Full wwPDB X-ray Structure Validation Report (i)

Mar 29, 2023 – 01:30 pm BST

PDB ID	:	8BT6
Title	:	Crystal structure of Toxoplasma gondii glideosome-associated connector
Authors	:	Hung, Y.F.; Kursula, I.
Deposited on	:	2022-11-27
Resolution	:	2.33 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

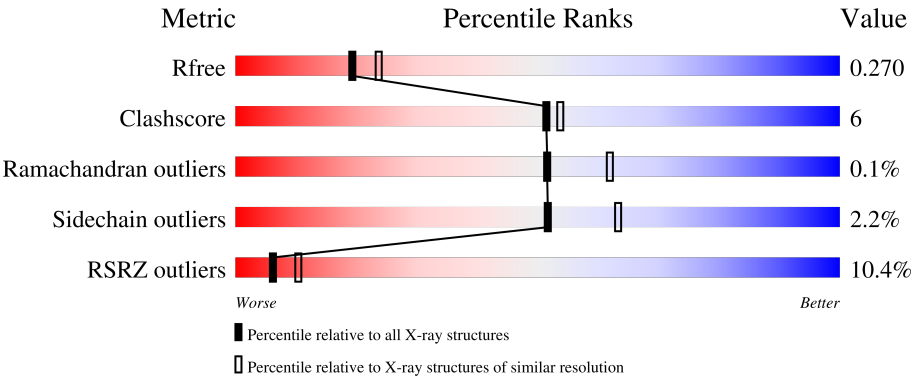
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 2.33 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	2646	10% 86% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	A	2701	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 40007 atoms, of which 19985 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.

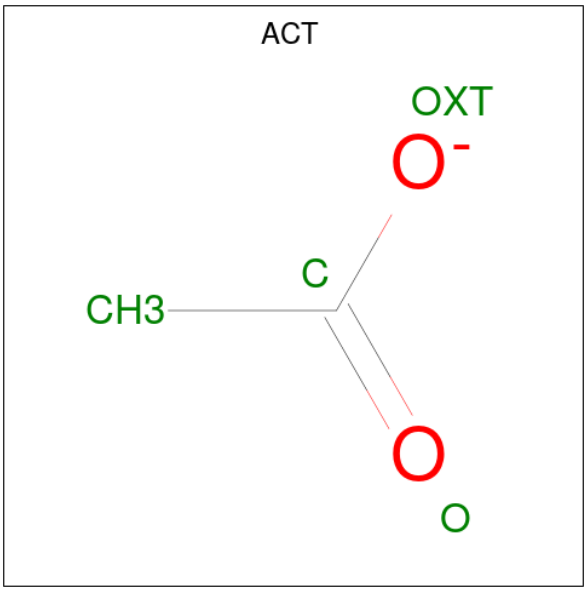
- Molecule 1 is a protein called Putative anonymous antigen-1.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trac
			Total	C	H	N	O	S	Se			
1	A	2633	39936	12477	19982	3407	3905	75	90	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP A0A151HKA5
A	2640	HIS	-	expression tag	UNP A0A151HKA5
A	2641	HIS	-	expression tag	UNP A0A151HKA5
A	2642	HIS	-	expression tag	UNP A0A151HKA5
A	2643	HIS	-	expression tag	UNP A0A151HKA5
A	2644	HIS	-	expression tag	UNP A0A151HKA5
A	2645	HIS	-	expression tag	UNP A0A151HKA5

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	K	0	0
			2	2		

- Molecule 4 is water.

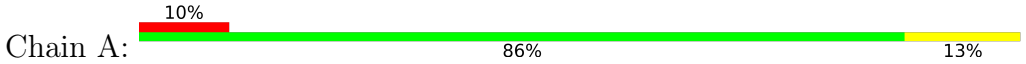
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	62	Total	O	0	0
			62	62		

