



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 05:44 am BST

PDB ID : 2Y25
Title : Crystal structure of the myomesin domains My11-My13
Authors : Pinotsis, N.; Chatziefthimiou, S.D.; Wilmanns, M.
Deposited on : 2010-12-13
Resolution : 3.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

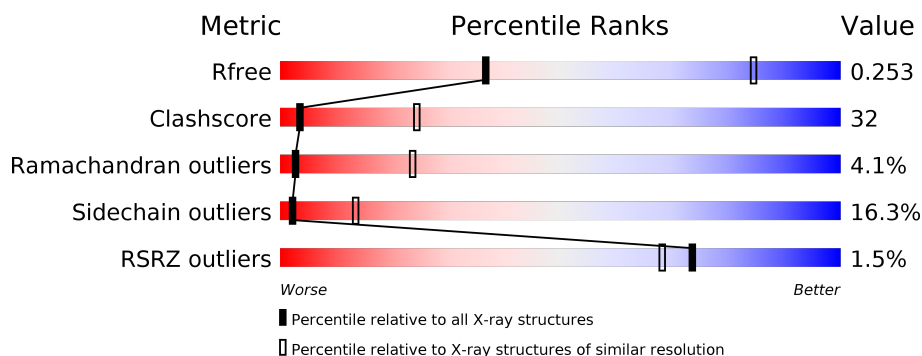
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 on 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	317	<div> <div>3%</div> <div>47%</div> <div>45%</div> <div>6%</div> <div>.</div> </div>
1	B	317	<div> <div>42%</div> <div>45%</div> <div>11%</div> <div>..</div> </div>
1	C	317	<div> <div>3%</div> <div>48%</div> <div>44%</div> <div>6%</div> <div>.</div> </div>
1	D	317	<div> <div>42%</div> <div>44%</div> <div>11%</div> <div>..</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9534 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 MYOMESIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2351	1492	391	459	9			
1	B	314	Total	C	N	O	S	0	0	0
			2416	1531	403	473	9			
1	C	310	Total	C	N	O	S	0	0	0
			2351	1492	391	459	9			
1	D	314	Total	C	N	O	S	0	0	0
			2416	1531	403	473	9			

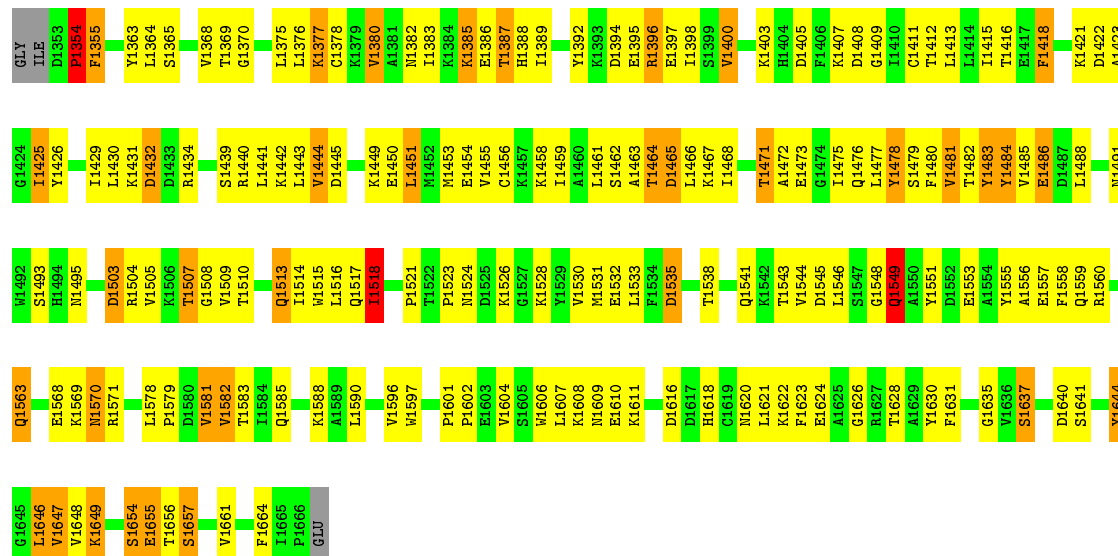
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1351	GLY	-	expression tag	UNP P52179
A	1352	ILE	-	expression tag	UNP P52179
A	1353	ASP	-	expression tag	UNP P52179
A	1354	PRO	-	expression tag	UNP P52179
A	1355	PHE	-	expression tag	UNP P52179
A	1356	THR	-	expression tag	UNP P52179
B	1351	GLY	-	expression tag	UNP P52179
B	1352	ILE	-	expression tag	UNP P52179
B	1353	ASP	-	expression tag	UNP P52179
B	1354	PRO	-	expression tag	UNP P52179
B	1355	PHE	-	expression tag	UNP P52179
B	1356	THR	-	expression tag	UNP P52179
C	1351	GLY	-	expression tag	UNP P52179
C	1352	ILE	-	expression tag	UNP P52179
C	1353	ASP	-	expression tag	UNP P52179
C	1354	PRO	-	expression tag	UNP P52179
C	1355	PHE	-	expression tag	UNP P52179
C	1356	THR	-	expression tag	UNP P52179
D	1351	GLY	-	expression tag	UNP P52179
D	1352	ILE	-	expression tag	UNP P52179
D	1353	ASP	-	expression tag	UNP P52179

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	1354	PRO	-	expression tag	UNP P52179
D	1355	PHE	-	expression tag	UNP P52179
D	1356	THR	-	expression tag	UNP P52179



4 Data and refinement statistics

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α , β , γ	155.20Å 155.20Å 106.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 3.50 19.95 – 3.50	Depositor EDS
% Data completeness (in resolution range)	93.8 (19.95-3.50) 93.8 (19.95-3.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 3.52Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.217 , 0.266 0.202 , 0.253	Depositor DCC
R_{free} test set	1234 reflections (4.12%)	wwPDB-VP
Wilson B-factor (Å ²)	92.9	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.408 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9534	wwPDB-VP
Average B, all atoms (Å ²)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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	0.62	0/2397	0.71	2/3261 (0.1%)
1	B	0.72	0/2464	0.84	3/3346 (0.1%)
1	C	0.62	1/2397 (0.0%)	0.71	3/3261 (0.1%)
1	D	0.72	1/2464 (0.0%)	0.85	3/3346 (0.1%)
All	All	0.67	2/9722 (0.0%)	0.78	11/13214 (0.1%)

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	B	0	2
1	D	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1563	GLN	CG-CD	5.40	1.63	1.51
1	C	1573	ARG	CG-CD	5.05	1.64	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1581	VAL	CB-CA-C	-6.54	98.98	111.40
1	B	1355	PHE	N-CA-C	6.40	128.28	111.00
1	D	1355	PHE	N-CA-C	6.26	127.91	111.00
1	D	1581	VAL	CB-CA-C	-6.04	99.92	111.40
1	C	1573	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	A	1573	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	1573	ARG	CA-CB-CG	5.61	125.73	113.40
1	C	1573	ARG	CA-CB-CG	5.60	125.73	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1616	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	1616	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	1616	ASP	CB-CG-OD2	5.15	122.94	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1354	PRO	Peptide
1	B	1483	TYR	Peptide
1	D	1354	PRO	Peptide
1	D	1483	TYR	Peptide

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	2351	0	2223	128	0
1	B	2416	0	2323	174	0
1	C	2351	0	2223	123	0
1	D	2416	0	2323	175	0
All	All	9534	0	9092	596	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 32.

