Full wwPDB X-ray Structure Validation Report ⓘ

Jul 11, 2023 – 10:43 am BST

PDB ID	:	8C4A
Title	:	Structural and interactional insights into the glideosome-associated connector from Toxoplasma gondii
Authors	:	Kumar, A.; Morgan, R.M.L.; Matthews, S.J.
Deposited on	:	2023-01-03
Resolution	:	2.67 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:

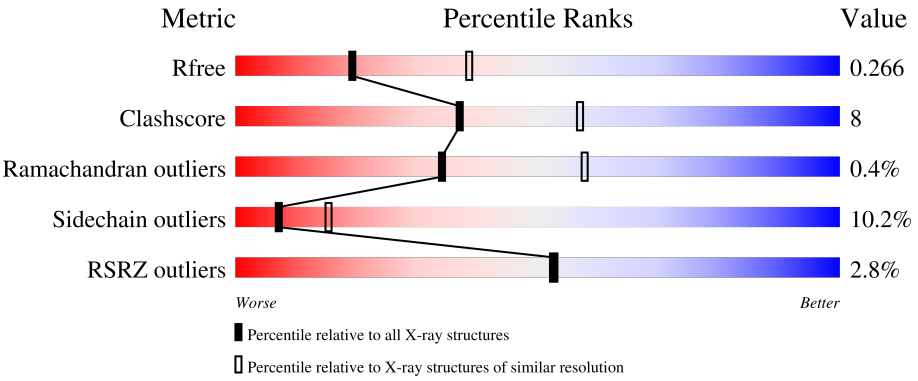
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.67 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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	2498	3% 77% 18%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 37731 atoms, of which 18940 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 Putative anonymous antigen-1.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trac
			Total	C	H	N	O	S	Se			
1	A	2474	37395	11670	18716	3181	3671	73	84	0	2	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	564	GLU	ALA	conflict	UNP A0A7J6JYP1

- Molecule 2 is water.

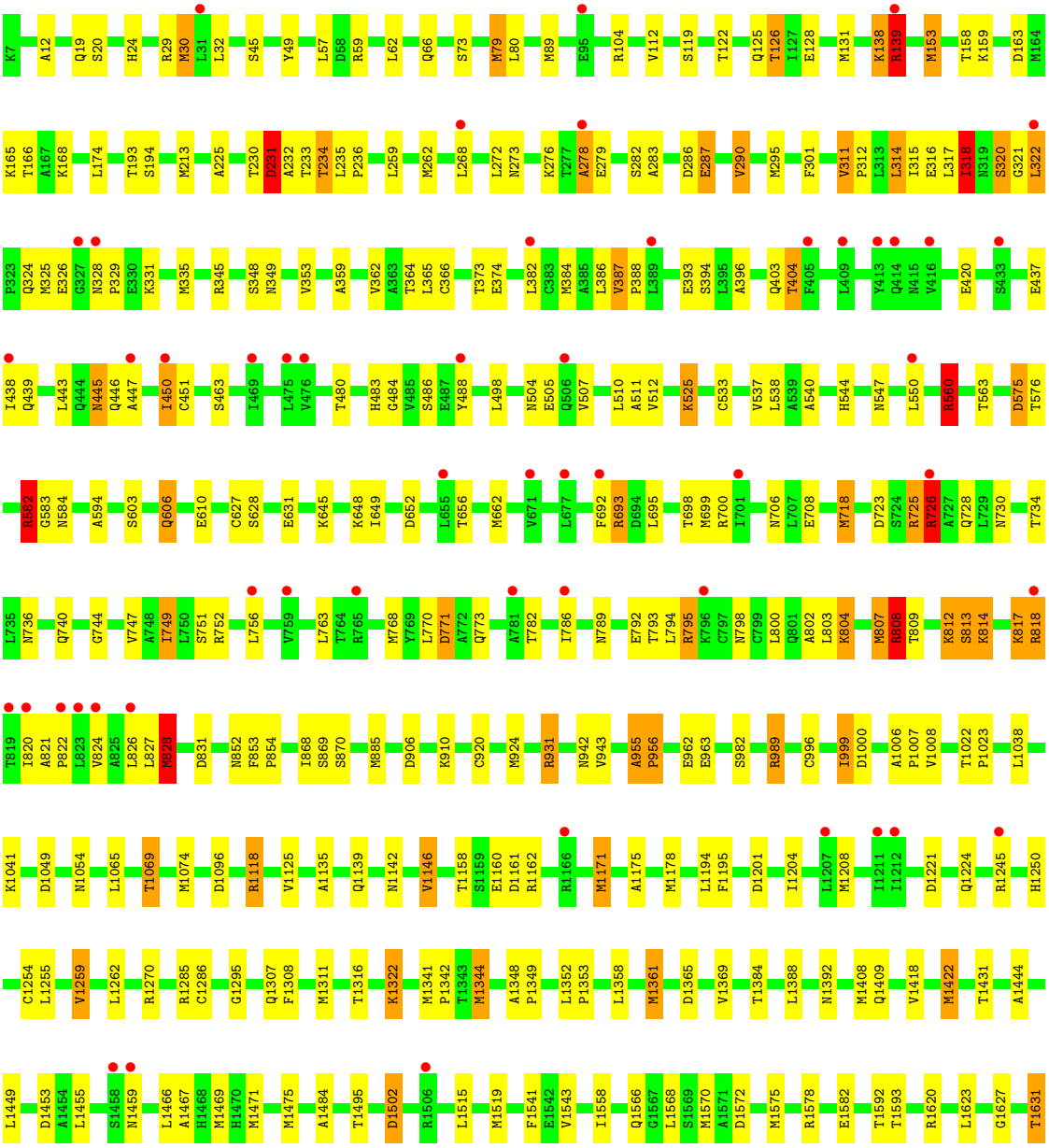
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	H	O		
2	A	112	336	224	112	0	0

