Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:29 PM GMT

PDB ID	:	1KF9
Title	:	PHAGE DISPLAY DERIVED VARIANT OF HUMAN GROWTH HORMONE COMPLEXED WITH TWO COPIES OF THE EXTRACELLULAR DOMAIN OF ITS RECEPTOR
Authors	:	Schiffer, C.A.; Ultsch, M.; Walsh, S.; Somers, W.; De Vos, A.M.; Kossiakoff, A.A.
Deposited on	:	2001-11-19
Resolution	:	2.60 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

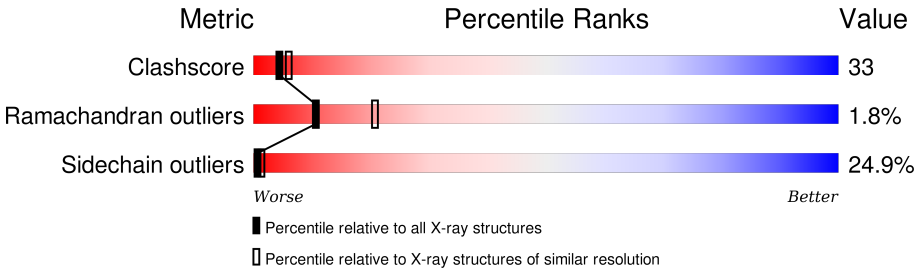
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	191	33% 38% 11% • 16%
1	D	191	37% 36% 9% • 17%
2	B	238	38% 30% 13% 19%
2	C	238	30% 32% 12% 26%
2	E	238	34% 35% 12% 19%
2	F	238	29% 36% 12% 23%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8678 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 PHAGE DISPLAY DERIVED VARIANT HUMAN GROWTH HORMONE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	0	0	0
			1284	825	211	242	6			
1	D	158	Total	C	N	O	S	0	0	0
			1264	811	208	239	6			

- Molecule 2 is a protein called EXTRACELLULAR DOMAIN HUMAN GROWTH HORMONE RECEPTOR (1-238).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	193	Total	C	N	O	S	0	0	0
			1577	1011	258	298	10			
2	C	175	Total	C	N	O	S	0	0	0
			1419	916	229	265	9			
2	E	193	Total	C	N	O	S	0	0	0
			1576	1011	258	298	9			
2	F	184	Total	C	N	O	S	0	0	0
			1484	952	239	284	9			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	13	Total	O	0	0
			13	13		
3	C	28	Total	O	0	0
			28	28		
3	D	3	Total	O	0	0
			3	3		
3	E	12	Total	O	0	0
			12	12		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	7	Total O 7 7	0	0

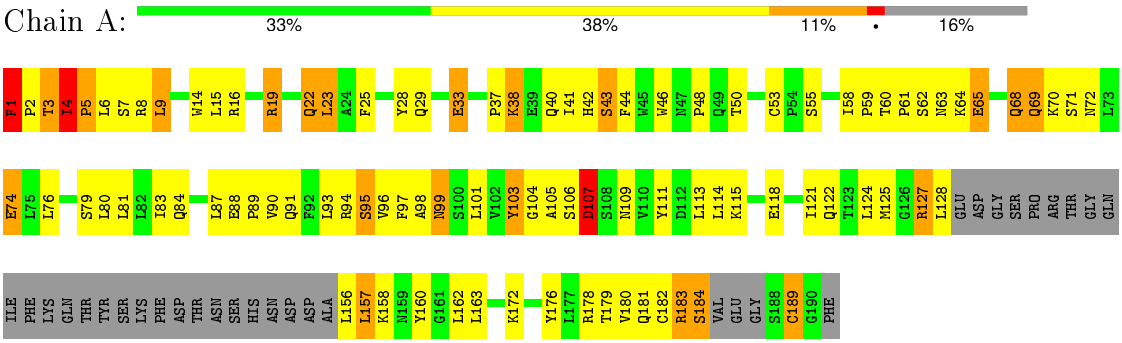
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

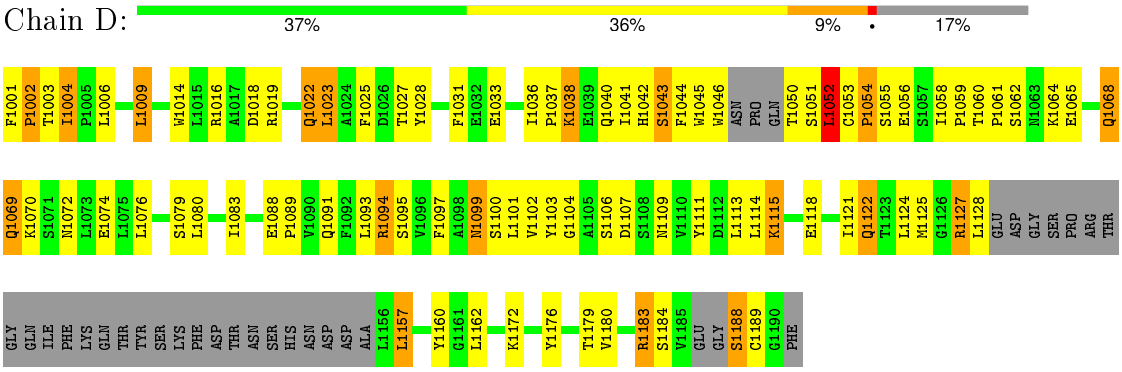
• Molecule 1: PHAGE DISPLAY DERIVED VARIANT HUMAN GROWTH HORMONE

Chain A:



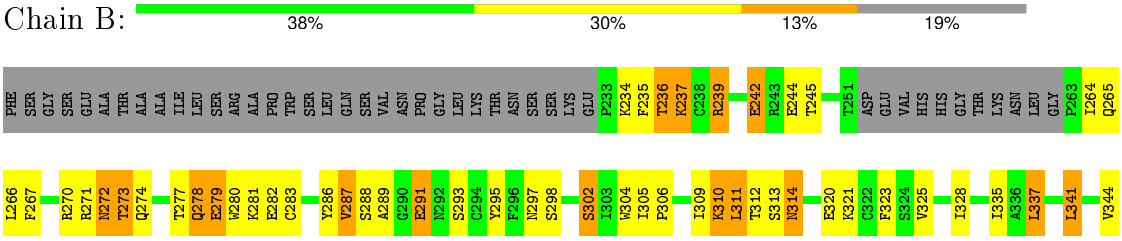
• Molecule 1: PHAGE DISPLAY DERIVED VARIANT HUMAN GROWTH HORMONE

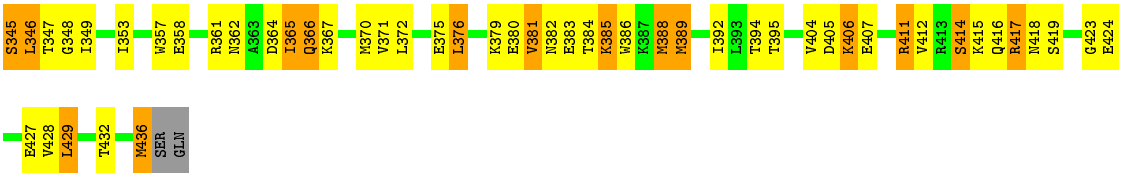
Chain D:



• Molecule 2: EXTRACELLULAR DOMAIN HUMAN GROWTH HORMONE RECEPTOR (1-238)

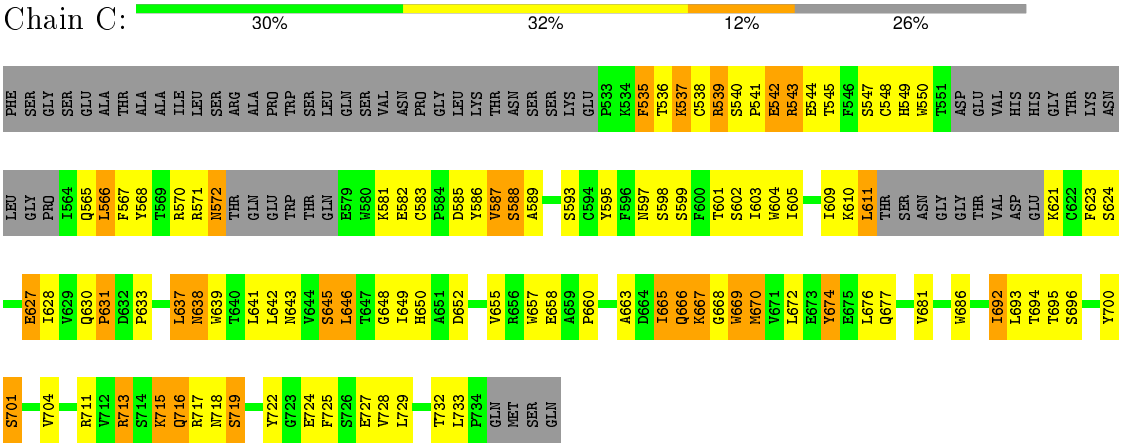
Chain B:





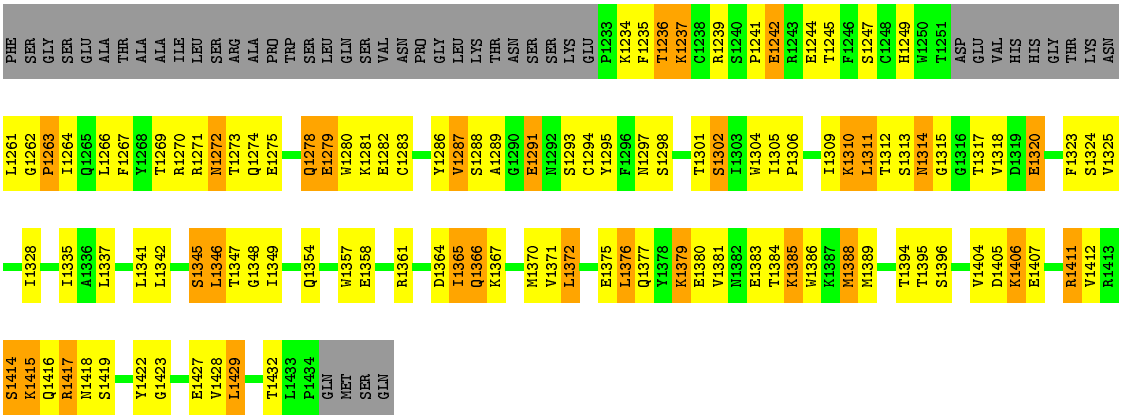
• Molecule 2: EXTRACELLULAR DOMAIN HUMAN GROWTH HORMONE RECEPTOR (1-238)

Chain C:



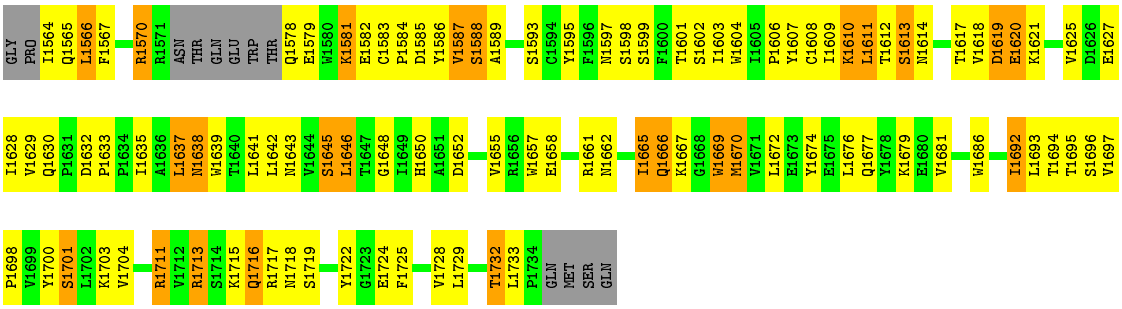
• Molecule 2: EXTRACELLULAR DOMAIN HUMAN GROWTH HORMONE RECEPTOR (1-238)

Chain E:



• Molecule 2: EXTRACELLULAR DOMAIN HUMAN GROWTH HORMONE RECEPTOR (1-238)

Chain F:


GLY PRO I1564 Q1565 L1566 F1567 R1570 R1571 ASN THR GLN GLU TRP THR Q1578 E1579 W1580 K1581 E1582 C1583 P1584 D1585 Y1586 V1587 S1588 A1589 S1593 C1594 Y1595 F1596 N1597 S1598 S1599 F1600 T1601 S1602 I1603 W1604 I1605 P1606 Y1607 C1608 I1609 K1610 L1611 T1612 S1613 N1614 T1617 V1618 D1619 E1620 K1621 V1625 D1626 E1627
I1628 V1629 Q1630 P1631 D1632 P1633 P1634 I1635 A1636 L1637 N1638 W1639 T1640 L1641 L1642 N1643 V1644 S1645 L1646 T1647 G1648 I1649 H1650 A1651 D1652 V1655 R1656 W1657 E1658 R1661 N1662 I1665 Q1666 K1667 G1668 W1669 M1670 V1671 L1672 E1673 Y1674 E1675 L1676 Q1677 Y1678 K1679 E1680 V1681 W1686 I1692 L1693 T1694 T1695 S1696 V1697
P1698 V1699 Y1700 S1701 L1702 K1703 V1704 R1711 V1712 R1713 S1714 K1715 Q1716 R1717 N1718 S1719 Y1722 G1723 E1724 F1725 V1728 L1729 T1732 L1733 P1734 GLN MET SER GLN

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.29Å 111.94Å 95.29Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	90.5 (20.00-2.60)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.234 , 0.326	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8678	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

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	0.67	0/1312	0.84	2/1781 (0.1%)
1	D	0.71	0/1289	0.84	2/1747 (0.1%)
2	B	0.70	0/1622	0.87	0/2208
2	C	0.67	0/1459	0.86	1/1987 (0.1%)
2	E	0.69	0/1621	0.86	1/2208 (0.0%)
2	F	0.65	0/1525	0.84	0/2078
All	All	0.68	0/8828	0.85	6/12009 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3	THR	N-CA-C	-9.03	86.61	111.00
1	D	1107	ASP	CB-CG-OD1	6.76	124.39	118.30
2	C	668	GLY	N-CA-C	-6.00	98.09	113.10
2	E	1324	SER	N-CA-C	-5.23	96.87	111.00
1	A	1	PHE	C-N-CD	5.20	139.32	128.40
1	D	1052	LEU	CA-CB-CG	5.13	127.10	115.30

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	1284	0	1257	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1264	0	1241	88	0
2	B	1577	0	1506	91	0
2	C	1419	0	1338	99	0
2	E	1576	0	1508	104	0
2	F	1484	0	1395	115	0
3	A	11	0	0	2	0
3	B	13	0	0	1	0
3	C	28	0	0	2	0
3	D	3	0	0	0	0
3	E	12	0	0	1	0
3	F	7	0	0	0	0
All	All	8678	0	8245	550	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 33.

