



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:37 AM UTC

PDB ID : 8C4A / pdb_00008c4a
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	:	4-5-2 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

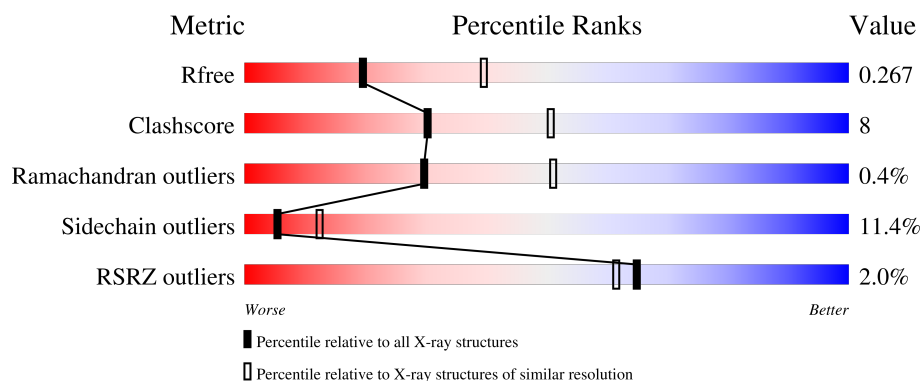
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (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 $\leq 5\%$. 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	2498	2% 75% 19% ..

2 Entry composition

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	Trace
1	A	2474	Total	C	H	N	O	S	Se		0	2	0
			37395	11670	18716	3181	3671	73	84				

There is a discrepancy between the modelled and reference sequences:

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

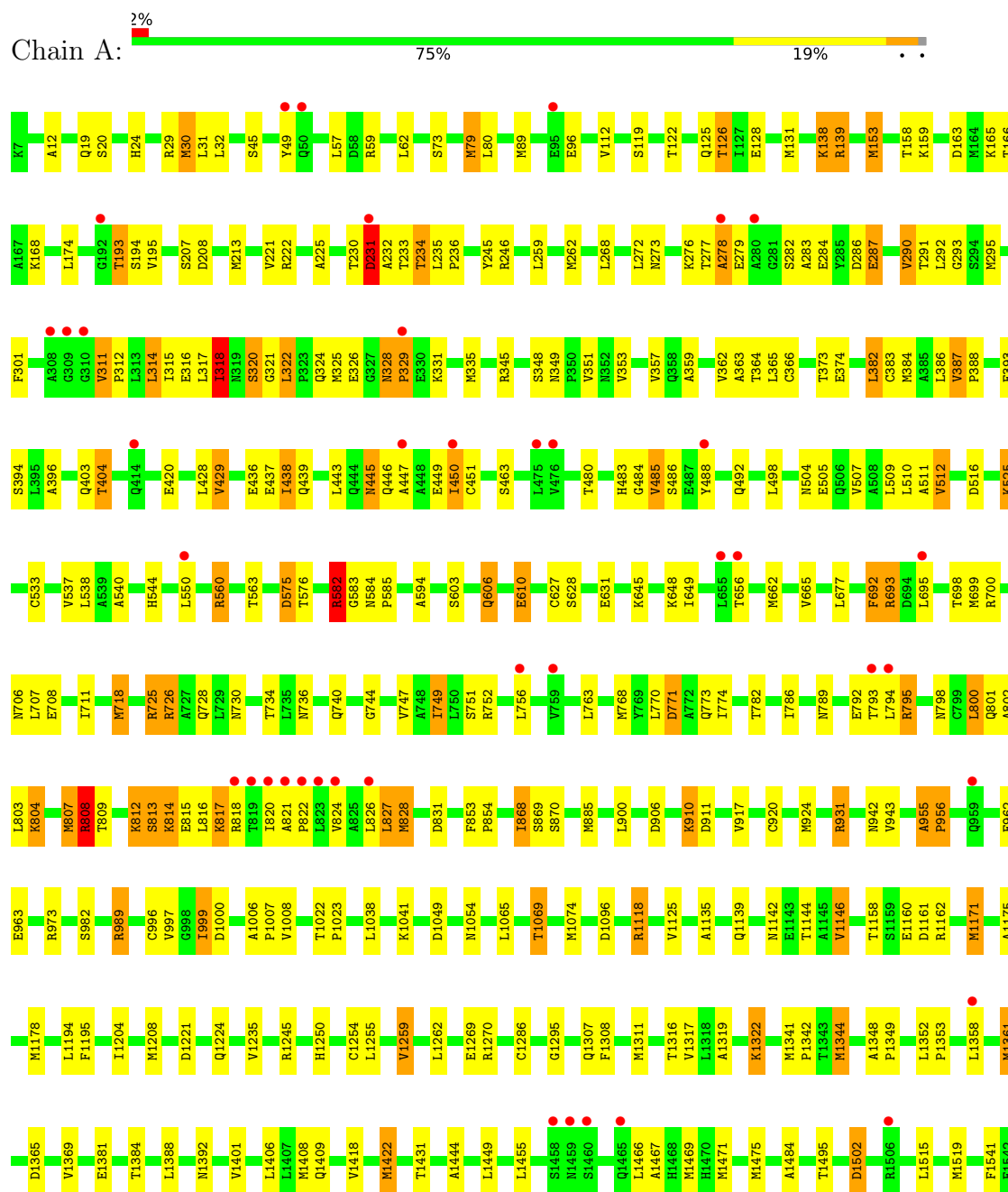
- Molecule 2 is water.