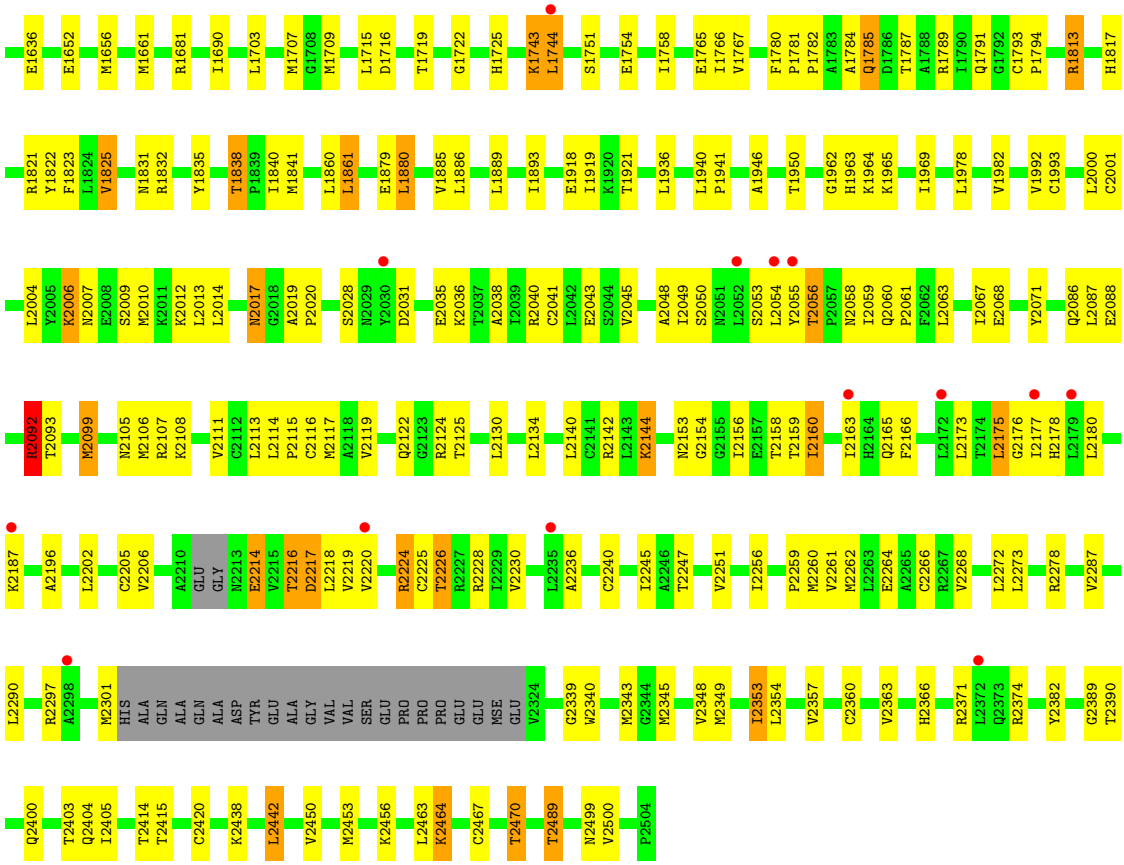
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: Putative anonymous antigen-1

Chain A:




E1636 E1652 M1656 M1661 R1681 I1690 L1703 M1707 G1708 M1709 L1715 D1716 T1719 G1722 H1725 K1743 L1744 S1751 E1754 I1758 E1765 I1766 V1767 F1780 P1781 P1782 A1783 A1784 Q1785 D1786 T1787 A1788 R1789 I1790 Q1791 G1792 C1793 P1794 R1813 H1817
R1821 Y1822 F1823 L1824 V1825 N1831 R1832 Y1835 T1838 P1839 I1840 M1841 L1860 L1861 E1879 L1880 V1885 L1886 L1889 I1893 E1918 I1919 K1920 T1921 L1936 L1940 P1941 A1946 T1950 G1962 H1963 K1964 K1965 I1969 L1978 V1982 V1992 C1993 L2000 C2001
L2004 Y2005 K2006 N2007 E2008 S2009 M2010 K2011 K2012 L2013 L2014 N2017 G2018 A2019 P2020 S2028 N2029 Y2030 D2031 E2035 K2036 T2037 A2038 I2039 R2040 C2041 L2042 E2043 S2044 V2045 A2048 I2049 S2050 N2051 L2052 S2053 L2054 Y2055 T2056 P2057 N2058 I2059 Q2060 P2061 F2062 L2063 I2067 E2068 Y2071 Q2086 L2087 E2088
R2092 T2093 M2099 N2105 M2106 R2107 K2108 V2111 C2112 L2113 L2114 P2115 C2116 M2117 A2118 V2119 Q2122 G2123 R2124 T2125 L2130 L2134 L2140 C2141 R2142 L2143 K2144 N2153 G2154 G2155 I2156 E2157 T2158 T2159 I2160 I2163 H2164 Q2165 F2166 L2172 L2173 T2174 L2175 G2176 I2177 H2178 L2179 L2180
K2187 A2196 L2202 C2205 V2206 A2210 GLU GLY N2213 E2214 Y2215 T2216 D2217 L2218 V2219 V2220 R2224 C2225 T2226 R2227 R2228 I2229 V2230 L2235 A2236 C2240 I2245 A2246 T2247 V2251 I2256 P2259 M2260 V2261 M2262 L2263 E2264 A2265 C2266 R2267 V2268 L2272 L2273 R2278 V2287
L2290 R2297 A2298 M2301 HIS ALA GLN ALA GLN ALA ASP TYR GLU ALA GLY VAL VAL SER GLU PRO PRO PRO GLU GLU MSE GLU V2324 G2339 W2340 M2343 G2344 M2345 V2348 M2349 I2353 L2354 V2357 C2360 V2363 H2366 R2371 L2372 Q2373 R2374 Y2382 G2389 T2390
Q2400 T2403 Q2404 I2405 T2414 T2415 C2420 K2438 L2442 V2450 M2453 K2456 L2463 K2464 C2467 T2470 T2489 N2499 V2500 P2504

