



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:12 AM UTC

PDB ID : 1KF9 / pdb_00001kf9
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

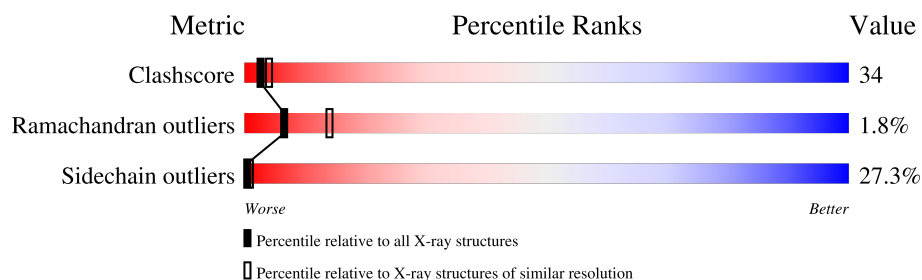
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	191	27% 42% 13% • 16%
1	D	191	33% 37% 12% • 17%
2	B	238	32% 32% 16% • 19%
2	C	238	24% 37% 11% • 26%
2	E	238	31% 34% 14% • 19%
2	F	238	24% 39% 14% 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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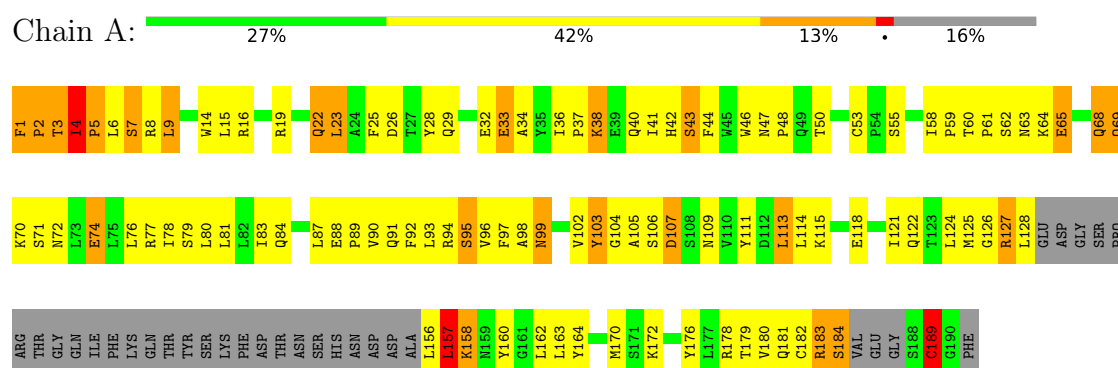
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	7	Total	O	0	0
			7	7		

3 Residue-property plots

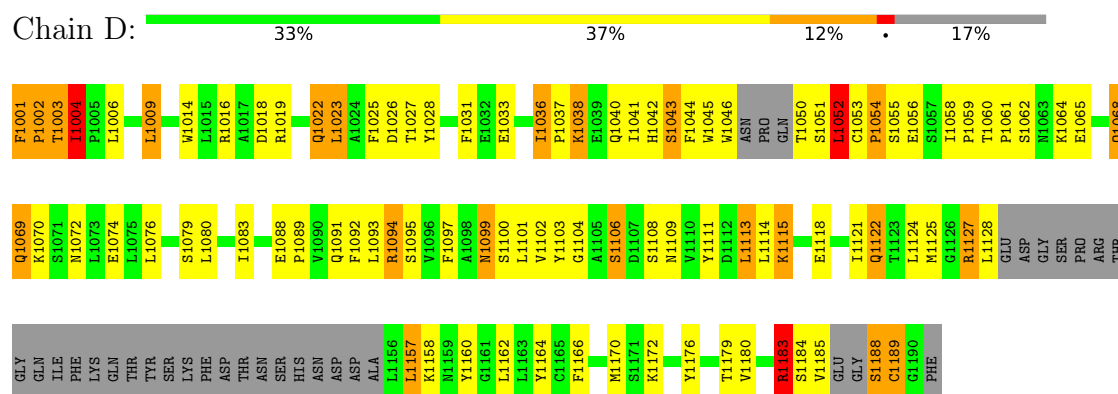
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

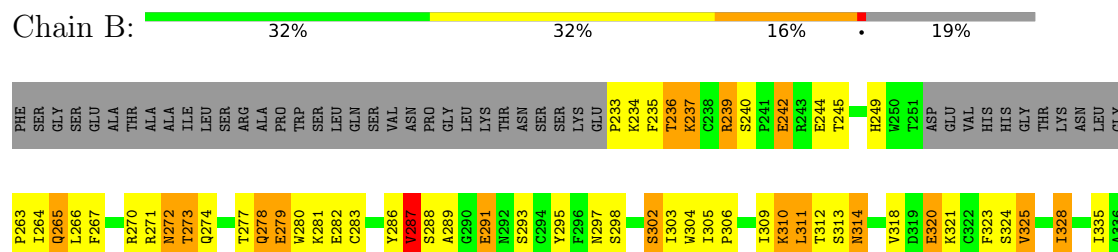
• Molecule 1: PHAGE DISPLAY DERIVED VARIANT HUMAN GROWTH HORMONE

