



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:11 AM UTC

PDB ID : 2VSK / pdb_00002vsk
Title : Hendra virus attachment glycoprotein in complex with human cell surface receptor ephrinB2
Authors : Bowden, T.A.; Aricescu, A.R.; Gilbert, R.J.; Grimes, J.M.; Jones, E.Y.; Stuart, D.I.
Deposited on : 2008-04-24
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

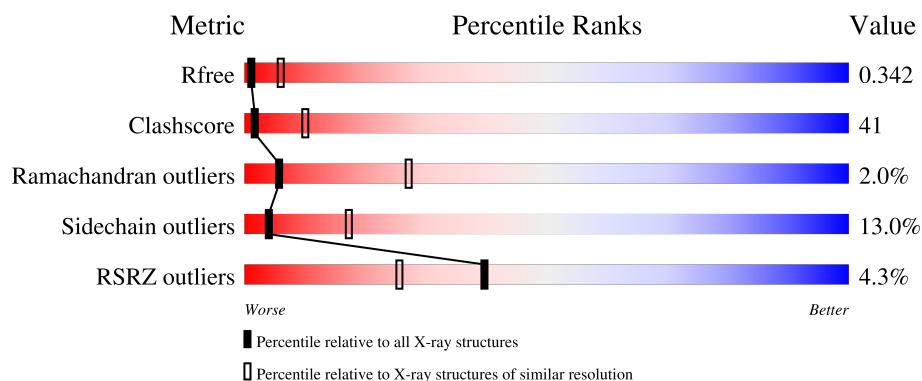
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

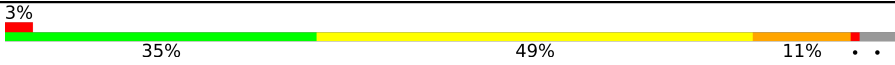
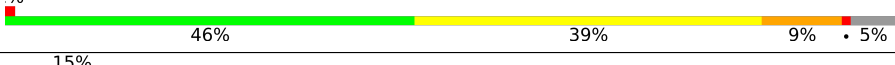
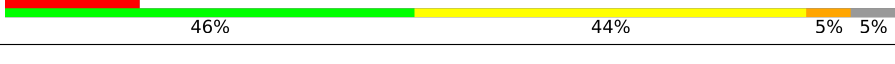
The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	416	
1	C	416	
2	B	138	
2	D	138	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8443 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 HEMAGGLUTININ-NEURAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	0	0
			3170	2025	530	596	19			
1	C	399	Total	C	N	O	S	0	0	0
			3161	2020	529	593	19			