All (596) 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:1485:VAL:HG21	1:A:1509:VAL:HG11	1.35	1.06
1:C:1485:VAL:HG21	1:C:1509:VAL:HG11	1.34	1.05
1:B:1615:SER:O	1:B:1616:ASP:OD1	1.76	1.02
1:D:1585:GLN:HB3	1:D:1588:LYS:HD2	1.39	1.02
1:B:1585:GLN:HB3	1:B:1588:LYS:HD2	1.41	1.00
1:D:1483:TYR:O	1:D:1484:TYR:CD1	2.15	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1483:TYR:O	1:B:1484:TYR:CD1	2.15	0.99
1:D:1363:TYR:HD1	1:D:1439:SER:HG	1.02	0.99
1:B:1363:TYR:HD1	1:B:1439:SER:HG	1.00	0.98
1:A:1581:VAL:HG13	1:B:1583:THR:HB	1.41	0.98
1:A:1486:GLU:HG3	1:A:1487:ASP:H	1.26	0.98
1:C:1486:GLU:HG3	1:C:1487:ASP:H	1.27	0.96
1:C:1581:VAL:HG13	1:D:1583:THR:HB	1.47	0.95
1:B:1483:TYR:O	1:B:1484:TYR:HD1	1.47	0.94
1:D:1477:LEU:HB2	1:D:1516:LEU:HB3	1.50	0.94
1:B:1477:LEU:HB2	1:B:1516:LEU:HB3	1.49	0.93
1:D:1483:TYR:O	1:D:1484:TYR:HD1	1.46	0.93
1:B:1425:ILE:HG23	1:B:1442:LYS:HG3	1.56	0.86
1:D:1425:ILE:HG23	1:D:1442:LYS:HG3	1.58	0.85
1:B:1631:PHE:HZ	1:B:1644:TYR:CE2	1.96	0.84
1:B:1518:ILE:O	1:B:1518:ILE:HG22	1.76	0.84
1:B:1385:LYS:H	1:B:1385:LYS:HD3	1.41	0.83
1:D:1385:LYS:H	1:D:1385:LYS:HD3	1.42	0.83
1:B:1375:LEU:HD11	1:B:1412:THR:HB	1.60	0.83
1:A:1485:VAL:HG21	1:A:1509:VAL:CG1	2.09	0.82
1:C:1485:VAL:HG21	1:C:1509:VAL:CG1	2.08	0.82
1:D:1631:PHE:HZ	1:D:1644:TYR:CE2	1.97	0.82
1:B:1482:THR:HA	1:B:1483:TYR:CB	2.10	0.81
1:D:1375:LEU:HD11	1:D:1412:THR:HB	1.62	0.81
1:C:1569:LYS:HG2	1:C:1569:LYS:O	1.80	0.81
1:B:1495:ASN:ND2	1:B:1528:LYS:H	1.79	0.80
1:D:1482:THR:HA	1:D:1483:TYR:CB	2.11	0.80
1:A:1569:LYS:HG2	1:A:1569:LYS:O	1.80	0.80
1:D:1518:ILE:O	1:D:1518:ILE:HG22	1.81	0.80
1:B:1604:VAL:HG11	1:B:1623:PHE:CE1	2.17	0.79
1:D:1398:ILE:HG22	1:D:1400:VAL:HG23	1.65	0.79
1:B:1615:SER:O	1:B:1616:ASP:CG	2.20	0.79
1:B:1606:TRP:O	1:B:1607:LEU:HD23	1.82	0.79
1:B:1398:ILE:HG22	1:B:1400:VAL:HG23	1.66	0.78
1:A:1552:ASP:O	1:A:1556:ALA:HB2	1.84	0.78
1:A:1493:SER:OG	1:A:1530:VAL:HB	1.85	0.77
1:C:1552:ASP:O	1:C:1556:ALA:HB2	1.84	0.77
1:D:1495:ASN:ND2	1:D:1528:LYS:H	1.84	0.77
1:D:1606:TRP:CD1	1:D:1621:LEU:HD13	2.20	0.76
1:C:1493:SER:OG	1:C:1530:VAL:HB	1.86	0.76
1:B:1518:ILE:CG2	1:B:1518:ILE:O	2.33	0.75
1:B:1415:ILE:HD11	1:B:1426:TYR:HE2	1.50	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1380:VAL:HG12	1:B:1430:LEU:HD11	1.67	0.75
1:D:1415:ILE:HD11	1:D:1426:TYR:HE2	1.49	0.75
1:D:1380:VAL:HG12	1:D:1430:LEU:HD11	1.69	0.75
1:B:1606:TRP:CD1	1:B:1621:LEU:HD13	2.21	0.75
1:C:1623:PHE:CZ	1:C:1626:GLY:HA2	2.22	0.75
1:B:1505:VAL:HG23	1:B:1517:GLN:O	1.87	0.74
1:C:1585:GLN:HB3	1:C:1664:PHE:CE1	2.22	0.74
1:A:1623:PHE:CZ	1:A:1626:GLY:HA2	2.23	0.74
1:D:1508:GLY:HA3	1:D:1515:TRP:CZ2	2.22	0.73
1:A:1486:GLU:HG3	1:A:1487:ASP:N	2.02	0.73
1:D:1389:ILE:HG12	1:D:1430:LEU:CD2	2.19	0.73
1:D:1606:TRP:O	1:D:1607:LEU:HD23	1.89	0.72
1:D:1604:VAL:HG11	1:D:1623:PHE:CE1	2.24	0.72
1:A:1585:GLN:HB3	1:A:1664:PHE:CE1	2.23	0.72
1:C:1443:LEU:HD22	1:C:1451:LEU:HD11	1.72	0.72
1:D:1606:TRP:CG	1:D:1621:LEU:HD13	2.23	0.72
1:D:1505:VAL:HG23	1:D:1517:GLN:O	1.88	0.72
1:C:1481:VAL:C	1:C:1483:TYR:H	1.92	0.72
1:D:1631:PHE:CZ	1:D:1644:TYR:CE2	2.78	0.71
1:B:1354:PRO:HB2	1:B:1355:PHE:HA	1.71	0.71
1:C:1610:GLU:OE1	1:C:1610:GLU:HA	1.88	0.71
1:A:1609:ASN:ND2	1:A:1643:LYS:HB2	2.05	0.71
1:B:1606:TRP:CG	1:B:1621:LEU:HD13	2.25	0.71
1:D:1354:PRO:HB2	1:D:1355:PHE:HA	1.71	0.71
1:D:1518:ILE:O	1:D:1518:ILE:CG2	2.38	0.71
1:D:1649:LYS:HB2	1:D:1654:SER:OG	1.91	0.71
1:B:1508:GLY:HA3	1:B:1515:TRP:CZ2	2.25	0.71
1:A:1481:VAL:C	1:A:1483:TYR:H	1.93	0.71
1:A:1610:GLU:HA	1:A:1610:GLU:OE1	1.91	0.71
1:A:1443:LEU:HD22	1:A:1451:LEU:HD11	1.71	0.70
1:B:1631:PHE:CZ	1:B:1644:TYR:CE2	2.78	0.70
1:A:1393:LYS:CB	1:A:1398:ILE:HD11	2.21	0.70
1:A:1456:CYS:HB3	1:A:1535:ASP:HB3	1.74	0.70
1:A:1553:GLU:O	1:A:1556:ALA:HB3	1.92	0.70
1:C:1393:LYS:CB	1:C:1398:ILE:HD11	2.21	0.70
1:D:1480:PHE:HE1	1:D:1513:GLN:HB2	1.57	0.69
1:B:1389:ILE:HG12	1:B:1430:LEU:CD2	2.21	0.69
1:C:1486:GLU:HG3	1:C:1487:ASP:N	2.02	0.69
1:D:1656:THR:HG22	1:D:1657:SER:H	1.57	0.69
1:B:1656:THR:HG22	1:B:1657:SER:H	1.57	0.69
1:C:1606:TRP:CD1	1:C:1621:LEU:HD13	2.27	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1380:VAL:CG1	1:B:1430:LEU:HD11	2.23	0.69
1:D:1582:VAL:HG23	1:D:1661:VAL:HA	1.74	0.68
1:A:1606:TRP:CD1	1:A:1621:LEU:HD13	2.29	0.68
1:B:1582:VAL:HG23	1:B:1661:VAL:HA	1.74	0.68
1:A:1509:VAL:HG22	1:A:1514:ILE:HA	1.74	0.68
1:C:1456:CYS:HB3	1:C:1535:ASP:HB3	1.76	0.68
1:C:1553:GLU:O	1:C:1556:ALA:HB3	1.94	0.67
1:A:1455:VAL:O	1:A:1459:ILE:HG13	1.94	0.67
1:B:1649:LYS:HB2	1:B:1654:SER:OG	1.95	0.67
1:C:1509:VAL:HG22	1:C:1514:ILE:HA	1.76	0.67