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	119.08Å 123.61Å 221.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	110.75 – 2.67 107.94 – 2.68	Depositor EDS
% Data completeness (in resolution range)	100.0 (110.75-2.67) 99.9 (107.94-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.69Å)	Xtriage
Refinement program	REFMAC v5.0	Depositor
R, R_{free}	0.209 , 0.268 0.232 , 0.266	Depositor DCC
R_{free} test set	4517 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	85.0	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 33.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	37731	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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	0.38	0/18847	0.66	7/25412 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	24

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	726	ARG	NE-CZ-NH2	-6.59	117.01	120.30
1	A	139	ARG	NE-CZ-NH1	-6.51	117.04	120.30
1	A	582	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	A	726	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	1285	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	808	ARG	NE-CZ-NH1	-5.92	117.34	120.30
1	A	560	ARG	NE-CZ-NH1	-5.69	117.45	120.30

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1118	ARG	Sidechain
1	A	1162	ARG	Sidechain
1	A	1245	ARG	Sidechain
1	A	139	ARG	Sidechain
1	A	1681	ARG	Sidechain
1	A	1813	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1832	ARG	Sidechain
1	A	2040	ARG	Sidechain
1	A	2092	ARG	Sidechain
1	A	2224	ARG	Sidechain
1	A	2228	ARG	Sidechain
1	A	2278	ARG	Sidechain
1	A	345	ARG	Sidechain
1	A	560	ARG	Sidechain
1	A	582	ARG	Sidechain
1	A	59	ARG	Sidechain
1	A	693	ARG	Sidechain
1	A	725	ARG	Sidechain
1	A	726	ARG	Sidechain
1	A	752	ARG	Sidechain
1	A	795	ARG	Sidechain
1	A	808	ARG	Sidechain
1	A	818	ARG	Sidechain
1	A	989	ARG	Sidechain