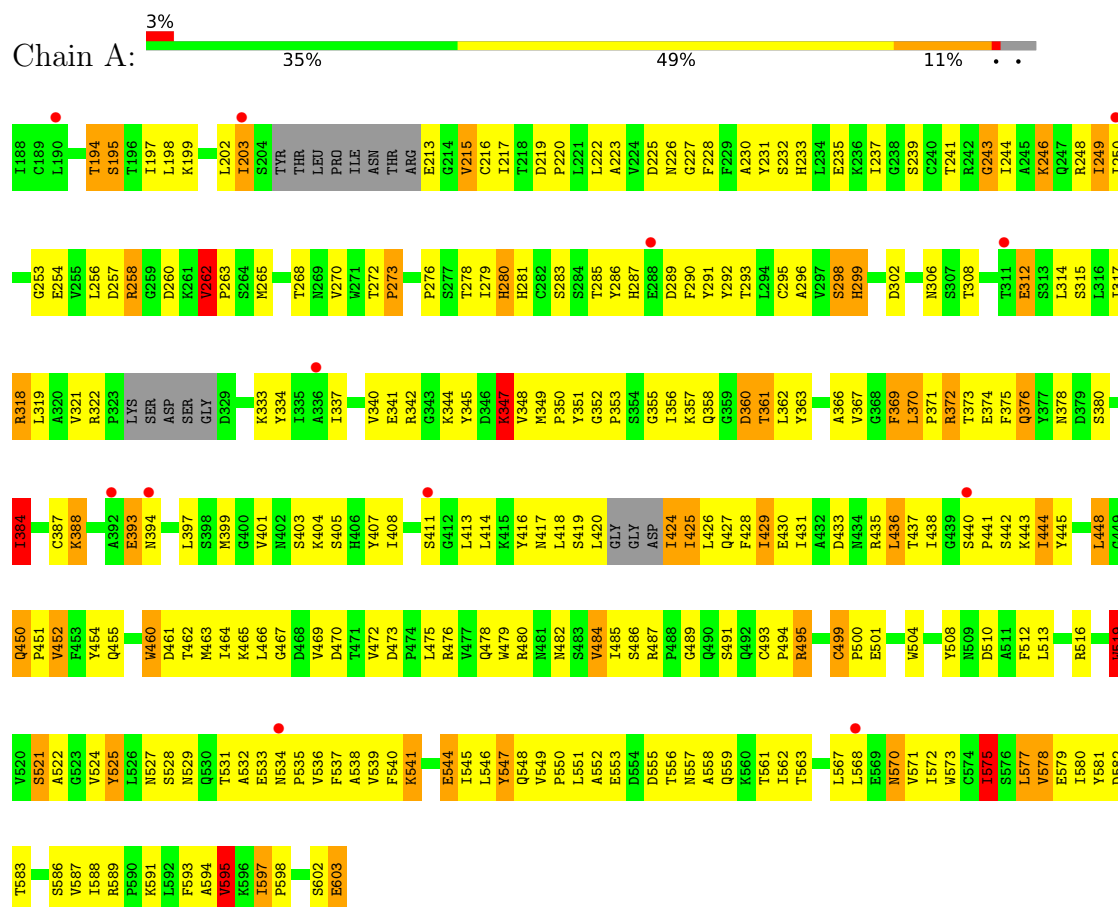
- Molecule 2 is a protein called EPHRIN-B2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	131	Total	C	N	O	S	0	0	0
			1056	681	169	199	7			
2	D	131	Total	C	N	O	S	0	0	0
			1056	681	169	199	7			