All (550) 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:104:GLY:CA	2:C:666:GLN:HB3	1.65	1.26
2:E:1346:LEU:HB2	2:F:1701:SER:HB3	1.24	1.17
1:A:104:GLY:HA2	2:C:666:GLN:HB3	1.25	1.14
2:F:1581:LYS:HZ3	2:F:1581:LYS:HB2	1.08	1.09
1:A:104:GLY:HA3	2:C:666:GLN:HB3	1.41	1.02
2:B:346:LEU:HB2	2:C:701:SER:HB3	1.37	1.01
1:D:1104:GLY:HA2	2:F:1666:GLN:HB3	1.42	1.01
1:D:1052:LEU:HB2	1:D:1056:GLU:HG3	1.38	1.00
2:F:1581:LYS:NZ	2:F:1581:LYS:HB2	1.76	0.98
2:F:1669:TRP:CE3	2:F:1669:TRP:HA	1.96	0.97
2:C:669:TRP:HA	2:C:669:TRP:CE3	1.97	0.94
1:D:1104:GLY:CA	2:F:1666:GLN:HB3	1.99	0.93
1:A:1:PHE:HB3	1:A:2:PRO:HD3	1.55	0.89
1:D:1006:LEU:HD21	1:D:1127:ARG:HG2	1.55	0.89
1:A:104:GLY:HA2	2:C:666:GLN:CB	2.03	0.88
2:C:605:ILE:HG13	3:C:2057:HOH:O	1.75	0.87
2:F:1669:TRP:HA	2:F:1669:TRP:HE3	1.37	0.86
2:C:669:TRP:HA	2:C:669:TRP:HE3	1.36	0.84
1:A:182:CYS:HG	1:A:189:CYS:HG	0.83	0.83
2:C:571:ARG:O	2:C:572:ASN:HB3	1.78	0.81
1:A:1:PHE:HB3	1:A:2:PRO:CD	2.10	0.81
1:D:1052:LEU:HB2	1:D:1056:GLU:CG	2.10	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1068:GLN:HE22	2:E:1367:LYS:HD2	1.48	0.78
1:A:93:LEU:HD21	1:A:162:LEU:HB3	1.64	0.78
2:F:1533:PRO:HB3	2:F:1618:VAL:HG21	1.64	0.78
1:D:1004:ILE:HG21	1:D:1009:LEU:HD21	1.65	0.78
1:A:6:LEU:HD12	3:A:2402:HOH:O	1.84	0.77
2:C:589:ALA:HB2	2:C:595:TYR:HB2	1.67	0.76
1:A:58:ILE:HG23	1:A:59:PRO:HD2	1.66	0.76
1:A:184:SER:O	3:A:2622:HOH:O	2.03	0.76
1:D:1006:LEU:HD21	1:D:1127:ARG:CG	2.15	0.76
2:F:1650:HIS:HE1	2:F:1703:LYS:NZ	1.83	0.75
1:D:1093:LEU:HD21	1:D:1162:LEU:HB3	1.69	0.75
2:E:1380:GLU:HB3	2:E:1383:GLU:HG2	1.69	0.75
1:D:1058:ILE:HG23	1:D:1059:PRO:HD2	1.68	0.74
2:F:1716:GLN:HG3	2:F:1717:ARG:N	2.02	0.73
1:A:1:PHE:CB	1:A:2:PRO:HD3	2.18	0.73
2:F:1686:TRP:CH2	2:F:1711:ARG:HD3	2.22	0.73
1:D:1006:LEU:CD2	1:D:1127:ARG:HG2	2.19	0.73
2:B:270:ARG:HE	2:B:272:ASN:HB3	1.53	0.73
2:C:655:VAL:HG12	2:C:657:TRP:CZ3	2.23	0.73
1:A:91:GLN:O	1:A:94:ARG:HG2	1.89	0.72
2:B:235:PHE:CE2	2:B:309:ILE:HG13	2.24	0.72
2:F:1541:PRO:HA	2:F:1630:GLN:O	1.89	0.72
2:E:1376:LEU:HD23	2:E:1376:LEU:C	2.10	0.72
1:D:1004:ILE:O	1:D:1127:ARG:NH1	2.21	0.72
2:E:1347:THR:HG22	2:F:1650:HIS:HB2	1.72	0.72
1:A:107:ASP:OD1	2:F:1578:GLN:N	2.23	0.72
2:F:1542:GLU:O	2:F:1670:MET:HG3	1.90	0.71
1:A:6:LEU:HD21	1:A:127:ARG:HG2	1.72	0.71
2:E:1272:ASN:HD22	2:E:1272:ASN:H	1.39	0.71
2:F:1542:GLU:HA	2:F:1670:MET:SD	2.31	0.70
1:A:4:ILE:HD12	2:C:604:TRP:O	1.91	0.70
2:F:1543:ARG:CD	2:F:1716:GLN:HE22	2.05	0.70
2:E:1235:PHE:CE2	2:E:1309:ILE:HG13	2.26	0.70
2:C:716:GLN:HG3	2:C:717:ARG:N	2.07	0.69
2:F:1638:ASN:C	2:F:1638:ASN:HD22	1.94	0.69
2:F:1543:ARG:NE	2:F:1716:GLN:HE22	1.90	0.69
1:D:1068:GLN:NE2	2:E:1367:LYS:HD2	2.07	0.69
2:E:1345:SER:HB2	2:F:1700:TYR:HB3	1.73	0.68
2:F:1581:LYS:CB	2:F:1581:LYS:NZ	2.53	0.68
1:A:109:ASN:OD1	1:A:113:LEU:HD21	1.94	0.68
1:D:1097:PHE:O	1:D:1100:SER:HB3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:631:PRO:HB3	2:C:670:MET:HE3	1.74	0.68
2:F:1582:GLU:HG3	2:F:1583:CYS:N	2.09	0.68
1:D:1004:ILE:HD12	2:F:1604:TRP:O	1.94	0.68
1:D:1043:SER:OG	1:D:1157:LEU:HD11	1.94	0.67
2:C:582:GLU:HG3	2:C:583:CYS:N	2.09	0.67
2:F:1536:THR:HG22	2:F:1549:HIS:C	2.14	0.67
1:D:1001:PHE:HB2	1:D:1002:PRO:HD2	1.77	0.67
1:D:1091:GLN:O	1:D:1094:ARG:HB3	1.94	0.67
2:C:665:ILE:HG12	2:C:666:GLN:N	2.10	0.67
2:F:1589:ALA:HB2	2:F:1595:TYR:HB2	1.77	0.67
2:F:1665:ILE:HG12	2:F:1666:GLN:N	2.09	0.66
2:B:376:LEU:C	2:B:376:LEU:HD23	2.15	0.66
2:E:1261:LEU:C	2:E:1261:LEU:HD23	2.15	0.66
2:F:1543:ARG:NE	2:F:1716:GLN:NE2	2.44	0.66
2:B:291:GLU:HA	2:B:291:GLU:OE2	1.94	0.66
2:C:543:ARG:CD	2:C:716:GLN:HE22	2.08	0.66
2:E:1241:PRO:O	3:E:2038:HOH:O	2.13	0.66
2:C:536:THR:HG22	2:C:549:HIS:C	2.16	0.65
1:A:1:PHE:CG	1:A:2:PRO:HD3	2.31	0.65
1:D:1004:ILE:HG22	1:D:1127:ARG:NH1	2.11	0.65
1:A:16:ARG:NH1	1:A:113:LEU:HD22	2.12	0.65
2:F:1655:VAL:HG12	2:F:1657:TRP:CZ3	2.30	0.65
2:F:1657:TRP:O	2:F:1695:THR:HB	1.97	0.65
1:A:1:PHE:CD1	1:A:2:PRO:HD3	2.31	0.65
2:E:1262:GLY:H	2:E:1263:PRO:HD2	1.61	0.65
2:E:1272:ASN:H	2:E:1272:ASN:ND2	1.94	0.65
2:C:657:TRP:HZ2	2:C:692:ILE:HD11	1.61	0.65
2:C:638:ASN:C	2:C:638:ASN:HD22	2.00	0.64
2:C:541:PRO:HA	2:C:630:GLN:O	1.97	0.64
2:B:323:PHE:CE1	2:B:328:ILE:HD13	2.32	0.64
2:F:1587:VAL:HG22	2:F:1588:SER:N	2.13	0.64
2:B:380:GLU:HB3	2:B:383:GLU:HG2	1.79	0.64
2:C:686:TRP:CH2	2:C:711:ARG:HD3	2.33	0.64
1:A:43:SER:OG	1:A:157:LEU:HD11	1.98	0.63
1:D:1001:PHE:HB2	1:D:1002:PRO:CD	2.28	0.63
1:D:1003:THR:HG21	2:F:1606:PRO:HG3	1.80	0.63
2:F:1579:GLU:HG2	2:F:1581:LYS:HZ1	1.63	0.63
2:B:345:SER:HB2	2:C:700:TYR:HB3	1.79	0.63
2:E:1310:LYS:NZ	2:E:1320:GLU:OE2	2.27	0.63
2:F:1535:PHE:CD2	2:F:1619:ASP:HB3	2.34	0.62
2:C:621:LYS:HD2	3:C:2506:HOH:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ASN:N	1:A:99:ASN:HD22	1.97	0.62
1:A:103:TYR:CD2	1:A:103:TYR:N	2.58	0.62
2:E:1376:LEU:HD22	2:E:1389:MET:HG3	1.81	0.62
1:D:1099:ASN:HD22	1:D:1099:ASN:N	1.98	0.62
1:A:178:ARG:HH21	1:A:181:GLN:NE2	1.97	0.62
2:F:1638:ASN:C	2:F:1638:ASN:ND2	2.49	0.62
2:E:1323:PHE:CE1	2:E:1328:ILE:HD13	2.35	0.62
2:F:1542:GLU:O	2:F:1543:ARG:HB2	2.00	0.62
2:C:544:GLU:O	2:C:601:THR:HB	1.99	0.62
1:D:1104:GLY:HA2	2:F:1666:GLN:CB	2.24	0.62
2:B:273:THR:HG23	2:B:277:THR:OG1	2.00	0.62
1:D:1027:THR:HG23	1:D:1102:VAL:HG21	1.80	0.61
1:A:19:ARG:O	1:A:22:GLN:HG3	1.99	0.61
2:C:660:PRO:O	2:C:663:ALA:HB3	1.99	0.61
2:F:1657:TRP:HZ2	2:F:1692:ILE:HD11	1.65	0.61
1:A:172:LYS:HE2	2:B:304:TRP:CE3	2.35	0.61
2:E:1261:LEU:HD23	2:E:1262:GLY:N	2.15	0.61
2:C:711:ARG:HG3	2:C:725:PHE:CD1	2.35	0.61
2:C:638:ASN:C	2:C:638:ASN:ND2	2.54	0.61
1:A:6:LEU:CD2	1:A:127:ARG:HG2	2.30	0.61
2:E:1380:GLU:HG3	2:E:1406:LYS:NZ	2.15	0.61
2:F:1716:GLN:HG3	2:F:1717:ARG:H	1.65	0.61
2:C:543:ARG:HD2	2:C:716:GLN:HE22	1.65	0.61
2:F:1564:ILE:HA	2:F:1612:THR:O	2.00	0.61
1:A:79:SER:O	1:A:83:ILE:HG12	2.01	0.60
1:A:4:ILE:HG21	1:A:9:LEU:HD21	1.82	0.60
1:A:16:ARG:HH12	1:A:113:LEU:HD22	1.66	0.60
2:F:1713:ARG:HG3	2:F:1722:TYR:CD2	2.36	0.60
2:E:1337:LEU:HB3	2:E:1429:LEU:HG	1.84	0.60
1:A:4:ILE:HD11	2:C:624:SER:HB2	1.84	0.60
2:C:655:VAL:HG12	2:C:657:TRP:CE3	2.36	0.60
2:B:380:GLU:HG3	2:B:406:LYS:HD2	1.83	0.60
2:E:1245:THR:HG22	2:E:1298:SER:N	2.17	0.60
2:B:337:LEU:HD22	2:B:357:TRP:CB	2.32	0.60
1:A:104:GLY:HA2	2:C:666:GLN:NE2	2.17	0.59
1:A:94:ARG:HG3	1:A:95:SER:H	1.66	0.59
2:B:236:THR:O	2:B:237:LYS:HB3	2.01	0.59
2:C:633:PRO:HB3	2:C:724:GLU:O	2.02	0.59
2:E:1272:ASN:N	2:E:1272:ASN:HD22	1.99	0.59
2:B:271:ARG:HD2	2:B:306:PRO:HG2	1.84	0.59
2:C:637:LEU:HD22	2:C:657:TRP:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1064:LYS:HZ1	2:E:1364:ASP:CG	2.05	0.59
2:B:376:LEU:HD22	2:B:389:MET:HG3	1.85	0.59
1:D:1070:LYS:O	1:D:1183:ARG:NH2	2.36	0.59
1:A:104:GLY:HA2	2:C:666:GLN:HE21	1.68	0.58
2:C:543:ARG:NE	2:C:716:GLN:NE2	2.52	0.58
2:C:631:PRO:HB3	2:C:670:MET:CE	2.32	0.58
2:E:1291:GLU:HA	2:E:1291:GLU:OE2	2.02	0.58
1:D:1080:LEU:HB2	1:D:1121:ILE:HG21	1.84	0.58
2:B:337:LEU:HD22	2:B:357:TRP:HB3	1.85	0.58
1:D:1113:LEU:N	1:D:1113:LEU:HD23	2.17	0.58
1:A:2:PRO:HG2	2:C:627:GLU:OE1	2.04	0.58
1:D:1027:THR:CG2	1:D:1102:VAL:HG21	2.33	0.58
2:C:657:TRP:O	2:C:695:THR:HB	2.03	0.58
2:C:587:VAL:HG22	2:C:588:SER:N	2.19	0.58
1:A:58:ILE:CG2	1:A:59:PRO:HD2	2.33	0.58
1:A:93:LEU:HD21	1:A:162:LEU:CB	2.34	0.58
1:A:69:GLN:OE1	1:A:70:LYS:HG2	2.03	0.58
2:F:1543:ARG:HB2	2:F:1670:MET:HG3	1.86	0.57
2:F:1650:HIS:HE1	2:F:1703:LYS:HZ1	1.50	0.57
2:F:1565:GLN:O	2:F:1611:LEU:HD23	2.04	0.57
2:F:1633:PRO:HB3	2:F:1724:GLU:O	2.05	0.57
1:D:1072:ASN:HA	1:D:1180:VAL:HG22	1.86	0.57
2:E:1264:ILE:HG22	2:E:1311:LEU:HD22	1.86	0.57
2:F:1655:VAL:HG12	2:F:1657:TRP:CE3	2.39	0.57
2:F:1535:PHE:HZ	2:F:1566:LEU:HD12	1.70	0.57
2:F:1618:VAL:HG13	2:F:1619:ASP:N	2.20	0.57
2:B:375:GLU:OE2	2:B:388:MET:HG2	2.05	0.57
2:E:1282:GLU:OE1	2:E:1286:TYR:OH	2.15	0.56
2:F:1536:THR:CG2	2:F:1549:HIS:HB2	2.36	0.56
2:C:540:SER:OG	2:C:545:THR:O	2.19	0.56
2:E:1380:GLU:HG3	2:E:1406:LYS:HD2	1.87	0.56
2:C:655:VAL:HG12	2:C:657:TRP:HZ3	1.68	0.56
2:C:543:ARG:NE	2:C:716:GLN:HE22	2.03	0.56
1:D:1019:ARG:NE	1:D:1022:GLN:OE1	2.31	0.56
1:A:2:PRO:HB2	2:C:627:GLU:OE1	2.05	0.56
2:C:642:LEU:HB2	2:C:652:ASP:O	2.06	0.56
2:F:1539:ARG:HA	2:F:1628:ILE:O	2.05	0.56
1:A:6:LEU:HD21	1:A:127:ARG:CG	2.35	0.56
2:E:1236:THR:HG22	2:E:1249:HIS:C	2.26	0.56
2:F:1692:ILE:HD12	2:F:1694:THR:O	2.06	0.56