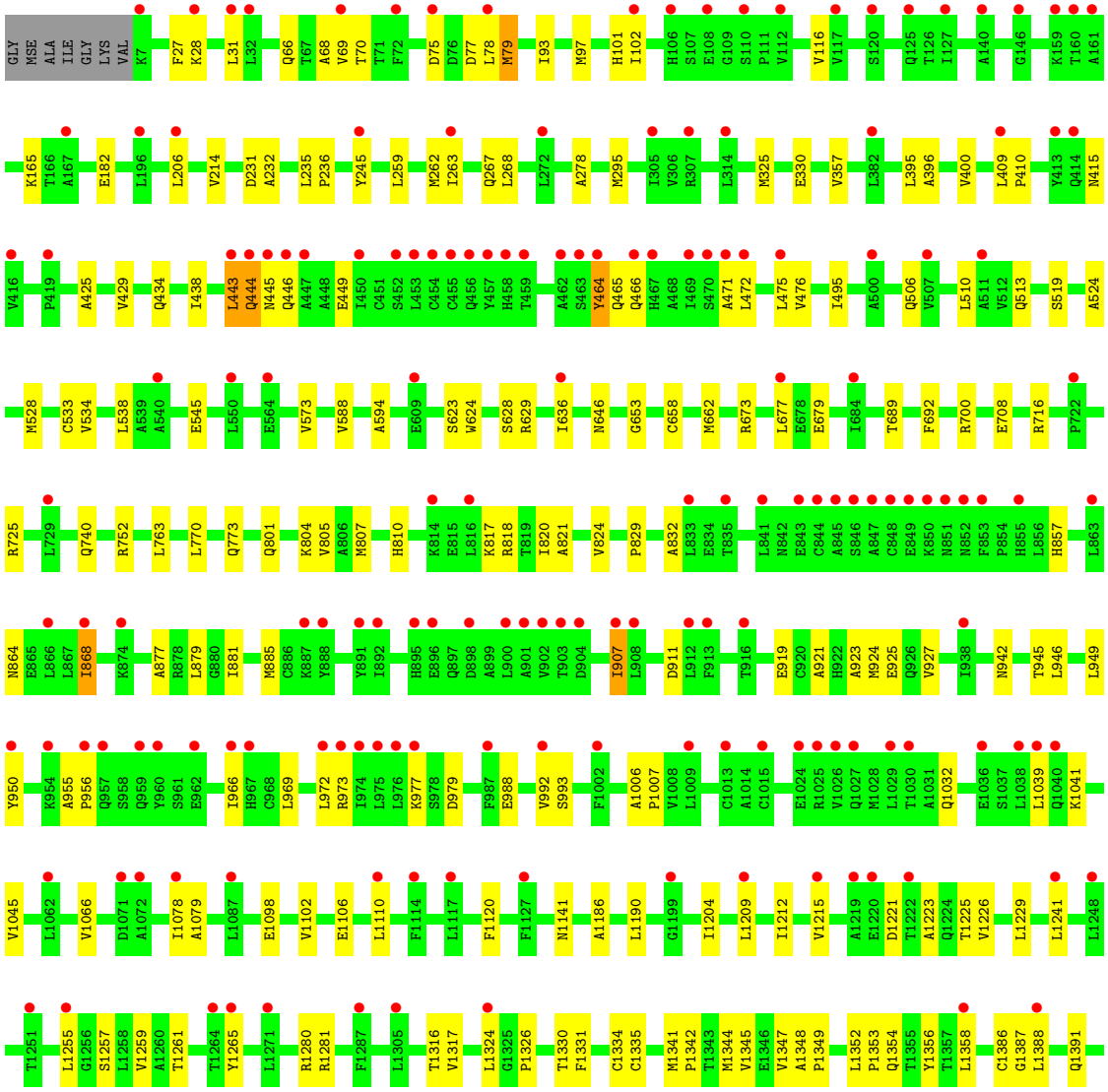
3 Residue-property plots (i)

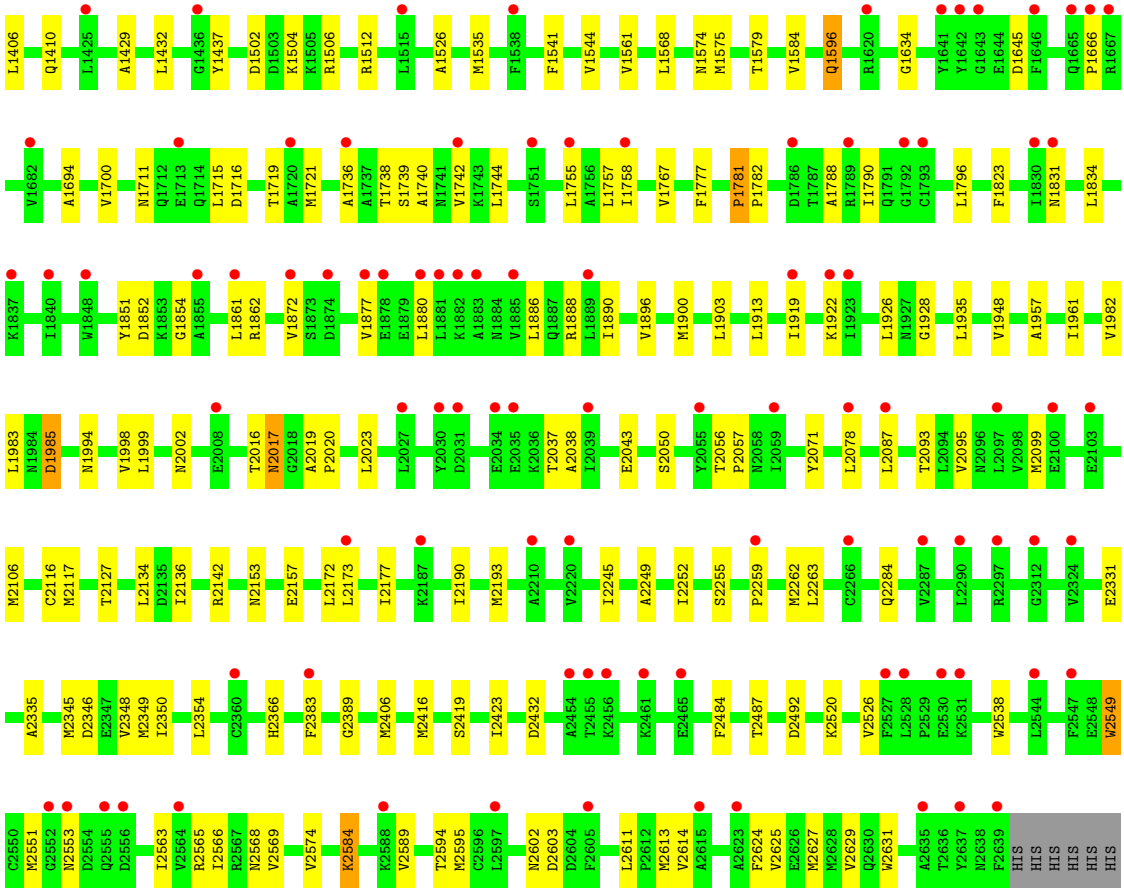
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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