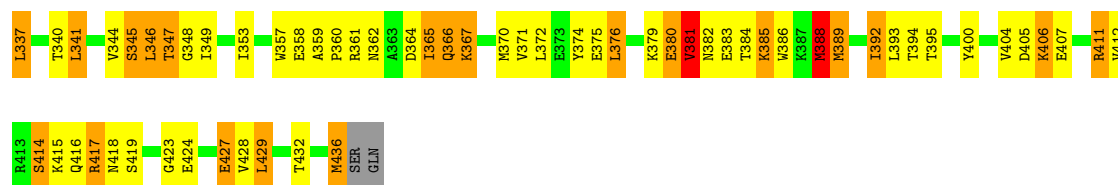


• Molecule 1: PHAGE DISPLAY DERIVED VARIANT HUMAN GROWTH HORMONE



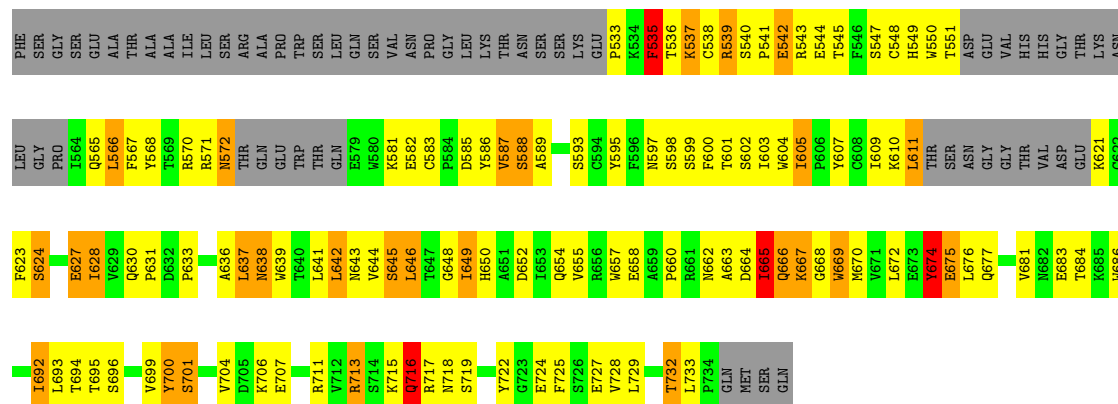
• Molecule 2: EXTRACELLULAR DOMAIN HUMAN GROWTH HORMONE RECEPTOR (1-238)





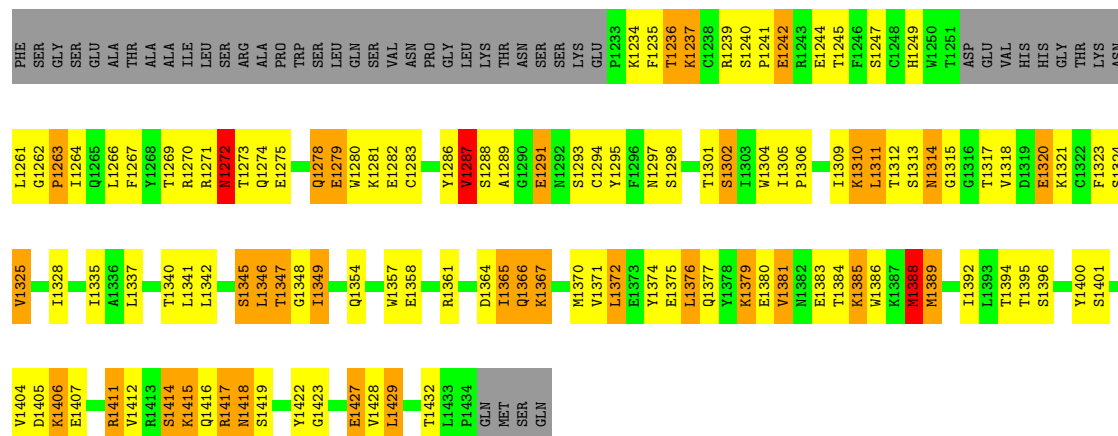
• Molecule 2: EXTRACELLULAR DOMAIN HUMAN GROWTH HORMONE RECEPTOR (1-238)

Chain C: 24% 37% 11% 26%



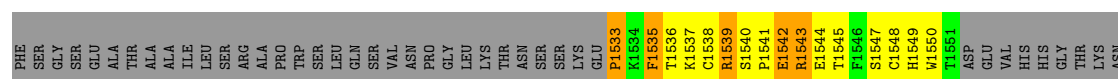
• Molecule 2: EXTRACELLULAR DOMAIN HUMAN GROWTH HORMONE RECEPTOR (1-238)

Chain E: 31% 34% 14% 19%



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

Chain F: 24% 39% 14% 23%



[illegible]

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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	0.79	0/1312	1.32	16/1781 (0.9%)
1	D	0.87	1/1289 (0.1%)	1.29	13/1747 (0.7%)
2	B	0.82	0/1622	1.24	16/2208 (0.7%)
2	C	0.80	1/1459 (0.1%)	1.25	17/1987 (0.9%)
2	E	0.84	0/1621	1.21	14/2208 (0.6%)
2	F	0.80	0/1525	1.19	13/2078 (0.6%)
All	All	0.82	2/8828 (0.0%)	1.25	89/12009 (0.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	665	ILE	CA-CB	6.36	1.63	1.54
1	D	1004	ILE	CA-CB	5.87	1.59	1.53