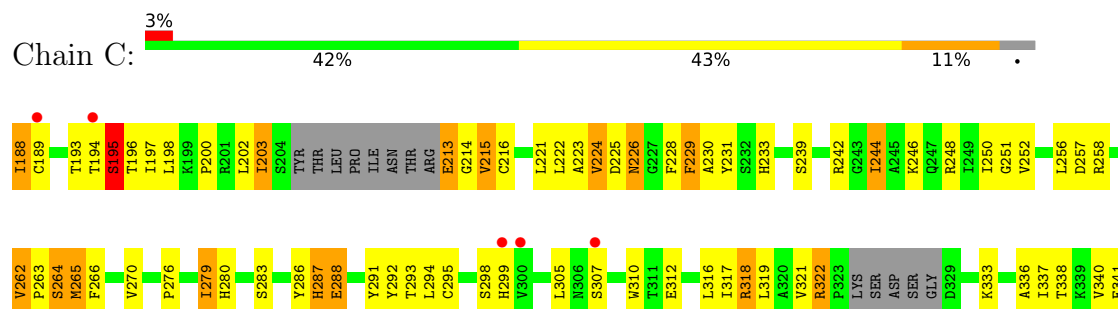
3 Residue-property plots

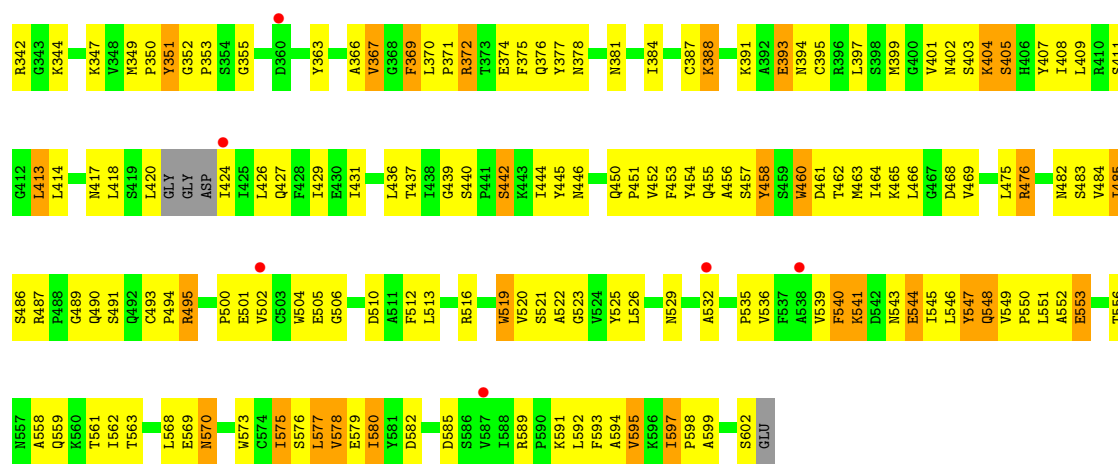
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: HEMAGGLUTININ-NEURAMINIDASE

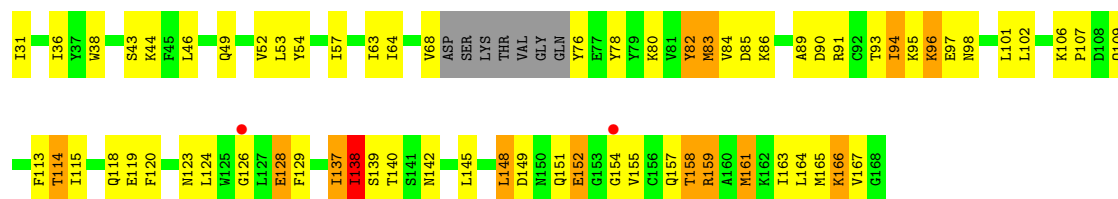


• Molecule 1: HEMAGGLUTININ-NEURAMINIDASE

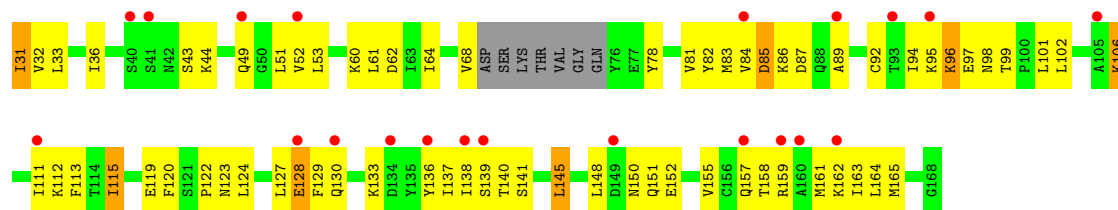




• Molecule 2: EPHRIN-B2



• Molecule 2: EPHRIN-B2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.25Å 106.17Å 196.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 20.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	82.7 (20.00-3.30) 93.0 (20.00-3.30)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 3.31Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.300 , 0.350 0.287 , 0.342	Depositor DCC
R_{free} test set	876 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 35.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.27$, $\langle L^2 \rangle = 0.11$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.70	EDS
Total number of atoms	8443	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.11	7/3245 (0.2%)	1.17	17/4415 (0.4%)
1	C	1.00	1/3236 (0.0%)	1.09	9/4403 (0.2%)
2	B	1.05	2/1078 (0.2%)	1.10	3/1454 (0.2%)
2	D	0.91	0/1078	1.04	4/1454 (0.3%)
All	All	1.04	10/8637 (0.1%)	1.12	33/11726 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	B	0	2
2	D	0	1
All	All	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	384	ILE	CA-CB	7.81	1.63	1.54
1	C	244	ILE	CA-CB	7.23	1.61	1.54
2	B	138	ILE	CA-CB	6.32	1.63	1.54
1	A	347	LYS	C-O	-5.95	1.16	1.23
1	A	270	VAL	CA-CB	-5.67	1.46	1.54
2	B	114	THR	CA-CB	5.20	1.60	1.53
1	A	244	ILE	CA-CB	5.19	1.60	1.54
1	A	203	ILE	CA-CB	5.17	1.61	1.54
1	A	597	ILE	CA-CB	-5.15	1.48	1.53
1	A	597	ILE	N-CA	-5.03	1.42	1.46