2:F:1535:PHE:CZ	2:F:1566:LEU:HD12	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1022:GLN:HG3	1:D:1023:LEU:N	2.21	0.56
2:B:289:ALA:HB2	2:B:295:TYR:HB2	1.88	0.56
2:E:1289:ALA:HB2	2:E:1295:TYR:HB2	1.88	0.56
1:D:1004:ILE:CG2	1:D:1009:LEU:HD21	2.34	0.56
2:B:380:GLU:CG	2:B:406:LYS:HD2	2.36	0.56
1:A:50:THR:HG21	1:A:158:LYS:HA	1.88	0.55
1:A:76:LEU:CD1	1:A:128:LEU:HD12	2.36	0.55
2:B:287:VAL:HG22	2:B:288:SER:N	2.21	0.55
2:F:1686:TRP:CD2	2:F:1711:ARG:NH2	2.75	0.55
2:F:1565:GLN:HB3	2:F:1586:TYR:OH	2.06	0.55
1:D:1109:ASN:OD1	1:D:1113:LEU:HD21	2.06	0.55
2:E:1269:THR:HA	2:E:1278:GLN:HG2	1.87	0.55
2:F:1544:GLU:O	2:F:1601:THR:HB	2.07	0.55
2:B:344:VAL:HG11	2:B:436:MET:CE	2.36	0.55
2:F:1657:TRP:CZ2	2:F:1692:ILE:HD11	2.42	0.55
2:F:1535:PHE:CZ	2:F:1609:ILE:HD12	2.41	0.55
2:F:1704:VAL:HG23	2:F:1733:LEU:HB3	1.89	0.55
1:D:1099:ASN:ND2	1:D:1099:ASN:N	2.53	0.55
1:D:1188:SER:O	1:D:1189:CYS:SG	2.65	0.55
1:D:1019:ARG:O	1:D:1022:GLN:HG3	2.08	0.54
1:A:42:HIS:HD2	1:A:44:PHE:CZ	2.25	0.54
2:B:267:PHE:HA	2:B:281:LYS:O	2.07	0.54
1:A:94:ARG:HG3	1:A:95:SER:N	2.22	0.54
2:B:380:GLU:HG3	2:B:406:LYS:NZ	2.22	0.54
2:B:266:LEU:C	2:B:266:LEU:HD23	2.27	0.54
1:D:1080:LEU:HD11	1:D:1118:GLU:HG3	1.88	0.54
1:D:1022:GLN:HG3	1:D:1023:LEU:H	1.71	0.54
1:A:111:TYR:CD1	1:A:111:TYR:C	2.81	0.54
1:D:1069:GLN:OE1	1:D:1070:LYS:HG2	2.08	0.54
2:E:1347:THR:OG1	2:E:1349:ILE:HG13	2.08	0.54
1:A:80:LEU:HB2	1:A:121:ILE:HG21	1.89	0.54
1:A:4:ILE:CG2	1:A:9:LEU:HD21	2.37	0.54
2:C:716:GLN:HG3	2:C:717:ARG:H	1.73	0.53
2:C:704:VAL:HG23	2:C:733:LEU:HB3	1.90	0.53
2:C:715:LYS:HZ1	2:C:719:SER:H	1.54	0.53
2:B:371:VAL:O	2:B:417:ARG:HB2	2.08	0.53
2:B:245:THR:HG22	2:B:298:SER:N	2.23	0.53
2:F:1533:PRO:HA	2:F:1618:VAL:HG11	1.90	0.53
2:F:1543:ARG:HD2	2:F:1716:GLN:HE22	1.73	0.53
2:C:542:GLU:O	2:C:543:ARG:HB2	2.07	0.53
1:A:72:ASN:HA	1:A:180:VAL:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:347:THR:HB	2:C:645:SER:CB	2.39	0.53
1:A:97:PHE:HB3	1:A:105:ALA:O	2.08	0.53
2:C:637:LEU:O	2:C:638:ASN:HB3	2.08	0.53
2:C:692:ILE:HD12	2:C:694:THR:O	2.08	0.53
2:C:677:GLN:HG3	2:C:725:PHE:HE1	1.74	0.53
1:A:68:GLN:HE22	2:B:367:LYS:HD2	1.74	0.53
2:C:539:ARG:HA	2:C:628:ILE:O	2.08	0.53
1:A:1:PHE:CB	1:A:2:PRO:CD	2.81	0.53
1:D:1004:ILE:HG22	1:D:1127:ARG:HH11	1.73	0.53
1:D:1093:LEU:HD21	1:D:1162:LEU:CB	2.38	0.53
2:E:1279:GLU:O	2:E:1280:TRP:C	2.46	0.53
1:A:70:LYS:O	1:A:183:ARG:NH2	2.42	0.53
2:E:1287:VAL:HG22	2:E:1288:SER:N	2.22	0.53
2:B:272:ASN:HD22	2:B:273:THR:H	1.57	0.52
2:C:657:TRP:CZ2	2:C:692:ILE:HD11	2.42	0.52
1:A:95:SER:O	1:A:98:ALA:N	2.41	0.52
2:B:388:MET:H	2:B:388:MET:HE2	1.73	0.52
2:F:1538:CYS:HA	2:F:1547:SER:O	2.10	0.52
2:C:713:ARG:HG3	2:C:722:TYR:CD2	2.45	0.52
1:A:113:LEU:HD23	1:A:113:LEU:N	2.24	0.52
1:A:9:LEU:N	1:A:9:LEU:HD23	2.24	0.52
2:E:1264:ILE:CG2	2:E:1311:LEU:HD22	2.40	0.52
2:C:637:LEU:N	2:C:637:LEU:HD23	2.25	0.52
2:B:280:TRP:CH2	2:B:310:LYS:HD2	2.45	0.52
1:D:1027:THR:HG22	1:D:1100:SER:OG	2.10	0.52
2:E:1310:LYS:HG2	2:E:1317:THR:HG23	1.92	0.52
1:A:103:TYR:HD2	1:A:103:TYR:H	1.51	0.52
2:E:1337:LEU:HD22	2:E:1357:TRP:CB	2.39	0.52
2:F:1535:PHE:HA	2:F:1550:TRP:HB3	1.91	0.52
2:C:589:ALA:CB	2:C:595:TYR:HB2	2.38	0.51
2:E:1371:VAL:O	2:E:1417:ARG:HB2	2.10	0.51
1:D:1058:ILE:CG2	1:D:1059:PRO:HD2	2.38	0.51
2:E:1347:THR:HB	2:F:1645:SER:CB	2.41	0.51
2:B:347:THR:OG1	2:B:349:ILE:HG13	2.10	0.51
2:E:1262:GLY:H	2:E:1263:PRO:CD	2.23	0.51
2:F:1677:GLN:HG3	2:F:1725:PHE:HE1	1.76	0.51
2:B:313:SER:OG	2:B:314:ASN:N	2.43	0.51
2:B:270:ARG:NE	2:B:272:ASN:HB3	2.25	0.51
2:C:637:LEU:HD22	2:C:657:TRP:CB	2.40	0.51
2:B:242:GLU:N	2:B:242:GLU:OE2	2.41	0.51
1:D:1104:GLY:HA3	2:F:1666:GLN:HB3	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:LEU:HG	1:A:84:GLN:OE1	2.10	0.51
1:D:1025:PHE:O	1:D:1028:TYR:HB3	2.10	0.51
2:F:1542:GLU:O	2:F:1543:ARG:CB	2.59	0.51
2:E:1262:GLY:O	2:E:1263:PRO:C	2.49	0.51
2:C:536:THR:CG2	2:C:549:HIS:HB2	2.41	0.51
2:E:1282:GLU:HG3	2:E:1283:CYS:N	2.25	0.51
2:F:1676:LEU:C	2:F:1676:LEU:HD23	2.31	0.51
1:D:1104:GLY:HA2	2:F:1666:GLN:HE21	1.75	0.51
2:B:347:THR:HG22	2:C:650:HIS:HB2	1.93	0.51
2:E:1380:GLU:CG	2:E:1406:LYS:HD2	2.41	0.50
2:B:279:GLU:O	2:B:280:TRP:C	2.48	0.50
2:C:727:GLU:HG2	1:D:1088:GLU:OE1	2.11	0.50
1:A:104:GLY:CA	2:C:666:GLN:CB	2.60	0.50
2:E:1235:PHE:CZ	2:E:1309:ILE:HD12	2.46	0.50
2:B:272:ASN:H	2:B:272:ASN:HD22	1.59	0.50
1:D:1016:ARG:HH12	1:D:1113:LEU:HD22	1.76	0.50
1:A:68:GLN:NE2	2:B:367:LYS:HD2	2.26	0.50
1:A:25:PHE:O	1:A:28:TYR:HB3	2.11	0.50
2:F:1713:ARG:HD2	2:F:1725:PHE:CE1	2.46	0.49
2:F:1637:LEU:HD23	2:F:1637:LEU:N	2.27	0.49
2:F:1686:TRP:CZ2	2:F:1711:ARG:HD3	2.47	0.49
2:C:638:ASN:HD22	2:C:639:TRP:N	2.11	0.49
1:A:76:LEU:HD11	1:A:128:LEU:HD12	1.94	0.49
2:E:1365:ILE:HG12	2:E:1366:GLN:N	2.26	0.49
2:E:1267:PHE:HA	2:E:1281:LYS:O	2.13	0.49
2:B:337:LEU:HB3	2:B:429:LEU:HG	1.95	0.49
1:D:1124:LEU:O	1:D:1128:LEU:HB2	2.13	0.49
2:C:571:ARG:O	2:C:572:ASN:CB	2.56	0.49
2:F:1655:VAL:HG12	2:F:1657:TRP:HZ3	1.78	0.49
2:E:1415:LYS:HB3	2:E:1422:TYR:CD2	2.48	0.49
2:B:273:THR:CG2	2:B:277:THR:OG1	2.61	0.48
2:E:1271:ARG:HA	2:E:1275:GLU:O	2.12	0.48
1:D:1093:LEU:HB2	1:D:1097:PHE:CE1	2.48	0.48
2:F:1638:ASN:HD22	2:F:1639:TRP:N	2.11	0.48
1:D:1080:LEU:CD1	1:D:1118:GLU:HG3	2.43	0.48
2:B:282:GLU:HG3	2:B:283:CYS:N	2.28	0.48
2:E:1272:ASN:N	2:E:1272:ASN:ND2	2.57	0.48
2:F:1567:PHE:CE2	2:F:1582:GLU:HB2	2.48	0.48
2:F:1618:VAL:CG1	2:F:1619:ASP:N	2.76	0.48
2:E:1380:GLU:HG3	2:E:1406:LYS:HZ2	1.77	0.48
2:E:1386:TRP:CZ3	2:E:1411:ARG:HG3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:417:ARG:O	2:B:418:ASN:HB2	2.14	0.48
2:B:278:GLN:HG3	2:B:278:GLN:O	2.13	0.48
1:D:1016:ARG:NH1	1:D:1113:LEU:HD22	2.29	0.47
1:A:109:ASN:O	1:A:113:LEU:HG	2.15	0.47
2:C:535:PHE:CZ	2:C:609:ILE:HD12	2.49	0.47
2:E:1337:LEU:HD22	2:E:1357:TRP:HB3	1.95	0.47
1:D:1080:LEU:HB2	1:D:1121:ILE:CG2	2.44	0.47
1:A:37:PRO:HG2	1:A:40:GLN:CB	2.45	0.47
2:E:1407:GLU:HG3	2:E:1432:THR:CG2	2.44	0.47
2:C:535:PHE:CE2	2:C:611:LEU:HB2	2.48	0.47
2:E:1236:THR:HG23	2:E:1237:LYS:N	2.30	0.47
1:D:1111:TYR:HA	1:D:1114:LEU:HD12	1.96	0.47
2:B:348:GLY:O	2:B:404:VAL:HG11	2.14	0.47
2:C:535:PHE:HA	2:C:550:TRP:HB3	1.95	0.47
2:F:1650:HIS:CE1	2:F:1703:LYS:NZ	2.73	0.47
2:B:272:ASN:H	2:B:272:ASN:ND2	2.13	0.47
2:E:1335:ILE:HG13	2:E:1358:GLU:HB3	1.96	0.47
2:C:676:LEU:C	2:C:676:LEU:HD23	2.35	0.47
1:D:1002:PRO:HD2	1:D:1127:ARG:HD2	1.97	0.47
2:B:325:VAL:O	2:B:328:ILE:HG12	2.14	0.47
1:A:22:GLN:HG3	1:A:23:LEU:H	1.79	0.47
2:B:265:GLN:HB3	2:B:286:TYR:OH	2.14	0.47
1:D:1037:PRO:HG2	1:D:1040:GLN:CB	2.45	0.47
2:E:1242:GLU:O	2:E:1242:GLU:HG2	2.14	0.47
1:D:1003:THR:CG2	2:F:1606:PRO:HG3	2.45	0.47
1:A:68:GLN:HA	1:A:183:ARG:HH12	1.79	0.47
1:A:88:GLU:N	1:A:89:PRO:HD2	2.30	0.47
1:A:1:PHE:CD1	1:A:2:PRO:CD	2.97	0.47
2:F:1609:ILE:O	2:F:1620:GLU:HA	2.15	0.47
1:A:64:LYS:HZ1	2:B:364:ASP:CG	2.18	0.47
1:D:1064:LYS:NZ	2:E:1364:ASP:OD2	2.46	0.47
1:D:1053:CYS:HB3	1:D:1054:PRO:HD2	1.96	0.47
1:D:1009:LEU:N	1:D:1009:LEU:HD23	2.30	0.46
1:A:4:ILE:O	1:A:127:ARG:NH1	2.47	0.46
2:C:582:GLU:HG3	2:C:583:CYS:H	1.79	0.46
2:C:535:PHE:CZ	2:C:566:LEU:HD12	2.49	0.46
1:D:1099:ASN:H	1:D:1099:ASN:HD22	1.62	0.46
2:E:1244:GLU:O	2:E:1298:SER:HA	2.14	0.46
1:A:124:LEU:O	1:A:128:LEU:HB2	2.15	0.46
2:C:565:GLN:HB3	2:C:586:TYR:OH	2.15	0.46
2:F:1637:LEU:O	2:F:1638:ASN:HB3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1386:TRP:CH2	2:E:1411:ARG:CG	2.97	0.46
2:B:364:ASP:OD1	2:B:366:GLN:NE2	2.49	0.46
1:A:60:THR:HA	1:A:61:PRO:HD3	1.85	0.46
2:E:1385:LYS:CD	2:E:1385:LYS:H	2.28	0.46
2:F:1732:THR:O	2:F:1732:THR:OG1	2.33	0.46
1:A:71:SER:H	1:A:74:GLU:HG3	1.81	0.46
2:C:548:CYS:O	2:C:593:SER:HA	2.15	0.46
1:A:22:GLN:HA	2:B:418:ASN:OD1	2.16	0.46
1:A:179:THR:O	1:A:183:ARG:HG3	2.15	0.46
1:A:90:VAL:HG21	1:A:114:LEU:HD11	1.98	0.46
1:A:44:PHE:HE2	1:A:160:TYR:CE2	2.34	0.46
2:E:1386:TRP:CH2	2:E:1411:ARG:HG2	2.51	0.46
2:F:1632:ASP:OD1	2:F:1662:ASN:ND2	2.49	0.46
2:F:1650:HIS:HE1	2:F:1703:LYS:HZ3	1.63	0.46
2:B:311:LEU:HD23	2:B:311:LEU:HA	1.86	0.46
1:A:58:ILE:HD13	1:A:81:LEU:HB3	1.98	0.46
2:B:287:VAL:CG2	2:B:288:SER:N	2.79	0.46
1:A:80:LEU:HD11	1:A:118:GLU:HG3	1.97	0.46
1:D:1115:LYS:HA	1:D:1115:LYS:HD2	1.46	0.46
1:A:22:GLN:HG3	1:A:23:LEU:N	2.31	0.46
2:B:337:LEU:HD22	2:B:357:TRP:HB2	1.98	0.46
2:C:538:CYS:HA	2:C:547:SER:O	2.16	0.46
