:A:840:LEU:HD23	1:A:843:ILE:HD11	1.93	0.51
1:B:2054:THR:HG23	1:B:2107:GLY:HA3	1.91	0.51
1:A:160:LYS:HA	1:A:163:ILE:HG12	1.92	0.51
1:A:1307:SER:HB2	1:A:1364:GLU:OE2	2.10	0.51
1:A:1345:LEU:HD13	1:A:1389:MET:HG3	1.92	0.51
1:A:2133:ARG:NH1	1:A:2236:TYR:HE2	2.08	0.51
1:B:1891:GLN:HG2	1:B:1927:LYS:NZ	2.26	0.51
1:B:1953:ARG:HD3	1:B:2061:ARG:HD2	1.92	0.51
1:A:718:GLU:HB3	1:A:776:TYR:OH	2.10	0.51
1:A:192:ALA:HA	1:A:198:TYR:HD1	1.76	0.51
1:A:284:ILE:HG23	1:A:289:ILE:HG23	1.92	0.51
1:A:1002:VAL:HG23	1:A:1011:LEU:HD11	1.92	0.51
1:B:983:VAL:HG12	1:B:983:VAL:O	2.11	0.51
1:B:1422:TYR:CE2	1:B:1426:ILE:HD11	2.45	0.51
1:B:2260:LEU:HG	1:B:2271:HIS:CE1	2.46	0.51
1:B:638:ASN:HB2	1:B:667:VAL:HG11	1.92	0.51
1:B:1326:HIS:ND1	1:B:1329:MET:HE3	2.25	0.51
1:B:1175:SER:HA	1:B:1178:ARG:HG3	1.91	0.51
1:B:1949:LYS:HG2	1:B:2002:ILE:HG21	1.93	0.51
1:B:2135:THR:HA	1:B:2165:LYS:HB2	1.93	0.51
1:B:973:LEU:HB3	1:B:1005:LYS:HD2	1.91	0.51
1:A:823:SER:OG	1:A:830:LYS:O	2.29	0.51
1:B:766:THR:HA	1:B:769:ILE:HG12	1.93	0.51
1:B:913:VAL:O	1:B:917:MET:HG3	2.10	0.51
1:A:1270:HIS:NE2	1:A:1274:LEU:HD11	2.26	0.50
1:A:2252:ARG:HG2	1:A:2339:LEU:HG	1.93	0.50
1:B:499:PHE:O	1:B:503:MET:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:TYR:HD1	1:B:184:CYS:HB3	1.76	0.50
1:B:2209:GLN:HB3	1:B:2246:THR:HG21	1.93	0.50
1:A:250:ILE:HD13	1:A:289:ILE:HD11	1.92	0.50
1:B:215:HIS:CD2	1:B:219:LEU:HD21	2.47	0.50
1:A:2135:THR:HA	1:A:2165:LYS:HB2	1.94	0.50
1:A:1142:VAL:O	1:A:1247:ASN:OD1	2.29	0.50
1:A:1257:HIS:CE1	1:A:1268:ARG:NH2	2.78	0.50
1:A:435:ASN:HD22	1:A:438:THR:H	1.58	0.50
1:A:791:LEU:HB3	1:A:817:TYR:CE2	2.47	0.50
1:B:687:MET:HE3	1:B:736:ILE:HG12	1.92	0.50
1:A:402:LEU:HB2	1:A:425:ILE:HG21	1.93	0.50
1:A:2209:GLN:HB3	1:A:2246:THR:HG21	1.94	0.50
1:B:2335:ILE:HG23	1:B:2339:LEU:HD23	1.94	0.50
1:B:1307:SER:HB2	1:B:1364:GLU:OE2	2.11	0.49
1:B:713:ASN:ND2	1:B:716:THR:OG1	2.46	0.49
1:B:1002:VAL:CG2	1:B:1011:LEU:HD11	2.43	0.49
1:A:1088:GLN:HE21	1:A:1114:HIS:HE1	1.60	0.49
1:A:1323:TRP:NE1	1:A:1537:LEU:CD1	2.75	0.49
1:A:2378:TRP:O	1:A:2382:THR:OG1	2.29	0.49
1:B:2247:ARG:NH1	1:B:2250:TYR:CD2	2.80	0.49
1:A:2335:ILE:HG23	1:A:2339:LEU:HD23	1.94	0.49
1:B:1277:VAL:HG22	1:B:1334:HIS:CE1	2.46	0.49
1:A:791:LEU:HB3	1:A:817:TYR:HE2	1.77	0.49
1:A:1326:HIS:ND1	1:A:1329:MET:HE3	2.28	0.49
1:B:192:ALA:HA	1:B:198:TYR:HD2	1.77	0.49
1:B:465:THR:HG22	1:B:466:PRO:HD2	1.94	0.49
1:B:1104:LEU:HD11	1:B:1106:ILE:HD12	1.94	0.49