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	577	LEU	N-CA-C	-7.61	96.87	109.80
2	B	54	TYR	CA-C-N	-7.28	112.13	119.92
2	B	54	TYR	C-N-CA	-7.28	112.13	119.92
1	A	273	PRO	CA-C-N	6.84	126.47	119.56
1	A	273	PRO	C-N-CA	6.84	126.47	119.56
1	A	577	LEU	N-CA-C	-6.48	100.15	109.29
1	A	262	VAL	N-CA-C	-6.41	100.48	108.05
1	A	298	SER	N-CA-C	6.32	119.55	108.75
2	D	120	PHE	N-CA-C	6.11	118.69	108.73
1	A	237	ILE	CB-CA-C	-5.99	105.45	111.80
1	A	529	ASN	N-CA-C	5.90	117.38	111.07
1	A	425	ILE	CB-CA-C	-5.77	102.49	111.26
1	C	485	ILE	CB-CA-C	-5.77	103.66	111.63
1	A	370	LEU	CA-C-N	-5.68	113.86	119.99
1	A	370	LEU	C-N-CA	-5.68	113.86	119.99
1	A	575	ILE	N-CA-C	-5.66	101.74	109.55
1	C	540	PHE	N-CA-C	5.63	116.82	108.60
1	C	224	VAL	CB-CA-C	-5.52	104.12	110.41
1	A	589	ARG	N-CA-C	5.50	114.63	108.25
2	D	106	LYS	O-C-N	5.48	126.31	121.32
1	C	264	SER	N-CA-C	5.43	116.53	108.60
1	C	460	TRP	N-CA-C	5.36	118.61	111.75
1	C	589	ARG	N-CA-C	5.35	115.01	108.11
1	A	467	GLY	N-CA-C	5.33	118.25	111.37
1	A	499	CYS	CA-C-N	5.33	125.63	119.93
1	A	499	CYS	C-N-CA	5.33	125.63	119.93
1	A	299	HIS	N-CA-C	-5.26	106.71	113.23
1	A	460	TRP	N-CA-C	5.22	118.43	111.75
1	C	287	HIS	N-CA-C	5.18	116.81	108.32
2	D	99	THR	N-CA-C	-5.13	102.58	110.32
1	C	458	TYR	N-CA-C	5.12	119.39	113.20
2	D	115	ILE	CB-CA-C	-5.09	103.53	110.96
2	B	159	ARG	N-CA-C	-5.02	102.63	110.42

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	138	ILE	Peptide
2	B	158	THR	Peptide
1	C	322	ARG	Peptide
2	D	158	THR	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3170	0	3117	290	2
1	C	3161	0	3111	279	3
2	B	1056	0	1053	64	0
2	D	1056	0	1053	71	0
All	All	8443	0	8334	687	3

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 41.