1:C:1623:PHE:CE1	1:C:1626:GLY:HA2	2.30	0.67
1:D:1380:VAL:CG1	1:D:1430:LEU:HD11	2.24	0.67
1:C:1427:GLU:HG2	1:C:1440:ARG:HG2	1.77	0.66
1:C:1455:VAL:O	1:C:1459:ILE:HG13	1.95	0.66
1:C:1609:ASN:ND2	1:C:1643:LYS:HB2	2.10	0.66
1:A:1606:TRP:CH2	1:A:1631:PHE:HB2	2.30	0.66
1:A:1649:LYS:HB2	1:A:1654:SER:HB2	1.76	0.66
1:D:1449:LYS:O	1:D:1453:MET:HG2	1.96	0.65
1:A:1623:PHE:CE1	1:A:1626:GLY:HA2	2.31	0.65
1:B:1495:ASN:HD21	1:B:1528:LYS:H	1.43	0.65
1:A:1637:SER:OG	1:A:1639:ALA:HB3	1.97	0.65
1:A:1427:GLU:HG2	1:A:1440:ARG:HG2	1.79	0.64
1:B:1394:ASP:C	1:B:1396:ARG:H	2.01	0.64
1:B:1631:PHE:CZ	1:B:1644:TYR:CD2	2.86	0.64
1:B:1449:LYS:O	1:B:1453:MET:HG2	1.96	0.64
1:A:1569:LYS:O	1:A:1570:ASN:ND2	2.31	0.64
1:D:1394:ASP:C	1:D:1396:ARG:H	2.00	0.64
1:B:1441:LEU:HD21	1:B:1443:LEU:HD21	1.79	0.63
1:B:1480:PHE:HE1	1:B:1513:GLN:HB2	1.63	0.63
1:C:1585:GLN:HB3	1:C:1664:PHE:CZ	2.33	0.63
1:D:1623:PHE:CZ	1:D:1626:GLY:HA2	2.33	0.63
1:A:1392:TYR:O	1:A:1426:TYR:HA	1.98	0.63
1:A:1649:LYS:CB	1:A:1654:SER:HB2	2.28	0.63
1:B:1385:LYS:CD	1:B:1385:LYS:H	2.09	0.63
1:A:1616:ASP:OD1	1:A:1616:ASP:N	2.30	0.63
1:D:1455:VAL:O	1:D:1459:ILE:HG13	1.99	0.63
1:D:1464:THR:OG1	1:D:1480:PHE:HB2	1.99	0.63
1:A:1585:GLN:HB3	1:A:1664:PHE:CZ	2.33	0.62
1:C:1392:TYR:O	1:C:1426:TYR:HA	1.98	0.62
1:D:1441:LEU:HD21	1:D:1443:LEU:HD21	1.81	0.62
1:B:1464:THR:OG1	1:B:1480:PHE:HB2	1.98	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1631:PHE:CZ	1:D:1644:TYR:CD2	2.88	0.62
1:C:1649:LYS:HB2	1:C:1654:SER:HB2	1.79	0.62
1:B:1656:THR:HG22	1:B:1657:SER:N	2.14	0.61
1:A:1476:GLN:HA	1:A:1476:GLN:OE1	1.99	0.61
1:B:1623:PHE:CZ	1:B:1626:GLY:HA2	2.35	0.61
1:B:1485:VAL:HG21	1:B:1509:VAL:HG21	1.83	0.61
1:D:1394:ASP:O	1:D:1396:ARG:N	2.33	0.60
1:C:1476:GLN:HA	1:C:1476:GLN:OE1	1.98	0.60
1:D:1485:VAL:HG21	1:D:1509:VAL:HG21	1.82	0.60
1:B:1509:VAL:CG1	1:B:1510:THR:N	2.64	0.60
1:D:1385:LYS:H	1:D:1385:LYS:CD	2.10	0.60
1:D:1509:VAL:CG1	1:D:1510:THR:N	2.64	0.60
1:B:1604:VAL:CG1	1:B:1623:PHE:CE1	2.84	0.60
1:B:1510:THR:HG22	1:B:1510:THR:O	2.02	0.60
1:D:1456:CYS:HB2	1:D:1535:ASP:HB3	1.84	0.60
1:B:1531:MET:O	1:B:1541:GLN:HA	2.02	0.60
1:C:1585:GLN:CB	1:C:1664:PHE:CE1	2.85	0.60
1:D:1656:THR:HG22	1:D:1657:SER:N	2.15	0.60
1:D:1376:LEU:HD21	1:D:1426:TYR:HD2	1.67	0.59
1:D:1609:ASN:O	1:D:1610:GLU:HB2	2.01	0.59
1:B:1455:VAL:O	1:B:1459:ILE:HG13	2.03	0.59
1:B:1546:LEU:HD11	1:B:1551:TYR:HD1	1.67	0.59
1:C:1649:LYS:CB	1:C:1654:SER:HB2	2.32	0.59
1:D:1531:MET:O	1:D:1541:GLN:HA	2.02	0.59
1:D:1495:ASN:HD21	1:D:1528:LYS:H	1.49	0.59
1:D:1407:LYS:HG3	1:D:1408:ASP:H	1.67	0.59
1:C:1606:TRP:CH2	1:C:1631:PHE:HB2	2.37	0.59
1:B:1407:LYS:HG3	1:B:1408:ASP:H	1.68	0.58
1:B:1604:VAL:HG12	1:B:1648:VAL:HG12	1.86	0.58
1:B:1609:ASN:O	1:B:1610:GLU:HB2	2.02	0.58
1:D:1485:VAL:HG12	1:D:1486:GLU:H	1.68	0.58
1:B:1394:ASP:O	1:B:1396:ARG:N	2.36	0.58
1:D:1456:CYS:HA	1:D:1459:ILE:HD12	1.85	0.58
1:C:1569:LYS:O	1:C:1570:ASN:ND2	2.37	0.58
1:A:1585:GLN:CB	1:A:1664:PHE:CE1	2.86	0.58
1:D:1568:GLU:O	1:D:1568:GLU:HG3	2.04	0.58
1:A:1574:VAL:O	1:A:1574:VAL:HG12	2.03	0.58
1:B:1456:CYS:HB2	1:B:1535:ASP:HB3	1.86	0.58
1:C:1481:VAL:O	1:C:1483:TYR:N	2.36	0.58
1:B:1456:CYS:HA	1:B:1459:ILE:HD12	1.86	0.57
1:D:1455:VAL:HG12	1:D:1459:ILE:HD11	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1553:GLU:O	1:B:1556:ALA:HB3	2.04	0.57
1:B:1608:LYS:HD2	1:B:1644:TYR:CZ	2.39	0.57
1:A:1590:LEU:HD11	1:A:1592:LEU:HD21	1.87	0.57
1:A:1608:LYS:HD2	1:A:1644:TYR:CZ	2.40	0.57
1:B:1376:LEU:HD21	1:B:1426:TYR:HD2	1.70	0.57
1:B:1466:LEU:HD23	1:B:1479:SER:HB2	1.87	0.57
1:B:1382:ASN:ND2	1:B:1434:ARG:HH12	2.03	0.57
1:D:1407:LYS:HG3	1:D:1408:ASP:N	2.20	0.57
1:D:1604:VAL:HG12	1:D:1648:VAL:HG12	1.86	0.57
1:A:1481:VAL:O	1:A:1483:TYR:N	2.37	0.57
1:D:1462:SER:HB2	1:D:1482:THR:OG1	2.05	0.57
1:B:1407:LYS:HG3	1:B:1408:ASP:N	2.20	0.56
1:D:1485:VAL:HG12	1:D:1486:GLU:N	2.20	0.56
1:D:1398:ILE:CG2	1:D:1400:VAL:HG23	2.34	0.56
1:B:1473:GLU:HA	1:B:1473:GLU:OE1	2.04	0.56
1:B:1462:SER:HB2	1:B:1482:THR:OG1	2.05	0.56
1:D:1363:TYR:HD1	1:D:1439:SER:OG	1.80	0.56
1:B:1568:GLU:O	1:B:1568:GLU:HG3	2.05	0.56
1:C:1562:LYS:O	1:C:1566:ILE:HG12	2.05	0.56
1:C:1442:LYS:O	1:C:1443:LEU:HD23	2.06	0.56
1:D:1415:ILE:HD11	1:D:1426:TYR:CE2	2.37	0.56
1:D:1647:VAL:HG22	1:D:1656:THR:HG23	1.87	0.56
1:C:1389:ILE:HG12	1:C:1430:LEU:HD23	1.87	0.56
1:B:1380:VAL:HB	1:B:1383:ILE:HD11	1.87	0.56
1:B:1415:ILE:HD11	1:B:1426:TYR:CE2	2.38	0.56
1:D:1380:VAL:HB	1:D:1383:ILE:HD11	1.87	0.56
1:A:1519:ASN:O	1:A:1520:GLU:C	2.45	0.56
1:B:1385:LYS:N	1:B:1385:LYS:HD3	2.16	0.56
1:D:1553:GLU:O	1:D:1556:ALA:HB3	2.05	0.56
1:D:1462:SER:O	1:D:1481:VAL:HA	2.06	0.55
