



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:40 PM UTC

PDB ID : 1UX4 / pdb_00001ux4
Title : Crystal structures of a Formin Homology-2 domain reveal a tethered-dimer architecture
Authors : Xu, Y.; Moseley, J.B.; Sagot, I.; Poy, F.; Pellman, D.; Goode, B.L.; Eck, M.J.
Deposited on : 2004-02-19
Resolution : 3.30 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
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

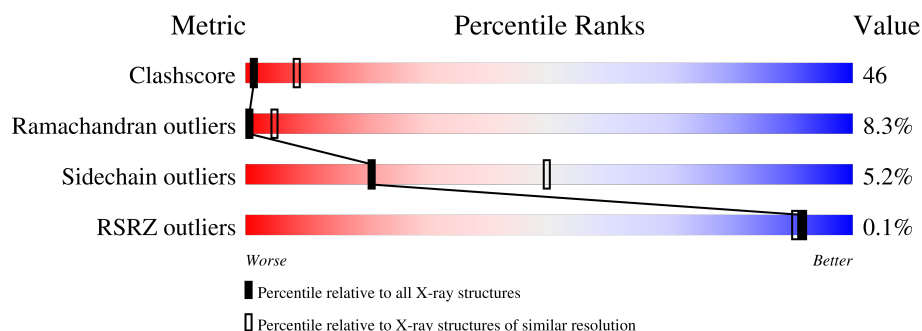
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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))
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	410	35% 55% 10%
1	B	410	33% 56% 12%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6644 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called BNI1 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	204	0	0
			3322	2119	555	638	10			
1	B	410	Total	C	N	O	S	197	0	0
			3322	2119	555	638	10			

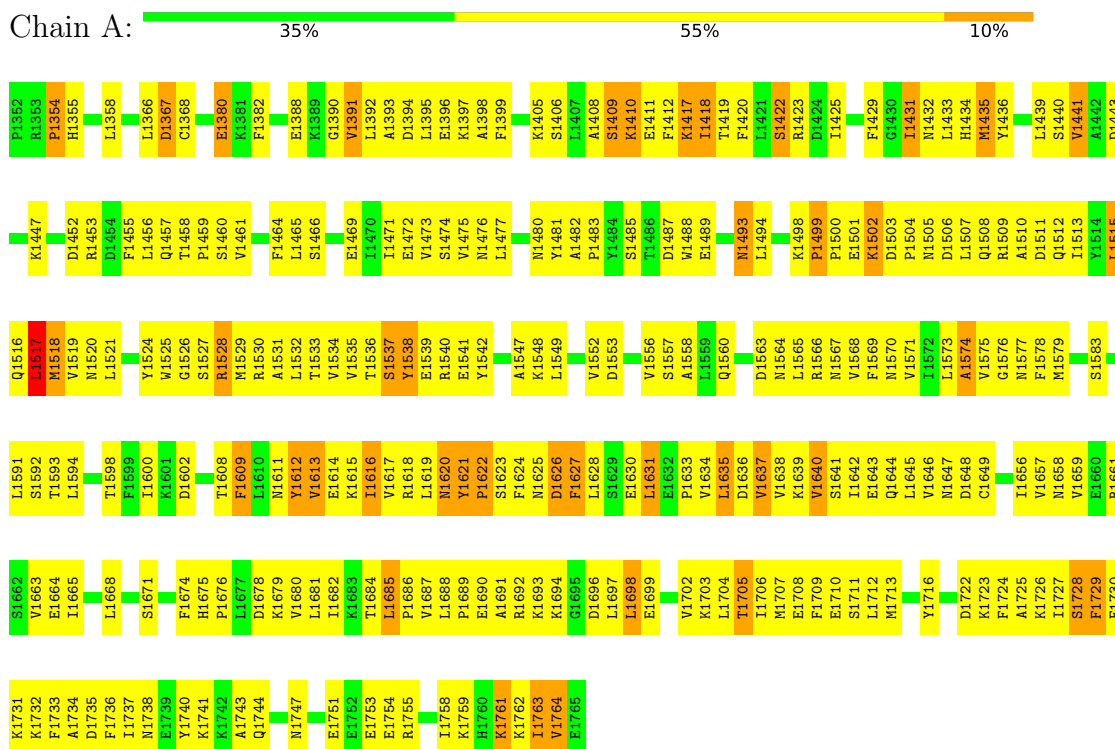
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1411	GLU	ARG	engineered mutation	UNP P41832
A	1412	PHE	LYS	engineered mutation	UNP P41832
B	2411	GLU	ARG	engineered mutation	UNP P41832
B	2412	PHE	LYS	engineered mutation	UNP P41832

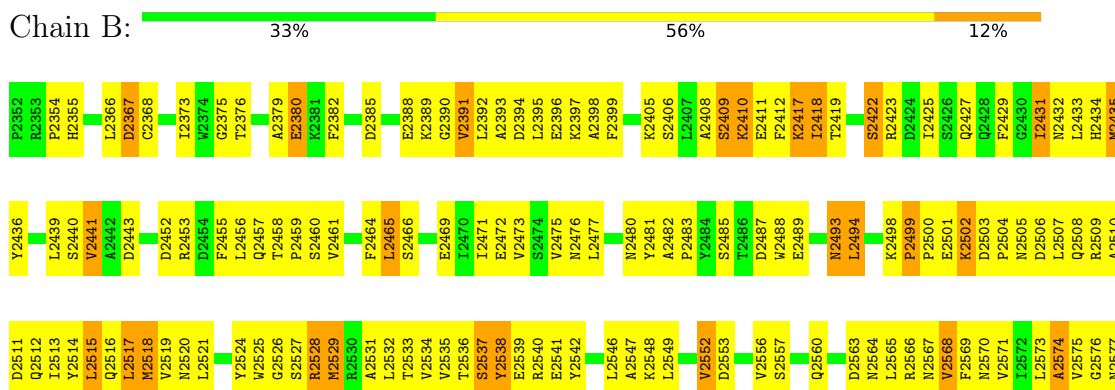
3 Residue-property plots

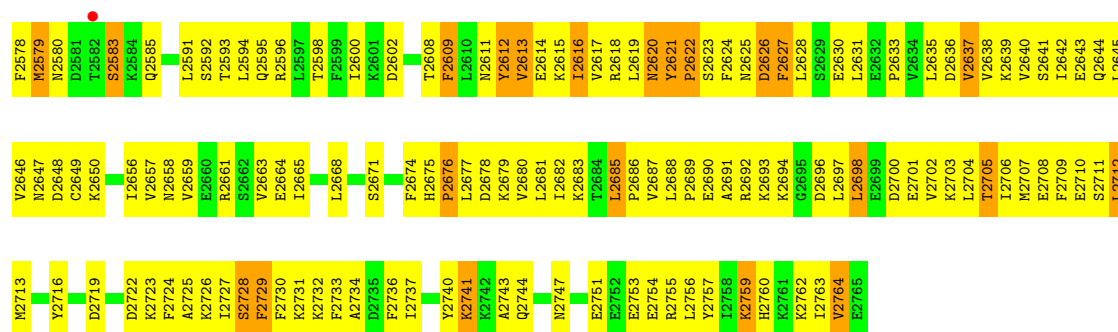
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: BNI1 PROTEIN



• Molecule 1: BNI1 PROTEIN





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	98.10Å 172.20Å 120.60Å 90.00° 112.30° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 20.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	81.0 (20.00-3.30) 75.2 (20.00-3.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.234 , 0.289 0.234 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	49.3	Xtriage
Anisotropy	1.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 115.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.186 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6644	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% 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