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	18679	18716	18693	290	0
2	A	112	224	0	3	0
All	All	18791	18940	18693	290	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 (290) 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:807:MSE:SE	1:A:868:ILE:HD13	1.85	1.27
1:A:1307:GLN:HG3	1:A:1311:MSE:HE2	1.18	1.07
1:A:885:MSE:HE1	1:A:920:CYS:SG	2.13	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:955:ALA:HB1	1:A:956:PRO:HD2	1.55	0.87
1:A:885:MSE:HE2	1:A:924:MSE:HE2	1.58	0.85
1:A:1408:MSE:HE2	1:A:1455:LEU:HD13	1.59	0.84
1:A:1707:MSE:HE1	1:A:1725:HIS:O	1.76	0.84
1:A:2420:CYS:HB3	1:A:2470:THR:HG21	1.60	0.82
1:A:1175:ALA:HA	1:A:1178:MSE:CE	2.12	0.80
1:A:1408:MSE:HE3	1:A:1418:VAL:HG13	1.65	0.78
1:A:1308:PHE:HD1	1:A:1311:MSE:HE3	1.46	0.78
1:A:2453:MSE:HE1	1:A:2467:CYS:HB2	1.65	0.77
1:A:1175:ALA:HA	1:A:1178:MSE:HE2	1.66	0.76
1:A:807:MSE:SE	1:A:868:ILE:CD1	2.78	0.74
1:A:1835:TYR:O	1:A:1838:THR:HG22	1.87	0.74
1:A:1307:GLN:HG3	1:A:1311:MSE:CE	2.08	0.73
1:A:1307:GLN:CG	1:A:1311:MSE:HE2	2.10	0.73
1:A:2259:PRO:HG3	1:A:2366:HIS:CE1	2.24	0.73
1:A:1578:ARG:HD2	1:A:1582:GLU:OE2	1.89	0.72
1:A:1171:MSE:HE1	1:A:1194:LEU:HB3	1.72	0.71
1:A:505:GLU:OE2	1:A:544:HIS:ND1	2.23	0.71
1:A:1541:PHE:HD1	1:A:1575:MSE:HE3	1.55	0.70
1:A:396:ALA:HB1	1:A:438:ILE:HD11	1.74	0.70
1:A:153:MSE:HE3	1:A:174:LEU:HD23	1.74	0.68
1:A:1158:THR:HG23	1:A:1160:GLU:H	1.59	0.67
1:A:2272:LEU:HD22	1:A:2343:MSE:HE1	1.76	0.67
1:A:1065:LEU:O	1:A:1069:THR:HB	1.94	0.67
1:A:1793:CYS:HB3	1:A:1794:PRO:HD3	1.76	0.67
1:A:2144:LYS:H	1:A:2144:LYS:HD2	1.60	0.66
1:A:2154:GLY:O	1:A:2158:THR:HG23	1.96	0.66
1:A:2240:CYS:SG	1:A:2343:MSE:HE2	2.36	0.65
1:A:999:ILE:HD11	1:A:1038:LEU:HD13	1.79	0.64
1:A:1758:ILE:HA	1:A:1767:VAL:HG23	1.80	0.64
1:A:1208:MSE:HG3	1:A:1254:CYS:SG	2.37	0.64
1:A:2262:MSE:HE1	1:A:2266:CYS:SG	2.38	0.63
1:A:885:MSE:CE	1:A:920:CYS:SG	2.85	0.63
1:A:2453:MSE:HE3	1:A:2464:LYS:HG2	1.81	0.63
1:A:1921:THR:HG22	1:A:1963:HIS:NE2	2.15	0.62
1:A:2489:THR:HG23	1:A:2489:THR:O	2.00	0.62
1:A:885:MSE:HE2	1:A:924:MSE:CE	2.30	0.61
1:A:1341:MSE:N	1:A:1342:PRO:HD2	2.14	0.61
1:A:163:ASP:HB3	1:A:166:THR:HG23	1.82	0.61
1:A:730:ASN:O	1:A:734:THR:OG1	2.19	0.61
1:A:235:LEU:HB3	1:A:236:PRO:HD3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:885:MSE:CE	1:A:924:MSE:HE2	2.30	0.59
1:A:1962:GLY:HA2	1:A:2006:LYS:HD2	1.83	0.59
1:A:80:LEU:HD12	1:A:126:THR:HG22	1.85	0.59
1:A:1495:THR:HG23	1:A:1519:MSE:HE2	1.84	0.59
1:A:1652:GLU:O	1:A:1656:MSE:HG3	2.03	0.59
1:A:2163:ILE:HG23	1:A:2173:LEU:HD12	1.85	0.59
1:A:504:ASN:HB3	1:A:507:VAL:HG22	1.84	0.58
1:A:2374:ARG:NH1	1:A:2414:THR:OG1	2.35	0.58
1:A:1262:LEU:HD13	1:A:1311:MSE:HE1	1.86	0.58
1:A:1950:THR:HG22	1:A:1992:VAL:HA	1.86	0.57
1:A:2259:PRO:HG3	1:A:2366:HIS:NE2	2.20	0.57
1:A:2405:ILE:HD13	1:A:2415:THR:HB	1.86	0.57
1:A:763:LEU:CD2	1:A:773:GLN:HA	2.35	0.57
1:A:1171:MSE:HE2	1:A:1195:PHE:HA	1.86	0.57
1:A:1568:LEU:HB3	1:A:1575:MSE:HG2	1.86	0.56
1:A:2354:LEU:HD12	1:A:2389:GLY:HA3	1.87	0.56
1:A:1886:LEU:HD11	1:A:1919:ILE:HG23	1.87	0.56
1:A:606:GLN:O	1:A:610:GLU:HG2	2.06	0.56
1:A:1822:TYR:HA	1:A:1825:VAL:HG13	1.88	0.55
1:A:2240:CYS:SG	1:A:2245:ILE:HG12	2.45	0.55
1:A:2340:TRP:HA	1:A:2345:MSE:HE3	1.87	0.55
1:A:268:LEU:HA	1:A:295:MSE:HE2	1.88	0.55
1:A:1572:ASP:HB3	1:A:1575:MSE:HB2	1.88	0.55
1:A:662:MSE:HE3	1:A:692:PHE:HB3	1.89	0.55
1:A:1208:MSE:HE3	1:A:1250:HIS:HB2	1.89	0.55
1:A:2262:MSE:CE	1:A:2266:CYS:SG	2.95	0.55
1:A:538:LEU:HD13	1:A:594:ALA:HA	1.89	0.54
1:A:2159:THR:O	1:A:2163:ILE:HG13	2.08	0.54
1:A:1408:MSE:HG2	1:A:1418:VAL:HA	1.89	0.54
1:A:2450:VAL:HA	1:A:2453:MSE:HE2	1.88	0.54
1:A:1880:LEU:HD22	1:A:1885:VAL:HG21	1.90	0.54
1:A:2114:LEU:N	1:A:2115:PRO:HD2	2.22	0.54
1:A:1422:MSE:CE	1:A:1467:ALA:HB3	2.38	0.53
1:A:2262:MSE:HE1	1:A:2357:VAL:HG12	1.90	0.53
1:A:853:PHE:HB3	1:A:854:PRO:HD3	1.91	0.53
1:A:782:THR:O	1:A:786:ILE:HG13	2.08	0.53
1:A:1993:CYS:HB3	1:A:2041:CYS:SG	2.49	0.53
1:A:318:ILE:HA	1:A:322:LEU:HG	1.90	0.53
1:A:443:LEU:O	1:A:447:ALA:HB2	2.09	0.53
1:A:1358:LEU:HA	1:A:1361:MSE:HE3	1.91	0.53
1:A:699:MSE:HG3	1:A:1409:GLN:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:CYS:SG	1:A:404:THR:HG21	2.50	0.52
1:A:1817:HIS:O	1:A:1821:ARG:HD3	2.10	0.52
1:A:1388:LEU:O	1:A:1392:ASN:HB2	2.10	0.52
1:A:2262:MSE:HG3	1:A:2360:CYS:SG	2.50	0.51
1:A:2230:VAL:HG13	1:A:2230:VAL:O	2.10	0.51
1:A:2403:THR:HG22	1:A:2442:LEU:HA	1.92	0.51
1:A:1307:GLN:O	1:A:1311:MSE:HG3	2.10	0.51