1:C:1557:GLU:OE2	1:C:1560:ARG:NH1	2.39	0.55
1:D:1604:VAL:CG1	1:D:1623:PHE:CE1	2.89	0.55
1:A:1389:ILE:HG12	1:A:1430:LEU:HD23	1.89	0.55
1:A:1571:ARG:NH1	1:A:1571:ARG:HG3	2.21	0.55
1:A:1471:THR:CG2	1:A:1476:GLN:HG2	2.36	0.55
1:D:1510:THR:HG22	1:D:1510:THR:O	2.06	0.55
1:D:1546:LEU:HD11	1:D:1551:TYR:HD1	1.71	0.55
1:D:1466:LEU:HD23	1:D:1479:SER:HB2	1.88	0.55
1:B:1488:LEU:HD21	1:B:1533:LEU:HB3	1.89	0.55
1:C:1582:VAL:HG23	1:C:1661:VAL:HA	1.89	0.55
1:C:1571:ARG:NH1	1:C:1571:ARG:HG3	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1389:ILE:HG12	1:D:1430:LEU:HD23	1.88	0.55
1:A:1360:PHE:HZ	1:A:1428:VAL:O	1.91	0.54
1:B:1398:ILE:CG2	1:B:1400:VAL:HG23	2.35	0.54
1:C:1557:GLU:CD	1:C:1560:ARG:NH1	2.61	0.54
1:B:1462:SER:O	1:B:1481:VAL:HA	2.07	0.54
1:B:1482:THR:CA	1:B:1483:TYR:CB	2.85	0.54
1:C:1476:GLN:HE22	1:C:1517:GLN:HA	1.72	0.54
1:D:1354:PRO:HB2	1:D:1355:PHE:CA	2.38	0.54
1:C:1360:PHE:HZ	1:C:1428:VAL:O	1.91	0.54
1:C:1519:ASN:O	1:C:1520:GLU:C	2.46	0.54
1:D:1473:GLU:HA	1:D:1473:GLU:OE1	2.06	0.54
1:D:1485:VAL:CG1	1:D:1486:GLU:H	2.19	0.54
1:B:1614:ALA:C	1:B:1615:SER:O	2.36	0.54
1:C:1471:THR:CG2	1:C:1476:GLN:HG2	2.37	0.54
1:A:1582:VAL:HG23	1:A:1661:VAL:HA	1.89	0.54
1:B:1364:LEU:HD12	1:B:1439:SER:O	2.08	0.54
1:B:1646:LEU:O	1:B:1656:THR:HG23	2.08	0.54
1:D:1608:LYS:HD2	1:D:1644:TYR:CZ	2.43	0.54
1:D:1488:LEU:HD21	1:D:1533:LEU:HB3	1.89	0.54
1:C:1485:VAL:CG2	1:C:1509:VAL:HG11	2.23	0.54
1:A:1442:LYS:O	1:A:1443:LEU:HD23	2.08	0.53
1:A:1641:SER:HA	1:A:1661:VAL:HG12	1.89	0.53
1:B:1455:VAL:HG12	1:B:1459:ILE:HD11	1.90	0.53
1:C:1637:SER:OG	1:C:1639:ALA:HB3	2.09	0.53
1:C:1494:HIS:O	1:C:1495:ASN:HB2	2.09	0.53
1:C:1522:THR:HB	1:C:1523:PRO:CD	2.39	0.53
1:D:1480:PHE:HE1	1:D:1513:GLN:HE21	1.55	0.53
1:B:1481:VAL:O	1:B:1483:TYR:HA	2.08	0.53
1:B:1623:PHE:CE2	1:B:1626:GLY:HA2	2.44	0.53
1:A:1494:HIS:O	1:A:1495:ASN:HB2	2.09	0.53
1:A:1543:THR:HG22	1:A:1544:VAL:N	2.24	0.53
1:B:1432:ASP:C	1:B:1432:ASP:OD1	2.47	0.53
1:C:1606:TRP:C	1:C:1607:LEU:HG	2.29	0.53
1:C:1518:ILE:O	1:C:1518:ILE:HG22	2.09	0.53
1:C:1518:ILE:O	1:C:1521:PRO:HG3	2.09	0.53
1:B:1389:ILE:HG12	1:B:1430:LEU:HD23	1.91	0.52
1:D:1388:HIS:HD2	1:D:1403:LYS:O	1.91	0.52
1:D:1646:LEU:O	1:D:1656:THR:HG23	2.09	0.52
1:A:1476:GLN:HE22	1:A:1517:GLN:HA	1.73	0.52
1:A:1575:LEU:HB2	1:A:1595:ASN:O	2.09	0.52
1:B:1647:VAL:HG22	1:B:1656:THR:HG23	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1623:PHE:CE2	1:D:1626:GLY:HA2	2.43	0.52
1:C:1567:ALA:O	1:C:1569:LYS:N	2.41	0.52
1:C:1574:VAL:O	1:C:1574:VAL:HG12	2.08	0.52
1:A:1557:GLU:CD	1:A:1560:ARG:NH1	2.63	0.52
1:B:1546:LEU:CD1	1:B:1551:TYR:HD1	2.23	0.52
1:D:1481:VAL:O	1:D:1483:TYR:HA	2.10	0.52
1:C:1641:SER:HA	1:C:1661:VAL:HG12	1.91	0.52
1:D:1385:LYS:HD3	1:D:1385:LYS:N	2.18	0.52
1:D:1364:LEU:HD12	1:D:1439:SER:O	2.10	0.52
1:B:1646:LEU:O	1:B:1656:THR:CG2	2.58	0.52
1:C:1590:LEU:HD11	1:C:1592:LEU:HD21	1.92	0.52
1:D:1477:LEU:O	1:D:1515:TRP:HA	2.09	0.52
1:A:1649:LYS:HB2	1:A:1654:SER:CB	2.40	0.52
1:C:1486:GLU:CG	1:C:1487:ASP:H	2.12	0.52
1:A:1562:LYS:O	1:A:1566:ILE:HG12	2.09	0.52
1:A:1571:ARG:HH11	1:A:1571:ARG:HG3	1.73	0.52
1:B:1464:THR:HG1	1:B:1480:PHE:HB2	1.75	0.52
1:A:1481:VAL:C	1:A:1483:TYR:N	2.63	0.51
1:B:1376:LEU:CD2	1:B:1426:TYR:HD2	2.23	0.51
1:B:1388:HIS:HD2	1:B:1403:LYS:O	1.92	0.51
1:B:1483:TYR:O	1:B:1484:TYR:CB	2.57	0.51
1:B:1491:ASN:HB2	1:B:1532:GLU:HB3	1.91	0.51
1:C:1533:LEU:N	1:C:1533:LEU:HD13	2.25	0.51
1:A:1522:THR:HB	1:A:1523:PRO:CD	2.40	0.51
1:C:1575:LEU:HB2	1:C:1595:ASN:O	2.10	0.51
1:D:1432:ASP:OD1	1:D:1432:ASP:C	2.48	0.51
1:D:1646:LEU:O	1:D:1656:THR:CG2	2.58	0.51
1:A:1615:SER:C	1:A:1616:ASP:OD1	2.47	0.51
1:B:1485:VAL:HG12	1:B:1486:GLU:N	2.26	0.51
1:C:1454:GLU:OE1	1:C:1457:LYS:HD3	2.10	0.51
1:D:1376:LEU:CD2	1:D:1426:TYR:HD2	2.23	0.51
1:D:1483:TYR:O	1:D:1484:TYR:CB	2.58	0.51
1:D:1491:ASN:HB2	1:D:1532:GLU:HB3	1.91	0.51
1:A:1454:GLU:OE1	1:A:1457:LYS:HD3	2.10	0.51
1:C:1531:MET:HE1	1:C:1542:LYS:HB2	1.93	0.51
1:C:1472:ALA:HA	1:C:1561:LEU:HB3	1.91	0.51
1:A:1557:GLU:OE2	1:A:1560:ARG:NH1	2.43	0.51
1:A:1590:LEU:HD12	1:A:1591:ASN:H	1.75	0.51
1:C:1543:THR:HG22	1:C:1544:VAL:N	2.25	0.51
1:D:1375:LEU:HD12	1:D:1376:LEU:N	2.26	0.51
1:D:1396:ARG:HD3	1:D:1397:GLU:N	2.26	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1608:LYS:HD2	1:C:1644:TYR:CZ	2.45	0.51
1:A:1491:ASN:O	1:A:1531:MET:HA	2.11	0.51
1:A:1606:TRP:C	1:A:1607:LEU:HG	2.30	0.51
1:B:1483:TYR:O	1:B:1484:TYR:CG	2.63	0.51
1:B:1421:LYS:C	1:B:1423:ALA:H	2.14	0.50
1:C:1481:VAL:C	1:C:1483:TYR:N	2.62	0.50
1:C:1522:THR:HB	1:C:1523:PRO:HD2	1.93	0.50
1:B:1368:VAL:CG1	1:B:1369:THR:N	2.74	0.50