L1406 Q1410 L1425 A1429 L1432 G1436 Y1437 D1502 D1503 K1504 K1505 R1506 R1512 L1515 A1526 M1535 F1538 F1541 V1544 V1561 L1568 N1574 M1575 T1579 V1584 Q1596 R1620 G1634 Y1641 Y1642 G1643 E1644 D1645 F1646 Q1665 P1666 R1667
V1682 A1694 V1700 N1711 Q1712 E1713 Q1714 L1715 D1716 T1719 A1720 M1721 A1736 A1737 T1738 S1739 A1740 N1741 V1742 K1743 L1744 S1751 L1755 A1756 L1757 I1758 V1767 F1777 P1781 P1782 D1786 T1787 A1788 R1789 I1790 Q1791 G1792 C1793 L1796 F1823 I1830 N1831 L1834
K1837 T1840 W1848 Y1851 D1852 K1853 G1854 A1855 L1861 R1862 V1872 S1873 D1874 V1877 E1878 E1879 L1880 L1881 K1882 A1883 N1884 V1885 L1886 Q1887 R1888 L1889 I1890 V1896 M1900 L1903 L1913 I1919 K1922 I1923 L1926 N1927 G1928 L1935 V1948 A1957 I1961 V1982
L1983 N1984 D1985 N1994 V1998 L1999 N2002 E2008 T2016 N2017 G2018 A2019 P2020 L2023 L2027 Y2030 D2031 E2034 E2035 K2036 T2037 A2038 I2039 E2043 S2050 Y2055 T2056 P2057 N2058 I2059 Y2071 L2078 L2087 T2093 L2094 V2095 N2096 L2097 V2098 M2099 E2100 E2103
M2106 C2116 M2117 T2127 L2134 D2135 I2136 R2142 N2153 E2157 L2172 L2173 I2177 K2187 I2190 M2193 A2210 V2220 I2245 A2249 I2252 S2255 P2259 M2262 L2263 C2266 Q2284 V2287 L2290 R2297 G2312 V2324 E2331
A2335 M2345 D2346 E2347 V2348 M2349 I2350 L2354 C2360 H2366 F2383 G2389 M2406 M2416 S2419 I2423 D2432 A2454 T2455 K2456 K2461 E2465 F2484 T2487 D2492 K2520 V2526 F2527 L2528 P2529 E2530 K2531 W2538 L2544 F2547 E2548 W2549
C2550 M2551 G2552 N2553 D2554 Q2555 D2556 I2563 V2564 R2565 I2566 R2567 N2568 V2569 V2574 K2584 K2588 V2589 T2594 M2595 C2596 L2597 N2602 D2603 D2604 F2605 L2611 P2612 M2613 V2614 A2615 A2623 F2624 V2625 E2626 M2627 M2628 V2629 Q2630 W2631 A2635 T2636 Y2637 N2638 F2639 HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	121.40Å 146.66Å 185.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.33 – 2.33 48.02 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.33-2.33) 99.9 (48.02-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.229 , 0.272 0.228 , 0.270	Depositor DCC
R_{free} test set	7088 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	55.7	Xtriage
Anisotropy	0.492	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	40007	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, K

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	0.24	0/20146	0.46	0/27155

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	19954	19982	19982	224	1
2	A	4	3	3	0	0
3	A	2	0	0	0	0
4	A	62	0	0	14	0
All	All	20022	19985	19985	224	1

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 6.