1:A:931:ARG:NH1	1:A:1502:ASP:OD2	2.44	0.51
1:A:311:VAL:N	1:A:312:PRO:HD2	2.26	0.51
1:A:999:ILE:CD1	1:A:1038:LEU:HD13	2.41	0.51
1:A:1408:MSE:HE1	1:A:1422:MSE:HG3	1.94	0.50
1:A:2349:MSE:O	1:A:2353:ILE:HG23	2.11	0.50
1:A:2117:MSE:HE1	1:A:2153:ASN:HB2	1.94	0.50
1:A:314:LEU:O	1:A:318:ILE:HG13	2.12	0.50
1:A:1719:THR:HG23	1:A:1722:GLY:H	1.76	0.50
1:A:1208:MSE:HG2	1:A:1254:CYS:HB2	1.94	0.50
1:A:1716:ASP:HB3	1:A:1719:THR:HG22	1.94	0.50
1:A:1946:ALA:O	1:A:1950:THR:HG23	2.11	0.50
1:A:62:LEU:HD12	1:A:62:LEU:H	1.77	0.49
1:A:2236:ALA:HB1	1:A:2343:MSE:CE	2.41	0.49
1:A:1135:ALA:O	1:A:1139:GLN:HB2	2.13	0.49
1:A:314:LEU:HD11	1:A:359:ALA:HB1	1.93	0.49
1:A:387:VAL:N	1:A:388:PRO:HD2	2.28	0.48
1:A:708:GLU:HA	1:A:749:ILE:HG21	1.95	0.48
1:A:812:LYS:HB3	1:A:813:SER:H	1.51	0.48
1:A:138:LYS:HE2	1:A:138:LYS:HB3	1.51	0.48
1:A:575:ASP:N	1:A:575:ASP:OD1	2.46	0.48
1:A:2144:LYS:HD2	1:A:2144:LYS:N	2.25	0.48
1:A:2001:CYS:HA	1:A:2004:LEU:HD12	1.94	0.48
1:A:2014:LEU:HA	1:A:2017:ASN:HB2	1.95	0.48
1:A:2177:ILE:HG13	1:A:2178:HIS:N	2.27	0.48
1:A:1308:PHE:CD1	1:A:1311:MSE:HE3	2.38	0.48
1:A:1703:LEU:O	1:A:1707:MSE:HB2	2.14	0.48
1:A:2247:THR:HG23	2:A:2618:HOH:O	2.12	0.48
1:A:512:VAL:HG21	1:A:550:LEU:CD1	2.44	0.48
1:A:1541:PHE:CD1	1:A:1575:MSE:HE3	2.42	0.48
1:A:1592:THR:OG1	1:A:1631:THR:HG22	2.14	0.48
1:A:2117:MSE:HE1	1:A:2153:ASN:CB	2.43	0.47
1:A:814:LYS:HB3	1:A:814:LYS:HE2	1.44	0.47
1:A:1344:MSE:CE	1:A:1344:MSE:HA	2.45	0.47
1:A:450:ILE:HG13	1:A:451:CYS:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:817:LYS:HE2	1:A:817:LYS:HB3	1.63	0.47
1:A:2019:ALA:O	1:A:2020:PRO:C	2.53	0.47
1:A:295:MSE:HE3	1:A:301:PHE:HD2	1.80	0.47
1:A:1781:PRO:HB2	1:A:1782:PRO:HD3	1.96	0.47
1:A:1568:LEU:HB3	1:A:1575:MSE:CG	2.44	0.47
1:A:2007:ASN:HD22	1:A:2010:MSE:HG2	1.79	0.47
1:A:1578:ARG:O	1:A:1582:GLU:HB2	2.15	0.47
1:A:1627:GLY:O	1:A:1631:THR:HG23	2.15	0.47
1:A:2043:GLU:HG3	1:A:2086:GLN:HE21	1.80	0.46
1:A:2224:ARG:O	1:A:2225:CYS:C	2.52	0.46
1:A:512:VAL:HG21	1:A:550:LEU:HD12	1.96	0.46
1:A:826:LEU:O	1:A:828:MSE:N	2.49	0.46
1:A:2214:GLU:O	1:A:2218:LEU:HG	2.14	0.46
1:A:57:LEU:HB2	1:A:89:MSE:HE2	1.96	0.46
1:A:583:GLY:O	1:A:584:ASN:C	2.53	0.46
1:A:1466:LEU:HA	1:A:1469:MSE:HE3	1.98	0.46
1:A:1568:LEU:HD13	1:A:1575:MSE:HE2	1.98	0.46
1:A:2216:THR:C	1:A:2218:LEU:N	2.69	0.46
1:A:2236:ALA:HB1	1:A:2343:MSE:HE1	1.97	0.46
1:A:1566:GLN:O	1:A:1570:MSE:HG3	2.16	0.46
1:A:1978:LEU:O	1:A:1982:VAL:HG23	2.16	0.46
1:A:287:GLU:O	1:A:290:VAL:N	2.48	0.46
1:A:1178:MSE:HE1	1:A:1195:PHE:CE2	2.51	0.46
1:A:1841:MSE:SE	1:A:1880:LEU:HD21	2.66	0.46
1:A:57:LEU:HD12	1:A:62:LEU:HD11	1.97	0.46
1:A:812:LYS:HB3	1:A:812:LYS:HE3	1.52	0.46
1:A:1049:ASP:CG	1:A:1054:ASN:HD22	2.19	0.46
1:A:1204:ILE:O	1:A:1208:MSE:HB2	2.16	0.45
1:A:1861:LEU:HD23	1:A:1861:LEU:HA	1.74	0.45
1:A:2000:LEU:HD22	1:A:2014:LEU:HD13	1.97	0.45
1:A:2264:GLU:O	1:A:2268:VAL:HG23	2.16	0.45
1:A:279:GLU:HB3	1:A:283:ALA:CB	2.45	0.45
1:A:213:MSE:HE3	1:A:213:MSE:HB3	1.92	0.45
1:A:656:THR:HG21	1:A:706:ASN:CG	2.37	0.45
1:A:1936:LEU:HD23	1:A:1978:LEU:HD13	1.99	0.45
1:A:1175:ALA:HA	1:A:1178:MSE:HE3	1.97	0.45
1:A:295:MSE:HE3	1:A:301:PHE:CD2	2.51	0.45
1:A:1449:LEU:CD2	1:A:1475:MSE:HE1	2.46	0.45
1:A:2060:GLN:O	1:A:2061:PRO:C	2.55	0.45
1:A:316:GLU:HA	1:A:320:SER:HB2	1.98	0.45
1:A:525:LYS:H	1:A:525:LYS:HG2	1.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1469:MSE:HE1	1:A:1515:LEU:HA	1.98	0.45
1:A:804:LYS:HA	1:A:807:MSE:HE3	1.98	0.45
1:A:885:MSE:HE2	1:A:924:MSE:SE	2.67	0.45
1:A:802:ALA:O	1:A:803:LEU:C	2.55	0.45
1:A:1348:ALA:N	1:A:1349:PRO:HD2	2.32	0.45
1:A:1743:LYS:HB3	1:A:1743:LYS:HE2	1.66	0.45
1:A:1767:VAL:HG13	1:A:1821:ARG:NH2	2.32	0.45
1:A:1623:LEU:HG	1:A:1661:MSE:HB3	1.99	0.44
1:A:1965:LYS:O	1:A:1969:ILE:HG12	2.17	0.44
1:A:2056:THR:HA	1:A:2059:ILE:HG13	1.98	0.44
1:A:384:MSE:HE1	2:A:2622:HOH:O	2.15	0.44
1:A:768:MSE:HE3	1:A:768:MSE:HB3	1.94	0.44
1:A:1568:LEU:HD13	1:A:1575:MSE:CE	2.47	0.44
1:A:2048:ALA:O	1:A:2049:ILE:C	2.56	0.44
1:A:2106:MSE:SE	1:A:2142:ARG:HH21	2.51	0.44
1:A:1270:ARG:HA	1:A:1270:ARG:HD3	1.72	0.44
1:A:1322:LYS:HB3	1:A:1322:LYS:HE2	1.69	0.44
1:A:2106:MSE:HG3	1:A:2140:LEU:HA	1.98	0.44
1:A:2013:LEU:HG	1:A:2017:ASN:ND2	2.32	0.44
1:A:2114:LEU:N	1:A:2115:PRO:CD	2.80	0.44
1:A:725:ARG:HE	1:A:725:ARG:HB2	1.72	0.44
1:A:2122:GLN:OE1	1:A:2124:ARG:NH1	2.51	0.44
1:A:2499:ASN:OD1	1:A:2499:ASN:N	2.51	0.44
1:A:311:VAL:O	1:A:312:PRO:C	2.56	0.44
1:A:393:GLU:O	1:A:394:SER:C	2.56	0.44