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	0.54	0/3382	1.04	21/4559 (0.5%)
1	B	0.54	0/3382	1.02	19/4559 (0.4%)
All	All	0.54	0/6764	1.03	40/9118 (0.4%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1754	GLU	N-CA-C	-9.60	102.79	112.97
1	A	1759	LYS	N-CA-C	-9.43	100.67	113.30
1	B	2757	TYR	N-CA-C	-8.51	103.49	114.04
1	A	1593	THR	N-CA-C	7.31	120.18	111.33
1	B	2423	ARG	N-CA-C	-7.17	103.46	111.71
1	A	1423	ARG	N-CA-C	-6.92	103.75	111.71
1	B	2593	THR	N-CA-C	6.79	119.54	111.33
1	A	1761	LYS	N-CA-C	-6.78	104.76	113.16
1	A	1626	ASP	N-CA-C	-6.71	105.06	113.18
1	B	2434	HIS	N-CA-C	6.68	118.56	111.28
1	B	2475	VAL	N-CA-C	-6.55	103.42	110.23
1	A	1475	VAL	N-CA-C	-6.51	103.52	110.36
1	A	1528	ARG	N-CA-C	-6.50	103.47	111.40
1	A	1671	SER	N-CA-C	6.42	118.36	111.36
1	B	2671	SER	N-CA-C	6.27	118.19	111.36
1	B	2728	SER	N-CA-C	6.18	118.81	111.71
1	A	1434	HIS	N-CA-C	6.07	117.90	111.28
1	B	2626	ASP	N-CA-C	-6.02	105.89	113.18
1	A	1728	SER	N-CA-C	5.83	119.50	112.38
1	A	1598	THR	N-CA-C	-5.78	106.13	112.72
1	B	2668	LEU	N-CA-C	-5.75	104.98	113.61
1	A	1422	SER	N-CA-C	-5.75	102.77	110.24
1	B	2754	GLU	N-CA-C	-5.71	104.96	112.72
1	A	1517	LEU	N-CA-C	5.66	117.82	108.48
1	A	1458	THR	CA-C-N	5.63	125.09	119.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1458	THR	C-N-CA	5.63	125.09	119.24
1	A	1640	VAL	N-CA-C	5.62	116.52	108.93
1	A	1635	LEU	N-CA-C	-5.56	106.63	113.41
1	B	2598	THR	N-CA-C	-5.53	106.42	112.72
1	B	2664	GLU	N-CA-C	5.49	118.10	111.40
1	B	2422	SER	N-CA-C	-5.48	102.90	110.35
1	B	2552	VAL	N-CA-C	-5.37	107.19	111.81
1	B	2528	ARG	N-CA-C	-5.37	104.85	111.40
1	B	2458	THR	CA-C-N	5.35	124.80	119.24
1	B	2458	THR	C-N-CA	5.35	124.80	119.24
1	A	1668	LEU	N-CA-C	-5.28	106.22	113.30
1	B	2373	ILE	N-CA-C	-5.28	106.73	112.80
1	A	1664	GLU	N-CA-C	5.26	117.81	111.40
1	A	1631	LEU	N-CA-C	-5.22	107.44	112.97
1	B	2517	LEU	N-CA-C	5.06	116.83	108.48

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	3322	0	3340	272	0
1	B	3322	0	3340	291	0
All	All	6644	0	6680	562	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 46.