All (224) 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:2345:MSE:HE3	1:A:2349:MSE:HE2	1.32	1.11
1:A:519:SER:HA	1:A:528:MSE:HE1	1.52	0.89
1:A:524:ALA:HB1	1:A:528:MSE:HE2	1.55	0.86
1:A:513:GLN:OE1	4:A:2801:HOH:O	1.94	0.84
1:A:817:LYS:NZ	4:A:2805:HOH:O	2.12	0.80
1:A:524:ALA:HB1	1:A:528:MSE:CE	2.12	0.78
1:A:946:LEU:HD22	1:A:972:LEU:HD13	1.68	0.74
1:A:2594:THR:HG22	1:A:2614:VAL:HG12	1.69	0.74
1:A:330:GLU:OE1	4:A:2802:HOH:O	2.06	0.74
1:A:396:ALA:O	1:A:400:VAL:HG23	1.87	0.74
1:A:1568:LEU:HD13	1:A:1575:MSE:CE	2.18	0.74
1:A:857:HIS:CE1	1:A:907:ILE:HD11	2.24	0.73
1:A:2245:ILE:HG23	1:A:2349:MSE:HE1	1.71	0.73
1:A:2249:ALA:HB2	1:A:2349:MSE:HE3	1.71	0.72
1:A:2419:SER:O	1:A:2423:ILE:HD12	1.89	0.72
1:A:2134:LEU:HD22	1:A:2172:LEU:HD11	1.71	0.71
1:A:2492:ASP:OD1	4:A:2803:HOH:O	2.08	0.71
1:A:1316:THR:HG23	1:A:1317:VAL:HG13	1.71	0.71
1:A:2117:MSE:HE1	1:A:2153:ASN:HB2	1.73	0.70
1:A:1852:ASP:OD2	4:A:2804:HOH:O	2.09	0.70
1:A:658:CYS:SG	1:A:662:MSE:HE3	2.32	0.70
1:A:231:ASP:OD1	1:A:232:ALA:N	2.25	0.69
1:A:259:LEU:HA	1:A:262:MSE:HE3	1.73	0.69
1:A:946:LEU:CD2	1:A:972:LEU:HD13	2.23	0.69
1:A:1324:LEU:HD22	1:A:1358:LEU:HD11	1.74	0.69
1:A:969:LEU:HA	1:A:972:LEU:HD12	1.76	0.68
1:A:495:ILE:HD11	1:A:533:CYS:SG	2.34	0.67
1:A:2406:MSE:HE3	1:A:2419:SER:HB3	1.77	0.67
1:A:2538:TRP:CZ2	1:A:2627:MSE:HE1	2.30	0.67
1:A:1334:CYS:HB2	1:A:1344:MSE:HE2	1.75	0.67
1:A:1851:TYR:CE2	1:A:1861:LEU:HD22	2.30	0.67
1:A:2106:MSE:HE3	1:A:2142:ARG:HD2	1.75	0.67
1:A:1755:LEU:HD12	1:A:1790:ILE:HD11	1.77	0.66
1:A:921:ALA:O	1:A:972:LEU:HD11	1.95	0.66
1:A:1215:VAL:HG11	1:A:1257:SER:HB2	1.77	0.65
1:A:1890:ILE:HD12	1:A:1928:GLY:HA2	1.78	0.65
1:A:425:ALA:O	1:A:429:VAL:HG13	1.97	0.65
1:A:992:VAL:HG21	1:A:1032:GLN:HG3	1.78	0.65
1:A:950:TYR:HE2	1:A:966:ILE:HG23	1.62	0.64
1:A:1429:ALA:O	4:A:2806:HOH:O	2.14	0.64
1:A:2406:MSE:HE2	1:A:2416:MSE:SE	2.47	0.64
1:A:2335:ALA:O	4:A:2808:HOH:O	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2331:GLU:O	4:A:2807:HOH:O	2.14	0.63
1:A:1985:ASP:OD1	1:A:1985:ASP:N	2.32	0.63
1:A:1223:ALA:HB2	1:A:1265:TYR:CG	2.35	0.62
1:A:1331:PHE:HA	1:A:1344:MSE:HE1	1.81	0.62
1:A:1900:MSE:HE1	1:A:1948:VAL:HG21	1.82	0.61
1:A:1326:PRO:O	1:A:1330:THR:HG23	2.00	0.61
1:A:770:LEU:HD13	1:A:810:HIS:CG	2.36	0.61
1:A:31:LEU:HD21	1:A:68:ALA:HB1	1.83	0.60
1:A:1281:ARG:O	4:A:2809:HOH:O	2.16	0.60
1:A:1739:SER:O	1:A:1742:VAL:HG12	2.00	0.60
1:A:278:ALA:O	4:A:2810:HOH:O	2.16	0.60
1:A:443:LEU:HD12	1:A:444:GLN:H	1.67	0.60
1:A:588:VAL:HG13	1:A:636:ILE:HD12	1.84	0.59
1:A:1983:LEU:HD21	1:A:2023:LEU:HD23	1.84	0.59
1:A:2484:PHE:O	1:A:2487:THR:HG22	2.02	0.59
1:A:2624:PHE:HA	1:A:2627:MSE:HE2	1.84	0.59
1:A:949:LEU:HB3	1:A:969:LEU:HD21	1.85	0.58
1:A:1872:VAL:HG23	1:A:1880:LEU:HD11	1.85	0.58
1:A:2134:LEU:HD22	1:A:2172:LEU:CD1	2.33	0.58
1:A:708:GLU:OE2	1:A:752:ARG:NH1	2.37	0.58
1:A:1758:ILE:HA	1:A:1767:VAL:HG13	1.84	0.57
1:A:1755:LEU:CD1	1:A:1790:ILE:HD11	2.33	0.57
1:A:763:LEU:HD22	1:A:773:GLN:HA	1.87	0.57
1:A:1526:ALA:CB	1:A:1535:MSE:HE2	2.35	0.57
1:A:2538:TRP:HZ2	1:A:2627:MSE:HE1	1.69	0.57
1:A:740:GLN:O	4:A:2811:HOH:O	2.18	0.56
1:A:79:MSE:HG3	1:A:116:VAL:HG13	1.87	0.56
1:A:573:VAL:HG12	1:A:573:VAL:O	2.04	0.56
1:A:925:GLU:N	1:A:972:LEU:HD21	2.21	0.56
1:A:1568:LEU:HD22	1:A:1575:MSE:HE2	1.87	0.55
1:A:877:ALA:HA	1:A:881:ILE:HG22	1.88	0.55
1:A:1106:GLU:O	1:A:1110:LEU:HD23	2.06	0.55
1:A:214:VAL:HG21	1:A:245:TYR:CZ	2.42	0.55