1:A:1365:ASP:O	1:A:1369:VAL:HG23	2.18	0.44
1:A:282:SER:HA	1:A:286:ASP:HB2	2.00	0.44
1:A:438:ILE:O	1:A:439:GLN:C	2.56	0.44
1:A:996:CYS:O	1:A:999:ILE:HG12	2.17	0.44
1:A:1000:ASP:OD1	1:A:1041:LYS:HE3	2.18	0.44
1:A:699:MSE:HE1	1:A:740:GLN:HG3	1.99	0.43
1:A:225:ALA:HB1	1:A:262:MSE:HG3	2.00	0.43
1:A:234:THR:OG1	1:A:262:MSE:SE	2.86	0.43
1:A:1308:PHE:HD1	1:A:1311:MSE:CE	2.21	0.43
1:A:1940:LEU:N	1:A:1941:PRO:HD2	2.34	0.43
1:A:2036:LYS:HE3	1:A:2036:LYS:HB3	1.67	0.43
1:A:231:ASP:HB2	1:A:232:ALA:H	1.61	0.43
1:A:235:LEU:HD23	1:A:259:LEU:HD22	2.00	0.43
1:A:386:LEU:O	1:A:387:VAL:C	2.56	0.43
1:A:962:GLU:O	1:A:963:GLU:C	2.57	0.43
1:A:2019:ALA:HB3	1:A:2020:PRO:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ASN:O	1:A:276:LYS:N	2.49	0.43
1:A:1422:MSE:HG2	1:A:1471:MSE:SE	2.67	0.43
1:A:2176:GLY:O	1:A:2180:LEU:HG	2.19	0.43
1:A:2339:GLY:O	1:A:2340:TRP:C	2.57	0.43
1:A:79:MSE:HE3	1:A:119:SER:HB3	2.01	0.43
1:A:662:MSE:HE2	1:A:695:LEU:HD22	2.00	0.43
1:A:2038:ALA:O	1:A:2041:CYS:HB3	2.19	0.43
1:A:2206:VAL:HG12	1:A:2251:VAL:HG21	2.01	0.43
1:A:1022:THR:HB	1:A:1023:PRO:HD2	1.99	0.43
1:A:789:ASN:O	1:A:792:GLU:HB2	2.19	0.43
1:A:999:ILE:HG22	1:A:1008:VAL:HG12	2.01	0.43
1:A:1255:LEU:O	1:A:1259:VAL:HG12	2.19	0.43
1:A:740:GLN:HA	1:A:744:GLY:HA2	2.00	0.43
1:A:2273:LEU:HD22	1:A:2382:TYR:CE2	2.54	0.43
1:A:2489:THR:O	1:A:2489:THR:CG2	2.65	0.43
1:A:312:PRO:O	1:A:315:ILE:HB	2.19	0.43
1:A:498:LEU:HD13	1:A:511:ALA:HB3	2.01	0.43
1:A:770:LEU:O	1:A:771:ASP:C	2.56	0.43
1:A:803:LEU:O	1:A:807:MSE:HG3	2.18	0.43
1:A:2092:ARG:HE	1:A:2092:ARG:HB2	1.61	0.43
1:A:2400:GLN:OE1	1:A:2400:GLN:N	2.51	0.43
1:A:955:ALA:O	1:A:956:PRO:C	2.58	0.42
1:A:1495:THR:HG22	1:A:1543:VAL:HG11	2.01	0.42
1:A:2217:ASP:O	1:A:2220:VAL:HG22	2.19	0.42
1:A:533:CYS:O	1:A:537:VAL:HG23	2.19	0.42
1:A:1690:ILE:HD13	1:A:1744:LEU:HD22	2.01	0.42
1:A:2202:LEU:HB3	1:A:2226:THR:HG22	2.01	0.42
1:A:193:THR:O	1:A:194:SER:C	2.57	0.42
1:A:29:ARG:HG3	1:A:29:ARG:HH11	1.84	0.42
1:A:804:LYS:O	1:A:808:ARG:HB2	2.20	0.42
1:A:821:ALA:HB3	1:A:822:PRO:HD3	2.02	0.42
1:A:318:ILE:HG13	1:A:318:ILE:H	1.45	0.42
1:A:364:THR:OG1	1:A:365:LEU:N	2.52	0.42
1:A:540:ALA:O	1:A:544:HIS:HD2	2.03	0.42
1:A:2134:LEU:HB2	1:A:2175:LEU:HD23	2.02	0.42
1:A:718:MSE:HE3	1:A:728:GLN:OE1	2.20	0.42
1:A:1006:ALA:N	1:A:1007:PRO:CD	2.83	0.42
1:A:1352:LEU:HD23	1:A:1352:LEU:HA	1.89	0.42
1:A:2290:LEU:HD23	1:A:2290:LEU:HA	1.90	0.42
1:A:645:LYS:O	1:A:649:ILE:HG12	2.20	0.41
1:A:1069:THR:HG21	1:A:1074:MSE:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1471:MSE:HG2	1:A:1475:MSE:HE2	2.01	0.41
1:A:445:ASN:C	1:A:447:ALA:H	2.23	0.41
1:A:942:ASN:HD22	1:A:942:ASN:HA	1.71	0.41
1:A:1142:ASN:O	1:A:1146:VAL:HG13	2.19	0.41
1:A:2450:VAL:HG22	1:A:2453:MSE:HE2	2.02	0.41
1:A:12:ALA:HB3	1:A:2256:ILE:HD13	2.03	0.41
1:A:2086:GLN:O	1:A:2087:LEU:C	2.59	0.41
1:A:1558:ILE:HD13	1:A:1558:ILE:HA	1.95	0.41
1:A:1118:ARG:NH2	1:A:1161:ASP:OD2	2.54	0.41
1:A:1751:SER:HB3	1:A:1787:THR:HG22	2.02	0.41
1:A:1838:THR:HG23	1:A:1840:ILE:H	1.86	0.41
1:A:2165:GLN:OE1	1:A:2166:PHE:CZ	2.74	0.41
1:A:73:SER:O	1:A:79:MSE:HE2	2.21	0.41
1:A:484:GLY:O	1:A:488:TYR:N	2.47	0.41
1:A:507:VAL:HA	1:A:510:LEU:HD12	2.02	0.41
1:A:2099:MSE:HE3	1:A:2099:MSE:HB3	1.97	0.41
1:A:2130:LEU:O	1:A:2134:LEU:HG	2.20	0.41
1:A:2160:ILE:HD11	1:A:2196:ALA:CB	2.50	0.41
1:A:648:LYS:O	1:A:700:ARG:NH2	2.41	0.41
1:A:763:LEU:HD22	1:A:773:GLN:HA	2.02	0.41
1:A:1352:LEU:N	1:A:1353:PRO:HD2	2.36	0.41
1:A:1715:LEU:HB2	1:A:1766:ILE:HD12	2.02	0.41
1:A:1889:LEU:O	1:A:1893:ILE:HG13	2.21	0.41
1:A:2260:MSE:HE3	1:A:2264:GLU:HG2	2.03	0.41
1:A:582:ARG:HH22	1:A:627:CYS:HB2	1.85	0.40
1:A:1784:ALA:O	1:A:1785:GLN:C	2.59	0.40
1:A:2113:LEU:C	1:A:2115:PRO:HD2	2.40	0.40
1:A:24:HIS:HE1	2:A:2642:HOH:O	2.04	0.40
1:A:30:MSE:HE3	1:A:30:MSE:HB3	1.92	0.40
1:A:2059:ILE:HG22	1:A:2063:LEU:HD11	2.02	0.40
1:A:2405:ILE:C	1:A:2405:ILE:HD12	2.41	0.40
1:A:278:ALA:O	1:A:279:GLU:HB2	2.21	0.40
1:A:550:LEU:HD12	1:A:550:LEU:O	2.22	0.40
1:A:1444:ALA:O	1:A:1484:ALA:HB2	2.21	0.40
1:A:49:TYR:HE1	1:A:768:MSE:HE2	1.87	0.40
1:A:1286:CYS:SG	1:A:1295:GLY:HA3	2.61	0.40
1:A:318:ILE:HG12	1:A:364:THR:HB	2.04	0.40
1:A:1171:MSE:HG3	1:A:1195:PHE:CE1	2.56	0.40
1:A:1780:PHE:HA	1:A:1781:PRO:HD3	1.98	0.40
1:A:2105:ASN:O	1:A:2108:LYS:HB3	2.21	0.40
1:A:2173:LEU:HD21	1:A:2205:CYS:HB2	2.04	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	2470/2498 (99%)	2312 (94%)	147 (6%)	11 (0%)	34 58