1:B:1623:PHE:O	1:B:1624:GLU:HG2	2.12	0.50
1:C:1491:ASN:O	1:C:1531:MET:HA	2.11	0.50
1:C:1590:LEU:HD12	1:C:1591:ASN:H	1.75	0.50
1:C:1572:ALA:HB1	1:C:1648:VAL:CG2	2.41	0.50
1:C:1649:LYS:HB2	1:C:1654:SER:CB	2.42	0.50
1:B:1354:PRO:HB2	1:B:1355:PHE:CA	2.39	0.50
1:B:1546:LEU:HD12	1:B:1551:TYR:HB2	1.91	0.50
1:A:1486:GLU:CG	1:A:1487:ASP:H	2.11	0.50
1:A:1509:VAL:HG22	1:A:1514:ILE:HG12	1.93	0.50
1:A:1572:ALA:HB1	1:A:1648:VAL:CG2	2.42	0.50
1:B:1481:VAL:C	1:B:1483:TYR:HA	2.32	0.50
1:A:1518:ILE:O	1:A:1521:PRO:HG3	2.10	0.50
1:A:1522:THR:HB	1:A:1523:PRO:HD2	1.94	0.50
1:C:1364:LEU:HB3	1:C:1441:LEU:HB2	1.93	0.50
1:C:1509:VAL:HG22	1:C:1514:ILE:HG12	1.93	0.50
1:C:1521:PRO:HA	1:C:1525:ASP:OD2	2.11	0.50
1:D:1546:LEU:CD1	1:D:1551:TYR:HD1	2.25	0.50
1:D:1387:THR:HG22	1:D:1388:HIS:H	1.78	0.49
1:A:1468:ILE:HG23	1:A:1477:LEU:HD23	1.93	0.49
1:C:1571:ARG:HG3	1:C:1571:ARG:HH11	1.75	0.49
1:A:1364:LEU:HB3	1:A:1441:LEU:HB2	1.94	0.49
1:A:1518:ILE:HG22	1:A:1518:ILE:O	2.12	0.49
1:A:1521:PRO:HA	1:A:1525:ASP:OD2	2.12	0.49
1:A:1495:ASN:ND2	1:A:1528:LYS:H	2.10	0.49
1:C:1495:ASN:ND2	1:C:1528:LYS:H	2.10	0.49
1:C:1570:ASN:O	1:C:1571:ARG:C	2.46	0.49
1:D:1382:ASN:ND2	1:D:1434:ARG:HH12	2.11	0.49
1:A:1533:LEU:N	1:A:1533:LEU:HD13	2.28	0.49
1:A:1630:TYR:CD1	1:A:1630:TYR:N	2.81	0.49
1:A:1358:PRO:HA	1:A:1382:ASN:HB3	1.94	0.49
1:D:1546:LEU:HD12	1:D:1551:TYR:HB2	1.95	0.49
1:B:1396:ARG:HD3	1:B:1397:GLU:N	2.28	0.49
1:D:1421:LYS:C	1:D:1423:ALA:H	2.16	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1480:PHE:HE1	1:B:1513:GLN:HE21	1.59	0.49
1:A:1633:ILE:HG21	1:A:1636:VAL:HG22	1.94	0.48
1:D:1596:VAL:HG11	1:D:1648:VAL:HG11	1.94	0.48
1:B:1387:THR:HG22	1:B:1388:HIS:H	1.78	0.48
1:C:1468:ILE:HG23	1:C:1477:LEU:HD23	1.94	0.48
1:B:1442:LYS:HE3	1:B:1444:VAL:HG22	1.95	0.48
1:B:1622:LYS:HB2	1:B:1630:TYR:HB2	1.95	0.48
1:D:1509:VAL:HG13	1:D:1510:THR:N	2.28	0.48
1:B:1485:VAL:CG1	1:B:1486:GLU:H	2.26	0.48
1:D:1478:TYR:HA	1:D:1514:ILE:O	2.14	0.48
1:A:1581:VAL:HG13	1:B:1583:THR:CB	2.29	0.48
1:B:1569:LYS:NZ	1:B:1570:ASN:HD21	2.11	0.48
1:C:1358:PRO:HA	1:C:1382:ASN:HB3	1.94	0.48
1:D:1376:LEU:HD21	1:D:1426:TYR:CD2	2.47	0.48
1:D:1481:VAL:C	1:D:1483:TYR:HA	2.33	0.48
1:A:1590:LEU:HD12	1:A:1591:ASN:N	2.28	0.48
1:B:1363:TYR:HD1	1:B:1439:SER:OG	1.80	0.48
1:B:1485:VAL:HG12	1:B:1486:GLU:H	1.77	0.48
1:C:1372:CYS:SG	1:C:1459:ILE:HG12	2.54	0.48
1:D:1644:TYR:N	1:D:1644:TYR:CD1	2.82	0.48
1:A:1372:CYS:SG	1:A:1459:ILE:HG12	2.54	0.48
1:B:1569:LYS:HZ2	1:B:1570:ASN:HD21	1.62	0.48
1:D:1623:PHE:O	1:D:1624:GLU:HG2	2.14	0.48
1:D:1368:VAL:CG1	1:D:1369:THR:N	2.76	0.47
1:D:1442:LYS:HE3	1:D:1444:VAL:HG22	1.95	0.47
1:C:1475:ILE:HD12	1:C:1521:PRO:HG2	1.95	0.47
1:C:1633:ILE:HG21	1:C:1636:VAL:HG22	1.97	0.47
1:A:1595:ASN:OD1	1:A:1595:ASN:N	2.46	0.47
1:C:1355:PHE:CG	1:C:1356:THR:N	2.79	0.47
1:C:1392:TYR:N	1:C:1427:GLU:O	2.47	0.47
1:A:1484:TYR:N	1:A:1484:TYR:CD1	2.83	0.47
1:D:1464:THR:O	1:D:1465:ASP:C	2.52	0.47
1:B:1544:VAL:HG22	1:B:1545:ASP:N	2.29	0.47
1:B:1644:TYR:N	1:B:1644:TYR:CD1	2.82	0.47
1:C:1507:THR:OG1	1:C:1508:GLY:N	2.48	0.47
1:D:1622:LYS:HB2	1:D:1630:TYR:HB2	1.96	0.47
1:D:1416:THR:C	1:D:1418:PHE:H	2.18	0.47
1:B:1376:LEU:HD21	1:B:1426:TYR:CD2	2.49	0.47
1:B:1382:ASN:HD21	1:B:1434:ARG:HH12	1.62	0.47
1:B:1478:TYR:HA	1:B:1514:ILE:O	2.14	0.47
1:B:1585:GLN:HB2	1:B:1664:PHE:CZ	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1654:SER:OG	1:C:1655:GLU:N	2.47	0.47
1:B:1407:LYS:CG	1:B:1408:ASP:H	2.27	0.47
1:B:1416:THR:C	1:B:1418:PHE:H	2.17	0.47
1:B:1477:LEU:O	1:B:1515:TRP:HA	2.14	0.47
1:B:1523:PRO:O	1:B:1526:LYS:HG3	2.14	0.47
1:D:1523:PRO:O	1:D:1526:LYS:HG3	2.15	0.47
1:A:1485:VAL:CG2	1:A:1509:VAL:HG11	2.25	0.47
1:B:1375:LEU:HD12	1:B:1376:LEU:N	2.30	0.47
1:C:1448:PHE:HA	1:C:1451:LEU:HG	1.97	0.47
1:A:1475:ILE:HD12	1:A:1521:PRO:HG2	1.96	0.46
1:A:1506:LYS:O	1:A:1516:LEU:HD12	2.14	0.46
1:A:1472:ALA:HA	1:A:1561:LEU:HB3	1.95	0.46
1:B:1596:VAL:HG11	1:B:1648:VAL:HG11	1.97	0.46
1:C:1367:GLU:HG2	1:C:1375:LEU:HB3	1.97	0.46
1:C:1557:GLU:OE1	1:C:1560:ARG:NH1	2.48	0.46
1:C:1630:TYR:N	1:C:1630:TYR:CD1	2.83	0.46
1:A:1448:PHE:HA	1:A:1451:LEU:HG	1.97	0.46
1:B:1421:LYS:O	1:B:1423:ALA:N	2.47	0.46
1:D:1485:VAL:CG1	1:D:1486:GLU:N	2.78	0.46
1:D:1544:VAL:HG22	1:D:1545:ASP:N	2.29	0.46
1:D:1418:PHE:CE2	1:D:1455:VAL:HG21	2.50	0.46
1:D:1421:LYS:O	1:D:1423:ALA:N	2.49	0.46
1:D:1482:THR:CA	1:D:1483:TYR:CB	2.85	0.46
1:A:1557:GLU:OE1	1:A:1560:ARG:NH1	2.49	0.46
1:B:1387:THR:HG22	1:B:1388:HIS:N	2.31	0.46
1:B:1388:HIS:CD2	1:B:1403:LYS:O	2.68	0.46
1:D:1601:PRO:HA	1:D:1602:PRO:HD3	1.55	0.46
1:B:1509:VAL:HG13	1:B:1510:THR:N	2.30	0.46