All (562) 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:B:2504:PRO:HA	1:B:2507:LEU:HD23	1.44	0.98
1:B:2528:ARG:HG3	1:B:2680:VAL:HG21	1.46	0.97
1:A:1504:PRO:HA	1:A:1507:LEU:HD23	1.44	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1713:MET:HE1	1:A:1726:LYS:HA	1.48	0.96
1:B:2713:MET:HE1	1:B:2726:LYS:HA	1.51	0.92
1:A:1528:ARG:HG3	1:A:1680:VAL:HG21	1.52	0.92
1:B:2552:VAL:O	1:B:2556:VAL:HG23	1.69	0.92
1:B:2529:MET:HE2	1:B:2529:MET:HA	1.51	0.91
1:A:1552:VAL:O	1:A:1556:VAL:HG23	1.74	0.88
1:B:2412:PHE:O	1:B:2417:LYS:HG2	1.73	0.87
1:A:1412:PHE:O	1:A:1417:LYS:HG2	1.76	0.86
1:A:1529:MET:HE2	1:A:1529:MET:HA	1.56	0.85
1:A:1659:VAL:O	1:A:1663:VAL:HG23	1.78	0.83
1:A:1744:GLN:HA	1:A:1747:ASN:ND2	1.93	0.83
1:A:1707:MET:HG3	1:A:1708:GLU:N	1.94	0.81
1:B:2707:MET:HG3	1:B:2708:GLU:N	1.94	0.81
1:B:2579:MET:SD	1:B:2609:PHE:HE1	2.04	0.81
1:A:1515:LEU:HD23	1:A:1516:GLN:N	1.96	0.79
1:B:2529:MET:O	1:B:2533:THR:HG23	1.83	0.79
1:B:2591:LEU:HD21	1:B:2733:PHE:CZ	2.17	0.78
1:A:1744:GLN:HA	1:A:1747:ASN:HD22	1.46	0.76
1:B:2517:LEU:CB	1:B:2518:MET:HE3	2.16	0.76
1:B:2482:ALA:HB3	1:B:2483:PRO:HD3	1.68	0.75
1:B:2564:ASN:HA	1:B:2567:ASN:HD22	1.52	0.74
1:A:1529:MET:O	1:A:1533:THR:HG23	1.87	0.74
1:B:2744:GLN:HA	1:B:2747:ASN:ND2	2.02	0.74
1:B:2517:LEU:HB2	1:B:2518:MET:HE3	1.70	0.73
1:A:1517:LEU:CB	1:A:1518:MET:HE3	2.20	0.72
1:B:2620:ASN:N	1:B:2620:ASN:HD22	1.85	0.72
1:A:1591:LEU:HD21	1:A:1733:PHE:CZ	2.24	0.72
1:A:1626:ASP:O	1:A:1630:GLU:HG3	1.88	0.72
1:A:1564:ASN:HA	1:A:1567:ASN:HD22	1.54	0.72
1:B:2626:ASP:O	1:B:2630:GLU:HG3	1.90	0.71
1:A:1620:ASN:N	1:A:1620:ASN:HD22	1.86	0.71
1:B:2744:GLN:HA	1:B:2747:ASN:HD22	1.56	0.70
1:A:1579:MET:SD	1:A:1609:PHE:HE1	2.15	0.70
1:B:2488:TRP:HH2	1:B:2494:LEU:HD22	1.57	0.70
1:B:2429:PHE:O	1:B:2433:LEU:HB2	1.92	0.70
1:B:2515:LEU:HD23	1:B:2516:GLN:N	2.07	0.70
1:A:1410:LYS:O	1:A:1411:GLU:HB2	1.91	0.69
1:B:2529:MET:HA	1:B:2529:MET:CE	2.21	0.69
1:B:2659:VAL:O	1:B:2663:VAL:HG23	1.91	0.69
1:B:2759:LYS:C	1:B:2759:LYS:HE2	2.17	0.68
1:B:2683:LYS:HE2	1:B:2683:LYS:HA	1.74	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1482:ALA:HB3	1:A:1483:PRO:HD3	1.73	0.68
1:B:2410:LYS:O	1:B:2411:GLU:HB2	1.92	0.68
1:B:2619:LEU:C	1:B:2620:ASN:HD22	2.01	0.68
1:A:1509:ARG:O	1:A:1513:ILE:HG12	1.94	0.68
1:A:1614:GLU:OE1	1:A:1744:GLN:HG3	1.94	0.68
1:B:2762:LYS:C	1:B:2764:VAL:H	2.01	0.67
1:B:2614:GLU:OE1	1:B:2744:GLN:HG3	1.94	0.67
1:A:1619:LEU:C	1:A:1620:ASN:HD22	2.01	0.67
1:A:1556:VAL:HG13	1:A:1712:LEU:HD23	1.76	0.67
1:A:1488:TRP:HH2	1:A:1494:LEU:HD22	1.59	0.66
1:B:2418:ILE:HG22	1:B:2419:THR:H	1.61	0.66
1:A:1627:PHE:CD1	1:A:1627:PHE:C	2.74	0.65
1:B:2627:PHE:CD1	1:B:2627:PHE:C	2.74	0.65
1:A:1642:ILE:HG23	1:A:1643:GLU:N	2.11	0.64
1:A:1517:LEU:HB3	1:A:1518:MET:HE3	1.79	0.64
1:A:1565:LEU:HD21	1:A:1569:PHE:CE1	2.33	0.64
1:A:1615:LYS:C	1:A:1617:VAL:H	2.03	0.64
1:A:1418:ILE:HD12	1:A:1418:ILE:N	2.12	0.64
1:B:2418:ILE:HD12	1:B:2418:ILE:N	2.12	0.64
1:B:2759:LYS:HE2	1:B:2760:HIS:N	2.11	0.64
1:B:2755:ARG:HG2	1:B:2756:LEU:HD23	1.80	0.64
1:A:1706:ILE:O	1:A:1710:GLU:HG3	1.98	0.63
1:B:2615:LYS:C	1:B:2617:VAL:H	2.04	0.63
1:B:2707:MET:HG3	1:B:2708:GLU:H	1.63	0.63
1:A:1517:LEU:HB2	1:A:1518:MET:HE3	1.80	0.62
1:A:1429:PHE:O	1:A:1433:LEU:HB2	1.99	0.62
1:B:2642:ILE:HG23	1:B:2643:GLU:N	2.14	0.62
1:A:1637:VAL:HG13	1:A:1637:VAL:O	1.99	0.62
1:B:2608:THR:HG22	1:B:2611:ASN:OD1	1.99	0.62
1:B:2637:VAL:O	1:B:2637:VAL:HG13	1.98	0.62
1:A:1418:ILE:HG22	1:A:1419:THR:H	1.63	0.62
1:A:1608:THR:HG22	1:A:1611:ASN:OD1	2.00	0.62
1:B:2644:GLN:HG3	1:B:2648:ASP:OD2	2.00	0.62
1:A:1740:TYR:O	1:A:1741:LYS:C	2.43	0.61
1:B:2504:PRO:CA	1:B:2507:LEU:HD23	2.27	0.61
1:A:1504:PRO:CA	1:A:1507:LEU:HD23	2.26	0.61
1:B:2397:LYS:C	1:B:2399:PHE:H	2.08	0.61
1:B:2556:VAL:HG13	1:B:2712:LEU:HD23	1.81	0.61
1:A:1480:ASN:O	1:A:1483:PRO:HD2	2.01	0.61
1:B:2615:LYS:HG3	1:B:2618:ARG:HH22	1.64	0.61
1:B:2517:LEU:HB3	1:B:2518:MET:HE3	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1453:ARG:HG2	1:A:1457:GLN:HE21	1.66	0.60
1:A:1649:CYS:SG	1:A:1698:LEU:HD21	2.41	0.60
1:A:1644:GLN:HG3	1:A:1648:ASP:OD2	2.01	0.60
1:B:2488:TRP:CH2	1:B:2494:LEU:HD22	2.36	0.60
1:B:2542:TYR:CD2	1:B:2694:LYS:HD2	2.36	0.60
1:B:2636:ASP:O	1:B:2639:LYS:HE2	2.01	0.60
1:B:2441:VAL:HG11	1:B:2512:GLN:HB3	1.83	0.60
1:B:2509:ARG:O	1:B:2513:ILE:HG12	2.02	0.60
1:B:2620:ASN:N	1:B:2620:ASN:ND2	2.50	0.60
1:A:1635:LEU:HD23	1:A:1734:ALA:HB1	1.83	0.59
1:B:2516:GLN:C	1:B:2517:LEU:HD23	2.27	0.59
1:B:2706:ILE:O	1:B:2710:GLU:HG3	2.02	0.59
1:A:1471:ILE:O	1:A:1473:VAL:HG23	2.03	0.59
1:A:1515:LEU:O	1:A:1519:VAL:HB	2.03	0.59
1:A:1642:ILE:CG2	1:A:1643:GLU:N	2.66	0.59
1:B:2471:ILE:O	1:B:2473:VAL:HG23	2.02	0.59
1:B:2579:MET:SD	1:B:2609:PHE:CE1	2.93	0.58
1:A:1441:VAL:HG11	1:A:1512:GLN:HB3	1.84	0.58
1:A:1487:ASP:O	1:A:1488:TRP:HB2	2.03	0.58
1:A:1516:GLN:HA	1:A:1520:ASN:HD22	1.68	0.58
1:B:2649:CYS:SG	1:B:2698:LEU:HD21	2.44	0.58
1:B:2722:ASP:OD1	1:B:2724:PHE:HB3	2.03	0.58
1:B:2740:TYR:O	1:B:2741:LYS:C	2.46	0.58
1:B:2453:ARG:HG2	1:B:2457:GLN:HE21	1.68	0.58
1:B:2728:SER:O	1:B:2731:LYS:HB3	2.02	0.58
1:A:1509:ARG:HG2	1:A:1509:ARG:HH11	1.68	0.58
1:A:1488:TRP:CH2	1:A:1494:LEU:HD22	2.38	0.58
1:B:2418:ILE:HG22	1:B:2419:THR:N	2.18	0.58
1:A:1615:LYS:C	1:A:1617:VAL:N	2.59	0.57
1:A:1456:LEU:HB3	1:A:1536:THR:HG21	1.87	0.57
1:A:1397:LYS:C	1:A:1399:PHE:H	2.12	0.57
1:A:1636:ASP:O	1:A:1639:LYS:HE2	2.03	0.57
1:A:1685:LEU:HB2	1:A:1686:PRO:HD3	1.87	0.57
1:A:1729:PHE:HA	1:A:1732:LYS:HZ2	1.68	0.57
1:A:1763:ILE:HG23	1:A:1763:ILE:O	2.05	0.57
1:B:2435:MET:HG2	1:B:2436:TYR:CE1	2.39	0.57
1:B:2487:ASP:O	1:B:2488:TRP:HB2	2.04	0.57
1:A:1435:MET:HG2	1:A:1436:TYR:CE1	2.40	0.57
1:A:1516:GLN:HA	1:A:1520:ASN:ND2	2.20	0.57
1:A:1542:TYR:CD2	1:A:1694:LYS:HD2	2.40	0.57
1:A:1722:ASP:OD1	1:A:1724:PHE:HB3	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1620:ASN:N	1:A:1620:ASN:ND2	2.51	0.56
1:A:1515:LEU:HA	1:A:1519:VAL:HB	1.86	0.56
1:B:2615:LYS:C	1:B:2617:VAL:N	2.63	0.56
1:A:1380:GLU:C	1:A:1382:PHE:H	2.14	0.56
1:A:1503:ASP:OD2	1:A:1505:ASN:HB2	2.05	0.56
1:B:2461:VAL:HG12	1:B:2465:LEU:HD12	1.85	0.56
1:B:2609:PHE:C	1:B:2609:PHE:CD2	2.83	0.56
1:B:2583:SER:N	1:B:2585:GLN:HE21	2.04	0.56
1:A:1504:PRO:HA	1:A:1507:LEU:CD2	2.29	0.56
1:A:1689:PRO:HA	1:A:1692:ARG:HG2	1.86	0.56
1:A:1707:MET:HG3	1:A:1708:GLU:H	1.69	0.56
1:B:2685:LEU:HB2	1:B:2686:PRO:HD3	1.87	0.56