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	827	LEU
1	A	318	ILE
1	A	348	SER
1	A	956	PRO
1	A	329	PRO
1	A	828	MSE
1	A	955	ALA
1	A	813	SER
1	A	231	ASP
1	A	278	ALA
1	A	321	GLY

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	2007/1944 (103%)	1802 (90%)	205 (10%)	7 15

All (205) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	20	SER
1	A	30	MSE
1	A	32	LEU
1	A	45	SER
1	A	66	GLN
1	A	79	MSE
1	A	104	ARG
1	A	112	VAL
1	A	122	THR
1	A	125	GLN
1	A	126	THR
1	A	128[A]	GLU
1	A	128[B]	GLU
1	A	131	MSE
1	A	138	LYS
1	A	139	ARG
1	A	153	MSE
1	A	158	THR
1	A	159	LYS
1	A	165	LYS
1	A	168	LYS
1	A	230	THR
1	A	231	ASP
1	A	233	THR
1	A	234	THR
1	A	272	LEU
1	A	287	GLU
1	A	290	VAL
1	A	311	VAL
1	A	314	LEU
1	A	317	LEU
1	A	318	ILE
1	A	320	SER
1	A	322	LEU
1	A	324	GLN
1	A	325	MSE
1	A	326	GLU
1	A	328	ASN
1	A	331	LYS
1	A	335	MSE
1	A	349	ASN
1	A	353	VAL

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Mol	Chain	Res	Type
1	A	362	VAL
1	A	373	THR
1	A	374	GLU
1	A	382	LEU
1	A	387	VAL
1	A	403	GLN
1	A	404	THR
1	A	420	GLU
1	A	437	GLU
1	A	445	ASN
1	A	446	GLN
1	A	450	ILE
1	A	463	SER
1	A	480	THR
1	A	483	HIS
1	A	486	SER
1	A	525	LYS
1	A	547	ASN
1	A	560	ARG
1	A	563	THR
1	A	575	ASP
1	A	576	THR
1	A	582	ARG
1	A	603	SER
1	A	606	GLN
1	A	628	SER
1	A	631	GLU
1	A	652	ASP
1	A	693	ARG
1	A	698	THR
1	A	718	MSE
1	A	723	ASP
1	A	726	ARG
1	A	736	ASN
1	A	747	VAL
1	A	749	ILE
1	A	751	SER
1	A	756	LEU
1	A	771	ASP
1	A	793	THR
1	A	794	LEU
1	A	795	ARG