1:B:1332:PHE:HA	1:B:1341:LYS:HE2	1.95	0.49
1:A:1949:LYS:HG2	1:A:2002:ILE:HG21	1.94	0.49
1:B:167:LYS:HD2	1:B:170:PRO:HB3	1.94	0.49
1:B:2049:PHE:O	1:B:2053:HIS:HD2	1.96	0.49
1:A:124:LEU:HD22	1:A:225:GLN:HB3	1.95	0.49
1:A:359:ASP:O	1:A:361:PRO:HD3	2.12	0.49
1:B:928:LEU:HD13	1:B:971:VAL:HG11	1.94	0.49
1:A:107:SER:HB3	1:A:147:ILE:HG22	1.93	0.49
1:A:1309:LYS:HZ3	1:A:1313:PHE:HE1	1.60	0.49
1:B:359:ASP:O	1:B:361:PRO:HD3	2.13	0.49
1:B:1089:GLY:HA3	1:B:1134:LEU:HD21	1.95	0.49
1:A:760:ASN:HD21	1:A:809:GLN:HE21	1.60	0.48
1:A:465:THR:HG22	1:A:466:PRO:HD2	1.96	0.48
1:A:687:MET:HE3	1:A:736:ILE:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2247:ARG:HA	1:A:2247:ARG:HD3	1.61	0.48
1:B:402:LEU:HB2	1:B:425:ILE:HG21	1.94	0.48
1:A:525:PHE:HB3	1:A:576:TYR:CE1	2.48	0.48
1:B:99:LEU:O	1:B:103:SER:OG	2.24	0.48
1:B:1133:ILE:HD13	1:B:1548:LYS:HD2	1.95	0.48
1:B:1323:TRP:NE1	1:B:1537:LEU:CD1	2.76	0.48
1:A:230:LYS:O	1:A:233:ARG:HG2	2.13	0.48
1:A:1323:TRP:NE1	1:A:1537:LEU:HD12	2.29	0.48
1:A:382:LEU:HB3	1:A:385:PRO:CD	2.44	0.48
1:B:791:LEU:HB3	1:B:817:TYR:CE2	2.48	0.48
1:A:215:HIS:CD2	1:A:219:LEU:HD21	2.49	0.48
1:A:910:LEU:HD23	1:A:964:LEU:HD13	1.96	0.48
1:B:791:LEU:HB3	1:B:817:TYR:HE2	1.78	0.48
1:B:1816:LEU:HB3	1:B:1865:LEU:HG	1.96	0.48
1:A:1104:LEU:HD11	1:A:1106:ILE:HD12	1.95	0.48
1:B:382:LEU:HB3	1:B:385:PRO:CD	2.43	0.48
1:B:622:TYR:H	1:B:632:THR:HG21	1.79	0.48
1:B:1323:TRP:NE1	1:B:1537:LEU:HD12	2.29	0.48
1:B:1429:VAL:HG21	1:B:1437:GLU:HG3	1.94	0.48
1:A:225:GLN:NE2	1:A:228:LYS:NZ	2.39	0.48
1:A:1133:ILE:HD13	1:A:1548:LYS:HD2	1.96	0.48
1:A:928:LEU:HD13	1:A:971:VAL:HG11	1.96	0.47
1:A:1816:LEU:HB3	1:A:1865:LEU:HG	1.96	0.47
1:B:837:GLN:HG2	1:B:841:MET:HE2	1.96	0.47
1:A:266:ILE:HA	1:A:274:ARG:HB2	1.96	0.47
1:A:1010:LEU:HD23	1:A:1011:LEU:HD12	1.96	0.47
1:A:1277:VAL:HG22	1:A:1334:HIS:CE1	2.49	0.47
1:A:623:ARG:H	1:A:628:ASN:ND2	2.13	0.47
1:A:622:TYR:H	1:A:632:THR:HG21	1.79	0.47
1:B:230:LYS:O	1:B:233:ARG:HG2	2.14	0.47
1:B:760:ASN:HD21	1:B:809:GLN:HE21	1.61	0.47
1:B:1326:HIS:CD2	1:B:1330:LEU:CD2	2.97	0.47
1:A:1326:HIS:ND1	1:A:1329:MET:CE	2.78	0.47
1:A:2272:ARG:HA	1:A:2275:VAL:HG22	1.97	0.47
1:B:903:CYS:SG	1:B:960:ARG:NH2	2.87	0.47
1:B:1016:ILE:HG12	1:B:1054:PHE:CE1	2.50	0.47
1:B:615:ARG:NH2	1:B:618:HIS:ND1	2.60	0.47
1:B:910:LEU:HD23	1:B:964:LEU:HD13	1.97	0.47
1:B:1905:LEU:HA	1:B:1908:VAL:HB	1.97	0.47
1:A:2361:LYS:HD3	1:A:2414:GLN:HG3	1.96	0.47
