



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 05:38 AM GMT

PDB ID : 1KF9
Title : PHAGE DISPLAY DERIVED VARIANT OF HUMAN GROWTH HORMONE COMPLEXED WITH TWO COPIES OF THE EXTRACELLULAR DOMAIN OF ITS RECEPTOR
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Deposited on : 2001-11-19
Resolution : 2.60 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

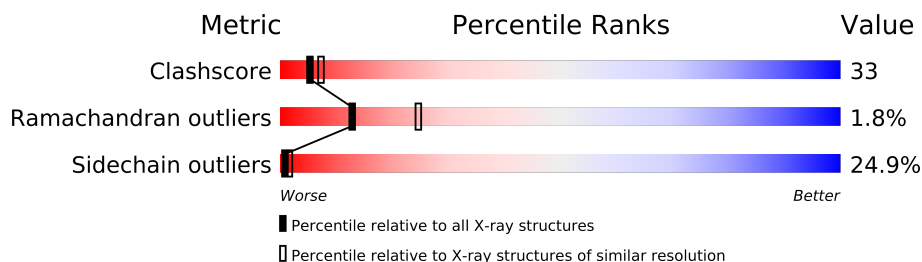
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	191	
1	D	191	
2	B	238	
2	C	238	
2	E	238	
2	F	238	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8678 atoms, of which 0 are hydrogen and 0 are deuterium.

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	0	0
			7	7		

3 Residue-property plots

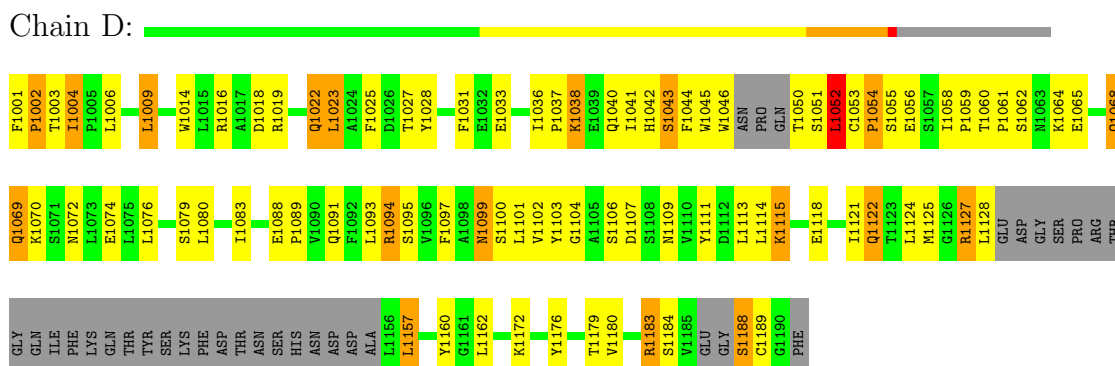
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

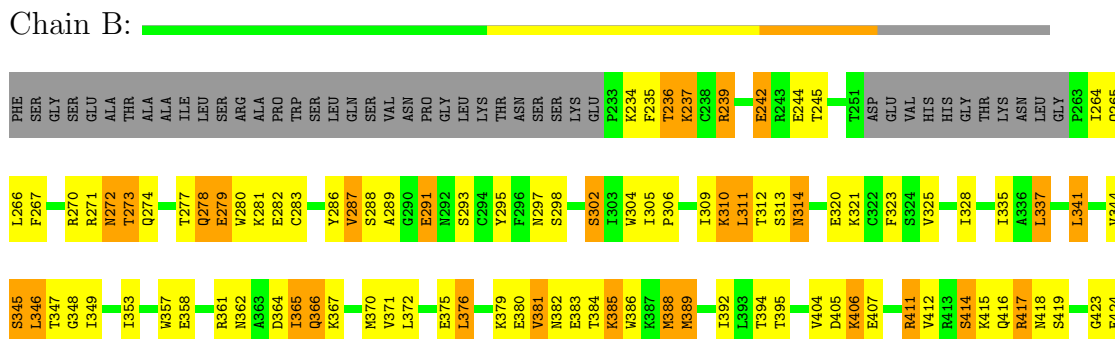
• Molecule 1: PHAGE DISPLAY DERIVED VARIANT HUMAN GROWTH HORMONE



• Molecule 1: PHAGE DISPLAY DERIVED VARIANT HUMAN GROWTH HORMONE



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



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
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4 Data and refinement statistics

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(°)	Ideal(°)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1284	0	1257	102	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 33.

All (550) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	154/191 (81%)	129 (84%)	19 (12%)	6 (4%)	5 6
1	D	150/191 (78%)	129 (86%)	17 (11%)	4 (3%)	8 13
2	B	189/238 (79%)	168 (89%)	20 (11%)	1 (0%)	38 67
2	C	167/238 (70%)	144 (86%)	21 (13%)	2 (1%)	19 39
2	E	189/238 (79%)	171 (90%)	16 (8%)	2 (1%)	21 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	178/238 (75%)	155 (87%)	20 (11%)	3 (2%)	14	26
All	All	1027/1334 (77%)	896 (87%)	113 (11%)	18 (2%)	13	25

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 ⓘ

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%)	1	1
2	C	157/218 (72%)	113 (72%)	44 (28%)	0	1
2	E	177/218 (81%)	134 (76%)	43 (24%)	1	2
2	F	165/218 (76%)	121 (73%)	44 (27%)	1	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	961/1222 (79%)	722 (75%)	239 (25%)	1 2

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 chains 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.