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Mol	Chain	Res	Type
1	A	798	ASN
1	A	800	LEU
1	A	804	LYS
1	A	807	MSE
1	A	808	ARG
1	A	809	THR
1	A	812	LYS
1	A	814	LYS
1	A	817	LYS
1	A	818	ARG
1	A	820	ILE
1	A	824	VAL
1	A	828	MSE
1	A	831	ASP
1	A	852	ASN
1	A	869	SER
1	A	870	SER
1	A	906	ASP
1	A	910	LYS
1	A	931	ARG
1	A	943	VAL
1	A	982	SER
1	A	989	ARG
1	A	999	ILE
1	A	1069	THR
1	A	1096	ASP
1	A	1125	VAL
1	A	1146	VAL
1	A	1171	MSE
1	A	1201	ASP
1	A	1221	ASP
1	A	1224	GLN
1	A	1259	VAL
1	A	1316	THR
1	A	1322	LYS
1	A	1344	MSE
1	A	1361	MSE
1	A	1384	THR
1	A	1422	MSE
1	A	1431	THR
1	A	1453	ASP
1	A	1459	ASN

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Mol	Chain	Res	Type
1	A	1502	ASP
1	A	1593	THR
1	A	1620	ARG
1	A	1631	THR
1	A	1636	GLU
1	A	1709	MSE
1	A	1743	LYS
1	A	1744	LEU
1	A	1754	GLU
1	A	1765	GLU
1	A	1785	GLN
1	A	1789	ARG
1	A	1791	GLN
1	A	1813	ARG
1	A	1823	PHE
1	A	1825	VAL
1	A	1831	ASN
1	A	1838	THR
1	A	1860	LEU
1	A	1861	LEU
1	A	1879	GLU
1	A	1880	LEU
1	A	1918	GLU
1	A	1964	LYS
1	A	2006	LYS
1	A	2009	SER
1	A	2012	LYS
1	A	2017	ASN
1	A	2028	SER
1	A	2031	ASP
1	A	2035	GLU
1	A	2045	VAL
1	A	2050	SER
1	A	2053	SER
1	A	2054	LEU
1	A	2055	TYR
1	A	2056	THR
1	A	2058	ASN
1	A	2067	ILE
1	A	2068	GLU
1	A	2071	TYR
1	A	2088	GLU

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Mol	Chain	Res	Type
1	A	2092	ARG
1	A	2093	THR
1	A	2099	MSE
1	A	2107	ARG
1	A	2111	VAL
1	A	2116	CYS
1	A	2119	VAL
1	A	2125	THR
1	A	2144	LYS
1	A	2156	ILE
1	A	2160	ILE
1	A	2175	LEU
1	A	2187	LYS
1	A	2214	GLU
1	A	2216	THR
1	A	2217	ASP
1	A	2219	VAL
1	A	2226	THR
1	A	2261	VAL
1	A	2287	VAL
1	A	2297	ARG
1	A	2301	MSE
1	A	2348	VAL
1	A	2353	ILE
1	A	2363	VAL
1	A	2371	ARG
1	A	2390	THR
1	A	2404	GLN
1	A	2438	LYS
1	A	2442	LEU
1	A	2456	LYS
1	A	2463	LEU
1	A	2464	LYS
1	A	2470	THR
1	A	2489	THR
1	A	2500	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	47	GLN

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Mol	Chain	Res	Type
1	A	189	ASN
1	A	324	GLN
1	A	414	GLN
1	A	446	GLN
1	A	517	ASN
1	A	789	ASN
1	A	798	ASN
1	A	959	GLN
1	A	1142	ASN
1	A	1224	GLN
1	A	1412	GLN
1	A	1596	GLN
1	A	1729	ASN
1	A	1785	GLN
1	A	2007	ASN
1	A	2029	ASN
1	A	2086	GLN
1	A	2096	ASN
1	A	2369	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 (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, 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	2390/2498 (95%)	0.32	66 (2%) 53 52	45, 74, 97, 121	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	822	PRO	5.9
1	A	488	TYR	5.8
1	A	475	LEU	5.0
1	A	476	VAL	4.6
1	A	389	LEU	4.1
1	A	322	LEU	4.0
1	A	819	THR	3.7
1	A	2298	ALA	3.6
1	A	414	GLN	3.6
1	A	450	ILE	3.6
1	A	826	LEU	3.6
1	A	2055	TYR	3.5
1	A	438	ILE	3.5
1	A	818	ARG	3.4
1	A	413	TYR	3.4
1	A	469	ILE	3.4
1	A	328	ASN	3.4
1	A	2187	LYS	3.2
1	A	823	LEU	3.1
1	A	409	LEU	3.1
1	A	765	ARG	2.9
1	A	1207	LEU	2.9
1	A	820	ILE	2.9
1	A	1245	ARG	2.9
1	A	1458	SER	2.8
1	A	506	GLN	2.8
1	A	2054	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	447	ALA	2.7
1	A	1166	ARG	2.7
1	A	2220	VAL	2.7
1	A	327	GLY	2.7
1	A	756	LEU	2.7
1	A	701	ILE	2.7
1	A	2052	LEU	2.6
1	A	677	LEU	2.5
1	A	1506	ARG	2.5
1	A	95	GLU	2.5
1	A	726	ARG	2.5
1	A	416	VAL	2.5
1	A	824	VAL	2.5
1	A	31	LEU	2.4
1	A	2235	LEU	2.3
1	A	692	PHE	2.3
1	A	278	ALA	2.3
1	A	139	ARG	2.3
1	A	759	VAL	2.3
1	A	2163	ILE	2.2
1	A	268	LEU	2.2
1	A	405	PHE	2.2
1	A	796	LYS	2.2
1	A	1459	ASN	2.2
1	A	550	LEU	2.2
1	A	2179	LEU	2.2
1	A	655	LEU	2.1
1	A	382	LEU	2.1
1	A	786	ILE	2.1
1	A	2177	ILE	2.1
1	A	2172	LEU	2.1
1	A	2030	TYR	2.1
1	A	1744	LEU	2.0
1	A	433	SER	2.0
1	A	781	ALA	2.0
1	A	2372	LEU	2.0
1	A	1211	ILE	2.0
1	A	1212	ILE	2.0
1	A	671	VAL	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.