1:B:2305:LEU:HD13	1:B:2325:LEU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:LEU:HB3	1:A:385:PRO:HD3	1.97	0.47
1:B:623:ARG:H	1:B:628:ASN:ND2	2.12	0.47
1:B:1326:HIS:ND1	1:B:1329:MET:CE	2.77	0.47
1:B:2059:ILE:HG23	1:B:2068:PHE:HB2	1.97	0.47
1:A:499:PHE:O	1:A:503:MET:HG2	2.15	0.46
1:B:1524:SER:HA	1:B:1527:GLN:HB3	1.97	0.46
1:B:238:SER:HB3	1:B:280:MET:HA	1.97	0.46
1:B:558:MET:SD	1:B:559:TYR:CE2	3.08	0.46
1:A:227:GLU:HB2	1:A:273:MET:SD	2.55	0.46
1:A:2047:LYS:O	1:A:2051:ILE:HG13	2.14	0.46
1:B:382:LEU:HB3	1:B:385:PRO:HD3	1.97	0.46
1:B:774:TYR:HD1	1:B:775:ARG:NH2	2.12	0.46
1:A:238:SER:HB3	1:A:280:MET:HA	1.96	0.46
1:A:487:LEU:N	1:A:488:PRO:HD2	2.31	0.46
1:A:840:LEU:HA	1:A:843:ILE:HG12	1.97	0.46
1:B:142:HIS:CE1	1:B:287:MET:CE	2.98	0.46
1:A:732:ILE:O	1:A:736:ILE:HG13	2.16	0.46
1:A:897:GLU:HB3	1:A:898:PRO:HD3	1.97	0.46
1:B:1161:HIS:CD2	1:B:1208:HIS:CE1	3.04	0.46
1:A:1002:VAL:CG2	1:A:1011:LEU:HD11	2.45	0.46
1:A:1323:TRP:HE1	1:A:1537:LEU:HD12	1.81	0.46
1:A:1905:LEU:HA	1:A:1908:VAL:HB	1.98	0.46
1:A:2084:GLU:HG2	1:A:2087:LYS:HD3	1.97	0.46
1:B:2101:LEU:HD21	1:B:2113:LEU:HD11	1.98	0.46
1:A:1087:ALA:HA	1:A:1090:ILE:HD12	1.98	0.46
1:B:645:LEU:HD13	1:B:705:ILE:HG21	1.97	0.46
1:B:732:ILE:O	1:B:736:ILE:HG13	2.16	0.46
1:B:1330:LEU:CD1	1:B:1334:HIS:CD2	2.99	0.46
1:B:2463:LEU:HD21	1:B:2472:LEU:HD11	1.97	0.46
1:A:73:LEU:HD12	1:A:117:PRO:HG3	1.97	0.45
1:A:1330:LEU:CD2	1:A:1334:HIS:CD2	2.99	0.45
1:A:351:GLN:O	1:A:355:ASN:OD1	2.33	0.45
1:A:1975:LEU:HD22	1:A:1978:LYS:HD3	1.97	0.45
1:B:847:GLU:HA	1:B:908:HIS:CE1	2.51	0.45
1:B:1882:ASN:CB	1:B:1885:LEU:HG	2.39	0.45
1:A:100:VAL:HG23	1:A:136:PHE:HE1	1.81	0.45
1:A:2433:GLN:H	1:A:2433:GLN:HG3	1.60	0.45
1:B:257:ARG:HG3	1:B:258:ASP:N	2.32	0.45
1:B:351:GLN:O	1:B:355:ASN:OD1	2.33	0.45
1:B:1363:SER:HB3	1:B:1395:MET:HE1	1.99	0.45
1:B:1123:GLU:HA	1:B:1263:MET:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:HIS:CE1	1:A:287:MET:CE	2.99	0.45
1:A:291:HIS:CE1	1:A:295:ILE:HD11	2.51	0.45
1:A:2305:LEU:HD13	1:A:2325:LEU:HB3	1.97	0.45
1:B:1161:HIS:CE1	1:B:1208:HIS:CE1	3.05	0.45
1:B:1323:TRP:HE1	1:B:1537:LEU:HD12	1.82	0.45
1:B:1975:LEU:HD22	1:B:1978:LYS:HD3	1.97	0.45
1:A:645:LEU:HD13	1:A:705:ILE:HG21	1.97	0.45
1:B:996:LYS:NZ	1:B:1024:HIS:CD2	2.80	0.45
1:B:1198:CYS:SG	1:B:1208:HIS:CD2	3.10	0.45
1:B:969:ILE:HD11	1:B:992:LEU:HD13	1.99	0.45
1:B:1768:ARG:O	1:B:1809:ARG:NH2	2.50	0.45
1:A:713:ASN:ND2	1:A:716:THR:OG1	2.50	0.45
1:A:844:ASN:HD21	1:A:901:LYS:HZ2	1.65	0.45