1:B:2528:ARG:HG3	1:B:2680:VAL:CG2	2.29	0.56
1:A:1447:LYS:HD2	1:A:1452:ASP:OD2	2.05	0.56
1:B:2549:LEU:HD13	1:B:2645:LEU:HD21	1.88	0.56
1:B:2642:ILE:CG2	1:B:2643:GLU:N	2.68	0.56
1:B:2747:ASN:O	1:B:2751:GLU:HG3	2.05	0.56
1:A:1419:THR:HA	1:A:1511:ASP:OD2	2.05	0.56
1:A:1628:LEU:HD21	1:A:1740:TYR:HD2	1.71	0.56
1:B:2594:LEU:HD13	1:B:2736:PHE:CG	2.40	0.56
1:B:2661:ARG:HE	1:B:2665:ILE:HD11	1.69	0.56
1:A:1461:VAL:HG12	1:A:1465:LEU:HD12	1.88	0.55
1:B:2528:ARG:CG	1:B:2680:VAL:HG21	2.29	0.55
1:A:1556:VAL:HG13	1:A:1712:LEU:CD2	2.37	0.55
1:A:1615:LYS:O	1:A:1617:VAL:N	2.39	0.55
1:B:2435:MET:SD	1:B:2435:MET:N	2.79	0.55
1:B:2509:ARG:HG2	1:B:2509:ARG:HH11	1.72	0.55
1:B:2515:LEU:HA	1:B:2519:VAL:HB	1.88	0.55
1:A:1624:PHE:C	1:A:1626:ASP:H	2.14	0.55
1:A:1698:LEU:O	1:A:1702:VAL:HG23	2.05	0.55
1:B:2516:GLN:HA	1:B:2520:ASN:HD22	1.71	0.55
1:B:2480:ASN:O	1:B:2483:PRO:HD2	2.07	0.55
1:B:2624:PHE:C	1:B:2626:ASP:H	2.15	0.55
1:A:1393:ALA:HA	1:A:1396:GLU:HG3	1.89	0.55
1:A:1609:PHE:C	1:A:1609:PHE:CD2	2.85	0.55
1:A:1615:LYS:HG2	1:A:1619:LEU:HD11	1.89	0.55
1:B:2515:LEU:O	1:B:2519:VAL:HB	2.07	0.55
1:B:2566:ARG:O	1:B:2569:PHE:HB2	2.07	0.55
1:A:1591:LEU:O	1:A:1592:SER:C	2.47	0.55
1:B:2567:ASN:O	1:B:2570:ASN:N	2.38	0.55
1:B:2656:ILE:HD13	1:B:2691:ALA:HB1	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2691:ALA:O	1:B:2694:LYS:N	2.40	0.55
1:B:2565:LEU:HD21	1:B:2569:PHE:CE1	2.42	0.55
1:B:2380:GLU:C	1:B:2382:PHE:H	2.14	0.55
1:B:2621:TYR:C	1:B:2623:SER:H	2.15	0.55
1:A:1393:ALA:O	1:A:1396:GLU:HB2	2.06	0.54
1:A:1656:ILE:HD13	1:A:1691:ALA:HB1	1.89	0.54
1:A:1728:SER:O	1:A:1731:LYS:HB3	2.07	0.54
1:A:1418:ILE:HG22	1:A:1419:THR:N	2.23	0.54
1:B:2393:ALA:HA	1:B:2396:GLU:HG3	1.89	0.54
1:A:1537:SER:O	1:A:1538:TYR:C	2.50	0.54
1:B:2564:ASN:HA	1:B:2567:ASN:ND2	2.20	0.54
1:B:2635:LEU:HD23	1:B:2734:ALA:HB1	1.89	0.54
1:B:2494:LEU:HD13	1:B:2494:LEU:O	2.07	0.54
1:A:1564:ASN:HA	1:A:1567:ASN:ND2	2.22	0.54
1:A:1753:GLU:C	1:A:1755:ARG:H	2.15	0.54
1:A:1758:ILE:HG22	1:A:1758:ILE:O	2.08	0.54
1:A:1528:ARG:HG3	1:A:1680:VAL:CG2	2.33	0.54
1:A:1529:MET:HA	1:A:1529:MET:CE	2.33	0.54
1:B:2517:LEU:HB2	1:B:2518:MET:CE	2.37	0.54
1:A:1642:ILE:HG22	1:A:1727:ILE:HD13	1.90	0.54
1:B:2548:LYS:HD2	1:B:2645:LEU:HD13	1.90	0.54
1:B:2366:LEU:O	1:B:2368:CYS:N	2.41	0.54
1:B:2431:ILE:O	1:B:2433:LEU:N	2.41	0.54
1:B:2439:LEU:HD12	1:B:2439:LEU:N	2.23	0.54
1:B:2481:TYR:O	1:B:2482:ALA:C	2.51	0.53
1:A:1441:VAL:HG13	1:A:1513:ILE:HD13	1.91	0.53
1:A:1678:ASP:OD2	1:A:1680:VAL:HG23	2.08	0.53
1:B:2616:ILE:HG22	1:B:2616:ILE:O	2.08	0.53
1:B:2658:ASN:O	1:B:2659:VAL:C	2.51	0.53
1:A:1435:MET:N	1:A:1435:MET:SD	2.81	0.53
1:A:1661:ARG:HE	1:A:1665:ILE:HD11	1.73	0.53
1:B:2435:MET:HG2	1:B:2436:TYR:CD1	2.43	0.53
1:A:1439:LEU:HD12	1:A:1439:LEU:N	2.23	0.53
1:A:1494:LEU:HD13	1:A:1494:LEU:O	2.08	0.53
1:B:2567:ASN:O	1:B:2568:VAL:C	2.52	0.53
1:A:1624:PHE:O	1:A:1626:ASP:N	2.42	0.53
1:A:1635:LEU:HD11	1:A:1737:ILE:HG21	1.91	0.53
1:B:2644:GLN:HE21	1:B:2644:GLN:HA	1.74	0.53
1:B:2681:LEU:HB3	1:B:2685:LEU:CD2	2.39	0.53
1:A:1690:GLU:O	1:A:1693:LYS:HB3	2.09	0.53
1:B:2524:TYR:CE2	1:B:2674:PHE:HA	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1435:MET:HG2	1:A:1436:TYR:CD1	2.44	0.53
1:A:1524:TYR:CE2	1:A:1674:PHE:HA	2.45	0.52
1:B:2690:GLU:O	1:B:2693:LYS:HB3	2.09	0.52
1:B:2618:ARG:HB3	1:B:2618:ARG:CZ	2.39	0.52
1:A:1366:LEU:O	1:A:1368:CYS:N	2.42	0.52
1:A:1408:ALA:O	1:A:1410:LYS:N	2.43	0.52
1:A:1506:ASP:C	1:A:1507:LEU:HD22	2.34	0.52
1:A:1621:TYR:C	1:A:1623:SER:H	2.18	0.52
1:A:1729:PHE:O	1:A:1730:PHE:C	2.52	0.52
1:B:2506:ASP:C	1:B:2507:LEU:HD22	2.35	0.52
1:B:2525:TRP:O	1:B:2528:ARG:N	2.40	0.52
1:A:1764:VAL:O	1:A:1764:VAL:HG12	2.09	0.52
1:B:2408:ALA:O	1:B:2410:LYS:N	2.43	0.52
1:B:2642:ILE:HG22	1:B:2727:ILE:HD13	1.92	0.52
1:B:2678:ASP:OD2	1:B:2680:VAL:HG23	2.10	0.52
1:A:1431:ILE:O	1:A:1433:LEU:N	2.43	0.52
1:B:2609:PHE:CD2	1:B:2609:PHE:O	2.63	0.52
1:A:1618:ARG:CZ	1:A:1618:ARG:HB3	2.39	0.52
1:B:2464:PHE:C	1:B:2466:SER:H	2.17	0.52
1:B:2540:ARG:O	1:B:2541:GLU:C	2.51	0.52
1:A:1447:LYS:HA	1:A:1452:ASP:OD2	2.10	0.52
1:B:2691:ALA:O	1:B:2692:ARG:C	2.53	0.52
1:A:1548:LYS:HD2	1:A:1645:LEU:HD13	1.91	0.51
1:B:2393:ALA:O	1:B:2396:GLU:HB2	2.09	0.51
1:A:1567:ASN:O	1:A:1570:ASN:N	2.44	0.51
1:A:1517:LEU:HB2	1:A:1518:MET:CE	2.40	0.51
1:A:1538:TYR:CG	1:A:1539:GLU:N	2.79	0.51
1:B:2516:GLN:HA	1:B:2520:ASN:ND2	2.26	0.51
1:B:2635:LEU:HD11	1:B:2737:ILE:HG21	1.92	0.51
1:A:1498:LYS:O	1:A:1500:PRO:HD3	2.10	0.51
1:B:2538:TYR:CG	1:B:2539:GLU:N	2.78	0.51
1:A:1549:LEU:HD13	1:A:1645:LEU:HD21	1.92	0.51
1:B:2504:PRO:HA	1:B:2507:LEU:CD2	2.30	0.51
1:B:2696:ASP:O	1:B:2697:LEU:C	2.54	0.51
1:B:2729:PHE:O	1:B:2730:PHE:C	2.52	0.51
1:A:1725:ALA:O	1:A:1726:LYS:C	2.52	0.51
1:B:2556:VAL:HG13	1:B:2712:LEU:CD2	2.41	0.51
1:A:1481:TYR:O	1:A:1482:ALA:C	2.54	0.51
1:A:1516:GLN:C	1:A:1517:LEU:HD23	2.36	0.51
1:B:2503:ASP:OD2	1:B:2505:ASN:HB2	2.10	0.51
1:A:1509:ARG:HG2	1:A:1509:ARG:NH1	2.26	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1531:ALA:O	1:A:1534:VAL:N	2.44	0.51
1:A:1380:GLU:C	1:A:1382:PHE:N	2.69	0.50
1:A:1612:TYR:O	1:A:1613:VAL:C	2.54	0.50
1:B:2380:GLU:C	1:B:2382:PHE:N	2.69	0.50
1:B:2637:VAL:HG22	1:B:2640:VAL:HB	1.92	0.50
1:B:2753:GLU:C	1:B:2755:ARG:H	2.18	0.50
1:A:1464:PHE:C	1:A:1466:SER:H	2.18	0.50
1:A:1565:LEU:HD12	1:A:1631:LEU:HD11	1.92	0.50
1:A:1644:GLN:HA	1:A:1644:GLN:HE21	1.75	0.50
1:B:2498:LYS:O	1:B:2500:PRO:HD3	2.12	0.50
1:B:2531:ALA:O	1:B:2534:VAL:N	2.43	0.50
1:A:1412:PHE:O	1:A:1417:LYS:CG	2.56	0.50
1:A:1540:ARG:O	1:A:1541:GLU:C	2.54	0.50
1:A:1600:ILE:HD12	1:A:1600:ILE:N	2.27	0.50
1:A:1704:LEU:O	1:A:1707:MET:HG2	2.12	0.50
1:B:2418:ILE:HD12	1:B:2418:ILE:H	1.75	0.50
1:B:2418:ILE:HD12	1:B:2506:ASP:O	2.11	0.50
1:A:1723:LYS:O	1:A:1724:PHE:C	2.54	0.50
1:A:1728:SER:O	1:A:1732:LYS:HG3	2.11	0.50
1:B:2419:THR:HA	1:B:2511:ASP:OD2	2.12	0.50
1:A:1647:ASN:O	1:A:1648:ASP:C	2.53	0.50
1:A:1519:VAL:HG12	1:A:1520:ASN:N	2.25	0.50
1:A:1567:ASN:O	1:A:1568:VAL:C	2.54	0.50
1:B:2531:ALA:O	1:B:2532:LEU:C	2.54	0.50
1:A:1418:ILE:HD12	1:A:1506:ASP:O	2.12	0.50
1:A:1637:VAL:HG22	1:A:1640:VAL:HB	1.93	0.50
1:A:1615:LYS:HG3	1:A:1618:ARG:HH22	1.76	0.49
1:B:2689:PRO:HA	1:B:2692:ARG:HG2	1.93	0.49
1:B:2704:LEU:O	1:B:2705:THR:C	2.55	0.49
1:B:2729:PHE:HA	1:B:2732:LYS:HZ2	1.77	0.49
1:B:2508:GLN:O	1:B:2509:ARG:C	2.55	0.49