1:B:1628:THR:HG21	1:B:1630:TYR:CZ	2.51	0.46
1:C:1590:LEU:HD12	1:C:1591:ASN:N	2.31	0.46
1:D:1517:GLN:HG2	1:D:1518:ILE:H	1.80	0.46
1:A:1507:THR:OG1	1:A:1508:GLY:N	2.48	0.46
1:A:1608:LYS:HD2	1:A:1644:TYR:OH	2.16	0.46
1:C:1506:LYS:O	1:C:1516:LEU:HD12	2.16	0.46
1:C:1476:GLN:OE1	1:C:1517:GLN:HA	2.15	0.46
1:C:1595:ASN:OD1	1:C:1595:ASN:N	2.49	0.46
1:D:1388:HIS:CD2	1:D:1403:LYS:O	2.68	0.46
1:B:1418:PHE:CE2	1:B:1455:VAL:HG21	2.51	0.46
1:B:1517:GLN:HG2	1:B:1518:ILE:H	1.81	0.46
1:D:1442:LYS:HE3	1:D:1444:VAL:CG2	2.46	0.46
1:C:1410:ILE:HG23	1:C:1410:ILE:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1628:THR:HG21	1:D:1630:TYR:CZ	2.51	0.45
1:A:1367:GLU:HG2	1:A:1375:LEU:HB3	1.98	0.45
1:A:1410:ILE:O	1:A:1410:ILE:HG23	2.16	0.45
1:A:1531:MET:HE1	1:A:1542:LYS:HB2	1.97	0.45
1:B:1429:ILE:HG22	1:B:1429:ILE:O	2.16	0.45
1:B:1509:VAL:HG13	1:B:1510:THR:H	1.81	0.45
1:B:1654:SER:O	1:B:1655:GLU:HB2	2.16	0.45
1:C:1476:GLN:OE1	1:C:1516:LEU:O	2.34	0.45
1:D:1483:TYR:O	1:D:1484:TYR:CG	2.64	0.45
1:D:1509:VAL:HG13	1:D:1510:THR:H	1.79	0.45
1:D:1513:GLN:HB2	1:D:1513:GLN:HE21	1.51	0.45
1:D:1618:HIS:O	1:D:1618:HIS:CG	2.69	0.45
1:B:1464:THR:O	1:B:1465:ASP:C	2.53	0.45
1:C:1484:TYR:N	1:C:1484:TYR:CD1	2.84	0.45
1:C:1476:GLN:NE2	1:C:1517:GLN:HA	2.31	0.45
1:A:1476:GLN:OE1	1:A:1517:GLN:HA	2.16	0.45
1:D:1461:LEU:HD23	1:D:1461:LEU:HA	1.81	0.45
1:B:1579:PRO:HG2	1:B:1582:VAL:HG13	1.98	0.45
1:D:1387:THR:HG22	1:D:1388:HIS:N	2.31	0.45
1:D:1481:VAL:CG2	1:D:1484:TYR:H	2.29	0.45
1:A:1360:PHE:CZ	1:A:1428:VAL:O	2.69	0.45
1:A:1456:CYS:HB3	1:A:1535:ASP:CB	2.43	0.45
1:B:1475:ILE:HG22	1:B:1476:GLN:N	2.32	0.45
1:D:1377:LYS:HB3	1:D:1377:LYS:HE2	1.73	0.45
1:D:1413:LEU:C	1:D:1413:LEU:HD23	2.36	0.45
1:A:1570:ASN:O	1:A:1571:ARG:C	2.53	0.44
1:A:1590:LEU:O	1:A:1591:ASN:OD1	2.35	0.44
1:B:1558:PHE:O	1:B:1559:GLN:C	2.53	0.44
1:A:1454:GLU:CD	1:A:1457:LYS:HD3	2.37	0.44
1:C:1493:SER:HG	1:C:1530:VAL:HB	1.82	0.44
1:C:1585:GLN:HG2	1:C:1588:LYS:HD2	1.99	0.44
1:D:1407:LYS:CG	1:D:1408:ASP:H	2.26	0.44
1:D:1585:GLN:HB2	1:D:1664:PHE:CZ	2.52	0.44
1:A:1476:GLN:NE2	1:A:1517:GLN:HA	2.32	0.44
1:C:1396:ARG:HD3	1:C:1397:GLU:N	2.32	0.44
1:C:1454:GLU:CD	1:C:1457:LYS:HD3	2.38	0.44
1:D:1456:CYS:HA	1:D:1459:ILE:CD1	2.48	0.44
1:B:1413:LEU:HD23	1:B:1413:LEU:C	2.37	0.44
1:B:1475:ILE:HG13	1:B:1521:PRO:HG3	1.99	0.44
1:B:1596:VAL:HG11	1:B:1648:VAL:CG1	2.48	0.44
1:D:1475:ILE:HG22	1:D:1476:GLN:N	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1507:THR:OG1	1:D:1508:GLY:N	2.48	0.44
1:A:1654:SER:OG	1:A:1655:GLU:N	2.48	0.44
1:D:1558:PHE:O	1:D:1559:GLN:C	2.55	0.44
1:A:1631:PHE:CZ	1:A:1633:ILE:HD11	2.52	0.44
1:D:1459:ILE:O	1:D:1462:SER:OG	2.35	0.44
1:A:1476:GLN:OE1	1:A:1516:LEU:O	2.36	0.44
1:B:1441:LEU:C	1:B:1441:LEU:HD23	2.38	0.44
1:D:1441:LEU:HD23	1:D:1441:LEU:C	2.38	0.44
1:D:1596:VAL:HG11	1:D:1648:VAL:CG1	2.48	0.44
1:A:1562:LYS:O	1:A:1563:GLN:C	2.56	0.44
1:A:1578:LEU:HD23	1:A:1593:THR:O	2.18	0.44
1:B:1473:GLU:O	1:B:1519:ASN:HA	2.18	0.44
1:D:1429:ILE:HG22	1:D:1429:ILE:O	2.18	0.44
1:D:1471:THR:OG1	1:D:1472:ALA:N	2.49	0.44
1:A:1396:ARG:HD3	1:A:1397:GLU:N	2.32	0.43
1:B:1569:LYS:HD2	1:B:1570:ASN:OD1	2.18	0.43
1:B:1464:THR:O	1:B:1465:ASP:O	2.36	0.43
1:D:1477:LEU:HD23	1:D:1477:LEU:HA	1.59	0.43
1:D:1654:SER:O	1:D:1655:GLU:HB2	2.18	0.43
1:B:1481:VAL:CG2	1:B:1484:TYR:H	2.31	0.43
1:B:1593:THR:HG22	1:B:1594:CYS:N	2.33	0.43
1:D:1464:THR:O	1:D:1465:ASP:O	2.35	0.43
1:B:1463:ALA:HA	1:B:1480:PHE:O	2.18	0.43
1:D:1578:LEU:HA	1:D:1579:PRO:HD3	1.81	0.43
1:A:1451:LEU:O	1:A:1455:VAL:HG23	2.19	0.43
1:A:1514:ILE:HG22	1:A:1515:TRP:N	2.34	0.43
1:B:1442:LYS:HE3	1:B:1444:VAL:CG2	2.48	0.43
1:B:1569:LYS:NZ	1:B:1570:ASN:ND2	2.66	0.43
1:C:1360:PHE:CZ	1:C:1428:VAL:O	2.69	0.43
1:D:1480:PHE:HA	1:D:1480:PHE:HD1	1.66	0.43
1:A:1355:PHE:CG	1:A:1356:THR:N	2.79	0.43
1:B:1461:LEU:HD23	1:B:1461:LEU:HA	1.81	0.43
1:C:1451:LEU:O	1:C:1455:VAL:HG23	2.19	0.43
1:C:1514:ILE:HG22	1:C:1515:TRP:N	2.34	0.43
1:D:1431:LYS:O	1:D:1432:ASP:HB3	2.19	0.43
1:A:1392:TYR:N	1:A:1427:GLU:O	2.48	0.43
1:A:1509:VAL:HG12	1:A:1509:VAL:O	2.18	0.43
1:C:1661:VAL:O	1:C:1661:VAL:HG12	2.16	0.43
1:D:1392:TYR:O	1:D:1426:TYR:HA	2.19	0.43
1:D:1463:ALA:HA	1:D:1480:PHE:O	2.19	0.43
1:D:1569:LYS:HZ2	1:D:1570:ASN:HD21	1.67	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1394:ASP:C	1:B:1396:ARG:N	2.69	0.42
1:B:1507:THR:OG1	1:B:1508:GLY:N	2.51	0.42
1:D:1385:LYS:O	1:D:1387:THR:N	2.51	0.42
1:D:1392:TYR:HE1	1:D:1429:ILE:HB	1.84	0.42
1:D:1475:ILE:HG13	1:D:1521:PRO:HG3	2.00	0.42
1:C:1421:LYS:C	1:C:1423:ALA:H	2.23	0.42
1:D:1450:GLU:O	1:D:1454:GLU:HB2	2.20	0.42
1:D:1354:PRO:CB	1:D:1355:PHE:HA	2.41	0.42