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

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



K2454	PR0	R2227	L2134	K2036	L1889	H1725	V1543
C2467	PR0	R2228	L2140	T2037	I1893	K1743	M1554
T2470	GLU	V2229	C2141	A2038	I1893	L1744	I1558
D2479	GLU	E2234	R2142	R2041	E1918	S1751	Q1566
T2489	GLU	L2235	L2143	L2042	I1919	E1754	G1567
N2499	V2324	A2236	K2144	E2043	K1920	I1758	L1568
V2500	G2339	C2240	N2153	S2044	T1921	E1765	S1569
P2504	W2340	G2155	G2154	V2045	L1936	I1766	M1570
	M2343	L2245	I2156	A2048	L1940	E1785	A1571
	G2344	A2246	F2157	I2049	P1941	V1767	D1572
	M2345	T2247	T2158	S2050	A1946		M1575
	V2348	V2251	T2159	S2053	T1950	F1780	R1578
	M2349	L2256	I2160	L2054	T1951	P1781	
	I2353	P2259	I2163	T2055	V1952	F1782	E1582
L2354	M2260	M2261	H2164	T2056	A1784	Q1785	T1592
V2357	V2262	M2262	Q2166	I2059	Q1785	D1786	T1593
C2360	L2263	E2264	L2173	Q2060	H1963	T1787	R1620
V2363	E2265	A2265	L2174	P2061	K1964	A1788	L1623
H2366	C2266	R2267	L2175	F2062	K1965	R1789	G1627
R2371	V2268	V2268	G2176	L2063	I1969	I1790	T1631
R2374	L2272	L2273	I2177	I2067	L1978	G1792	E1636
Y2382	L2278	R2278	H2178	Q2086	L1982	C1793	E1652
G2389	V2287	V2287	L2179	L2087	V1982	P1794	K1653
T2390	L2280	L2280	L2180	E2088	V1992	R1813	V1654
Q2400	Q2295	Q2295	K2187	R2092	C1993	H1817	M1655
T2403	R2296	R2296	I2190	L2094	L2000	R1821	M1656
Q2404	A2298	A2298	Q2191	M2099	C2001	Y1822	M1661
I2405	M2301	M2301	A2196	N2105	L2004	V1825	E1662
T2414	HIS	HIS	L2202	M2106	T2005	N1831	R1681
T2415	ALA	ALA	C2205	R2107	K2006	Y1835	T1690
C2420	GLN	GLN	V2206	K2108	N2007	T1838	L1703
K2438	ALA	ALA	A2210	V2111	E2008	I1840	M1707
L2442	GLN	GLN	GLU	C2112	M2009	M1841	G1708
S2449	ASP	ASP	GLY	L2113	M2010	K1853	M1709
V2450	TYR	TYR	N2213	L2114	K2011	L1715	D1716
M2453	GLU	GLU	E2214	P2115	L2012	D1716	T1719
L2463	VAL	VAL	V2215	C2116	L2013	E1879	A1720
	ALA	ALA	T2216	M2117	L2014	L1880	M1721
	GLN	GLN	D2217	A2118	N2017	T1719	G1722
	ASP	ASP	L2218	V2119	G2018	L1715	
	TYR	TYR	V2219	Q2122	A2019	D1716	
	GLU	GLU	V2220	G2123	P2020	E1879	
	ALA	ALA	G2221	R2124	S2028	L1880	
	GLY	GLY	G2222	T2125	D2031	A1720	
	VAL	VAL	L2223	L2130	E2035	G1722	
	SER	SER	R2224				
	GLU	GLU	T2226				