1:B:2762:LYS:C	1:B:2764:VAL:N	2.68	0.49
1:A:1500:PRO:O	1:A:1501:GLU:HB2	2.13	0.49
1:B:2498:LYS:O	1:B:2500:PRO:CD	2.60	0.49
1:B:2642:ILE:CG2	1:B:2643:GLU:H	2.25	0.49
1:B:2456:LEU:HB3	1:B:2536:THR:HG21	1.94	0.49
1:A:1704:LEU:O	1:A:1705:THR:C	2.56	0.49
1:B:2624:PHE:O	1:B:2626:ASP:N	2.45	0.49
1:A:1498:LYS:O	1:A:1500:PRO:CD	2.61	0.49
1:A:1525:TRP:O	1:A:1528:ARG:N	2.38	0.49
1:A:1535:VAL:HG12	1:A:1535:VAL:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1616:ILE:HG22	1:A:1616:ILE:O	2.12	0.49
1:B:2509:ARG:HG2	1:B:2509:ARG:NH1	2.29	0.48
1:A:1397:LYS:O	1:A:1398:ALA:HB3	2.12	0.48
1:A:1452:ASP:O	1:A:1455:PHE:HB3	2.12	0.48
1:A:1646:VAL:HG22	1:A:1706:ILE:HD11	1.95	0.48
1:B:2565:LEU:O	1:B:2566:ARG:C	2.56	0.48
1:B:2728:SER:O	1:B:2732:LYS:HG3	2.13	0.48
1:A:1641:SER:HB3	1:A:1644:GLN:HB3	1.95	0.48
1:A:1682:ILE:HG12	1:A:1682:ILE:O	2.13	0.48
1:B:2493:ASN:HD22	1:B:2494:LEU:H	1.62	0.48
1:B:2628:LEU:HD21	1:B:2740:TYR:HD2	1.78	0.48
1:A:1366:LEU:O	1:A:1367:ASP:C	2.55	0.48
1:B:2575:VAL:HG11	1:B:2609:PHE:HZ	1.77	0.48
1:B:2723:LYS:O	1:B:2724:PHE:C	2.57	0.48
1:A:1579:MET:SD	1:A:1609:PHE:CE1	3.02	0.48
1:A:1691:ALA:O	1:A:1694:LYS:N	2.46	0.48
1:B:2564:ASN:O	1:B:2565:LEU:C	2.57	0.48
1:B:2591:LEU:CD1	1:B:2716:TYR:HB3	2.44	0.48
1:B:2621:TYR:O	1:B:2623:SER:N	2.46	0.48
1:B:2704:LEU:O	1:B:2707:MET:HG2	2.12	0.48
1:A:1642:ILE:CG2	1:A:1643:GLU:H	2.24	0.48
1:B:2385:ASP:OD2	1:B:2389:LYS:HE3	2.14	0.48
1:B:2538:TYR:CD2	1:B:2539:GLU:N	2.80	0.48
1:B:2591:LEU:HD11	1:B:2716:TYR:HB3	1.94	0.48
1:B:2755:ARG:O	1:B:2759:LYS:HB3	2.13	0.48
1:A:1751:GLU:O	1:A:1755:ARG:HB2	2.13	0.48
1:B:2687:VAL:O	1:B:2688:LEU:C	2.57	0.48
1:A:1493:ASN:HD22	1:A:1494:LEU:H	1.62	0.48
1:B:2397:LYS:O	1:B:2398:ALA:HB3	2.14	0.48
1:A:1392:LEU:O	1:A:1393:ALA:C	2.57	0.48
1:B:2563:ASP:O	1:B:2564:ASN:C	2.55	0.48
1:B:2656:ILE:O	1:B:2657:VAL:C	2.57	0.48
1:B:2441:VAL:HG13	1:B:2513:ILE:HD13	1.95	0.48
1:B:2566:ARG:HG3	1:B:2566:ARG:HH11	1.78	0.48
1:B:2698:LEU:O	1:B:2702:VAL:HG23	2.13	0.48
1:B:2529:MET:HE3	1:B:2532:LEU:HD12	1.95	0.47
1:B:2647:ASN:O	1:B:2648:ASP:C	2.56	0.47
1:A:1573:LEU:HD11	1:A:1577:ASN:HD21	1.79	0.47
1:B:2570:ASN:O	1:B:2573:LEU:N	2.47	0.47
1:A:1390:GLY:O	1:A:1393:ALA:HB3	2.13	0.47
1:A:1574:ALA:O	1:A:1575:VAL:C	2.56	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2390:GLY:O	1:B:2393:ALA:HB3	2.14	0.47
1:B:2422:SER:HB2	1:B:2425:ILE:HG12	1.96	0.47
1:B:2690:GLU:OE1	1:B:2690:GLU:HA	2.13	0.47
1:A:1531:ALA:O	1:A:1532:LEU:C	2.56	0.47
1:A:1573:LEU:CD1	1:A:1577:ASN:HD21	2.27	0.47
1:A:1696:ASP:O	1:A:1697:LEU:C	2.55	0.47
1:B:2573:LEU:HD12	1:B:2573:LEU:O	2.15	0.47
1:A:1504:PRO:C	1:A:1507:LEU:HD23	2.39	0.47
1:A:1614:GLU:HG3	1:A:1744:GLN:HB2	1.96	0.47
1:B:2519:VAL:HG12	1:B:2520:ASN:N	2.29	0.47
1:A:1418:ILE:HD12	1:A:1418:ILE:H	1.77	0.47
1:A:1579:MET:HE2	1:A:1579:MET:HB3	1.84	0.47
1:A:1609:PHE:CD2	1:A:1609:PHE:O	2.67	0.47
1:A:1709:PHE:O	1:A:1713:MET:HG3	2.15	0.47
1:A:1762:LYS:C	1:A:1764:VAL:H	2.23	0.47
1:B:2366:LEU:O	1:B:2367:ASP:C	2.57	0.47
1:B:2409:SER:O	1:B:2411:GLU:N	2.48	0.47
1:B:2537:SER:O	1:B:2538:TYR:C	2.57	0.47
1:B:2583:SER:H	1:B:2585:GLN:HE21	1.62	0.47
1:B:2615:LYS:O	1:B:2617:VAL:N	2.48	0.47
1:B:2759:LYS:C	1:B:2759:LYS:CE	2.87	0.47
1:A:1566:ARG:O	1:A:1569:PHE:HB2	2.15	0.47
1:B:2570:ASN:O	1:B:2571:VAL:C	2.58	0.47
1:A:1529:MET:HE2	1:A:1532:LEU:HB2	1.97	0.47
1:A:1591:LEU:CD1	1:A:1716:TYR:HB3	2.44	0.47
1:A:1591:LEU:HD11	1:A:1716:TYR:HB3	1.97	0.47
1:B:2498:LYS:N	1:B:2499:PRO:CD	2.78	0.47
1:A:1498:LYS:N	1:A:1499:PRO:CD	2.78	0.46
1:B:2440:SER:O	1:B:2441:VAL:C	2.58	0.46
1:B:2641:SER:HB3	1:B:2644:GLN:HB3	1.96	0.46
1:B:2412:PHE:O	1:B:2417:LYS:CG	2.54	0.46
1:B:2529:MET:HE2	1:B:2532:LEU:HB2	1.98	0.46
1:B:2397:LYS:C	1:B:2399:PHE:N	2.73	0.46
1:B:2600:ILE:HD12	1:B:2600:ILE:N	2.29	0.46
1:B:2466:SER:OG	1:B:2529:MET:HB3	2.14	0.46
1:A:1547:ALA:C	1:A:1549:LEU:H	2.23	0.46
1:B:2521:LEU:HD21	1:B:2675:HIS:HB2	1.97	0.46
1:A:1477:LEU:O	1:A:1481:TYR:HD1	1.99	0.46
1:A:1691:ALA:O	1:A:1692:ARG:C	2.58	0.46
1:B:2379:ALA:HB3	1:B:2380:GLU:OE1	2.15	0.46
1:B:2436:TYR:HA	1:B:2439:LEU:HD13	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2638:VAL:CG2	1:B:2731:LYS:HA	2.45	0.46
1:A:1459:PRO:O	1:A:1460:SER:C	2.59	0.46
1:B:2500:PRO:O	1:B:2501:GLU:HB2	2.16	0.46
1:B:2573:LEU:CD1	1:B:2577:ASN:HD21	2.29	0.46
1:A:1656:ILE:O	1:A:1657:VAL:C	2.58	0.46
1:B:2576:GLY:O	1:B:2580:ASN:ND2	2.48	0.46
1:A:1395:LEU:C	1:A:1397:LYS:N	2.72	0.45
1:A:1594:LEU:HD13	1:A:1736:PHE:CG	2.50	0.45
1:A:1618:ARG:HG2	1:A:1618:ARG:HH11	1.81	0.45
1:B:2575:VAL:HG11	1:B:2609:PHE:CZ	2.51	0.45
1:A:1419:THR:HG23	1:A:1511:ASP:OD1	2.17	0.45
1:A:1538:TYR:CD2	1:A:1539:GLU:N	2.81	0.45
1:A:1628:LEU:HD21	1:A:1740:TYR:CD2	2.50	0.45
1:A:1417:LYS:HA	1:A:1417:LYS:HD3	1.76	0.45
1:A:1436:TYR:HA	1:A:1439:LEU:HD13	1.98	0.45
1:A:1702:VAL:C	1:A:1704:LEU:N	2.74	0.45
1:B:2547:ALA:C	1:B:2549:LEU:H	2.23	0.45
1:B:2547:ALA:C	1:B:2549:LEU:N	2.71	0.45
1:B:2566:ARG:HG3	1:B:2566:ARG:NH1	2.31	0.45
1:A:1521:LEU:HD21	1:A:1675:HIS:HB2	1.97	0.45
1:A:1565:LEU:O	1:A:1566:ARG:C	2.59	0.45
1:A:1658:ASN:O	1:A:1659:VAL:C	2.58	0.45
1:A:1687:VAL:O	1:A:1688:LEU:C	2.59	0.45
1:B:2477:LEU:O	1:B:2481:TYR:HD1	2.00	0.45
1:B:2681:LEU:HB3	1:B:2685:LEU:HD22	1.97	0.45
1:A:1553:ASP:O	1:A:1556:VAL:N	2.50	0.45
1:B:2390:GLY:O	1:B:2391:VAL:C	2.58	0.45
1:B:2591:LEU:O	1:B:2592:SER:C	2.58	0.45
1:B:2616:ILE:O	1:B:2616:ILE:CG2	2.64	0.45
1:A:1390:GLY:O	1:A:1391:VAL:C	2.58	0.45
1:B:2464:PHE:C	1:B:2466:SER:N	2.74	0.45
1:B:2618:ARG:O	1:B:2622:PRO:HB3	2.17	0.45
1:A:1388:GLU:C	1:A:1390:GLY:H	2.23	0.45
1:A:1539:GLU:O	1:A:1542:TYR:HB3	2.17	0.45
1:A:1569:PHE:CZ	1:A:1594:LEU:HD11	2.52	0.45
1:B:2685:LEU:N	1:B:2686:PRO:CD	2.80	0.45
1:B:2751:GLU:O	1:B:2755:ARG:HB2	2.17	0.45
1:A:1464:PHE:C	1:A:1466:SER:N	2.75	0.45
1:A:1644:GLN:HA	1:A:1644:GLN:NE2	2.32	0.45
1:A:1409:SER:O	1:A:1411:GLU:N	2.49	0.45
1:A:1761:LYS:O	1:A:1761:LYS:HG2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1440:SER:O	1:A:1441:VAL:C	2.59	0.44
1:B:2471:ILE:O	1:B:2472:GLU:C	2.61	0.44
1:B:2679:LYS:HB3	1:B:2682:ILE:CG2	2.46	0.44
1:A:1504:PRO:O	1:A:1507:LEU:HD23	2.16	0.44
1:A:1557:SER:O	1:A:1560:GLN:HB3	2.18	0.44
1:B:2455:PHE:CD1	1:B:2455:PHE:C	2.94	0.44
1:B:2614:GLU:HG3	1:B:2744:GLN:HB2	1.99	0.44
1:A:1474:SER:OG	1:A:1477:LEU:HB2	2.18	0.44
1:A:1547:ALA:C	1:A:1549:LEU:N	2.73	0.44
1:A:1633:PRO:HA	1:A:1636:ASP:HB2	1.97	0.44