1:A:772:THR:HG22	1:A:775:ARG:HH11	1.82	0.44
1:B:1166:ARG:H	1:B:1166:ARG:HG3	1.60	0.44
1:A:1549:GLU:O	1:A:1552:ILE:HG12	2.18	0.44
1:B:291:HIS:CE1	1:B:295:ILE:HD11	2.52	0.44
1:A:2448:SER:HB2	1:A:2471:GLN:OE1	2.17	0.44
1:B:1426:ILE:HG23	1:B:1434:ALA:HB1	1.98	0.44
1:B:2334:VAL:O	1:B:2335:ILE:HD12	2.16	0.44
1:A:257:ARG:HG3	1:A:258:ASP:N	2.32	0.44
1:B:487:LEU:N	1:B:488:PRO:HD2	2.32	0.44
1:B:2056:GLN:HB2	1:B:2058:TYR:CE1	2.53	0.44
1:A:801:GLN:NE2	1:A:810:ARG:NH2	2.66	0.44
1:A:1945:CYS:O	1:A:1949:LYS:HG3	2.18	0.44
1:B:288:ARG:HA	1:B:291:HIS:CD2	2.52	0.44
1:B:910:LEU:HD13	1:B:963:ILE:HD11	1.98	0.44
1:A:109:PHE:O	1:A:150:SER:OG	2.36	0.44
1:A:2101:LEU:HD21	1:A:2113:LEU:HD11	2.00	0.44
1:A:350:VAL:HG21	1:A:385:PRO:HB3	2.00	0.44
1:B:2448:SER:HB2	1:B:2471:GLN:OE1	2.17	0.44
1:A:173:MET:HB3	1:A:186:ARG:HB2	2.00	0.44
1:B:2258:VAL:HG21	1:B:2331:LEU:HD11	1.99	0.44
1:B:1549:GLU:O	1:B:1552:ILE:HG12	2.18	0.44
1:A:910:LEU:HD13	1:A:963:ILE:HD11	1.99	0.43
1:A:827:TYR:CD2	1:A:830:LYS:HB2	2.49	0.43
1:A:1895:LYS:HZ2	1:A:1896:ARG:CZ	2.31	0.43
1:B:2052:VAL:HG23	1:B:2053:HIS:CD2	2.53	0.43
1:B:2212:HIS:NE2	1:B:2334:VAL:CG1	2.78	0.43
1:B:2332:VAL:O	1:B:2336:GLU:HB2	2.18	0.43
1:B:2396:TRP:CD1	1:B:2469:TYR:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2025:TYR:CZ	1:A:2045:LEU:HD13	2.54	0.43
1:B:825:GLN:NE2	1:B:831:ASN:ND2	2.53	0.43
1:A:1422:TYR:O	1:A:1426:ILE:HG12	2.18	0.43
1:B:350:VAL:HG21	1:B:385:PRO:HB3	2.00	0.43
1:B:1929:ILE:HG13	1:B:1962:TYR:CD2	2.53	0.43
1:B:2133:ARG:HD3	1:B:2165:LYS:HZ3	1.83	0.43
1:A:225:GLN:HG3	1:A:228:LYS:NZ	2.33	0.43
1:B:162:LEU:HD23	1:B:215:HIS:CE1	2.54	0.43
1:B:1309:LYS:NZ	1:B:1313:PHE:HE1	2.16	0.43
1:A:558:MET:SD	1:A:559:TYR:CE1	3.12	0.43
1:A:891:LEU:HG	1:A:892:PHE:CD1	2.49	0.43
1:A:2116:ASP:O	1:A:2120:ILE:HG13	2.18	0.43
1:A:162:LEU:HD23	1:A:215:HIS:CE1	2.54	0.43
1:A:1403:ASP:HA	1:A:1409:TYR:HE2	1.83	0.43
1:A:2332:VAL:O	1:A:2336:GLU:HB2	2.19	0.43
1:B:2025:TYR:CZ	1:B:2045:LEU:HD13	2.54	0.43
1:B:2116:ASP:O	1:B:2120:ILE:HG13	2.18	0.43
1:A:215:HIS:O	1:A:219:LEU:HG	2.19	0.43
1:A:1122:VAL:HG11	1:A:1267:VAL:HG21	2.00	0.43
1:A:1309:LYS:NZ	1:A:1313:PHE:HE1	2.17	0.43
1:B:2446:GLY:HA3	1:B:2450:ARG:HD2	2.01	0.43
1:A:1123:GLU:HA	1:A:1263:MET:HG2	2.00	0.43
1:B:215:HIS:O	1:B:219:LEU:HG	2.19	0.43
1:B:1085:VAL:HA	1:B:1088:GLN:HE21	1.84	0.43
1:A:140:LYS:HD3	1:A:143:ILE:HD12	2.01	0.42
1:A:1999:LEU:HD23	1:A:2002:ILE:HD12	2.00	0.42
1:A:2396:TRP:CD1	1:A:2469:TYR:HB2	2.54	0.42