4 Data and refinement statistics

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 – 2.67 110.75 – 2.67	Depositor EDS
% Data completeness (in resolution range)	100.0 (110.75-2.67) 99.9 (110.75-2.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.69Å)	Xtriage
Refinement program	REFMAC v5.0	Depositor
R, R_{free}	0.209 , 0.268 0.232 , 0.267	Depositor DCC
R_{free} test set	4517 reflections (4.86%)	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)	0.36 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

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	0.56	2/18847 (0.0%)	1.02	10/25412 (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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	492[A]	GLN	C-O	5.72	1.31	1.24
1	A	492[B]	GLN	C-O	5.72	1.31	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2479	ASP	CA-CB-CG	7.76	120.36	112.60
1	A	692	PHE	CA-CB-CG	6.59	120.39	113.80
1	A	1144	THR	CA-CB-OG1	-5.71	101.04	109.60
1	A	585	PRO	N-CA-C	-5.57	106.90	113.86
1	A	516	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	1791	GLN	CB-CA-C	5.25	118.30	109.89
1	A	1269	GLU	CB-CG-CD	5.09	121.25	112.60
1	A	492[A]	GLN	CA-C-O	5.05	127.73	120.51
1	A	492[B]	GLN	CA-C-O	5.05	127.73	120.51
1	A	1620	ARG	CB-CA-C	-5.03	102.99	110.88

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
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

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	314	0
2	A	112	224	0	3	0
All	All	18791	18940	18693	314	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 (314) 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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:2019:ALA:O	1:A:2020:PRO:C	2.53	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:583:GLY:O	1:A:584:ASN:C	2.53	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:1049:ASP:CG	1:A:1054:ASN:HD22	2.19	0.50
1:A:656:THR:HG21	1:A:706:ASN:CG	2.37	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:2224:ARG:O	1:A:2225:CYS:C	2.52	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:2060:GLN:O	1:A:2061:PRO:C	2.55	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:802:ALA:O	1:A:803:LEU:C	2.55	0.49
1:A:314:LEU:HD11	1:A:359:ALA:HB1	1.93	0.49
1:A:2048:ALA:O	1:A:2049:ILE:C	2.56	0.49
1:A:311:VAL:O	1:A:312:PRO:C	2.56	0.48
1:A:387:VAL:N	1:A:388:PRO:HD2	2.28	0.48
1:A:393:GLU:O	1:A:394:SER:C	2.56	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:438:ILE:O	1:A:439:GLN:C	2.56	0.48
1:A:575:ASP:OD1	1:A:575:ASP:N	2.46	0.48
1:A:2144:LYS:HD2	1:A:2144:LYS:N	2.25	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:962:GLU:O	1:A:963:GLU:C	2.57	0.48
1:A:386:LEU:O	1:A:387:VAL:C	2.56	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:2339:GLY:O	1:A:2340:TRP:C	2.57	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:770:LEU:O	1:A:771:ASP:C	2.56	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
1:A:817:LYS:HE2	1:A:817:LYS:HB3	1.63	0.47
1:A:193:THR:O	1:A:194:SER:C	2.57	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:955:ALA:O	1:A:956:PRO:C	2.58	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: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: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:2236:ALA:HB1	1:A:2343:MSE:HE1	1.97	0.46