All (687) 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:C:310:TRP:HB3	1:C:347:LYS:NZ	1.34	1.38
1:A:577:LEU:O	1:A:578:VAL:HG23	1.36	1.20
2:B:63:ILE:HD11	2:B:163:ILE:HD12	1.26	1.15
1:A:203:ILE:HD11	1:A:575:ILE:CD1	1.77	1.14
2:D:62:ASP:HB3	2:D:64:ILE:HD11	1.28	1.14
1:A:203:ILE:CD1	1:A:575:ILE:HD11	1.78	1.14
2:B:164:LEU:HD21	2:B:166:LYS:HZ1	1.08	1.13
1:A:347:LYS:HZ2	1:A:347:LYS:HB3	1.12	1.12
1:C:310:TRP:HE3	1:C:347:LYS:CE	1.64	1.09
1:C:310:TRP:CE3	1:C:347:LYS:HD2	1.87	1.08
1:A:451:PRO:HG2	1:A:469:VAL:HG21	1.33	1.08
1:A:420:LEU:HD13	1:A:424:ILE:HG23	1.16	1.06
1:A:552:ALA:HB1	1:A:556:THR:HG21	1.37	1.05
2:B:164:LEU:HD21	2:B:166:LYS:NZ	1.70	1.05
1:C:257:ASP:HB3	1:C:568:LEU:HD21	1.39	1.05
1:A:451:PRO:HG2	1:A:469:VAL:CG2	1.87	1.04
1:C:287:HIS:HD2	1:C:418:LEU:CD1	1.69	1.03
1:C:417:ASN:O	1:C:420:LEU:HD12	1.60	1.02
1:C:293:THR:O	1:C:316:LEU:HD12	1.56	1.01
1:A:287:HIS:ND1	1:A:418:LEU:HD12	1.76	1.01
1:A:203:ILE:HD11	1:A:575:ILE:HD11	0.99	0.99
1:A:577:LEU:HG	1:A:578:VAL:H	1.27	0.98
1:C:287:HIS:HD2	1:C:418:LEU:HD12	1.29	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:LEU:CD1	1:A:424:ILE:HG23	1.93	0.97
1:C:413:LEU:HD11	1:C:475:LEU:HD22	1.47	0.96
1:C:287:HIS:CD2	1:C:418:LEU:HD12	2.01	0.95
1:A:408:ILE:HD12	1:A:408:ILE:C	1.91	0.94
1:A:197:ILE:HG22	1:A:602:SER:O	1.68	0.94
2:B:84:VAL:HG23	2:B:85:ASP:O	1.69	0.93
1:A:370:LEU:HD22	1:A:375:PHE:HB2	1.48	0.93
1:C:293:THR:N	1:C:316:LEU:HD11	1.84	0.92
1:A:411:SER:O	1:A:431:ILE:HG22	1.68	0.92
1:C:198:LEU:HB2	1:C:549:VAL:HG21	1.50	0.91
1:C:310:TRP:HB3	1:C:347:LYS:HZ1	1.35	0.91
1:C:548:GLN:O	1:C:549:VAL:HG23	1.69	0.91
1:A:408:ILE:HD12	1:A:408:ILE:O	1.69	0.91
1:C:310:TRP:CB	1:C:347:LYS:NZ	2.29	0.91
1:A:448:LEU:HD23	1:A:448:LEU:H	1.36	0.90
1:C:552:ALA:HB1	1:C:556:THR:HG21	1.52	0.90
1:A:287:HIS:ND1	1:A:418:LEU:CD1	2.33	0.90
1:C:310:TRP:HB3	1:C:347:LYS:HZ2	1.10	0.89
1:C:310:TRP:CB	1:C:347:LYS:HZ2	1.84	0.89
1:A:573:TRP:CZ3	1:A:594:ALA:HB1	2.08	0.89
1:C:413:LEU:CD1	1:C:475:LEU:HD22	2.02	0.89
1:C:310:TRP:CE3	1:C:347:LYS:CD	2.55	0.88