2:B:386:TRP:CH2	2:B:411:ARG:CG	2.98	0.46
1:A:156:LEU:HD23	1:A:156:LEU:C	2.36	0.46
2:E:1407:GLU:HG3	2:E:1432:THR:HG22	1.97	0.45
1:D:1045:TRP:O	1:D:1051:SER:OG	2.29	0.45
2:F:1548:CYS:O	2:F:1593:SER:HA	2.16	0.45
2:B:289:ALA:HB3	2:B:293:SER:OG	2.16	0.45
2:F:1666:GLN:H	2:F:1666:GLN:HG2	1.45	0.45
2:E:1270:ARG:HB2	2:E:1306:PRO:O	2.16	0.45
2:E:1309:ILE:O	2:E:1320:GLU:HA	2.15	0.45
1:A:172:LYS:HD3	1:A:176:TYR:OH	2.17	0.45
2:C:542:GLU:O	2:C:543:ARG:CB	2.64	0.45
2:E:1325:VAL:O	2:E:1328:ILE:HG12	2.16	0.45
1:A:19:ARG:HG2	2:C:667:LYS:O	2.16	0.45
2:B:386:TRP:CZ3	2:B:411:ARG:HG3	2.51	0.45
2:B:385:LYS:H	2:B:385:LYS:CD	2.30	0.45
1:D:1001:PHE:CB	1:D:1002:PRO:CD	2.92	0.45
1:D:1076:LEU:CD1	1:D:1128:LEU:HD12	2.47	0.45
2:F:1715:LYS:HG3	2:F:1716:GLN:O	2.17	0.45
2:E:1348:GLY:O	2:E:1404:VAL:HG11	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1297:ASN:C	2:E:1297:ASN:OD1	2.55	0.45
1:D:1079:SER:O	1:D:1083:ILE:HG12	2.16	0.45
2:C:549:HIS:CE1	2:C:593:SER:HB2	2.52	0.45
2:B:282:GLU:OE1	2:B:286:TYR:OH	2.29	0.45
2:E:1376:LEU:HD23	2:E:1376:LEU:O	2.17	0.45
2:E:1245:THR:HA	2:E:1301:THR:OG1	2.16	0.45
2:B:267:PHE:CA	2:B:281:LYS:O	2.65	0.45
2:E:1313:SER:OG	2:E:1314:ASN:N	2.48	0.45
2:E:1266:LEU:HD23	2:E:1266:LEU:C	2.37	0.45
1:D:1064:LYS:HD2	2:E:1244:GLU:OE1	2.17	0.45
2:C:585:ASP:CG	2:C:588:SER:HB2	2.38	0.45
1:A:96:VAL:HG11	1:A:163:LEU:HD11	1.97	0.45
2:C:713:ARG:HD2	2:C:725:PHE:CE1	2.51	0.44
2:B:392:ILE:HG13	2:B:392:ILE:H	1.67	0.44
2:F:1657:TRP:CH2	2:F:1697:VAL:HG12	2.52	0.44
2:B:244:GLU:O	2:B:298:SER:HA	2.17	0.44
2:F:1642:LEU:HB2	2:F:1652:ASP:O	2.18	0.44
2:E:1261:LEU:CD2	2:E:1261:LEU:C	2.84	0.44
2:F:1536:THR:H	2:F:1550:TRP:HA	1.81	0.44
2:B:365:ILE:HG12	2:B:366:GLN:N	2.32	0.44
2:B:424:GLU:N	3:B:2015:HOH:O	2.45	0.44
2:E:1354:GLN:NE2	2:E:1396:SER:OG	2.48	0.44
2:E:1280:TRP:CH2	2:E:1310:LYS:HD2	2.52	0.44
2:B:337:LEU:HD11	2:B:412:VAL:HG23	1.99	0.44
1:A:84:GLN:HA	1:A:87:LEU:HG	1.98	0.44
2:E:1388:MET:H	2:E:1388:MET:HE2	1.81	0.44
2:B:414:SER:O	2:B:423:GLY:N	2.49	0.44
1:D:1009:LEU:HB3	1:D:1124:LEU:HG	1.99	0.44
2:F:1620:GLU:HG3	2:F:1620:GLU:O	2.17	0.44
2:B:380:GLU:HG3	2:B:406:LYS:HZ2	1.81	0.44
2:E:1337:LEU:HD22	2:E:1357:TRP:HB2	2.00	0.44
1:A:115:LYS:HD2	1:A:115:LYS:HA	1.58	0.44
1:A:4:ILE:CG2	1:A:9:LEU:CD2	2.96	0.44
2:E:1270:ARG:HE	2:E:1272:ASN:HB3	1.83	0.44
2:F:1637:LEU:HD22	2:F:1657:TRP:HB3	2.00	0.44
2:C:713:ARG:HH21	2:C:713:ARG:HD3	1.70	0.43
1:D:1080:LEU:HD21	1:D:1122:GLN:HG3	1.99	0.43
1:A:80:LEU:HD12	1:A:80:LEU:O	2.17	0.43
2:B:264:ILE:CG2	2:B:311:LEU:HD22	2.48	0.43
2:B:381:VAL:HG12	2:B:382:ASN:OD1	2.17	0.43
2:C:677:GLN:HG3	2:C:725:PHE:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1287:VAL:O	2:E:1288:SER:C	2.57	0.43
2:F:1716:GLN:CG	2:F:1717:ARG:N	2.78	0.43
2:B:272:ASN:ND2	2:B:273:THR:H	2.16	0.43
2:E:1417:ARG:O	2:E:1418:ASN:HB2	2.18	0.43
2:F:1610:LYS:HG2	2:F:1617:THR:HG23	2.00	0.43
2:E:1289:ALA:HB3	2:E:1293:SER:OG	2.17	0.43
2:E:1385:LYS:HD3	2:E:1385:LYS:O	2.19	0.43
2:B:407:GLU:HG3	2:B:432:THR:CG2	2.48	0.43
2:C:549:HIS:ND1	2:C:593:SER:HB2	2.34	0.43
1:A:64:LYS:HE3	2:B:364:ASP:OD2	2.18	0.43
2:B:366:GLN:HG3	2:B:366:GLN:H	1.51	0.43
2:E:1287:VAL:CG2	2:E:1288:SER:N	2.82	0.43
2:F:1625:VAL:O	2:F:1629:VAL:HG23	2.19	0.43
1:D:1001:PHE:CD2	1:D:1006:LEU:HG	2.53	0.43
2:E:1379:LYS:HG3	2:E:1383:GLU:HB2	2.00	0.43
1:D:1080:LEU:HD12	1:D:1080:LEU:O	2.18	0.43
2:C:623:PHE:CD2	2:C:623:PHE:N	2.87	0.43
1:D:1162:LEU:HD23	1:D:1162:LEU:HA	1.83	0.43
2:E:1376:LEU:C	2:E:1376:LEU:CD2	2.80	0.43
2:C:704:VAL:HG23	2:C:733:LEU:CB	2.49	0.43
1:D:1044:PHE:HE2	1:D:1160:TYR:CE2	2.36	0.43
2:E:1239:ARG:HG2	2:E:1239:ARG:O	2.19	0.43
2:E:1247:SER:HB2	2:E:1294:CYS:O	2.19	0.43
1:A:29:GLN:O	1:A:33:GLU:HB2	2.19	0.43
2:E:1414:SER:O	2:E:1423:GLY:N	2.51	0.42
2:B:297:ASN:C	2:B:297:ASN:OD1	2.57	0.42
2:C:666:GLN:OE1	2:F:1579:GLU:HG3	2.19	0.42
1:A:93:LEU:HB2	1:A:97:PHE:CE1	2.54	0.42
2:E:1375:GLU:OE2	2:E:1388:MET:HG2	2.19	0.42
2:E:1388:MET:HB2	2:E:1388:MET:HE3	1.92	0.42
2:F:1697:VAL:HG22	2:F:1698:PRO:HD2	2.01	0.42
2:B:386:TRP:CH2	2:B:411:ARG:HG2	2.54	0.42
2:E:1302:SER:HB3	2:E:1305:ILE:HG13	2.01	0.42
2:F:1635:ILE:HD13	2:F:1661:ARG:HG3	2.00	0.42
2:C:649:ILE:HG22	2:C:650:HIS:CE1	2.54	0.42
1:D:1088:GLU:N	1:D:1089:PRO:HD2	2.34	0.42
2:E:1365:ILE:H	2:E:1366:GLN:NE2	2.18	0.42
2:E:1366:GLN:NE2	2:E:1366:GLN:H	2.17	0.42
2:F:1611:LEU:HD23	2:F:1611:LEU:HA	1.85	0.42
2:C:674:TYR:N	2:C:674:TYR:CD2	2.88	0.42
1:D:1064:LYS:HE3	2:E:1364:ASP:OD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:385:LYS:HD3	2:B:385:LYS:O	2.20	0.42
1:D:1042:HIS:HD2	1:D:1044:PHE:CZ	2.37	0.42
2:F:1608:CYS:HA	2:F:1621:LYS:O	2.19	0.42
1:A:6:LEU:HD21	1:A:127:ARG:HE	1.85	0.42
2:B:357:TRP:O	2:B:395:THR:HB	2.19	0.42
2:E:1314:ASN:CG	2:E:1315:GLY:N	2.72	0.42
2:F:1677:GLN:HG3	2:F:1725:PHE:CE1	2.55	0.42
1:D:1060:THR:HA	1:D:1061:PRO:HD3	1.82	0.42
1:A:14:TRP:CZ3	1:A:15:LEU:HD23	2.54	0.42
1:D:1019:ARG:HG3	1:D:1023:LEU:HD22	2.01	0.41
2:B:337:LEU:HD11	2:B:412:VAL:CG2	2.49	0.41
2:B:302:SER:HB3	2:B:305:ILE:HG13	2.02	0.41
2:C:536:THR:HG22	2:C:549:HIS:O	2.19	0.41
2:F:1566:LEU:HD11	2:F:1609:ILE:HB	2.02	0.41
1:D:1111:TYR:CD1	1:D:1111:TYR:C	2.94	0.41
2:E:1345:SER:HB2	2:F:1700:TYR:CG	2.55	0.41
2:C:567:PHE:CE2	2:C:582:GLU:HB2	2.55	0.41
1:A:80:LEU:HB2	1:A:121:ILE:CG2	2.50	0.41
2:F:1613:SER:HB3	2:F:1614:ASN:H	1.68	0.41
1:D:1172:LYS:HE2	2:E:1304:TRP:CE3	2.55	0.41
2:F:1713:ARG:HD3	2:F:1713:ARG:HH21	1.71	0.41
2:B:280:TRP:CZ2	2:B:310:LYS:HD2	2.55	0.41
1:D:1031:PHE:HE2	1:D:1160:TYR:HB2	1.86	0.41
1:A:16:ARG:NH2	2:C:669:TRP:CD1	2.88	0.41
2:C:536:THR:HG23	2:C:537:LYS:N	2.35	0.41
2:E:1337:LEU:HD11	2:E:1412:VAL:CG2	2.50	0.41
1:A:22:GLN:HB2	1:A:22:GLN:HE21	1.54	0.41
2:E:1357:TRP:O	2:E:1395:THR:HB	2.20	0.41
1:D:1179:THR:O	1:D:1183:ARG:HG3	2.20	0.41
1:D:1016:ARG:NH2	2:F:1669:TRP:CD1	2.89	0.41
1:A:2:PRO:HA	1:A:5:PRO:HD3	2.02	0.41
2:F:1566:LEU:HG	2:F:1567:PHE:N	2.36	0.41
2:B:266:LEU:O	2:B:266:LEU:HD23	2.21	0.41
2:B:235:PHE:CZ	2:B:309:ILE:HG13	2.55	0.41
2:E:1376:LEU:HD23	2:E:1377:GLN:N	2.36	0.41
2:F:1589:ALA:CB	2:F:1595:TYR:HB2	2.48	0.41
2:F:1585:ASP:CG	2:F:1588:SER:HB2	2.42	0.41
2:C:715:LYS:HE2	2:C:715:LYS:HB2	1.83	0.41
2:E:1282:GLU:O	2:E:1283:CYS:C	2.59	0.41
1:A:64:LYS:NZ	2:B:364:ASP:OD2	2.53	0.41
2:F:1642:LEU:HA	2:F:1642:LEU:HD23	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1172:LYS:HD3	1:D:1176:TYR:OH	2.21	0.41
2:C:732:THR:O	2:C:732:THR:OG1	2.30	0.41
2:F:1674:TYR:N	2:F:1674:TYR:CD2	2.89	0.41
1:D:1014:TRP:O	1:D:1018:ASP:N	2.47	0.41
2:E:1346:LEU:HA	2:E:1346:LEU:HD12	1.85	0.41
2:B:235:PHE:CE1	2:B:266:LEU:HD12	2.56	0.41
2:E:1345:SER:HB2	2:F:1700:TYR:CB	2.46	0.41
2:F:1570:ARG:HD2	2:F:1607:TYR:CE2	2.56	0.41
2:B:239:ARG:O	2:B:239:ARG:HG2	2.20	0.41
2:C:646:LEU:C	2:C:648:GLY:H	2.23	0.41
1:D:1072:ASN:O	1:D:1076:LEU:HD12	2.21	0.40
2:B:270:ARG:HB2	2:B:306:PRO:O	2.21	0.40
2:B:436:MET:HE3	2:B:436:MET:HB3	1.89	0.40
1:A:63:ASN:OD1	1:A:65:GLU:HB2	2.21	0.40
1:A:162:LEU:HA	1:A:162:LEU:HD23	1.89	0.40
2:F:1583:CYS:HA	2:F:1584:PRO:HD3	1.90	0.40
2:C:535:PHE:HZ	2:C:566:LEU:HD12	1.84	0.40
1:A:7:SER:O	1:A:8:ARG:C	2.58	0.40
2:F:1679:LYS:HG2	2:F:1686:TRP:CE3	2.56	0.40
2:E:1337:LEU:HD11	2:E:1412:VAL:HG23	2.03	0.40
2:B:341:LEU:HD23	2:B:353:ILE:HG22	2.02	0.40
2:F:1646:LEU:C	2:F:1648:GLY:H	2.24	0.40
2:F:1618:VAL:CG1	2:F:1619:ASP:H	2.34	0.40
2:C:692:ILE:HG13	2:C:692:ILE:H	1.59	0.40
2:F:1565:GLN:O	2:F:1611:LEU:CD2	2.69	0.40
1:D:1036:ILE:HG13	1:D:1160:TYR:CE1	2.55	0.40
2:B:335:ILE:HG13	2:B:358:GLU:HB3	2.03	0.40
2:E:1342:LEU:HD23	2:E:1342:LEU:HA	1.87	0.40
2:C:568:TYR:C	2:C:568:TYR:CD1	2.94	0.40
2:C:536:THR:H	2:C:550:TRP:HA	1.86	0.40
2:C:715:LYS:HB3	2:C:722:TYR:HA	2.04	0.40
1:A:128:LEU:HA	1:A:128:LEU:HD23	1.93	0.40
1:A:111:TYR:HA	1:A:114:LEU:HD12	2.04	0.40
2:B:407:GLU:HG3	2:B:432:THR:HG22	2.03	0.40
2:E:1372:LEU:HD12	2:E:1372:LEU:HA	1.71	0.40
2:B:362:ASN:N	2:B:362:ASN:OD1	2.54	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	154/191 (81%)	129 (84%)	19 (12%)	6 (4%)	4 5
1	D	150/191 (78%)	129 (86%)	17 (11%)	4 (3%)	6 10
2	B	189/238 (79%)	168 (89%)	20 (11%)	1 (0%)	34 60
2	C	167/238 (70%)	144 (86%)	21 (13%)	2 (1%)	16 33
2	E	189/238 (79%)	171 (90%)	16 (8%)	2 (1%)	17 36
2	F	178/238 (75%)	155 (87%)	20 (11%)	3 (2%)	11 22
All	All	1027/1334 (77%)	896 (87%)	113 (11%)	18 (2%)	11 21