1:B:188:SER:O	1:B:199:SER:O	2.37	0.42
1:B:382:LEU:HG	1:B:383:PRO:HD2	2.01	0.42
1:B:2047:LYS:O	1:B:2051:ILE:HG13	2.19	0.42
1:A:382:LEU:HG	1:A:383:PRO:HD2	2.01	0.42
1:A:1891:GLN:CG	1:A:1927:LYS:NZ	2.82	0.42
1:B:307:ILE:HD13	1:B:344:LEU:HD21	2.01	0.42
1:A:49:ASP:HB3	1:A:51:LEU:HD12	2.01	0.42
1:A:892:PHE:CD2	1:A:961:ARG:HB3	2.52	0.42
1:A:1330:LEU:HD23	1:A:1330:LEU:HA	1.96	0.42
1:B:584:LYS:HZ2	1:B:633:ASP:HB2	1.84	0.42
1:B:1891:GLN:CG	1:B:1927:LYS:NZ	2.83	0.42
1:A:248:LEU:HG	1:A:249:PRO:CD	2.40	0.42
1:A:527:ASN:HB3	1:A:530:LEU:HG	2.02	0.42
1:A:890:ASN:HB2	1:A:893:VAL:CB	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:896:LYS:HA	1:A:899:LYS:HE3	2.00	0.42
1:B:556:ILE:HA	1:B:561:ILE:HB	2.01	0.42
1:B:841:MET:HG2	1:B:905:ILE:HD11	2.00	0.42
1:B:2286:LEU:HG	1:B:2288:MET:HB2	2.00	0.42
1:A:360:GLN:HE21	1:A:362:ASP:HB2	1.85	0.42
1:B:1429:VAL:HG12	1:B:1431:GLU:HG2	2.00	0.42
1:B:82:LYS:HZ1	1:B:84:SER:HB3	1.81	0.42
1:B:1118:ILE:HG21	1:B:1135:ALA:HB2	2.01	0.42
1:B:1567:GLU:HA	1:B:1570:ILE:HD12	2.01	0.42
1:B:2030:LEU:CG	1:B:2034:LYS:HE3	2.47	0.42
1:A:1302:ALA:HA	1:A:1361:ILE:HG21	2.01	0.42
1:A:2258:VAL:HG21	1:A:2331:LEU:HD11	2.01	0.42
1:B:237:PHE:O	1:B:241:VAL:HG23	2.20	0.42
1:B:288:ARG:HH11	1:B:337:SER:HB2	1.84	0.42
1:B:1330:LEU:CD1	1:B:1334:HIS:NE2	2.83	0.42
1:B:519:ASN:O	1:B:522:GLU:HG2	2.20	0.42
1:B:2372:GLU:HA	1:B:2406:MET:CG	2.50	0.42
1:A:1136:ASN:HD21	1:A:1271:SER:HA	1.85	0.41
1:B:140:LYS:HD3	1:B:143:ILE:HD12	2.02	0.41
1:B:360:GLN:HE21	1:B:362:ASP:HB2	1.85	0.41
1:B:1122:VAL:HG11	1:B:1267:VAL:HG21	2.02	0.41
1:B:2282:ILE:HD13	1:B:2282:ILE:HA	1.96	0.41
1:B:2397:TYR:HA	1:B:2472:LEU:HD21	2.02	0.41
1:A:307:ILE:HD13	1:A:344:LEU:HD21	2.01	0.41
1:A:479:TYR:CD2	1:A:490:ILE:HD11	2.54	0.41
1:A:1059:ASP:HA	1:A:1063:LYS:CB	2.21	0.41
1:B:1059:ASP:HA	1:B:1063:LYS:CB	2.21	0.41
1:B:1136:ASN:HD21	1:B:1271:SER:HA	1.85	0.41
1:A:128:ILE:CD1	1:A:231:ILE:HG13	2.47	0.41
1:A:844:ASN:HD21	1:A:901:LYS:NZ	2.18	0.41
1:A:1330:LEU:CD2	1:A:1334:HIS:NE2	2.83	0.41
1:A:2061:ARG:HG3	1:A:2067:GLU:HG2	2.02	0.41
1:B:49:ASP:HB3	1:B:51:LEU:HD12	2.02	0.41
1:B:1999:LEU:HD23	1:B:2002:ILE:HD12	2.01	0.41
1:B:2455:HIS:HB2	1:B:2460:GLN:HB3	2.01	0.41
1:A:584:LYS:HZ1	1:A:633:ASP:HB2	1.85	0.41
1:A:1770:ALA:O	1:A:1805:ASN:HB3	2.20	0.41
1:B:579:ILE:H	1:B:579:ILE:HG13	1.75	0.41
1:B:1792:ARG:HH21	1:B:1860:ARG:NE	2.19	0.41
1:A:1387:LYS:HG3	1:A:1427:LEU:HD13	2.02	0.41