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	THR	N-CA-C	-16.82	86.61	113.19
2	C	668	GLY	N-CA-C	-12.92	98.09	114.37
1	D	1003	THR	N-CA-C	9.91	121.77	110.97
2	C	664	ASP	N-CA-C	9.76	124.48	108.96
1	D	1108	SER	N-CA-C	9.53	123.07	112.97
2	F	1668	GLY	N-CA-C	-9.31	103.61	114.69
2	B	287	VAL	N-CA-C	8.80	119.12	111.56
1	A	7	SER	N-CA-C	-8.26	102.22	111.14
2	F	1642	LEU	N-CA-C	-8.04	100.63	111.96
2	C	649	ILE	N-CA-C	8.02	118.80	110.62
2	C	642	LEU	N-CA-C	-7.95	100.75	111.96
1	D	1189	CYS	N-CA-C	7.89	122.69	108.48
2	C	605	ILE	N-CA-C	7.76	115.30	108.63
2	F	1605	ILE	N-CA-C	7.56	115.13	108.63
2	E	1272	ASN	N-CA-C	7.53	122.70	112.68
1	A	47	ASN	CA-C-N	7.45	129.15	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	ASN	C-N-CA	7.45	129.15	119.84
2	F	1649	ILE	N-CA-C	7.29	118.94	110.62
2	B	381	VAL	N-CA-C	7.26	118.90	110.62
2	E	1324	SER	N-CA-C	-7.17	96.87	109.06
1	A	1	PHE	CA-C-N	-6.89	111.22	119.84
1	A	1	PHE	C-N-CA	-6.89	111.22	119.84
2	E	1287	VAL	N-CA-C	6.82	118.15	111.67
2	C	662	ASN	N-CA-C	-6.53	105.31	113.28
2	B	240	SER	CA-C-N	6.52	126.10	119.19
2	B	240	SER	C-N-CA	6.52	126.10	119.19
2	B	325	VAL	N-CA-C	6.50	122.87	109.34
1	A	36	ILE	N-CA-C	6.46	114.28	107.76
2	B	324	SER	N-CA-C	-6.39	98.20	109.06
1	D	1052	LEU	N-CA-C	6.21	118.99	110.24
1	D	1106	SER	N-CA-C	6.20	119.46	110.28
2	E	1240	SER	CA-C-N	6.12	126.02	119.28
2	E	1240	SER	C-N-CA	6.12	126.02	119.28
2	E	1325	VAL	N-CA-C	6.12	122.07	109.34
1	A	92	PHE	N-CA-C	-6.07	104.78	111.82
1	D	1036	ILE	N-CA-C	6.06	113.88	107.76
2	E	1374	TYR	N-CA-C	6.01	119.34	109.72
1	A	158	LYS	N-CA-C	-6.01	104.81	111.36
1	A	164	TYR	N-CA-C	-5.95	104.72	111.14
2	F	1605	ILE	CA-C-N	5.80	126.13	119.92
2	F	1605	ILE	C-N-CA	5.80	126.13	119.92
2	C	605	ILE	CA-C-N	5.80	126.13	119.92
2	C	605	ILE	C-N-CA	5.80	126.13	119.92
2	C	535	PHE	N-CA-C	-5.79	101.08	109.59
2	E	1418	ASN	N-CA-C	5.77	120.27	113.23
1	D	1001	PHE	CA-C-N	5.76	127.03	119.84
1	D	1001	PHE	C-N-CA	5.76	127.03	119.84
2	C	700	TYR	N-CA-C	5.75	118.22	109.95
1	A	2	PRO	N-CA-C	5.73	124.28	112.47
2	E	1347	THR	N-CA-C	-5.65	105.88	112.89
1	D	1092	PHE	N-CA-C	-5.61	105.31	111.82
2	C	624	SER	N-CA-C	-5.55	99.26	108.75
2	E	1427	GLU	N-CA-C	-5.55	102.07	110.28
1	A	2	PRO	CA-C-N	5.54	130.27	121.18
1	A	2	PRO	C-N-CA	5.54	130.27	121.18
2	E	1400	TYR	N-CA-C	5.54	119.00	110.42
1	D	1158	LYS	N-CA-C	-5.52	105.34	111.36
2	B	347	THR	N-CA-C	-5.51	106.06	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	674	TYR	N-CA-C	5.50	118.42	109.24
2	B	388	MET	N-CA-C	5.49	118.19	109.24
2	E	1388	MET	N-CA-C	5.49	118.18	109.24
2	C	683	GLU	N-CA-C	-5.47	103.16	110.55
1	D	1183	ARG	N-CA-C	-5.46	105.05	112.26
2	B	374	TYR	N-CA-C	5.46	118.45	109.72
2	F	1707	GLU	N-CA-C	-5.44	100.83	109.59
2	F	1674	TYR	N-CA-C	5.39	118.02	109.50
2	E	1381	VAL	N-CA-C	5.38	118.59	111.17
2	C	707	GLU	N-CA-C	-5.37	100.95	109.59
2	B	380	GLU	N-CA-C	-5.34	102.48	110.23
2	F	1700	TYR	N-CA-C	5.32	117.96	110.14
2	B	400	TYR	N-CA-C	5.30	118.64	110.42
2	F	1673	GLU	N-CA-C	-5.26	101.07	109.23
2	B	328	ILE	N-CA-C	5.26	116.59	111.91
2	B	263	PRO	N-CA-CB	5.24	108.77	103.00
2	C	636	ALA	N-CA-C	5.23	118.65	111.54
2	F	1535	PHE	N-CA-C	-5.22	101.92	109.59
2	C	533	PRO	N-CA-CB	5.20	108.72	103.00
1	A	189	CYS	N-CA-C	5.20	116.74	108.79
1	A	26	ASP	N-CA-C	5.17	117.59	111.33
2	B	233	PRO	N-CA-CB	5.13	108.65	103.00
2	F	1716	GLN	N-CA-C	-5.13	103.76	110.53
2	C	716	GLN	N-CA-C	-5.12	103.78	110.53
2	E	1349	ILE	CB-CA-C	-5.08	105.71	111.55
2	B	287	VAL	CB-CA-C	-5.07	106.62	111.44
2	F	1533	PRO	N-CA-CB	5.06	108.57	103.00
1	A	157	LEU	N-CA-C	-5.06	107.06	113.18
1	D	1026	ASP	N-CA-C	5.06	117.45	111.33
1	D	1164	TYR	N-CA-C	-5.05	105.68	111.14
2	B	427	GLU	N-CA-C	-5.05	102.81	110.28

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	109	0
1	D	1264	0	1241	89	0
2	B	1577	0	1506	98	0
2	C	1419	0	1338	100	0
2	E	1576	0	1508	102	0
2	F	1484	0	1395	117	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	566	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 34.