1:B:2525:TRP:O	1:B:2526:GLY:C	2.60	0.44
1:B:2725:ALA:O	1:B:2726:LYS:C	2.59	0.44
1:A:1390:GLY:O	1:A:1393:ALA:N	2.50	0.44
1:A:1508:GLN:O	1:A:1509:ARG:C	2.60	0.44
1:A:1740:TYR:O	1:A:1743:ALA:N	2.51	0.44
1:B:2417:LYS:HA	1:B:2417:LYS:HD3	1.83	0.44
1:B:2557:SER:O	1:B:2560:GLN:HB3	2.17	0.44
1:A:1528:ARG:CG	1:A:1680:VAL:HG21	2.36	0.44
1:A:1575:VAL:O	1:A:1578:PHE:HB3	2.17	0.44
1:B:2624:PHE:C	1:B:2626:ASP:N	2.75	0.44
1:B:2631:LEU:CD1	1:B:2737:ILE:HD11	2.48	0.44
1:B:2702:VAL:C	1:B:2704:LEU:N	2.74	0.44
1:A:1524:TYR:HE1	1:A:1528:ARG:HD2	1.83	0.44
1:A:1688:LEU:HD23	1:A:1688:LEU:HA	1.80	0.44
1:B:2594:LEU:HD13	1:B:2736:PHE:CD1	2.52	0.44
1:B:2633:PRO:HA	1:B:2636:ASP:HB2	1.99	0.44
1:A:1455:PHE:CD1	1:A:1455:PHE:C	2.95	0.44
1:A:1618:ARG:O	1:A:1622:PRO:HB3	2.17	0.44
1:A:1722:ASP:OD1	1:A:1724:PHE:N	2.50	0.44
1:B:2539:GLU:O	1:B:2542:TYR:HB3	2.18	0.44
1:B:2691:ALA:C	1:B:2693:LYS:N	2.73	0.44
1:A:1684:THR:O	1:A:1685:LEU:C	2.61	0.44
1:B:2461:VAL:HG12	1:B:2465:LEU:CD1	2.48	0.44
1:B:2569:PHE:CZ	1:B:2594:LEU:HD11	2.52	0.44
1:A:1408:ALA:O	1:A:1409:SER:C	2.61	0.44
1:B:2504:PRO:C	1:B:2507:LEU:HD23	2.42	0.44
1:B:2574:ALA:O	1:B:2575:VAL:C	2.60	0.44
1:B:2390:GLY:O	1:B:2393:ALA:N	2.51	0.43
1:B:2487:ASP:C	1:B:2489:GLU:H	2.26	0.43
1:B:2644:GLN:HA	1:B:2644:GLN:NE2	2.32	0.43
1:B:2649:CYS:O	1:B:2650:LYS:C	2.60	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1564:ASN:ND2	1:A:1630:GLU:OE1	2.51	0.43
1:A:1570:ASN:O	1:A:1571:VAL:C	2.59	0.43
1:B:2524:TYR:HE1	1:B:2528:ARG:HD2	1.82	0.43
1:B:2535:VAL:HG12	1:B:2535:VAL:O	2.18	0.43
1:B:2707:MET:HE3	1:B:2707:MET:HB2	1.85	0.43
1:B:2579:MET:HE2	1:B:2579:MET:HB3	1.81	0.43
1:B:2594:LEU:N	1:B:2594:LEU:HD23	2.33	0.43
1:A:1573:LEU:HD12	1:A:1573:LEU:O	2.18	0.43
1:A:1679:LYS:HB3	1:A:1682:ILE:CG2	2.49	0.43
1:A:1743:ALA:O	1:A:1747:ASN:ND2	2.51	0.43
1:B:2513:ILE:O	1:B:2514:TYR:C	2.61	0.43
1:B:2553:ASP:O	1:B:2556:VAL:N	2.51	0.43
1:B:2565:LEU:HD12	1:B:2631:LEU:HD11	2.00	0.43
1:B:2612:TYR:O	1:B:2613:VAL:C	2.61	0.43
1:B:2733:PHE:O	1:B:2737:ILE:HG13	2.18	0.43
1:A:1638:VAL:CG2	1:A:1731:LYS:HA	2.48	0.43
1:A:1735:ASP:O	1:A:1738:ASN:N	2.51	0.43
1:A:1392:LEU:O	1:A:1395:LEU:N	2.52	0.43
1:B:2689:PRO:O	1:B:2690:GLU:C	2.61	0.43
1:A:1466:SER:OG	1:A:1529:MET:HB3	2.19	0.43
1:A:1708:GLU:O	1:A:1711:SER:HB3	2.19	0.43
1:B:2524:TYR:CE1	1:B:2528:ARG:HD2	2.54	0.43
1:B:2709:PHE:O	1:B:2713:MET:HG3	2.18	0.43
1:B:2453:ARG:CG	1:B:2457:GLN:HE21	2.30	0.43
1:B:2682:ILE:O	1:B:2682:ILE:HG12	2.18	0.43
1:B:2708:GLU:O	1:B:2711:SER:HB3	2.19	0.43
1:A:1536:THR:O	1:A:1537:SER:HB2	2.19	0.42
1:B:2573:LEU:HD11	1:B:2577:ASN:HD21	1.84	0.42
1:A:1526:GLY:O	1:A:1530:ARG:HB2	2.20	0.42
1:B:2507:LEU:HD22	1:B:2507:LEU:N	2.35	0.42
1:B:2583:SER:H	1:B:2585:GLN:NE2	2.16	0.42
1:B:2764:VAL:O	1:B:2764:VAL:HG13	2.19	0.42
1:B:2452:ASP:O	1:B:2455:PHE:HB3	2.19	0.42
1:B:2459:PRO:O	1:B:2460:SER:C	2.60	0.42
1:B:2502:LYS:HB3	1:B:2503:ASP:H	1.63	0.42
1:B:2537:SER:OG	1:B:2541:GLU:HG3	2.20	0.42
1:A:1528:ARG:NH1	1:A:1529:MET:HE3	2.34	0.42
1:A:1681:LEU:O	1:A:1685:LEU:HD22	2.20	0.42
1:B:2392:LEU:O	1:B:2395:LEU:N	2.52	0.42
1:B:2595:GLN:HG3	1:B:2596:ARG:N	2.33	0.42
1:B:2681:LEU:HB3	1:B:2685:LEU:HD21	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2488:TRP:CE3	1:B:2676:PRO:CD	3.03	0.42
1:B:2546:LEU:O	1:B:2549:LEU:N	2.46	0.42
1:B:2628:LEU:HD21	1:B:2740:TYR:CD2	2.54	0.42
1:B:2631:LEU:HD13	1:B:2737:ILE:HD11	2.01	0.42
1:A:1699:GLU:HG2	1:A:1703:LYS:HE3	2.01	0.42
1:B:2731:LYS:O	1:B:2732:LYS:C	2.62	0.42
1:A:1535:VAL:HG13	1:A:1687:VAL:HG21	2.00	0.42
1:B:2675:HIS:CE1	1:B:2677:LEU:HB2	2.54	0.42
1:A:1397:LYS:C	1:A:1399:PHE:N	2.78	0.42
1:A:1628:LEU:HD22	1:A:1741:LYS:HG3	2.01	0.42
1:A:1624:PHE:C	1:A:1626:ASP:N	2.75	0.42
1:B:2388:GLU:C	1:B:2390:GLY:H	2.27	0.42
1:B:2700:ASP:O	1:B:2701:GLU:C	2.62	0.42
1:A:1391:VAL:O	1:A:1392:LEU:C	2.63	0.42
1:A:1441:VAL:HG13	1:A:1513:ILE:CD1	2.48	0.41
1:B:2408:ALA:O	1:B:2409:SER:C	2.62	0.41
1:A:1621:TYR:O	1:A:1623:SER:N	2.53	0.41
1:A:1731:LYS:O	1:A:1732:LYS:C	2.63	0.41
1:A:1537:SER:O	1:A:1540:ARG:N	2.53	0.41
1:B:2395:LEU:C	1:B:2397:LYS:N	2.74	0.41
1:B:2524:TYR:OH	1:B:2678:ASP:OD1	2.33	0.41
1:A:1524:TYR:CE1	1:A:1528:ARG:HD2	2.55	0.41
1:A:1525:TRP:O	1:A:1526:GLY:C	2.63	0.41
1:A:1525:TRP:O	1:A:1528:ARG:HB3	2.20	0.41
1:A:1563:ASP:O	1:A:1564:ASN:C	2.62	0.41
1:A:1634:VAL:O	1:A:1634:VAL:HG12	2.19	0.41
1:A:1681:LEU:HB3	1:A:1685:LEU:CD2	2.49	0.41
1:B:2575:VAL:O	1:B:2578:PHE:HB3	2.20	0.41
1:B:2621:TYR:C	1:B:2623:SER:N	2.77	0.41
1:B:2488:TRP:CE3	1:B:2676:PRO:HD2	2.55	0.41
1:B:2646:VAL:O	1:B:2649:CYS:HB2	2.20	0.41
1:A:1633:PRO:C	1:A:1635:LEU:N	2.75	0.41
1:B:2688:LEU:HD23	1:B:2688:LEU:HA	1.81	0.41
1:B:2691:ALA:O	1:B:2693:LYS:N	2.53	0.41
1:A:1631:LEU:CD1	1:A:1737:ILE:HD11	2.50	0.41
1:A:1391:VAL:O	1:A:1394:ASP:HB2	2.20	0.41
1:A:1412:PHE:HB3	1:B:2418:ILE:HG23	2.03	0.41
1:A:1471:ILE:O	1:A:1472:GLU:C	2.63	0.41
1:A:1487:ASP:C	1:A:1489:GLU:H	2.28	0.41
1:A:1564:ASN:O	1:A:1565:LEU:C	2.64	0.41
1:A:1621:TYR:CD1	1:A:1621:TYR:N	2.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2391:VAL:O	1:B:2394:ASP:HB2	2.21	0.41
1:B:2425:ILE:C	1:B:2427:GLN:N	2.78	0.41
1:B:2504:PRO:O	1:B:2507:LEU:HD23	2.20	0.41
1:B:2595:GLN:CG	1:B:2596:ARG:N	2.83	0.41
1:B:2621:TYR:CD1	1:B:2621:TYR:N	2.89	0.41
1:B:2640:VAL:O	1:B:2640:VAL:HG12	2.20	0.41
1:A:1420:PHE:CE2	1:A:1480:ASN:HB3	2.55	0.41
1:A:1707:MET:HE3	1:A:1707:MET:HB2	1.92	0.41
1:B:2419:THR:HG23	1:B:2511:ASP:OD1	2.21	0.41
1:A:1537:SER:O	1:A:1539:GLU:N	2.53	0.40
1:A:1538:TYR:O	1:A:1539:GLU:C	2.64	0.40
1:B:2431:ILE:C	1:B:2433:LEU:N	2.79	0.40
1:B:2728:SER:O	1:B:2729:PHE:C	2.64	0.40
1:A:1727:ILE:HD13	1:A:1727:ILE:HA	1.93	0.40
1:B:2618:ARG:HG2	1:B:2618:ARG:HH11	1.86	0.40
1:A:1453:ARG:CG	1:A:1457:GLN:HE21	2.32	0.40
1:A:1502:LYS:HB3	1:A:1503:ASP:H	1.67	0.40
1:A:1422:SER:HB2	1:A:1425:ILE:HG12	2.01	0.40
1:B:2391:VAL:O	1:B:2392:LEU:C	2.64	0.40
1:B:2392:LEU:O	1:B:2393:ALA:C	2.63	0.40
1:B:2743:ALA:O	1:B:2747:ASN:ND2	2.54	0.40
1:A:1354:PRO:HB3	1:A:1358:LEU:HD11	2.02	0.40
1:A:1557:SER:O	1:A:1558:ALA:C	2.65	0.40
1:A:1576:GLY:O	1:A:1577:ASN:C	2.64	0.40
1:A:1696:ASP:O	1:A:1699:GLU:N	2.55	0.40
1:B:2375:GLY:O	1:B:2376:THR:C	2.64	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	408/410 (100%)	280 (69%)	97 (24%)	31 (8%)	1	6
1	B	408/410 (100%)	272 (67%)	99 (24%)	37 (9%)	0	3
All	All	816/820 (100%)	552 (68%)	196 (24%)	68 (8%)	0	5