1:A:2335:ILE:HG23	1:A:2335:ILE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2397:TYR:HA	1:A:2472:LEU:HD21	2.02	0.41
1:A:798:LYS:HG2	1:A:810:ARG:NE	2.35	0.41
1:A:1814:GLU:HA	1:A:1817:VAL:HG12	2.03	0.41
1:B:288:ARG:HA	1:B:291:HIS:HD2	1.84	0.41
1:B:2335:ILE:HG23	1:B:2335:ILE:O	2.21	0.41
1:A:237:PHE:O	1:A:241:VAL:HG23	2.20	0.41
1:A:685:ARG:HA	1:A:688:LYS:CE	2.48	0.41
1:A:2267:ASP:HB2	1:A:2330:LYS:NZ	2.36	0.41
1:B:112:PHE:CE1	1:B:134:VAL:HG22	2.56	0.41
1:B:310:LEU:HD12	1:B:313:LYS:HD2	2.03	0.41
1:B:895:VAL:HG12	1:B:897:GLU:H	1.86	0.41
1:B:928:LEU:HD22	1:B:968:PHE:HD1	1.85	0.41
1:A:1089:GLY:HA3	1:A:1134:LEU:HD21	2.02	0.41
1:A:2030:LEU:CG	1:A:2034:LYS:HE3	2.48	0.41
1:B:140:LYS:HB2	1:B:147:ILE:HD13	2.03	0.41
1:B:685:ARG:HA	1:B:688:LYS:CE	2.49	0.41
1:B:844:ASN:HD21	1:B:901:LYS:HZ2	1.67	0.41
1:B:1302:ALA:HA	1:B:1361:ILE:HG21	2.02	0.41
1:B:1811:PHE:HA	1:B:1814:GLU:HG2	2.03	0.41
1:A:594:LEU:HD22	1:A:613:LEU:HD22	2.02	0.41
1:A:798:LYS:CE	1:A:810:ARG:HE	2.21	0.41
1:A:914:GLU:HA	1:A:917:MET:HE3	2.03	0.41
1:B:85:ASP:O	1:B:89:VAL:HG12	2.21	0.41
1:B:231:ILE:HG21	1:B:273:MET:HA	2.03	0.41
1:B:1404:ASN:HD22	1:B:1404:ASN:HA	1.78	0.40
1:B:2051:ILE:O	1:B:2055:ILE:HG13	2.20	0.40
1:A:479:TYR:HD2	1:A:490:ILE:HD11	1.86	0.40
1:A:799:THR:HG22	1:A:810:ARG:HD2	2.03	0.40
1:B:2267:ASP:HB2	1:B:2330:LYS:NZ	2.36	0.40
1:B:2351:ASP:HB3	1:B:2354:MET:HB2	2.03	0.40
1:A:162:LEU:HD23	1:A:215:HIS:ND1	2.36	0.40
1:A:844:ASN:ND2	1:A:901:LYS:NZ	2.69	0.40
1:A:2359:ASN:HB3	1:A:2362:GLU:H	1.86	0.40
1:A:2474:LYS:HD3	1:A:2474:LYS:HA	1.83	0.40
1:B:142:HIS:ND1	1:B:287:MET:HE3	2.36	0.40
1:B:844:ASN:HD21	1:B:901:LYS:NZ	2.19	0.40
1:B:1387:LYS:HG3	1:B:1427:LEU:HD13	2.02	0.40
1:B:1814:GLU:HA	1:B:1817:VAL:HG12	2.03	0.40
1:B:2136:ILE:HG12	1:B:2164:ALA:HB1	2.04	0.40
1:A:1:MET:SD	1:A:54:VAL:HG12	2.62	0.40
1:A:142:HIS:ND1	1:A:287:MET:CE	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:841:MET:HG2	1:A:905:ILE:HD11	2.03	0.40
1:A:1404:ASN:HD22	1:A:1404:ASN:HA	1.76	0.40
1:B:621:VAL:HB	1:B:632:THR:HG22	2.03	0.40
1:B:850:MET:HA	1:B:912:ILE:HG12	2.03	0.40
1:B:1825:VAL:HG23	1:B:1826:GLU:HG3	2.03	0.40
1:A:473:PHE:CD1	1:A:520:LEU:HD22	2.56	0.40
1:A:525:PHE:HE1	1:A:534:ILE:HG21	1.87	0.40
1:A:1779:VAL:CG2	1:A:1811:PHE:HD2	2.34	0.40
1:B:1251:PHE:HD2	1:B:1275:LEU:HD13	1.86	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	2129/2492 (85%)	2019 (95%)	106 (5%)	4 (0%)	47 80
1	B	2128/2492 (85%)	2011 (94%)	112 (5%)	5 (0%)	47 80