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	SER
1	A	107	ASP
2	B	274	GLN
1	D	1002	PRO
2	E	1274	GLN
2	C	597	ASN
2	C	667	LYS
1	D	1103	TYR
1	A	38	LYS
1	D	1038	LYS
2	E	1263	PRO
2	F	1597	ASN
2	F	1613	SER
1	A	4	ILE
1	A	48	PRO
2	F	1667	LYS
1	D	1054	PRO
1	A	5	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	143/175 (82%)	112 (78%)	31 (22%)	1	2
1	D	142/175 (81%)	112 (79%)	30 (21%)	1	2
2	B	177/218 (81%)	130 (73%)	47 (27%)	0	1
2	C	157/218 (72%)	113 (72%)	44 (28%)	0	1
2	E	177/218 (81%)	134 (76%)	43 (24%)	1	1
2	F	165/218 (76%)	121 (73%)	44 (27%)	0	1
All	All	961/1222 (79%)	722 (75%)	239 (25%)	1	1

All (239) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	PHE
1	A	3	THR
1	A	4	ILE
1	A	9	LEU
1	A	19	ARG
1	A	22	GLN
1	A	23	LEU
1	A	33	GLU
1	A	38	LYS
1	A	41	ILE
1	A	43	SER
1	A	46	TRP
1	A	53	CYS
1	A	55	SER
1	A	62	SER
1	A	65	GLU
1	A	68	GLN
1	A	69	GLN
1	A	74	GLU
1	A	95	SER
1	A	99	ASN
1	A	101	LEU