All (566) 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:HB2	2:F:1581:LYS:NZ	1.76	0.98
2:F:1669:TRP:HA	2:F:1669:TRP:CE3	1.96	0.97
2:C:669:TRP:CE3	2:C:669:TRP:HA	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:E:1376:LEU:C	2:E:1376:LEU:HD23	2.10	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:1638:ASN:C	2:F:1638:ASN:HD22	1.94	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
2:B:344:VAL:HG11	2:B:436:MET:HE1	1.71	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
1:D:1004:ILE:O	1:D:1127:ARG:NH1	2.21	0.72
2:F:1536:THR:HG22	2:F:1549:HIS:C	2.14	0.72
1:A:107:ASP:OD1	2:F:1578:GLN:N	2.23	0.72
2:E:1347:THR:HG22	2:F:1650:HIS:HB2	1.72	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:B:376:LEU:HD23	2:B:376:LEU:C	2.15	0.71
2:E:1261:LEU:C	2:E:1261:LEU:HD23	2.15	0.71
2:E:1272:ASN:H	2:E:1272:ASN:HD22	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:536:THR:HG22	2:C:549:HIS:C	2.16	0.69
2:C:716:GLN:HG3	2:C:717:ARG:N	2.07	0.69
2:C:638:ASN:C	2:C:638:ASN:HD22	2.00	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NZ	2:F:1581:LYS:CB	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
1:D:1004:ILE:HD12	2:F:1604:TRP:O	1.94	0.68
2:C:582:GLU:HG3	2:C:583:CYS:N	2.09	0.67
1:D:1043:SER:OG	1:D:1157:LEU:HD11	1.94	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:F:1582:GLU:HG3	2:F:1583:CYS:N	2.09	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:C:631:PRO:HB3	2:C:670:MET:HE3	1.76	0.66
2:B:291:GLU:OE2	2:B:291:GLU:HA	1.94	0.66
2:F:1543:ARG:NE	2:F:1716:GLN:NE2	2.44	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:638:ASN:C	2:C:638:ASN:ND2	2.54	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:F:1638:ASN:C	2:F:1638:ASN:ND2	2.49	0.65
2:C:541:PRO:HA	2:C:630:GLN:O	1.97	0.64
2:F:1650:HIS:HE1	2:F:1703:LYS:HZ1	1.43	0.64
2:B:323:PHE:CE1	2:B:328:ILE:HD13	2.32	0.64
2:B:380:GLU:HB3	2:B:383:GLU:HG2	1.79	0.64
1:D:1064:LYS:HZ1	2:E:1364:ASP:CG	2.05	0.64
2:F:1587:VAL:HG22	2:F:1588:SER:N	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:621:LYS:HD2	3:C:2506:HOH:O	1.98	0.62
2:F:1535:PHE:CD2	2:F:1619:ASP:HB3	2.34	0.62
1:A:99:ASN:HD22	1:A:99:ASN:N	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:A:178:ARG:HH21	1:A:181:GLN:NE2	1.97	0.62
1:D:1099:ASN:N	1:D:1099:ASN:HD22	1.98	0.62
2:E:1323:PHE:CE1	2:E:1328:ILE:HD13	2.35	0.62
2:C:544:GLU:O	2:C:601:THR:HB	1.99	0.62
2:F:1542:GLU:O	2:F:1543:ARG:HB2	2.00	0.62
2:B:273:THR:HG23	2:B:277:THR:OG1	2.00	0.62
1:D:1104:GLY:HA2	2:F:1666:GLN:CB	2.24	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:C:711:ARG:HG3	2:C:725:PHE:CD1	2.35	0.61
2:E:1261:LEU:HD23	2:E:1262:GLY:N	2.15	0.61
1:A:6:LEU:CD2	1:A:127:ARG:HG2	2.30	0.61
2:C:543:ARG:HD2	2:C:716:GLN:HE22	1.65	0.61
2:E:1236:THR:HG22	2:E:1249:HIS:C	2.26	0.61
2:E:1380:GLU:HG3	2:E:1406:LYS:NZ	2.15	0.61
2:F:1564:ILE:HA	2:F:1612:THR:O	2.00	0.61
2:F:1716:GLN:HG3	2:F:1717:ARG:H	1.65	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:1380:GLU:HG3	2:E:1406:LYS:HZ2	1.66	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:B:380:GLU:HG3	2:B:406:LYS:HD2	1.83	0.60
2:C:655:VAL:HG12	2:C:657:TRP:CE3	2.36	0.60
2:B:337:LEU:HD22	2:B:357:TRP:CB	2.32	0.60
2:E:1245:THR:HG22	2:E:1298:SER:N	2.17	0.60
1:A:94:ARG:HG3	1:A:95:SER:H	1.66	0.59
1:A:104:GLY:HA2	2:C:666:GLN:NE2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD22	2:E:1272:ASN:N	1.99	0.59
2:B:266:LEU:C	2:B:266:LEU:HD23	2.27	0.59
2:B:271:ARG:HD2	2:B:306:PRO:HG2	1.84	0.59
1:A:111:TYR:C	1:A:111:TYR:CD1	2.81	0.59
2:C:637:LEU:HD22	2:C:657:TRP:HB3	1.85	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
1:D:1080:LEU:HB2	1:D:1121:ILE:HG21	1.84	0.58
2:E:1291:GLU:OE2	2:E:1291:GLU:HA	2.02	0.58
2:B:337:LEU:HD22	2:B:357:TRP:HB3	1.85	0.58
1:A:2:PRO:HG2	2:C:627:GLU:OE1	2.04	0.58
1:D:1113:LEU:N	1:D:1113:LEU:HD23	2.17	0.58
2:C:587:VAL:HG22	2:C:588:SER:N	2.19	0.58
2:C:657:TRP:O	2:C:695:THR:HB	2.03	0.58
1:D:1027:THR:CG2	1:D:1102:VAL:HG21	2.33	0.58
1:A:58:ILE:CG2	1:A:59:PRO:HD2	2.33	0.58
1:A:69:GLN:OE1	1:A:70:LYS:HG2	2.03	0.58
1:A:93:LEU:HD21	1:A:162:LEU:CB	2.34	0.58
2:F:1543:ARG:HB2	2:F:1670:MET:HG3	1.86	0.57
2:E:1279:GLU:O	2:E:1280:TRP:C	2.46	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:B:375:GLU:OE2	2:B:388:MET:HG2	2.05	0.57
2:F:1618:VAL:HG13	2:F:1619:ASP:N	2.20	0.57
2:E:1282:GLU:OE1	2:E:1286:TYR:OH	2.15	0.56
2:C:540:SER:OG	2:C:545:THR:O	2.19	0.56
2:F:1536:THR:CG2	2:F:1549:HIS:HB2	2.36	0.56
2:C:543:ARG:NE	2:C:716:GLN:HE22	2.03	0.56
2:C:655:VAL:HG12	2:C:657:TRP:HZ3	1.68	0.56
1:D:1019:ARG:NE	1:D:1022:GLN:OE1	2.31	0.56
2:E:1380:GLU:HG3	2:E:1406:LYS:HD2	1.87	0.56
1:A:2:PRO:HB2	2:C:627:GLU:OE1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:B:289:ALA:HB2	2:B:295:TYR:HB2	1.88	0.56
1:D:1022:GLN:HG3	1:D:1023:LEU:N	2.21	0.56
2:E:1289:ALA:HB2	2:E:1295:TYR:HB2	1.88	0.56