1:A:1567:ALA:O	1:A:1569:LYS:N	2.47	0.42
1:A:1571:ARG:HA	1:A:1652:TYR:HB2	2.01	0.42
1:B:1513:GLN:HB2	1:B:1513:GLN:HE21	1.52	0.42
1:C:1665:ILE:HG22	1:C:1665:ILE:O	2.19	0.42
1:D:1416:THR:C	1:D:1418:PHE:N	2.73	0.42
1:B:1483:TYR:C	1:B:1484:TYR:HD1	2.19	0.42
1:B:1567:ALA:O	1:B:1571:ARG:HG2	2.19	0.42
1:C:1434:ARG:HG2	1:C:1434:ARG:H	1.69	0.42
1:C:1590:LEU:O	1:C:1591:ASN:OD1	2.37	0.42
1:D:1596:VAL:CG1	1:D:1648:VAL:HG11	2.49	0.42
1:B:1416:THR:C	1:B:1418:PHE:N	2.72	0.42
1:C:1578:LEU:HD23	1:C:1593:THR:O	2.20	0.42
1:C:1575:LEU:HA	1:C:1575:LEU:HD23	1.70	0.42
1:A:1471:THR:HG22	1:A:1476:GLN:HG2	2.02	0.42
1:C:1608:LYS:HD2	1:C:1644:TYR:OH	2.20	0.42
1:B:1503:ASP:N	1:B:1503:ASP:OD1	2.53	0.42
1:D:1475:ILE:O	1:D:1518:ILE:HB	2.20	0.42
1:B:1480:PHE:HA	1:B:1480:PHE:HD1	1.66	0.41
1:B:1485:VAL:CG1	1:B:1486:GLU:N	2.83	0.41
1:C:1571:ARG:HA	1:C:1652:TYR:HB2	2.02	0.41
1:C:1647:VAL:HG13	1:C:1656:THR:OG1	2.20	0.41
1:D:1451:LEU:O	1:D:1454:GLU:HB3	2.20	0.41
1:B:1382:ASN:HD21	1:B:1434:ARG:NH1	2.18	0.41
1:C:1583:THR:HA	1:C:1662:SER:O	2.20	0.41
1:D:1394:ASP:C	1:D:1396:ARG:N	2.68	0.41
1:D:1656:THR:CG2	1:D:1657:SER:H	2.31	0.41
1:A:1400:VAL:HB	1:A:1401:ASP:H	1.66	0.41
1:A:1492:TRP:HB3	1:A:1499:ILE:HD12	2.02	0.41
1:B:1354:PRO:CB	1:B:1355:PHE:HA	2.40	0.41
1:B:1483:TYR:O	1:B:1484:TYR:HB3	2.19	0.41
1:C:1608:LYS:O	1:C:1609:ASN:HB2	2.20	0.41
1:D:1375:LEU:CD1	1:D:1412:THR:HB	2.43	0.41
1:D:1456:CYS:HA	1:D:1459:ILE:CG1	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1583:THR:HA	1:A:1662:SER:O	2.20	0.41
1:B:1392:TYR:O	1:B:1426:TYR:HA	2.19	0.41
1:A:1468:ILE:HG23	1:A:1477:LEU:CD2	2.51	0.41
1:B:1456:CYS:HA	1:B:1459:ILE:CG1	2.51	0.41
1:D:1464:THR:HG1	1:D:1480:PHE:HB2	1.84	0.41
1:D:1483:TYR:O	1:D:1484:TYR:HB3	2.20	0.41
1:D:1480:PHE:CE1	1:D:1513:GLN:HB2	2.46	0.41
1:A:1424:GLY:O	1:A:1443:LEU:HB2	2.21	0.41
1:B:1408:ASP:HA	1:B:1409:GLY:HA2	1.84	0.41
1:B:1471:THR:OG1	1:B:1472:ALA:N	2.53	0.41
1:C:1460:ALA:C	1:C:1462:SER:H	2.24	0.41
1:C:1613:LEU:O	1:C:1613:LEU:HG	2.20	0.41
1:A:1421:LYS:C	1:A:1423:ALA:H	2.23	0.41
1:B:1548:GLY:O	1:B:1549:GLN:C	2.58	0.41
1:C:1471:THR:HG22	1:C:1476:GLN:HG2	2.03	0.41
1:D:1579:PRO:HG2	1:D:1582:VAL:HG13	2.01	0.41
1:B:1574:VAL:HG23	1:B:1655:GLU:HG2	2.03	0.41
1:D:1408:ASP:HA	1:D:1409:GLY:HA2	1.85	0.41
1:D:1590:LEU:HA	1:D:1590:LEU:HD12	1.78	0.41
1:D:1644:TYR:N	1:D:1644:TYR:HD1	2.19	0.41
1:A:1591:ASN:HB3	1:B:1593:THR:HB	2.02	0.41
1:B:1596:VAL:CG1	1:B:1648:VAL:HG11	2.50	0.41
1:D:1656:THR:CG2	1:D:1657:SER:N	2.83	0.41
1:A:1585:GLN:HG2	1:A:1588:LYS:HD2	2.02	0.41
1:A:1661:VAL:O	1:A:1661:VAL:HG12	2.19	0.41
1:B:1451:LEU:O	1:B:1454:GLU:HB3	2.21	0.41
1:D:1569:LYS:NZ	1:D:1570:ASN:HD21	2.19	0.41
1:D:1637:SER:O	1:D:1640:ASP:N	2.40	0.41
1:B:1450:GLU:O	1:B:1454:GLU:HB2	2.22	0.40
1:C:1358:PRO:HB3	1:C:1383:ILE:HD13	2.03	0.40
1:C:1424:GLY:O	1:C:1443:LEU:HB2	2.20	0.40
1:A:1358:PRO:HB3	1:A:1383:ILE:HD13	2.03	0.40
1:A:1614:ALA:O	1:A:1616:ASP:OD1	2.39	0.40
1:B:1392:TYR:HE1	1:B:1429:ILE:HB	1.85	0.40
1:B:1431:LYS:O	1:B:1432:ASP:HB3	2.21	0.40
1:B:1481:VAL:HG22	1:B:1483:TYR:HA	2.04	0.40
1:D:1548:GLY:O	1:D:1549:GLN:C	2.60	0.40
1:D:1551:TYR:C	1:D:1553:GLU:N	2.73	0.40
1:A:1366:TRP:CE2	1:A:1451:LEU:HD22	2.57	0.40
1:A:1647:VAL:HG13	1:A:1656:THR:OG1	2.21	0.40
1:B:1513:GLN:HG2	1:B:1515:TRP:HD1	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1373:ASN:HB3	1:C:1414:LEU:HD11	2.03	0.40
1:C:1474:GLY:HA2	1:C:1558:PHE:CE1	2.56	0.40
1:C:1648:VAL:HG23	1:C:1649:LYS:N	2.35	0.40
1:D:1364:LEU:HB3	1:D:1441:LEU:HB2	2.03	0.40
1:D:1425:ILE:HG23	1:D:1442:LYS:CG	2.42	0.40
1:D:1503:ASP:N	1:D:1503:ASP:OD1	2.54	0.40
1:D:1555:TYR:CZ	1:D:1559:GLN:NE2	2.88	0.40
1:A:1575:LEU:HD23	1:A:1575:LEU:HA	1.72	0.40
1:B:1456:CYS:HA	1:B:1459:ILE:CD1	2.49	0.40
1:B:1644:TYR:N	1:B:1644:TYR:HD1	2.19	0.40
1:C:1578:LEU:HA	1:C:1579:PRO:HD3	1.68	0.40
1:C:1570:ASN:HD22	1:C:1597:TRP:HH2	1.69	0.40
1:A:1354:PRO:HA	1:A:1355:PHE:HA	1.55	0.40
1:A:1373:ASN:HB3	1:A:1414:LEU:HD11	2.04	0.40
1:A:1609:ASN:O	1:A:1611:LYS:HG3	2.22	0.40
1:B:1466:LEU:HA	1:B:1466:LEU:HD23	1.71	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	306/317 (96%)	250 (82%)	47 (15%)	9 (3%)	4	31
1	B	312/317 (98%)	244 (78%)	51 (16%)	17 (5%)	2	17
1	C	306/317 (96%)	248 (81%)	49 (16%)	9 (3%)	4	31
1	D	312/317 (98%)	242 (78%)	54 (17%)	16 (5%)	2	19
All	All	1236/1268 (98%)	984 (80%)	201 (16%)	51 (4%)	3	23

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1482	THR
1	B	1354	PRO
1	B	1400	VAL
1	B	1418	PHE
1	B	1484	TYR
1	B	1549	GLN
1	C	1482	THR
1	D	1354	PRO
1	D	1386	GLU
1	D	1400	VAL
1	D	1418	PHE
1	D	1484	TYR
1	D	1549	GLN