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1354	PRO
1	A	1367	ASP
1	A	1409	SER
1	A	1417	LYS
1	A	1432	ASN
1	A	1485	SER
1	A	1602	ASP
1	A	1625	ASN
1	B	2354	PRO
1	B	2367	ASP
1	B	2409	SER
1	B	2410	LYS
1	B	2417	LYS
1	B	2432	ASN
1	B	2602	ASP
1	B	2625	ASN
1	A	1355	HIS
1	A	1405	LYS
1	A	1406	SER
1	A	1410	LYS
1	A	1431	ILE
1	A	1502	LYS
1	A	1537	SER
1	A	1583	SER
1	A	1613	VAL
1	B	2355	HIS
1	B	2405	LYS
1	B	2406	SER
1	B	2431	ILE
1	B	2485	SER
1	B	2502	LYS
1	B	2583	SER
1	B	2729	PHE
1	A	1469	GLU
1	A	1499	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1510	ALA
1	A	1729	PHE
1	B	2499	PRO
1	B	2510	ALA
1	B	2537	SER
1	A	1476	ASN
1	A	1612	TYR
1	A	1616	ILE
1	B	2465	LEU
1	B	2476	ASN
1	B	2538	TYR
1	B	2574	ALA
1	B	2579	MET
1	B	2622	PRO
1	B	2763	ILE
1	B	2764	VAL
1	A	1538	TYR
1	A	1574	ALA
1	A	1609	PHE
1	A	1622	PRO
1	A	1763	ILE
1	B	2469	GLU
1	B	2609	PHE
1	B	2612	TYR
1	B	2613	VAL
1	A	1764	VAL
1	B	2703	LYS
1	B	2719	ASP
1	B	2741	LYS
1	A	1391	VAL
1	B	2616	ILE
1	B	2391	VAL
1	B	2568	VAL