2:B:380:GLU:CG	2:B:406:LYS:HD2	2.36	0.56
1:D:1004:ILE:CG2	1:D:1009:LEU:HD21	2.34	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:380:GLU:HG3	2:B:406:LYS:HZ2	1.70	0.55
2:E:1262:GLY:O	2:E:1263:PRO:C	2.49	0.55
2:F:1676:LEU:HD23	2:F:1676:LEU:C	2.31	0.55
2:B:287:VAL:HG22	2:B:288:SER:N	2.21	0.55
2:B:279:GLU:O	2:B:280:TRP:C	2.48	0.55
2:F:1565:GLN:HB3	2:F:1586:TYR:OH	2.06	0.55
2:F:1686:TRP:CD2	2:F:1711:ARG:NH2	2.75	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: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:N	1:D:1099:ASN:ND2	2.53	0.55
1:D:1188:SER:O	1:D:1189:CYS:SG	2.65	0.55
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:D:1019:ARG:O	1:D:1022:GLN:HG3	2.08	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
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:D:1069:GLN:OE1	1:D:1070:LYS:HG2	2.08	0.54
2:B:344:VAL:HG11	2:B:436:MET:CE	2.36	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:704:VAL:HG23	2:C:733:LEU:HB3	1.90	0.53
2:C:716:GLN:HG3	2:C:717:ARG:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:245:THR:HG22	2:B:298:SER:N	2.23	0.53
2:B:371:VAL:O	2:B:417:ARG:HB2	2.08	0.53
1:A:72:ASN:HA	1:A:180:VAL:HG22	1.90	0.53
2:C:542:GLU:O	2:C:543:ARG:HB2	2.07	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:B:347:THR:HB	2:C:645:SER:CB	2.39	0.53
1:A:68:GLN:HE22	2:B:367:LYS:HD2	1.74	0.53
1:A:97:PHE:HB3	1:A:105:ALA:O	2.08	0.53
2:C:539:ARG:HA	2:C:628:ILE:O	2.08	0.53
2:C:637:LEU:O	2:C:638:ASN:HB3	2.08	0.53
2:C:677:GLN:HG3	2:C:725:PHE:HE1	1.74	0.53
2:C:692:ILE:HD12	2:C:694:THR: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
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
1:A:95:SER:O	1:A:98:ALA:N	2.41	0.52
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
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:9:LEU:N	1:A:9:LEU:HD23	2.24	0.52
1:A:113:LEU:HD23	1:A:113:LEU:N	2.24	0.52
2:E:1264:ILE:CG2	2:E:1311:LEU:HD22	2.40	0.52
2:B:280:TRP:CH2	2:B:310:LYS:HD2	2.45	0.52
2:C:637:LEU:HD23	2:C:637:LEU:N	2.25	0.52
1:D:1027:THR:HG22	1:D:1100:SER:OG	2.10	0.52
2:C:676:LEU:C	2:C:676:LEU:HD23	2.35	0.52
2:E:1310:LYS:HG2	2:E:1317:THR:HG23	1.92	0.52
1:A:103:TYR:H	1:A:103:TYR:HD2	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:B:347:THR:OG1	2:B:349:ILE:HG13	2.10	0.51
2:E:1347:THR:HB	2:F:1645:SER:CB	2.41	0.51
2:B:313:SER:OG	2:B:314:ASN:N	2.43	0.51
2:E:1262:GLY:H	2:E:1263:PRO:CD	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1677:GLN:HG3	2:F:1725:PHE:HE1	1.76	0.51
2:B:242:GLU:OE2	2:B:242:GLU:N	2.41	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
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
1:D:1104:GLY:HA3	2:F:1666:GLN:HB3	1.90	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:1542:GLU:O	2:F:1543:ARG:CB	2.59	0.51
2:B:347:THR:HG22	2:C:650:HIS:HB2	1.93	0.51
1:D:1104:GLY:HA2	2:F:1666:GLN:HE21	1.75	0.51
2:C:727:GLU:HG2	1:D:1088:GLU:OE1	2.11	0.50
2:E:1380:GLU:CG	2:E:1406:LYS:HD2	2.41	0.50
1:A:104:GLY:CA	2:C:666:GLN:CB	2.60	0.50
1:A:156:LEU:C	1:A:156:LEU:HD23	2.36	0.50
2:E:1235:PHE:CZ	2:E:1309:ILE:HD12	2.46	0.50
2:B:272:ASN:HD22	2:B:272:ASN:H	1.59	0.50
1:D:1016:ARG:HH12	1:D:1113:LEU:HD22	1.76	0.50
1:A:25:PHE:O	1:A:28:TYR:HB3	2.11	0.50
1:A:68:GLN:NE2	2:B:367:LYS:HD2	2.26	0.50
2:F:1713:ARG:HD2	2:F:1725:PHE:CE1	2.46	0.49
1:A:64:LYS:HZ1	2:B:364:ASP:CG	2.20	0.49
2:F:1637:LEU:N	2:F:1637:LEU:HD23	2.27	0.49
1:A:76:LEU:HD11	1:A:128:LEU:HD12	1.94	0.49
2:C:585:ASP:CG	2:C:588:SER:HB2	2.38	0.49
2:C:638:ASN:HD22	2:C:639:TRP:N	2.11	0.49
2:E:1267:PHE:HA	2:E:1281:LYS:O	2.13	0.49
2:E:1297:ASN:OD1	2:E:1297:ASN:C	2.55	0.49
2:E:1365:ILE:HG12	2:E:1366:GLN:N	2.26	0.49
2:F:1686:TRP:CZ2	2:F:1711:ARG:HD3	2.47	0.49
2:B:337:LEU:HB3	2:B:429:LEU:HG	1.95	0.49
2:E:1261:LEU:C	2:E:1261:LEU:CD2	2.84	0.49
2:C:571:ARG:O	2:C:572:ASN:CB	2.56	0.49
1:D:1124:LEU:O	1:D:1128:LEU:HB2	2.13	0.49
2:E:1415:LYS:HB3	2:E:1422:TYR:CD2	2.48	0.49
2:F:1655:VAL:HG12	2:F:1657:TRP:HZ3	1.78	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:1080:LEU:CD1	1:D:1118:GLU:HG3	2.43	0.48
1:D:1093:LEU:HB2	1:D:1097:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1266:LEU:C	2:E:1266:LEU:HD23	2.37	0.48
2:F:1638:ASN:HD22	2:F:1639:TRP:N	2.11	0.48
2:B:282:GLU:HG3	2:B:283:CYS:N	2.28	0.48
2:E:1272:ASN:ND2	2:E:1272:ASN:N	2.57	0.48
2:E:1287:VAL:O	2:E:1288:SER:C	2.57	0.48
2:E:1386:TRP:CZ3	2:E:1411:ARG:HG3	2.48	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:B:278:GLN:O	2:B:278:GLN:HG3	2.13	0.48
2:B:417:ARG:O	2:B:418:ASN:HB2	2.14	0.48
1:D:1016:ARG:NH1	1:D:1113:LEU:HD22	2.29	0.47
1:A:37:PRO:HG2	1:A:40:GLN:CB	2.45	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
1:D:1080:LEU:HB2	1:D:1121:ILE:CG2	2.44	0.47
2:E:1337:LEU:HD22	2:E:1357:TRP:HB3	1.95	0.47
2:E:1407:GLU:HG3	2:E:1432:THR:CG2	2.44	0.47
2:B:348:GLY:O	2:B:404:VAL:HG11	2.14	0.47