1:A:445:ASN:C	1:A:447:ALA:H	2.23	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:2086:GLN:O	1:A:2087:LEU:C	2.59	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:LEU:HD12	1:A:62:LEU:HD11	1.97	0.46
1:A:2216:THR:C	1:A:2218:LEU:N	2.69	0.46
1:A:812:LYS:HB3	1:A:812:LYS:HE3	1.52	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: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:1784:ALA:O	1:A:1785:GLN:C	2.59	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:2113:LEU:C	1:A:2115:PRO:HD2	2.40	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
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: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:2405:ILE:C	1:A:2405:ILE:HD12	2.41	0.44
1:A:1568:LEU:HD13	1:A:1575:MSE:CE	2.47	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:1554:ASN:OD1	1:A:1554:ASN:C	2.60	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:1365:ASP:O	1:A:1369:VAL:HG23	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:THR:O	1:A:278:ALA:C	2.60	0.44
1:A:282:SER:HA	1:A:286:ASP:HB2	2.00	0.44
1:A:827:LEU:C	1:A:828:MSE:SE	3.10	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:194:SER:O	1:A:195:VAL:C	2.61	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:800:LEU:O	1:A:801:GLN:C	2.61	0.43
1:A:2019:ALA:HB3	1:A:2020:PRO:HD3	1.99	0.43
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:79:MSE:HE3	1:A:119:SER:HB3	2.01	0.43
1:A:363:ALA:O	1:A:364:THR:C	2.62	0.43
1:A:484:GLY:O	1:A:485:VAL:C	2.60	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:1789:ARG:O	1:A:1790:ILE:C	2.61	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:1317:VAL:C	1:A:1319:ALA:H	2.27	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: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:815:GLU:O	1:A:816:LEU:C	2.62	0.42
1:A:1495:THR:HG22	1:A:1543:VAL:HG11	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2217:ASP:O	1:A:2220:VAL:HG22	2.19	0.42
1:A:221:VAL:O	1:A:222:ARG:C	2.61	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:292:LEU:O	1:A:293:GLY:C	2.61	0.42
1:A:2216:THR:C	1:A:2218:LEU:H	2.27	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:910:LYS:O	1:A:911:ASP:C	2.63	0.42
1:A:2093:THR:O	1:A:2094:LEU:C	2.62	0.42
1:A:318:ILE:HG13	1:A:318:ILE:H	1.45	0.42
1:A:328:ASN:O	1:A:329:PRO:C	2.63	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:707:LEU:O	1:A:708:GLU:C	2.63	0.42
1:A:2290:LEU:HD23	1:A:2290:LEU:HA	1.90	0.42
1:A:245:TYR:O	1:A:246:ARG:C	2.62	0.41
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
1:A:1471:MSE:HG2	1:A:1475:MSE:HE2	2.01	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:2449:SER:O	1:A:2450:VAL:C	2.63	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:428:LEU:O	1:A:429:VAL:C	2.63	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:207:SER:O	1:A:208:ASP:C	2.64	0.40
1:A:2059:ILE:HG22	1:A:2063:LEU:HD11	2.02	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:291:THR:O	1:A:292:LEU:C	2.64	0.40
1:A:1286:CYS:SG	1:A:1295:GLY:HA3	2.61	0.40
1:A:1406:LEU:C	1:A:1406:LEU:HD13	2.47	0.40
1:A:318:ILE:HG12	1:A:364:THR:HB	2.04	0.40
1:A:382:LEU:O	1:A:383:CYS:C	2.64	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