1:A:864:ASN:O	1:A:868:ILE:HD12	2.07	0.55
1:A:2569:VAL:O	1:A:2569:VAL:HG13	2.07	0.55
1:A:2406:MSE:HE3	1:A:2419:SER:CB	2.37	0.54
1:A:1596:GLN:HG2	1:A:1634:GLY:HA3	1.87	0.54
1:A:2568:ASN:OD1	1:A:2569:VAL:N	2.41	0.54
1:A:804:LYS:HA	1:A:807:MSE:HE3	1.89	0.54
1:A:1888:ARG:HD3	4:A:2804:HOH:O	2.06	0.54
1:A:1141:ASN:ND2	4:A:2801:HOH:O	2.18	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:MSE:HA	1:A:102:ILE:HD11	1.90	0.53
1:A:1255:LEU:O	1:A:1259:VAL:HG23	2.08	0.53
1:A:1922:LYS:O	1:A:1926:LEU:HD23	2.08	0.53
1:A:1541:PHE:HD1	1:A:1575:MSE:HE1	1.74	0.53
1:A:1851:TYR:HE2	1:A:1861:LEU:HD22	1.72	0.53
1:A:263:ILE:CG2	1:A:295:MSE:HE2	2.38	0.53
1:A:1349:PRO:HG3	1:A:1388:LEU:HD13	1.90	0.53
1:A:1341:MSE:O	1:A:1345:VAL:HG23	2.09	0.53
1:A:263:ILE:HG21	1:A:295:MSE:HE2	1.90	0.53
1:A:2050:SER:HB2	1:A:2093:THR:HG22	1.92	0.52
1:A:1994:ASN:O	1:A:1998:VAL:HG23	2.09	0.52
1:A:2574:VAL:HG12	1:A:2574:VAL:O	2.08	0.52
1:A:2017:ASN:ND2	1:A:2017:ASN:O	2.43	0.52
1:A:2099:MSE:HE3	1:A:2565:ARG:HG3	1.91	0.52
1:A:2563:ILE:HD12	1:A:2566:ILE:HD12	1.90	0.52
1:A:2602:ASN:OD1	1:A:2603:ASP:N	2.42	0.52
1:A:471:ALA:O	1:A:475:LEU:HD13	2.10	0.52
1:A:829:PRO:HB2	1:A:832:ALA:HB3	1.92	0.52
1:A:2549:TRP:HE1	1:A:2551:MSE:HE3	1.75	0.52
1:A:1526:ALA:HB3	1:A:1535:MSE:HE2	1.92	0.51
1:A:1900:MSE:HE1	1:A:1948:VAL:CG2	2.41	0.51
1:A:1502:ASP:OD1	1:A:1512:ARG:NE	2.44	0.51
1:A:2346:ASP:OD1	1:A:2348:VAL:HG12	2.11	0.50
1:A:1280:ARG:HA	1:A:1330:THR:HG22	1.94	0.50
1:A:357:VAL:HG21	1:A:395:LEU:HD11	1.93	0.50
1:A:409:LEU:HB2	1:A:410:PRO:HD3	1.93	0.50
1:A:2190:ILE:HA	1:A:2193:MSE:HE3	1.93	0.50
1:A:2252:ILE:HG23	1:A:2262:MSE:SE	2.61	0.50
1:A:1226:VAL:HG21	1:A:1261:THR:HG21	1.94	0.49
1:A:28:LYS:NZ	1:A:75:ASP:OD2	2.45	0.49
1:A:538:LEU:HD13	1:A:594:ALA:HA	1.94	0.49
1:A:2245:ILE:CG2	1:A:2349:MSE:HE1	2.42	0.49
1:A:1796:LEU:C	1:A:1796:LEU:HD23	2.33	0.49
1:A:1872:VAL:HG21	1:A:1913:LEU:HD22	1.95	0.49
1:A:66:GLN:O	1:A:70:THR:HG23	2.13	0.48
1:A:93:ILE:CD1	1:A:101:HIS:HB3	2.43	0.48
1:A:1204:ILE:CD1	1:A:1241:LEU:HD21	2.43	0.48
1:A:506:GLN:O	1:A:510:LEU:HD22	2.14	0.48
1:A:807:MSE:SE	1:A:868:ILE:HD13	2.64	0.48
1:A:1039:LEU:HD11	1:A:1078:ILE:HG12	1.96	0.48
1:A:2056:THR:OG1	1:A:2057:PRO:HD3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1738:THR:HG22	1:A:1740:ALA:H	1.79	0.48
1:A:2071:TYR:OH	1:A:2093:THR:OG1	2.31	0.48
1:A:2526:VAL:HG11	1:A:2551:MSE:HE2	1.95	0.48
1:A:588:VAL:CG1	1:A:636:ILE:HD12	2.44	0.47
1:A:69:VAL:HA	1:A:78:LEU:HD21	1.95	0.47
1:A:79:MSE:HE3	1:A:116:VAL:HA	1.95	0.47
1:A:1098:GLU:O	1:A:1102:VAL:HG23	2.15	0.47
1:A:2350:ILE:HD13	1:A:2383:PHE:CE1	2.50	0.47
1:A:818:ARG:O	1:A:1504:LYS:NZ	2.34	0.47
1:A:1221:ASP:OD1	1:A:1221:ASP:N	2.47	0.47
1:A:2255:SER:O	1:A:2262:MSE:HE2	2.15	0.47
1:A:2037:THR:HG23	1:A:2038:ALA:N	2.29	0.47
1:A:950:TYR:HA	1:A:969:LEU:HD13	1.97	0.46
1:A:545:GLU:OE2	1:A:646:ASN:ND2	2.44	0.46
1:A:942:ASN:O	1:A:945:THR:HG22	2.16	0.46
1:A:1886:LEU:O	1:A:1890:ILE:HG12	2.15	0.46
1:A:206:LEU:HD22	1:A:206:LEU:N	2.31	0.46
1:A:472:LEU:O	1:A:476:VAL:HG23	2.16	0.46
1:A:1225:THR:O	1:A:1229:LEU:HD23	2.16	0.46
1:A:1574:ASN:OD1	1:A:1694:ALA:N	2.49	0.45
1:A:801:GLN:O	1:A:805:VAL:HG23	2.16	0.45
1:A:2078:LEU:CD1	1:A:2087:LEU:HD13	2.46	0.45
1:A:624:TRP:CE3	1:A:636:ILE:HG22	2.52	0.45
1:A:689:THR:HA	1:A:692:PHE:CE2	2.52	0.45
1:A:2263:LEU:C	1:A:2263:LEU:HD23	2.37	0.45
1:A:629:ARG:NH1	1:A:677:LEU:HD11	2.32	0.45