1	A	1400	VAL
1	A	1511	GLY
1	A	1569	LYS
1	A	1625	ALA
1	B	1370	GLY
1	B	1386	GLU
1	B	1465	ASP
1	B	1486	GLU
1	B	1518	ILE
1	B	1655	GLU
1	C	1400	VAL
1	C	1511	GLY
1	C	1569	LYS
1	D	1370	GLY
1	D	1465	ASP
1	D	1486	GLU
1	D	1518	ILE
1	D	1655	GLU
1	A	1356	THR
1	A	1461	LEU
1	A	1594	CYS
1	B	1395	GLU
1	B	1422	ASP
1	C	1356	THR
1	C	1461	LEU
1	C	1594	CYS
1	D	1395	GLU
1	D	1422	ASP
1	A	1623	PHE
1	B	1432	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1623	PHE
1	C	1625	ALA
1	D	1378	CYS
1	D	1432	ASP
1	B	1378	CYS
1	B	1601	PRO
1	B	1635	GLY
1	D	1635	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	242/274 (88%)	211 (87%)	31 (13%)	4	22
1	B	255/274 (93%)	203 (80%)	52 (20%)	1	6
1	C	242/274 (88%)	213 (88%)	29 (12%)	5	24
1	D	255/274 (93%)	205 (80%)	50 (20%)	1	7
All	All	994/1096 (91%)	832 (84%)	162 (16%)	2	13

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1376	LEU
1	A	1432	ASP
1	A	1434	ARG
1	A	1468	ILE
1	A	1470	SER
1	A	1471	THR
1	A	1485	VAL
1	A	1488	LEU
1	A	1490	VAL
1	A	1500	ARG
1	A	1507	THR
1	A	1512	GLU
1	A	1533	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1558	PHE
1	A	1561	LEU
1	A	1563	GLN
1	A	1580	ASP
1	A	1581	VAL
1	A	1586	GLU
1	A	1593	THR
1	A	1595	ASN
1	A	1607	LEU
1	A	1613	LEU
1	A	1615	SER
1	A	1616	ASP
1	A	1627	ARG
1	A	1634	ASN
1	A	1648	VAL
1	A	1654	SER
1	A	1663	VAL
1	A	1665	ILE
1	B	1365	SER
1	B	1377	LYS
1	B	1380	VAL
1	B	1385	LYS
1	B	1387	THR
1	B	1396	ARG
1	B	1405	ASP
1	B	1411	CYS
1	B	1425	ILE
1	B	1440	ARG
1	B	1444	VAL
1	B	1445	ASP
1	B	1451	LEU
1	B	1458	LYS
1	B	1464	THR
1	B	1467	LYS
1	B	1468	ILE
1	B	1471	THR
1	B	1478	TYR
1	B	1481	VAL
1	B	1493	SER
1	B	1503	ASP
1	B	1504	ARG
1	B	1507	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1513	GLN
1	B	1518	ILE
1	B	1524	ASN
1	B	1530	VAL
1	B	1535	ASP
1	B	1538	THR
1	B	1543	THR
1	B	1546	LEU
1	B	1549	GLN
1	B	1557	GLU
1	B	1560	ARG
1	B	1563	GLN
1	B	1570	ASN
1	B	1571	ARG
1	B	1581	VAL
1	B	1582	VAL
1	B	1597	TRP
1	B	1611	LYS
1	B	1615	SER
1	B	1620	ASN
1	B	1637	SER
1	B	1638	THR
1	B	1641	SER
1	B	1646	LEU
1	B	1647	VAL
1	B	1649	LYS
1	B	1654	SER
1	B	1657	SER
1	C	1376	LEU
1	C	1432	ASP
1	C	1434	ARG
1	C	1468	ILE
1	C	1470	SER
1	C	1471	THR
1	C	1485	VAL
1	C	1488	LEU
1	C	1490	VAL
1	C	1500	ARG
1	C	1507	THR
1	C	1512	GLU
1	C	1533	LEU
1	C	1558	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1561	LEU
1	C	1563	GLN
1	C	1580	ASP
1	C	1581	VAL
1	C	1586	GLU
1	C	1593	THR
1	C	1595	ASN
1	C	1607	LEU
1	C	1613	LEU
1	C	1627	ARG
1	C	1634	ASN
1	C	1648	VAL
1	C	1654	SER
1	C	1663	VAL
1	C	1665	ILE
1	D	1365	SER
1	D	1377	LYS
1	D	1380	VAL
1	D	1385	LYS
1	D	1387	THR
1	D	1396	ARG
1	D	1405	ASP
1	D	1411	CYS
1	D	1425	ILE
1	D	1440	ARG
1	D	1444	VAL
1	D	1445	ASP
1	D	1451	LEU
1	D	1458	LYS
1	D	1464	THR
1	D	1467	LYS
1	D	1468	ILE
1	D	1471	THR
1	D	1478	TYR
1	D	1481	VAL
1	D	1493	SER
1	D	1503	ASP
1	D	1504	ARG
1	D	1507	THR
1	D	1513	GLN
1	D	1518	ILE
1	D	1524	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1530	VAL
1	D	1535	ASP
1	D	1538	THR
1	D	1543	THR
1	D	1549	GLN
1	D	1557	GLU
1	D	1560	ARG
1	D	1563	GLN
1	D	1570	ASN
1	D	1571	ARG
1	D	1581	VAL
1	D	1582	VAL
1	D	1597	TRP
1	D	1611	LYS
1	D	1620	ASN
1	D	1637	SER
1	D	1641	SER
1	D	1644	TYR
1	D	1646	LEU
1	D	1647	VAL
1	D	1649	LYS
1	D	1654	SER
1	D	1657	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1491	ASN
1	A	1495	ASN
1	A	1513	GLN
1	A	1570	ASN
1	A	1609	ASN
1	B	1359	HIS
1	B	1388	HIS
1	B	1476	GLN
1	B	1495	ASN
1	B	1513	GLN
1	B	1524	ASN
1	B	1570	ASN
1	B	1609	ASN
1	C	1491	ASN
1	C	1495	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1513	GLN
1	C	1559	GLN
1	C	1570	ASN
1	C	1609	ASN
1	D	1359	HIS
1	D	1388	HIS
1	D	1476	GLN
1	D	1495	ASN
1	D	1513	GLN
1	D	1524	ASN
1	D	1570	ASN
1	D	1609	ASN

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 carbohydrates 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	310/317 (97%)	-0.20	10 (3%) 47 42	43, 158, 290, 454	0
1	B	314/317 (99%)	-0.44	0 100 100	49, 95, 169, 308	0
1	C	310/317 (97%)	-0.18	9 (2%) 51 45	48, 161, 288, 455	0
1	D	314/317 (99%)	-0.43	0 100 100	51, 95, 172, 325	0
All	All	1248/1268 (98%)	-0.31	19 (1%) 73 68	43, 111, 259, 455	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1436	LYS	4.1
1	C	1403	LYS	3.1
1	C	1481	VAL	3.1
1	A	1401	ASP	3.1
1	A	1444	VAL	2.9
1	C	1435	GLY	2.9
1	C	1400	VAL	2.8
1	A	1372	CYS	2.8
1	C	1463	ALA	2.6
1	A	1375	LEU	2.6
1	C	1402	GLU	2.5
1	A	1403	LYS	2.5
1	A	1481	VAL	2.5
1	A	1463	ALA	2.4
1	C	1372	CYS	2.3
1	A	1436	LYS	2.2
1	C	1376	LEU	2.2
1	A	1537	LYS	2.2
1	A	1376	LEU	2.1

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 carbohydrates 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.