2:C:535:PHE:CE2	2:C:611:LEU:HB2	2.48	0.47
1:D:1111:TYR:HA	1:D:1114:LEU:HD12	1.96	0.47
2:E:1236:THR:HG23	2:E:1237:LYS:N	2.30	0.47
2:B:297:ASN:C	2:B:297:ASN:OD1	2.57	0.47
2:C:535:PHE:HA	2:C:550:TRP:HB3	1.95	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:F:1650:HIS:CE1	2:F:1703:LYS:NZ	2.73	0.47
1:D:1002:PRO:HD2	1:D:1127:ARG:HD2	1.97	0.47
2:E:1376:LEU:C	2:E:1376:LEU:CD2	2.80	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
2:B:325:VAL:O	2:B:328:ILE:HG12	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: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:D:1003:THR:CG2	2:F:1606:PRO:HG3	2.45	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:D:1053:CYS:HB3	1:D:1054:PRO:HD2	1.96	0.47
1:D:1064:LYS:NZ	2:E:1364:ASP:OD2	2.46	0.47
2:E:1314:ASN:CG	2:E:1315:GLY:N	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ILE:O	1:A:127:ARG:NH1	2.47	0.46
2:C:535:PHE:CZ	2:C:566:LEU:HD12	2.49	0.46
2:C:582:GLU:HG3	2:C:583:CYS:H	1.79	0.46
1:D:1009:LEU:N	1:D:1009:LEU:HD23	2.30	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
1:D:1099:ASN:HD22	1:D:1099:ASN:H	1.62	0.46
2:E:1244:GLU:O	2:E:1298:SER:HA	2.14	0.46
2:E:1386:TRP:CH2	2:E:1411:ARG:CG	2.97	0.46
2:F:1637:LEU:O	2:F:1638:ASN:HB3	2.14	0.46
1:A:60:THR:HA	1:A:61:PRO:HD3	1.85	0.46
1:A:71:SER:H	1:A:74:GLU:HG3	1.81	0.46
2:B:364:ASP:OD1	2:B:366:GLN:NE2	2.49	0.46
2:E:1385:LYS:H	2:E:1385:LYS:CD	2.28	0.46
2:F:1732:THR:O	2:F:1732:THR:OG1	2.33	0.46
1:A:22:GLN:HA	2:B:418:ASN:OD1	2.16	0.46
1:A:90:VAL:HG21	1:A:114:LEU:HD11	1.98	0.46
1:A:179:THR:O	1:A:183:ARG:HG3	2.15	0.46
2:C:548:CYS:O	2:C:593:SER:HA	2.15	0.46
1:D:1111:TYR:CD1	1:D:1111:TYR:C	2.94	0.46
1:A:44:PHE:HE2	1:A:160:TYR:CE2	2.34	0.46
2:C:600:PHE:O	2:C:607:TYR:OH	2.30	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: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
1:A:80:LEU:HD11	1:A:118:GLU:HG3	1.97	0.46
1:D:1115:LYS:HD2	1:D:1115:LYS:HA	1.46	0.46
1:A:22:GLN:HG3	1:A:23:LEU:N	2.31	0.46
1:A:170:MET:HE2	1:A:170:MET:HA	1.98	0.46
2:B:337:LEU:HD22	2:B:357:TRP:HB2	1.98	0.46
2:B:386:TRP:CH2	2:B:411:ARG:CG	2.98	0.46
2:C:538:CYS:HA	2:C:547:SER:O	2.16	0.46
1:D:1045:TRP:O	1:D:1051:SER:OG	2.29	0.45
2:E:1282:GLU:O	2:E:1283:CYS:C	2.59	0.45
2:E:1407:GLU:HG3	2:E:1432:THR:HG22	1.97	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:C:646:LEU:C	2:C:648:GLY:H	2.23	0.45
2:F:1585:ASP:CG	2:F:1588:SER:HB2	2.42	0.45
1:A:172:LYS:HD3	1:A:176:TYR:OH	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:1666:GLN:H	2:F:1666:GLN:HG2	1.45	0.45
1:A:19:ARG:HG2	2:C:667:LYS:O	2.16	0.45
2:C:542:GLU:O	2:C:543:ARG:CB	2.64	0.45
1:D:1166:PHE:CE2	1:D:1170:MET:HE3	2.52	0.45
2:E:1325:VAL:O	2:E:1328:ILE:HG12	2.16	0.45
1:A:7:SER:O	1:A:8:ARG:C	2.58	0.45
2:B:385:LYS:CD	2:B:385:LYS:H	2.30	0.45
2:B:386:TRP:CZ3	2:B:411:ARG:HG3	2.51	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:1646:LEU:C	2:F:1648:GLY:H	2.24	0.45
2:F:1715:LYS:HG3	2:F:1716:GLN:O	2.17	0.45
2:C:568:TYR:C	2:C:568:TYR:CD1	2.94	0.45
1:D:1079:SER:O	1:D:1083:ILE:HG12	2.16	0.45
2:E:1348:GLY:O	2:E:1404:VAL:HG11	2.17	0.45
2:B:282:GLU:OE1	2:B:286:TYR:OH	2.29	0.45
2:C:549:HIS:CE1	2:C:593:SER:HB2	2.52	0.45
2:B:267:PHE:CA	2:B:281:LYS:O	2.65	0.45
2:E:1245:THR:HA	2:E:1301:THR:OG1	2.16	0.45
2:E:1313:SER:OG	2:E:1314:ASN:N	2.48	0.45
2:E:1376:LEU:HD23	2:E:1376:LEU:O	2.17	0.45
1:A:96:VAL:HG11	1:A:163:LEU:HD11	1.97	0.45
1:D:1064:LYS:HD2	2:E:1244:GLU:OE1	2.17	0.45
2:B:392:ILE:H	2:B:392:ILE:HG13	1.67	0.44
2:C:713:ARG:HD2	2:C:725:PHE:CE1	2.51	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:F:1657:TRP:CH2	2:F:1697:VAL:HG12	2.52	0.44
1:A:93:LEU:O	1:A:94:ARG:C	2.60	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:F:1536:THR:H	2:F:1550:TRP:HA	1.81	0.44
1:A:84:GLN:HA	1:A:87:LEU:HG	1.98	0.44
2:B:337:LEU:HD11	2:B:412:VAL:HG23	1.99	0.44
2:E:1280:TRP:CH2	2:E:1310:LYS:HD2	2.52	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:1540:SER:OG	2:F:1545:THR:O	2.26	0.44
2:F:1620:GLU:O	2:F:1620:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LYS:HD2	1:A:115:LYS:HA	1.58	0.44
2:B:287:VAL:O	2:B:288:SER:C	2.61	0.44
2:B:365:ILE:HG12	2:B:366:GLN:N	2.32	0.44
2:E:1337:LEU:HD22	2:E:1357:TRP:HB2	2.00	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
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: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
2:C:677:GLN:HG3	2:C:725:PHE:CE1	2.53	0.43
2:B:272:ASN:ND2	2:B:273:THR:H	2.16	0.43
2:F:1716:GLN:CG	2:F:1717:ARG:N	2.78	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
1:A:32:GLU:C	1:A:34:ALA:H	2.27	0.43
2:B:407:GLU:HG3	2:B:432:THR:CG2	2.48	0.43
2:E:1289:ALA:HB3	2:E:1293:SER:OG	2.17	0.43
2:E:1385:LYS:O	2:E:1385:LYS:HD3	2.19	0.43
2:F:1718:ASN:HD22	2:F:1718:ASN:C	2.27	0.43
1:A:64:LYS:HE3	2:B:364:ASP:OD2	2.18	0.43
2:B:366:GLN:H	2:B:366:GLN:HG3	1.51	0.43