1:A:821:ALA:O	1:A:824:VAL:HG22	2.16	0.45
1:A:973:ARG:HB3	1:A:977:LYS:HG3	1.99	0.45
1:A:1335:CYS:O	1:A:1341:MSE:HE2	2.16	0.45
1:A:396:ALA:HB1	1:A:438:ILE:CD1	2.47	0.45
1:A:2116:CYS:SG	1:A:2136:ILE:HD11	2.57	0.44
1:A:2589:VAL:HG12	1:A:2589:VAL:O	2.17	0.44
1:A:818:ARG:HD2	1:A:1506:ARG:HB3	1.99	0.44
1:A:1354:GLN:OE1	1:A:1354:GLN:N	2.49	0.44
1:A:534:VAL:HG12	1:A:538:LEU:HD11	1.98	0.44
1:A:1209:LEU:HA	1:A:1212:ILE:HD12	1.99	0.44
1:A:653:GLY:O	1:A:700:ARG:NH1	2.50	0.44
1:A:857:HIS:HD2	1:A:919:GLU:HG3	1.83	0.44
1:A:885:MSE:HG2	1:A:924:MSE:SE	2.68	0.44
1:A:1544:VAL:CG1	1:A:1561:VAL:HG13	2.47	0.44
1:A:2549:TRP:NE1	1:A:2551:MSE:HE3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1331:PHE:CA	1:A:1344:MSE:HE1	2.47	0.44
1:A:1568:LEU:HD13	1:A:1575:MSE:HE3	1.99	0.44
1:A:1700:VAL:HG11	1:A:1744:LEU:HD21	1.99	0.44
1:A:1579:THR:O	1:A:1584:VAL:HG23	2.19	0.43
1:A:1877:VAL:HG23	1:A:1919:ILE:HD11	1.99	0.43
1:A:2569:VAL:O	1:A:2569:VAL:CG1	2.65	0.43
1:A:1851:TYR:O	1:A:1854:GLY:N	2.51	0.43
1:A:1903:LEU:HD21	1:A:1935:LEU:HD21	2.00	0.43
1:A:2563:ILE:HD13	1:A:2631:TRP:CE3	2.54	0.43
1:A:1890:ILE:HD12	1:A:1928:GLY:CA	2.46	0.43
1:A:2173:LEU:O	1:A:2177:ILE:HG12	2.19	0.43
1:A:1961:ILE:HD12	1:A:2002:ASN:ND2	2.33	0.43
1:A:1716:ASP:HB3	1:A:1719:THR:HG23	1.99	0.42
1:A:2625:VAL:O	1:A:2629:VAL:HG23	2.18	0.42
1:A:679:GLU:N	1:A:679:GLU:OE1	2.52	0.42
1:A:923:ALA:O	1:A:927:VAL:HG23	2.20	0.42
1:A:1041:LYS:O	1:A:1045:VAL:HG23	2.20	0.42
1:A:2611:LEU:O	1:A:2613:MSE:HE2	2.20	0.42
1:A:2584:LYS:HD3	1:A:2584:LYS:N	2.35	0.42
1:A:268:LEU:C	1:A:268:LEU:HD13	2.40	0.42
1:A:1066:VAL:HG22	1:A:1078:ILE:HD12	2.02	0.42
1:A:263:ILE:HG23	1:A:267:GLN:OE1	2.19	0.42
1:A:534:VAL:HG12	1:A:538:LEU:CD1	2.49	0.42
1:A:235:LEU:HB3	1:A:236:PRO:HD3	2.01	0.42
1:A:1186:ALA:O	1:A:1190:LEU:HD22	2.20	0.42
1:A:955:ALA:N	1:A:956:PRO:HD3	2.35	0.41
1:A:1387:GLY:O	1:A:1391:GLN:HG2	2.20	0.41
1:A:464:TYR:N	4:A:2826:HOH:O	2.51	0.41
1:A:1352:LEU:N	1:A:1353:PRO:CD	2.83	0.41
1:A:1711:ASN:OD1	1:A:1757:LEU:HD21	2.20	0.41
1:A:2019:ALA:N	1:A:2020:PRO:CD	2.84	0.41
1:A:1535:MSE:HE1	1:A:1568:LEU:CD2	2.51	0.41
1:A:1788:ALA:HB1	1:A:1834:LEU:HD21	2.03	0.41
1:A:2354:LEU:HD12	1:A:2389:GLY:HA3	2.03	0.41
1:A:624:TRP:CZ3	1:A:636:ILE:HG22	2.56	0.41
1:A:817:LYS:HD3	1:A:820:ILE:HD11	2.02	0.41
1:A:857:HIS:HE1	1:A:907:ILE:HD11	1.79	0.41
1:A:1079:ALA:HB1	1:A:1120:PHE:CZ	2.56	0.41
1:A:182:GLU:OE1	1:A:182:GLU:N	2.48	0.41
1:A:885:MSE:HG2	1:A:924:MSE:CG	2.50	0.41
1:A:946:LEU:HD21	1:A:972:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:924:MSE:C	1:A:972:LEU:HD21	2.41	0.41
1:A:2345:MSE:CE	1:A:2349:MSE:HE2	2.24	0.41
1:A:1781:PRO:N	1:A:1782:PRO:HD2	2.36	0.41
1:A:1896:VAL:O	1:A:1896:VAL:HG12	2.21	0.41
1:A:2259:PRO:HG3	1:A:2366:HIS:NE2	2.36	0.41
1:A:1957:ALA:HB2	1:A:1999:LEU:HA	2.03	0.40
1:A:534:VAL:CG1	1:A:538:LEU:HD11	2.50	0.40
1:A:992:VAL:HG23	1:A:993:SER:N	2.36	0.40
1:A:1348:ALA:N	1:A:1349:PRO:CD	2.84	0.40
1:A:1386:CYS:SG	1:A:1432:LEU:HD23	2.60	0.40
1:A:1982:VAL:O	1:A:1985:ASP:O	2.39	0.40
1:A:2157:GLU:OE1	1:A:2157:GLU:N	2.49	0.40
1:A:1006:ALA:N	1:A:1007:PRO:CD	2.85	0.40
1:A:1341:MSE:N	1:A:1342:PRO:CD	2.84	0.40
1:A:1736:ALA:HB1	1:A:1777:PHE:HA	2.03	0.40
1:A:2117:MSE:HE1	1:A:2153:ASN:CB	2.46	0.40
1:A:2016:THR:HG22	1:A:2016:THR:O	2.21	0.40
1:A:2095:VAL:HG23	1:A:2136:ILE:HG22	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1437:TYR:OH	1:A:2520:LYS:NZ[3_655]	2.18	0.02