All	All	4257/4984 (85%)	4030 (95%)	218 (5%)	9 (0%)	47 80

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1064	THR
1	B	1064	THR
1	A	170	PRO
1	A	2481	GLU
1	B	170	PRO
1	B	1168	TYR
1	B	1207	ARG
1	B	243	TYR
1	A	243	TYR

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	1955/2267 (86%)	1879 (96%)	76 (4%)	32	66
1	B	1955/2267 (86%)	1878 (96%)	77 (4%)	32	66
All	All	3910/4534 (86%)	3757 (96%)	153 (4%)	32	66

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	LEU
1	A	112	PHE
1	A	113	ASP
1	A	124	LEU
1	A	137	PHE
1	A	257	ARG
1	A	263	LEU
1	A	272	GLN
1	A	306	MET
1	A	326	VAL
1	A	382	LEU
1	A	396	ARG
1	A	446	LEU
1	A	461	SER
1	A	465	THR
1	A	529	GLU
1	A	560	ASP
1	A	593	ASN
1	A	626	THR
1	A	679	ILE
1	A	695	ASN
1	A	718	GLU
1	A	779	THR
1	A	803	ASP
1	A	857	VAL
1	A	920	ILE
1	A	928	LEU

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Mol	Chain	Res	Type
1	A	940	LEU
1	A	976	PRO
1	A	993	VAL
1	A	994	LYS
1	A	997	LYS
1	A	1010	LEU
1	A	1055	VAL
1	A	1122	VAL
1	A	1166	ARG
1	A	1196	PHE
1	A	1206	ILE
1	A	1320	LEU
1	A	1372	MET
1	A	1373	ARG
1	A	1375	SER
1	A	1403	ASP
1	A	1404	ASN
1	A	1431	GLU
1	A	1537	LEU
1	A	1539	ILE
1	A	1549	GLU
1	A	1574	LEU
1	A	1779	VAL
1	A	1915	ASP
1	A	1925	VAL
1	A	1974	CYS
1	A	2005	ILE
1	A	2008	THR
1	A	2052	VAL
1	A	2084	GLU
1	A	2099	ASP
1	A	2105	PHE
1	A	2131	GLN
1	A	2216	ILE
1	A	2217	ASN
1	A	2220	HIS
1	A	2247	ARG
1	A	2286	LEU
1	A	2325	LEU
1	A	2331	LEU
1	A	2335	ILE
1	A	2355	LEU

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Mol	Chain	Res	Type
1	A	2368	SER
1	A	2379	ARG
1	A	2425	GLU
1	A	2433	GLN
1	A	2458	PHE
1	A	2479	SER
1	A	2480	LEU
1	B	112	PHE
1	B	113	ASP
1	B	137	PHE
1	B	145	ARG
1	B	189	ILE
1	B	227	GLU
1	B	257	ARG
1	B	272	GLN
1	B	288	ARG
1	B	289	ILE
1	B	306	MET
1	B	326	VAL
1	B	341	VAL
1	B	382	LEU
1	B	446	LEU
1	B	447	GLU
1	B	455	SER
1	B	461	SER
1	B	462	GLU
1	B	465	THR
1	B	512	ASP
1	B	528	SER
1	B	529	GLU
1	B	560	ASP
1	B	593	ASN
1	B	626	THR
1	B	672	GLN
1	B	679	ILE
1	B	695	ASN
1	B	718	GLU
1	B	779	THR
1	B	899	LYS
1	B	900	LYS
1	B	928	LEU
1	B	940	LEU

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Mol	Chain	Res	Type
1	B	1010	LEU
1	B	1055	VAL
1	B	1122	VAL
1	B	1166	ARG
1	B	1168	TYR
1	B	1198	CYS
1	B	1257	HIS
1	B	1320	LEU
1	B	1372	MET
1	B	1373	ARG
1	B	1403	ASP
1	B	1404	ASN
1	B	1438	GLU
1	B	1439	VAL
1	B	1537	LEU
1	B	1539	ILE
1	B	1549	GLU
1	B	1574	LEU
1	B	1779	VAL
1	B	1915	ASP
1	B	1925	VAL
1	B	1961	LEU
1	B	1974	CYS
1	B	2005	ILE