2:C:549:HIS:ND1	2:C:593:SER:HB2	2.34	0.43
2:B:376:LEU:C	2:B:376:LEU:CD2	2.84	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:A:77:ARG:O	1:A:78:ILE:C	2.62	0.43
2:C:623:PHE:CD2	2:C:623:PHE:N	2.87	0.43
1:D:1001:PHE:CD2	1:D:1006:LEU:HG	2.53	0.43
1:D:1080:LEU:HD12	1:D:1080:LEU:O	2.18	0.43
2:E:1379:LYS:HG3	2:E:1383:GLU:HB2	2.00	0.43
1:A:29:GLN:O	1:A:33:GLU:HB2	2.19	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
1:D:1162:LEU:HD23	1:D:1162:LEU:HA	1.83	0.43
2:E:1239:ARG:O	2:E:1239:ARG:HG2	2.19	0.43
2:E:1247:SER:HB2	2:E:1294:CYS:O	2.19	0.43
2:F:1675:GLU:CD	2:F:1713:ARG:NH2	2.77	0.43
2:E:1414:SER:O	2:E:1423:GLY:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:LEU:HB2	1:A:97:PHE:CE1	2.54	0.42
2:C:666:GLN:OE1	2:F:1579:GLU:HG3	2.19	0.42
2:E:1375:GLU:OE2	2:E:1388:MET:HG2	2.19	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:F:1697:VAL:HG22	2:F:1698:PRO:HD2	2.01	0.42
1:A:94:ARG:O	1:A:95:SER:C	2.62	0.42
2:B:388:MET:HE2	2:B:388:MET:H	1.84	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:H	2:E:1366:GLN:NE2	2.17	0.42
2:C:674:TYR:CD2	2:C:674:TYR:N	2.88	0.42
2:F:1611:LEU:HD23	2:F:1611:LEU:HA	1.85	0.42
2:B:385:LYS:O	2:B:385:LYS:HD3	2.20	0.42
1:D:1042:HIS:HD2	1:D:1044:PHE:CZ	2.37	0.42
1:D:1064:LYS:HE3	2:E:1364:ASP:OD2	2.19	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
1:A:14:TRP:CZ3	1:A:15:LEU:HD23	2.54	0.42
1:D:1060:THR:HA	1:D:1061:PRO:HD3	1.82	0.42
2:F:1677:GLN:HG3	2:F:1725:PHE:CE1	2.55	0.42
1:D:1019:ARG:HG3	1:D:1023:LEU:HD22	2.01	0.41
2:B:302:SER:HB3	2:B:305:ILE:HG13	2.02	0.41
2:B:310:LYS:NZ	2:B:320:GLU:OE2	2.39	0.41
2:B:337:LEU:HD11	2:B:412:VAL:CG2	2.49	0.41
2:B:282:GLU:O	2:B:283:CYS:C	2.63	0.41
2:C:536:THR:HG22	2:C:549:HIS:O	2.19	0.41
2:B:236:THR:HG22	2:B:249:HIS:C	2.45	0.41
2:F:1566:LEU:HD11	2:F:1609:ILE:HB	2.02	0.41
1:A:80:LEU:HB2	1:A:121:ILE:CG2	2.50	0.41
2:C:567:PHE:CE2	2:C:582:GLU:HB2	2.55	0.41
1:D:1172:LYS:HE2	2:E:1304:TRP:CE3	2.55	0.41
2:E:1345:SER:HB2	2:F:1700:TYR:CG	2.55	0.41
2:F:1613:SER:HB3	2:F:1614:ASN:H	1.68	0.41
2:B:280:TRP:CZ2	2:B:310:LYS:HD2	2.55	0.41
2:B:388:MET:HB2	2:B:388:MET:HE3	1.71	0.41
2:C:675:GLU:CD	2:C:713:ARG:NH2	2.79	0.41
1:D:1031:PHE:HE2	1:D:1160:TYR:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1713:ARG:HH21	2:F:1713:ARG:HD3	1.71	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:HE21	1:A:22:GLN:HB2	1.54	0.41
1:D:1179:THR:O	1:D:1183:ARG:HG3	2.20	0.41
2:E:1357:TRP:O	2:E:1395:THR:HB	2.20	0.41
1:A:2:PRO:HA	1:A:5:PRO:HD3	2.02	0.41
1:A:64:LYS:NZ	2:B:364:ASP:OD2	2.53	0.41
2:B:235:PHE:CZ	2:B:309:ILE:HG13	2.55	0.41
2:C:715:LYS:HB2	2:C:715:LYS:HE2	1.83	0.41
2:C:732:THR:O	2:C:732:THR:OG1	2.30	0.41
1:D:1014:TRP:O	1:D:1018:ASP:N	2.47	0.41
1:D:1016:ARG:NH2	2:F:1669:TRP:CD1	2.89	0.41
1:D:1172:LYS:HD3	1:D:1176:TYR:OH	2.21	0.41
2:E:1376:LEU:HD23	2:E:1377:GLN:N	2.36	0.41
2:F:1566:LEU:HG	2:F:1567:PHE:N	2.36	0.41
2:F:1589:ALA:CB	2:F:1595:TYR:HB2	2.48	0.41
2:F:1642:LEU:HD23	2:F:1642:LEU:HA	1.83	0.41
2:F:1674:TYR:CD2	2:F:1674:TYR:N	2.89	0.41
2:B:235:PHE:CE1	2:B:266:LEU:HD12	2.56	0.41
2:B:239:ARG:O	2:B:239:ARG:HG2	2.20	0.41
2:E:1345:SER:HB2	2:F:1700:TYR:CB	2.46	0.41
2:E:1346:LEU:HD12	2:E:1346:LEU:HA	1.85	0.41
2:F:1570:ARG:HD2	2:F:1607:TYR:CE2	2.56	0.41
1:A:63:ASN:OD1	1:A:65:GLU:HB2	2.21	0.40
2:B:266:LEU:HD23	2:B:266:LEU:O	2.21	0.40
2:B:270:ARG:HB2	2:B:306:PRO:O	2.21	0.40
1:D:1072:ASN:O	1:D:1076:LEU:HD12	2.21	0.40
1:A:126:GLY:C	1:A:128:LEU:N	2.78	0.40
1:A:162:LEU:HA	1:A:162:LEU:HD23	1.89	0.40
2:B:359:ALA:O	2:B:360:PRO:C	2.62	0.40
2:C:535:PHE:HZ	2:C:566:LEU:HD12	1.84	0.40
2:F:1583:CYS:HA	2:F:1584:PRO:HD3	1.90	0.40
1:A:170:MET:HE2	1:A:170:MET:CA	2.52	0.40
2:B:341:LEU:HD23	2:B:353:ILE:HG22	2.02	0.40
2:E:1337:LEU:HD11	2:E:1412:VAL:HG23	2.03	0.40
2:F:1679:LYS:HG2	2:F:1686:TRP:CE3	2.56	0.40
2:B:335:ILE:HG13	2:B:358:GLU:HB3	2.03	0.40
2:C:692:ILE:H	2:C:692:ILE:HG13	1.59	0.40
1:D:1036:ILE:HG13	1:D:1160:TYR:CE1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1342:LEU:HD23	2:E:1342:LEU:HA	1.87	0.40
2:F:1565:GLN:O	2:F:1611:LEU:CD2	2.69	0.40
2:F:1618:VAL:CG1	2:F:1619:ASP:H	2.34	0.40
1:A:111:TYR:HA	1:A:114:LEU:HD12	2.04	0.40
1:A:128:LEU:HD23	1:A:128:LEU:HA	1.93	0.40
2:B:362:ASN:OD1	2:B:362:ASN:N	2.54	0.40
2:B:380:GLU:CD	2:B:406:LYS:HD2	2.46	0.40
2:B:407:GLU:HG3	2:B:432:THR:HG22	2.03	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
2:E:1372:LEU:HD12	2:E:1372:LEU:HA	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	154/191 (81%)	129 (84%)	19 (12%)	6 (4%)	2	3
1	D	150/191 (78%)	129 (86%)	17 (11%)	4 (3%)	4	7
2	B	189/238 (79%)	168 (89%)	20 (11%)	1 (0%)	24	46
2	C	167/238 (70%)	144 (86%)	21 (13%)	2 (1%)	10	23
2	E	189/238 (79%)	171 (90%)	16 (8%)	2 (1%)	11	25
2	F	178/238 (75%)	155 (87%)	20 (11%)	3 (2%)	7	15
All	All	1027/1334 (77%)	896 (87%)	113 (11%)	18 (2%)	6	14