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	2631/2646 (99%)	2542 (97%)	87 (3%)	2 (0%)	51 62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	415	ASN
1	A	1666	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	2145/2064 (104%)	2098 (98%)	47 (2%)	52 63

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	PHE
1	A	77	ASP
1	A	79	MSE
1	A	165	LYS
1	A	325	MSE
1	A	434	GLN
1	A	443	LEU
1	A	444	GLN
1	A	445	ASN
1	A	446	GLN
1	A	449	GLU
1	A	464	TYR
1	A	465	GLN
1	A	466	GLN
1	A	623	SER
1	A	628	SER
1	A	673	ARG
1	A	716	ARG
1	A	725	ARG
1	A	868	ILE
1	A	879	LEU
1	A	907	ILE
1	A	911	ASP
1	A	979	ASP
1	A	988	GLU

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Mol	Chain	Res	Type
1	A	1347	VAL
1	A	1356	TYR
1	A	1406	LEU
1	A	1410	GLN
1	A	1596	GLN
1	A	1645	ASP
1	A	1715	LEU
1	A	1721	MSE
1	A	1781	PRO
1	A	1823	PHE
1	A	1831	ASN
1	A	1862	ARG
1	A	1985	ASP
1	A	2017	ASN
1	A	2043	GLU
1	A	2127	THR
1	A	2284	GLN
1	A	2432	ASP
1	A	2549	TRP
1	A	2553	ASN
1	A	2584	LYS
1	A	2595	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ACT	A	2701	-	3,3,3	1.10	0	3,3,3	1.48	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	2543/2646 (96%)	0.78	265 (10%)	6	10	45, 74, 118, 169	0