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	373/373 (100%)	355 (95%)	18 (5%)	23	52
1	B	373/373 (100%)	352 (94%)	21 (6%)	19	47
All	All	746/746 (100%)	707 (95%)	39 (5%)	21	49

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1380	GLU
1	A	1418	ILE
1	A	1435	MET
1	A	1441	VAL
1	A	1443	ASP
1	A	1493	ASN
1	A	1515	LEU
1	A	1517	LEU
1	A	1518	MET
1	A	1527	SER
1	A	1620	ASN
1	A	1621	TYR
1	A	1627	PHE
1	A	1637	VAL
1	A	1676	PRO
1	A	1685	LEU
1	A	1698	LEU
1	A	1705	THR
1	B	2380	GLU
1	B	2418	ILE
1	B	2435	MET
1	B	2441	VAL
1	B	2443	ASP
1	B	2493	ASN
1	B	2494	LEU
1	B	2515	LEU
1	B	2518	MET
1	B	2527	SER
1	B	2529	MET
1	B	2620	ASN
1	B	2621	TYR
1	B	2627	PHE
1	B	2637	VAL
1	B	2676	PRO
1	B	2685	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2698	LEU
1	B	2705	THR
1	B	2712	LEU
1	B	2759	LYS

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	1457	GLN
1	A	1493	ASN
1	A	1516	GLN
1	A	1567	ASN
1	A	1570	ASN
1	A	1577	ASN
1	A	1580	ASN
1	A	1620	ASN
1	A	1644	GLN
1	A	1747	ASN
1	A	1760	HIS
1	B	2457	GLN
1	B	2493	ASN
1	B	2516	GLN
1	B	2567	ASN
1	B	2577	ASN
1	B	2580	ASN
1	B	2585	GLN
1	B	2620	ASN
1	B	2644	GLN
1	B	2747	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	408/410 (99%)	-1.30	0 100 100	14, 44, 134, 199	48 (11%)
1	B	410/410 (100%)	-1.28	1 (0%) 91 86	12, 47, 149, 199	49 (11%)
All	All	818/820 (99%)	-1.29	1 (0%) 92 90	12, 45, 144, 199	97 (11%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2582	THR	2.4

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.