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	SER

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Mol	Chain	Res	Type
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%)	114 (80%)	29 (20%)	1	2
1	D	142/175 (81%)	110 (78%)	32 (22%)	1	1
2	B	177/218 (81%)	123 (70%)	54 (30%)	0	0
2	C	157/218 (72%)	108 (69%)	49 (31%)	0	0
2	E	177/218 (81%)	128 (72%)	49 (28%)	0	1
2	F	165/218 (76%)	116 (70%)	49 (30%)	0	0
All	All	961/1222 (79%)	699 (73%)	262 (27%)	0	1

All (262) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR

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Mol	Chain	Res	Type
1	A	4	ILE
1	A	9	LEU
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	102	VAL
1	A	103	TYR
1	A	113	LEU
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	265	GLN
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	303	ILE

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Mol	Chain	Res	Type
2	B	310	LYS
2	B	311	LEU
2	B	312	THR
2	B	314	ASN
2	B	318	VAL
2	B	320	GLU
2	B	321	LYS
2	B	337	LEU
2	B	340	THR
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	367	LYS
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	392	ILE
2	B	393	LEU
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

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Mol	Chain	Res	Type
2	C	539	ARG
2	C	542	GLU
2	C	551	THR
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	628	ILE
2	C	637	LEU
2	C	638	ASN
2	C	641	LEU
2	C	643	ASN
2	C	644	VAL
2	C	645	SER
2	C	646	LEU
2	C	654	GLN
2	C	658	GLU
2	C	665	ILE
2	C	666	GLN
2	C	669	TRP
2	C	672	LEU
2	C	674	TYR
2	C	675	GLU
2	C	681	VAL
2	C	684	THR
2	C	692	ILE
2	C	693	LEU
2	C	696	SER
2	C	699	VAL
2	C	701	SER
2	C	706	LYS
2	C	713	ARG
2	C	716	GLN

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Mol	Chain	Res	Type
2	C	718	ASN
2	C	719	SER
2	C	728	VAL
2	C	729	LEU
2	C	732	THR
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	1113	LEU
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	1185	VAL
1	D	1188	SER
2	E	1234	LYS
2	E	1236	THR
2	E	1237	LYS
2	E	1242	GLU
2	E	1272	ASN

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Mol	Chain	Res	Type
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	1321	LYS
2	E	1340	THR
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	1367	LYS
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	1389	MET
2	E	1392	ILE
2	E	1394	THR
2	E	1401	SER
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

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Mol	Chain	Res	Type
2	E	1428	VAL
2	E	1429	LEU
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	1640	THR
2	F	1641	LEU
2	F	1643	ASN
2	F	1644	VAL
2	F	1646	LEU
2	F	1658	GLU
2	F	1661	ARG
2	F	1665	ILE
2	F	1666	GLN
2	F	1669	TRP
2	F	1670	MET
2	F	1672	LEU
2	F	1675	GLU
2	F	1681	VAL
2	F	1684	THR
2	F	1692	ILE
2	F	1693	LEU
2	F	1696	SER
2	F	1699	VAL
2	F	1701	SER

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Mol	Chain	Res	Type
2	F	1706	LYS
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	68	GLN
1	A	91	GLN
1	A	99	ASN
1	A	122	GLN
1	A	167	ASN
2	B	272	ASN
2	B	314	ASN
2	B	343	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	1091	GLN
1	D	1099	ASN
1	D	1122	GLN
2	E	1265	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	1650	HIS
2	F	1716	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.