All (265) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	853	PHE	10.5
1	A	443	LEU	9.2
1	A	2553	ASN	8.2
1	A	464	TYR	8.1
1	A	902	VAL	8.0
1	A	848	CYS	7.2
1	A	160	THR	7.0
1	A	972	LEU	6.4
1	A	852	ASN	6.2
1	A	2528	LEU	6.1
1	A	1855	ALA	6.0
1	A	973	ARG	5.8
1	A	895	HIS	5.7
1	A	850	LYS	5.5
1	A	1877	VAL	5.5
1	A	453	LEU	5.4
1	A	1222	THR	5.3
1	A	454	CYS	5.3
1	A	903	THR	5.3
1	A	896	GLU	5.2
1	A	956	PRO	5.2
1	A	1880	LEU	5.2
1	A	846	SER	5.1
1	A	954	LYS	5.0
1	A	457	TYR	5.0
1	A	1220	GLU	5.0
1	A	866	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	849	GLU	4.9
1	A	841	LEU	4.8
1	A	32	LEU	4.7
1	A	1265	TYR	4.7
1	A	1881	LEU	4.7
1	A	855	HIS	4.6
1	A	898	ASP	4.6
1	A	912	LEU	4.4
1	A	2597	LEU	4.3
1	A	1026	VAL	4.3
1	A	450	ILE	4.3
1	A	444	GLN	4.3
1	A	414	GLN	4.1
1	A	950	TYR	4.0
1	A	1755	LEU	4.0
1	A	69	VAL	4.0
1	A	1002	PHE	4.0
1	A	957	GLN	4.0
1	A	2527	PHE	4.0
1	A	907	ILE	4.0
1	A	967	HIS	4.0
1	A	1078	ILE	3.9
1	A	1071	ASP	3.9
1	A	900	LEU	3.9
1	A	1039	LEU	3.9
1	A	938	ILE	3.9
1	A	314	LEU	3.8
1	A	463	SER	3.8
1	A	161	ALA	3.8
1	A	7	LYS	3.8
1	A	72	PHE	3.8
1	A	835	THR	3.8
1	A	916	THR	3.8
1	A	1666	PRO	3.7
1	A	469	ILE	3.7
1	A	1305	LEU	3.7
1	A	2531	LYS	3.7
1	A	2639	PHE	3.7
1	A	2290	LEU	3.7
1	A	1030	THR	3.6
1	A	462	ALA	3.6
1	A	272	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	1271	LEU	3.6
1	A	966	ILE	3.6
1	A	960	TYR	3.5
1	A	2031	ASP	3.5
1	A	1922	LYS	3.4
1	A	1667	ARG	3.4
1	A	1013	CYS	3.4
1	A	1062	LEU	3.4
1	A	472	LEU	3.4
1	A	847	ALA	3.4
1	A	28	LYS	3.4
1	A	419	PRO	3.4
1	A	196	LEU	3.4
1	A	455	CYS	3.4
1	A	977	LYS	3.3
1	A	1199	GLY	3.3
1	A	2547	PHE	3.3
1	A	470	SER	3.3
1	A	2187	LYS	3.3
1	A	892	ILE	3.2
1	A	974	ILE	3.2
1	A	962	GLU	3.2
1	A	863	LEU	3.2
1	A	1720	ALA	3.2
1	A	1029	LEU	3.2
1	A	992	VAL	3.2
1	A	887	LYS	3.2
1	A	1919	ILE	3.1
1	A	409	LEU	3.1
1	A	475	LEU	3.1
1	A	305	ILE	3.1
1	A	891	TYR	3.1
1	A	1885	VAL	3.1
1	A	1861	LEU	3.1
1	A	2552	GLY	3.0
1	A	140	ALA	3.0
1	A	1219	ALA	3.0
1	A	913	PHE	3.0
1	A	452	SER	3.0
1	A	445	ASN	3.0
1	A	416	VAL	3.0
1	A	1883	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	1215	VAL	3.0
1	A	127	ILE	2.9
1	A	500	ALA	2.9
1	A	908	LEU	2.9
1	A	901	ALA	2.9
1	A	844	CYS	2.9
1	A	1792	GLY	2.9
1	A	1038	LEU	2.9
1	A	1127	PHE	2.9
1	A	888	TYR	2.9
1	A	1758	ILE	2.8
1	A	2455	THR	2.8
1	A	456	GLN	2.8
1	A	471	ALA	2.8
1	A	1889	LEU	2.8
1	A	1665	GLN	2.8
1	A	2454	ALA	2.8
1	A	120	SER	2.8
1	A	1830	ILE	2.8
1	A	382	LEU	2.8
1	A	1072	ALA	2.7
1	A	1248	LEU	2.7
1	A	2556	ASP	2.7
1	A	1848	TRP	2.6
1	A	1027	GLN	2.6
1	A	459	THR	2.6
1	A	1538	PHE	2.6
1	A	2461	LYS	2.6
1	A	106	HIS	2.6
1	A	609	GLU	2.6
1	A	1264	THR	2.6
1	A	2027	LEU	2.6
1	A	2087	LEU	2.6
1	A	1789	ARG	2.6
1	A	2039	ILE	2.6
1	A	845	ALA	2.6
1	A	1641	TYR	2.6
1	A	1874	ASP	2.6
1	A	814	LYS	2.6
1	A	975	LEU	2.6
1	A	987	PHE	2.5
1	A	1025	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1024	GLU	2.5
1	A	2555	GLN	2.5
1	A	206	LEU	2.5
1	A	1087	LEU	2.5
1	A	245	TYR	2.5
1	A	125	GLN	2.5
1	A	1751	SER	2.5
1	A	868	ILE	2.5
1	A	1878	GLU	2.5
1	A	1209	LEU	2.5
1	A	507	VAL	2.5
1	A	540	ALA	2.5
1	A	2530	GLU	2.5
1	A	78	LEU	2.5
1	A	976	LEU	2.5
1	A	2324	VAL	2.4
1	A	851	ASN	2.4
1	A	2456	LYS	2.4
1	A	467	HIS	2.4
1	A	833	LEU	2.4
1	A	1255	LEU	2.4
1	A	2034	GLU	2.4
1	A	2605	PHE	2.4
1	A	677	LEU	2.4
1	A	1515	LEU	2.4
1	A	102	ILE	2.4
1	A	2097	LEU	2.4
1	A	1114	PHE	2.4
1	A	1251	THR	2.4
1	A	2287	VAL	2.4
1	A	446	GLN	2.4
1	A	636	ILE	2.4
1	A	904	ASP	2.4
1	A	564	GLU	2.4
1	A	1642	TYR	2.4
1	A	550	LEU	2.4
1	A	2210	ALA	2.4
1	A	263	ILE	2.3
1	A	1646	PHE	2.3
1	A	1436	GLY	2.3
1	A	466	GLN	2.3
1	A	2637	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1110	LEU	2.3
1	A	2173	LEU	2.3
1	A	2623	ALA	2.3
1	A	816	LEU	2.3
1	A	843	GLU	2.3
1	A	2564	VAL	2.3
1	A	108	GLU	2.3
1	A	2312	GLY	2.3
1	A	1742	VAL	2.3
1	A	2220	VAL	2.3
1	A	2297	ARG	2.3
1	A	2615	ALA	2.3
1	A	112	VAL	2.3
1	A	722	PRO	2.3
1	A	458	HIS	2.2
1	A	117	VAL	2.2
1	A	31	LEU	2.2
1	A	1682	VAL	2.2
1	A	1620	ARG	2.2
1	A	2078	LEU	2.2
1	A	2259	PRO	2.2
1	A	1643	GLY	2.2
1	A	1831	ASN	2.2
1	A	307	ARG	2.2
1	A	2360	CYS	2.2
1	A	1036	GLU	2.2
1	A	1713	GLU	2.2
1	A	1040	GLN	2.2
1	A	511	ALA	2.1
1	A	1241	LEU	2.1
1	A	1324	LEU	2.1
1	A	1786	ASP	2.1
1	A	2635	ALA	2.1
1	A	75	ASP	2.1
1	A	159	LYS	2.1
1	A	959	GLN	2.1
1	A	2059	ILE	2.1
1	A	1015	CYS	2.1
1	A	2008	GLU	2.1
1	A	2103	GLU	2.1
1	A	2465	GLU	2.1
1	A	2055	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1287	PHE	2.1
1	A	1117	LEU	2.1
1	A	1837	LYS	2.1
1	A	1736	ALA	2.1
1	A	2383	PHE	2.1
1	A	874	LYS	2.1
1	A	1358	LEU	2.1
1	A	1388	LEU	2.1
1	A	2588	LYS	2.1
1	A	1793	CYS	2.1
1	A	1872	VAL	2.1
1	A	110	SER	2.1
1	A	413	TYR	2.1
1	A	1923	ILE	2.1
1	A	1882	LYS	2.1
1	A	2035	GLU	2.0
1	A	2100	GLU	2.0
1	A	1425	LEU	2.0
1	A	1840	ILE	2.0
1	A	167	ALA	2.0
1	A	2030	TYR	2.0
1	A	2266	CYS	2.0
1	A	729	LEU	2.0
1	A	1009	LEU	2.0
1	A	447	ALA	2.0
1	A	684	ILE	2.0
1	A	2544	LEU	2.0
1	A	146	GLY	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ACT	A	2701	4/4	0.76	0.50	95,114,137,137	0
3	K	A	2702	1/1	0.94	0.29	81,81,81,81	0
3	K	A	2703	1/1	0.98	0.10	81,81,81,81	0

6.5 Other polymers (i)

There are no such residues in this entry.