1	B	2084	GLU
1	B	2086	GLU
1	B	2099	ASP
1	B	2131	GLN
1	B	2216	ILE
1	B	2217	ASN
1	B	2220	HIS
1	B	2325	LEU
1	B	2331	LEU
1	B	2335	ILE
1	B	2355	LEU
1	B	2359	ASN
1	B	2368	SER
1	B	2379	ARG
1	B	2425	GLU
1	B	2433	GLN
1	B	2458	PHE
1	B	2479	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	A	225	GLN
1	A	244	ASN
1	A	267	ASN
1	A	272	GLN
1	A	291	HIS
1	A	322	HIS
1	A	355	ASN
1	A	360	GLN
1	A	416	HIS
1	A	435	ASN
1	A	593	ASN
1	A	628	ASN
1	A	672	GLN
1	A	713	ASN
1	A	731	GLN
1	A	742	ASN
1	A	755	ASN
1	A	801	GLN
1	A	809	GLN
1	A	844	ASN
1	A	890	ASN
1	A	908	HIS
1	A	943	GLN
1	A	995	ASN
1	A	1001	GLN
1	A	1024	HIS
1	A	1088	GLN
1	A	1136	ASN
1	A	1161	HIS
1	A	1247	ASN
1	A	1404	ASN
1	A	1554	ASN
1	A	1563	GLN
1	A	1800	HIS
1	A	1801	ASN
1	A	1922	ASN
1	A	1982	ASN
1	A	2091	ASN
1	A	2131	GLN
1	A	2151	HIS

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Mol	Chain	Res	Type
1	A	2217	ASN
1	A	2381	ASN
1	A	2414	GLN
1	B	244	ASN
1	B	291	HIS
1	B	322	HIS
1	B	355	ASN
1	B	360	GLN
1	B	416	HIS
1	B	435	ASN
1	B	593	ASN
1	B	628	ASN
1	B	672	GLN
1	B	713	ASN
1	B	731	GLN
1	B	742	ASN
1	B	755	ASN
1	B	801	GLN
1	B	809	GLN
1	B	831	ASN
1	B	844	ASN
1	B	890	ASN
1	B	908	HIS
1	B	995	ASN
1	B	1024	HIS
1	B	1088	GLN
1	B	1136	ASN
1	B	1208	HIS
1	B	1247	ASN
1	B	1334	HIS
1	B	1404	ASN
1	B	1554	ASN
1	B	1563	GLN
1	B	1801	ASN
1	B	1922	ASN
1	B	1982	ASN
1	B	2053	HIS
1	B	2131	GLN
1	B	2151	HIS
1	B	2217	ASN
1	B	2359	ASN
1	B	2381	ASN

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Mol	Chain	Res	Type
1	B	2414	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	2143/2492 (85%)	-0.11	13 (0%)	89	72	45, 101, 157, 222	0
1	B	2144/2492 (86%)	-0.12	20 (0%)	84	62	44, 105, 152, 223	0
All	All	4287/4984 (86%)	-0.12	33 (0%)	86	65	44, 103, 155, 223	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1168	TYR	4.6
1	A	2064	ASN	4.2
1	A	1205	GLU	4.0
1	B	2286	LEU	3.4
1	B	1162	LEU	3.3
1	A	1311	SER	3.2
1	B	1198	CYS	3.0
1	B	2064	ASN	2.9
1	A	208	GLN	2.9
1	B	1207	ARG	2.9
1	B	1205	GLU	2.8
1	A	2065	ILE	2.7
1	B	1167	MET	2.7
1	B	2287	ASP	2.6
1	A	2313	ALA	2.6
1	B	1202	GLY	2.6
1	B	2063	GLU	2.5
1	B	1193	SER	2.5
1	B	189	ILE	2.5
1	B	1197	GLU	2.4
1	A	1312	ALA	2.4
1	B	1166	ARG	2.4
1	B	213	PHE	2.3
1	A	246	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	289	ILE	2.3
1	A	1441	GLN	2.2
1	B	1570	ILE	2.2
1	A	829	GLN	2.2
1	A	1203	TRP	2.2
1	A	81	MET	2.1
1	B	2062	ASN	2.1
1	B	143	ILE	2.1
1	B	1239	GLN	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.