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Mol	Chain	Res	Type
1	A	103	TYR
1	A	107	ASP
1	A	122	GLN
1	A	125	MET
1	A	127	ARG
1	A	157	LEU
1	A	183	ARG
1	A	184	SER
1	A	189	CYS
2	B	234	LYS
2	B	236	THR
2	B	237	LYS
2	B	239	ARG
2	B	242	GLU
2	B	272	ASN
2	B	273	THR
2	B	278	GLN
2	B	279	GLU
2	B	287	VAL
2	B	291	GLU
2	B	302	SER
2	B	310	LYS
2	B	311	LEU
2	B	312	THR
2	B	314	ASN
2	B	320	GLU
2	B	321	LYS
2	B	337	LEU
2	B	341	LEU
2	B	345	SER
2	B	346	LEU
2	B	361	ARG
2	B	365	ILE
2	B	366	GLN
2	B	370	MET
2	B	372	LEU
2	B	376	LEU
2	B	379	LYS
2	B	381	VAL
2	B	384	THR
2	B	385	LYS
2	B	388	MET

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Mol	Chain	Res	Type
2	B	389	MET
2	B	394	THR
2	B	405	ASP
2	B	406	LYS
2	B	411	ARG
2	B	414	SER
2	B	415	LYS
2	B	416	GLN
2	B	417	ARG
2	B	419	SER
2	B	427	GLU
2	B	428	VAL
2	B	429	LEU
2	B	436	MET
2	C	535	PHE
2	C	537	LYS
2	C	539	ARG
2	C	542	GLU
2	C	543	ARG
2	C	566	LEU
2	C	570	ARG
2	C	572	ASN
2	C	581	LYS
2	C	587	VAL
2	C	588	SER
2	C	598	SER
2	C	599	SER
2	C	602	SER
2	C	603	ILE
2	C	610	LYS
2	C	611	LEU
2	C	627	GLU
2	C	631	PRO
2	C	637	LEU
2	C	638	ASN
2	C	641	LEU
2	C	643	ASN
2	C	645	SER
2	C	646	LEU
2	C	658	GLU
2	C	665	ILE
2	C	666	GLN