5.3.1 Protein backbone

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%)	30 51

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 ⓘ

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%)	1778 (89%)	229 (11%)	5 12

All (229) 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	31	LEU
1	A	32	LEU
1	A	45	SER
1	A	79	MSE
1	A	96	GLU
1	A	112	VAL
1	A	122	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	193	THR
1	A	230	THR
1	A	231	ASP
1	A	233	THR
1	A	234	THR
1	A	272	LEU
1	A	284	GLU
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	351	VAL
1	A	353	VAL
1	A	357	VAL
1	A	362	VAL
1	A	373	THR
1	A	374	GLU
1	A	382	LEU
1	A	387	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	403	GLN
1	A	404	THR
1	A	420	GLU
1	A	429	VAL
1	A	436	GLU
1	A	437	GLU
1	A	438	ILE
1	A	445	ASN
1	A	446	GLN
1	A	449	GLU
1	A	450	ILE
1	A	463	SER
1	A	480	THR
1	A	483	HIS
1	A	485	VAL
1	A	486	SER
1	A	509	LEU
1	A	512	VAL
1	A	525	LYS
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	610	GLU
1	A	628	SER
1	A	631	GLU
1	A	665	VAL
1	A	677	LEU
1	A	693	ARG
1	A	698	THR
1	A	711	ILE
1	A	718	MSE
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	774	ILE
1	A	793	THR
1	A	794	LEU
1	A	795	ARG
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	820	ILE
1	A	824	VAL
1	A	831	ASP
1	A	868	ILE
1	A	869	SER
1	A	870	SER
1	A	900	LEU
1	A	906	ASP
1	A	910	LYS
1	A	917	VAL
1	A	931	ARG
1	A	943	VAL
1	A	973	ARG
1	A	982	SER
1	A	989	ARG
1	A	997	VAL
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	1221	ASP
1	A	1224	GLN
1	A	1235	VAL
1	A	1259	VAL
1	A	1316	THR
1	A	1322	LYS
1	A	1344	MSE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1361	MSE
1	A	1381	GLU
1	A	1384	THR
1	A	1401	VAL
1	A	1422	MSE
1	A	1431	THR
1	A	1502	ASP
1	A	1593	THR
1	A	1620	ARG
1	A	1631	THR
1	A	1636	GLU
1	A	1654	VAL
1	A	1662	GLU
1	A	1681	ARG
1	A	1690	ILE
1	A	1709	MSE
1	A	1721	MSE
1	A	1743	LYS
1	A	1744	LEU
1	A	1754	GLU
1	A	1765	GLU
1	A	1766	ILE
1	A	1785	GLN
1	A	1789	ARG
1	A	1791	GLN
1	A	1813	ARG
1	A	1825	VAL
1	A	1831	ASN
1	A	1838	THR
1	A	1853	LYS
1	A	1861	LEU
1	A	1879	GLU
1	A	1880	LEU
1	A	1918	GLU
1	A	1952	VAL
1	A	1961	ILE
1	A	1964	LYS
1	A	2006	LYS
1	A	2009	SER
1	A	2012	LYS
1	A	2017	ASN
1	A	2020	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2028	SER
1	A	2031	ASP
1	A	2035	GLU
1	A	2036	LYS
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	2067	ILE
1	A	2088	GLU
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	2156	ILE
1	A	2160	ILE
1	A	2175	LEU
1	A	2187	LYS
1	A	2190	ILE
1	A	2191	GLN
1	A	2216	THR
1	A	2219	VAL
1	A	2220	VAL
1	A	2226	THR
1	A	2234	GLU
1	A	2245	ILE
1	A	2261	VAL
1	A	2287	VAL
1	A	2290	LEU
1	A	2295	GLN
1	A	2297	ARG
1	A	2301	MSE
1	A	2348	VAL
1	A	2353	ILE
1	A	2363	VAL
1	A	2371	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2390	THR
1	A	2404	GLN
1	A	2438	LYS
1	A	2442	LEU
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 (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	ASN
1	A	324	GLN
1	A	397	HIS
1	A	414	GLN
1	A	506	GLN
1	A	517	ASN
1	A	547	ASN
1	A	798	ASN
1	A	810	HIS
1	A	859	ASN
1	A	889	GLN
1	A	959	GLN
1	A	1076	ASN
1	A	1123	ASN
1	A	1130	GLN
1	A	1139	GLN
1	A	1224	GLN
1	A	1412	GLN
1	A	1489	GLN
1	A	1596	GLN
1	A	1615	GLN
1	A	1785	GLN
1	A	1937	GLN
1	A	1984	ASN
1	A	2007	ASN
1	A	2017	ASN
1	A	2029	ASN
1	A	2086	GLN
1	A	2096	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2104	ASN
1	A	2191	GLN
1	A	2296	GLN
1	A	2369	GLN
1	A	2387	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	2390/2498 (95%)	0.02	48 (2%) 65 61	36, 74, 97, 121	2 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	822	PRO	5.6
1	A	476	VAL	4.0
1	A	475	LEU	3.7
1	A	329	PRO	3.7
1	A	95	GLU	3.7
1	A	818	ARG	3.4
1	A	450	ILE	3.4
1	A	1458	SER	3.3
1	A	819	THR	3.3
1	A	278	ALA	3.3
1	A	447	ALA	3.2
1	A	1459	ASN	3.1
1	A	826	LEU	2.9
1	A	309	GLY	2.8
1	A	308	ALA	2.8
1	A	2298	ALA	2.7
1	A	824	VAL	2.7
1	A	655	LEU	2.7
1	A	231	ASP	2.7
1	A	2055	TYR	2.6
1	A	280	ALA	2.6
1	A	488	TYR	2.6
1	A	959	GLN	2.6
1	A	820	ILE	2.5
1	A	695	LEU	2.5
1	A	1465	GLN	2.5
1	A	2220	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1506	ARG	2.4
1	A	2222	GLY	2.4
1	A	1460	SER	2.4
1	A	1358	LEU	2.3
1	A	192	GLY	2.3
1	A	310	GLY	2.3
1	A	823	LEU	2.3
1	A	759	VAL	2.3
1	A	821	ALA	2.2
1	A	793	THR	2.2
1	A	794	LEU	2.2
1	A	2221	GLY	2.2
1	A	49	TYR	2.2
1	A	2123	GLY	2.2
1	A	2215	VAL	2.1
1	A	2217	ASP	2.1
1	A	50	GLN	2.1
1	A	550	LEU	2.1
1	A	656	THR	2.0
1	A	414	GLN	2.0
1	A	756	LEU	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.