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Mol	Chain	Res	Type
2	C	669	TRP
2	C	670	MET
2	C	672	LEU
2	C	674	TYR
2	C	681	VAL
2	C	692	ILE
2	C	693	LEU
2	C	696	SER
2	C	701	SER
2	C	713	ARG
2	C	715	LYS
2	C	716	GLN
2	C	718	ASN
2	C	719	SER
2	C	728	VAL
2	C	729	LEU
1	D	1004	ILE
1	D	1009	LEU
1	D	1022	GLN
1	D	1023	LEU
1	D	1033	GLU
1	D	1038	LYS
1	D	1041	ILE
1	D	1043	SER
1	D	1046	TRP
1	D	1050	THR
1	D	1052	LEU
1	D	1055	SER
1	D	1062	SER
1	D	1065	GLU
1	D	1068	GLN
1	D	1069	GLN
1	D	1074	GLU
1	D	1094	ARG
1	D	1095	SER
1	D	1099	ASN
1	D	1101	LEU
1	D	1106	SER
1	D	1115	LYS
1	D	1122	GLN
1	D	1125	MET
1	D	1127	ARG

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Mol	Chain	Res	Type
1	D	1157	LEU
1	D	1183	ARG
1	D	1184	SER
1	D	1188	SER
2	E	1234	LYS
2	E	1236	THR
2	E	1237	LYS
2	E	1242	GLU
2	E	1272	ASN
2	E	1273	THR
2	E	1278	GLN
2	E	1279	GLU
2	E	1287	VAL
2	E	1291	GLU
2	E	1302	SER
2	E	1310	LYS
2	E	1311	LEU
2	E	1312	THR
2	E	1314	ASN
2	E	1318	VAL
2	E	1320	GLU
2	E	1341	LEU
2	E	1345	SER
2	E	1346	LEU
2	E	1361	ARG
2	E	1365	ILE
2	E	1366	GLN
2	E	1370	MET
2	E	1372	LEU
2	E	1376	LEU
2	E	1379	LYS
2	E	1381	VAL
2	E	1384	THR
2	E	1385	LYS
2	E	1388	MET
2	E	1394	THR
2	E	1405	ASP
2	E	1406	LYS
2	E	1411	ARG
2	E	1414	SER
2	E	1415	LYS
2	E	1416	GLN

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Mol	Chain	Res	Type
2	E	1417	ARG
2	E	1419	SER
2	E	1427	GLU
2	E	1428	VAL
2	E	1429	LEU
2	F	1535	PHE
2	F	1537	LYS
2	F	1539	ARG
2	F	1542	GLU
2	F	1543	ARG
2	F	1566	LEU
2	F	1570	ARG
2	F	1581	LYS
2	F	1587	VAL
2	F	1588	SER
2	F	1598	SER
2	F	1599	SER
2	F	1602	SER
2	F	1603	ILE
2	F	1610	LYS
2	F	1611	LEU
2	F	1619	ASP
2	F	1620	GLU
2	F	1627	GLU
2	F	1637	LEU
2	F	1638	ASN
2	F	1641	LEU
2	F	1643	ASN
2	F	1645	SER
2	F	1646	LEU
2	F	1658	GLU
2	F	1665	ILE
2	F	1666	GLN
2	F	1669	TRP
2	F	1670	MET
2	F	1672	LEU
2	F	1681	VAL
2	F	1692	ILE
2	F	1693	LEU
2	F	1696	SER
2	F	1701	SER
2	F	1711	ARG

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Mol	Chain	Res	Type
2	F	1713	ARG
2	F	1716	GLN
2	F	1718	ASN
2	F	1719	SER
2	F	1728	VAL
2	F	1729	LEU
2	F	1732	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	68	GLN
1	A	99	ASN
1	A	122	GLN
1	A	167	ASN
1	A	181	GLN
2	B	272	ASN
2	B	314	ASN
2	B	354	GLN
2	B	416	GLN
2	C	638	ASN
2	C	643	ASN
2	C	716	GLN
1	D	1068	GLN
1	D	1099	ASN
1	D	1122	GLN
1	D	1181	GLN
2	E	1272	ASN
2	E	1314	ASN
2	E	1354	GLN
2	E	1366	GLN
2	E	1416	GLN
2	F	1578	GLN
2	F	1630	GLN
2	F	1638	ASN
2	F	1643	ASN
2	F	1650	HIS
2	F	1716	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.