1:C:310:TRP:HE3	1:C:347:LYS:CD	1.87	0.87
1:C:548:GLN:O	1:C:549:VAL:CG2	2.23	0.87
2:B:63:ILE:HD11	2:B:163:ILE:CD1	2.04	0.87
1:A:367:VAL:HG13	1:A:369:PHE:CE2	2.09	0.87
1:A:429:ILE:HG21	1:A:473:ASP:OD1	1.74	0.87
1:C:337:ILE:HG21	1:C:426:LEU:HD12	1.56	0.86
1:C:310:TRP:CE3	1:C:347:LYS:CE	2.55	0.86
1:C:310:TRP:HE3	1:C:347:LYS:NZ	1.74	0.85
1:A:347:LYS:HZ2	1:A:347:LYS:CB	1.84	0.85
1:A:577:LEU:O	1:A:578:VAL:CG2	2.23	0.84
1:C:197:ILE:HG22	1:C:602:SER:O	1.77	0.84
1:C:575:ILE:HD12	1:C:592:LEU:HD22	1.59	0.84
1:C:293:THR:C	1:C:316:LEU:HD12	2.02	0.84
1:C:293:THR:C	1:C:316:LEU:CD1	2.50	0.83
1:C:310:TRP:CZ3	1:C:347:LYS:HD2	2.12	0.83
1:A:448:LEU:HD23	1:A:448:LEU:N	1.94	0.83
1:A:347:LYS:HB3	1:A:347:LYS:NZ	1.93	0.83
2:B:63:ILE:HG22	2:B:102:LEU:HD12	1.60	0.83
1:A:420:LEU:HD13	1:A:424:ILE:CG2	2.07	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:LEU:HD12	1:C:502:VAL:HG21	1.61	0.83
1:C:462:THR:HG22	1:C:487:ARG:CZ	2.09	0.82
1:A:197:ILE:HD11	1:A:547:TYR:CD1	2.14	0.82
1:C:198:LEU:HB2	1:C:549:VAL:CG2	2.09	0.82
1:A:370:LEU:HD23	1:A:371:PRO:O	1.78	0.81
2:B:137:ILE:HG13	2:B:165:MET:HE2	1.61	0.81
1:C:553:GLU:HB2	1:C:556:THR:HG23	1.63	0.80
1:A:287:HIS:CE1	1:A:418:LEU:HD12	2.15	0.79
2:D:82:TYR:CZ	2:D:94:ILE:HD12	2.16	0.79
2:D:62:ASP:HB3	2:D:64:ILE:CD1	2.11	0.79
1:A:337:ILE:HG21	1:A:426:LEU:HD12	1.62	0.79
1:C:420:LEU:HD13	1:C:424:ILE:HG23	1.65	0.79
1:A:567:LEU:HD22	1:A:570:ASN:C	2.07	0.79
1:A:553:GLU:HB2	1:A:556:THR:HG23	1.64	0.78
2:D:82:TYR:CE2	2:D:94:ILE:CD1	2.67	0.78
1:A:197:ILE:HD11	1:A:547:TYR:CG	2.19	0.77
1:C:221:LEU:C	1:C:221:LEU:HD23	2.09	0.77
1:C:408:ILE:HD12	1:C:408:ILE:O	1.84	0.77
2:D:62:ASP:CB	2:D:64:ILE:HD11	2.13	0.77
1:C:197:ILE:HD12	1:C:598:PRO:HG3	1.65	0.77
1:A:384:ILE:HG22	1:A:500:PRO:HG2	1.67	0.77
1:A:213:GLU:O	1:A:587:VAL:HG22	1.84	0.77
1:A:480:ARG:HG3	1:A:519:TRP:CZ3	2.20	0.77
1:C:535:PRO:HD3	1:C:558:ALA:HB3	1.67	0.77
2:B:155:VAL:HG23	2:B:161:MET:HB2	1.67	0.76
2:B:164:LEU:CD2	2:B:166:LYS:NZ	2.47	0.76
1:C:310:TRP:CE3	1:C:347:LYS:NZ	2.51	0.76
2:D:122:PRO:O	2:D:124:LEU:CD2	2.33	0.76
1:A:583:THR:HG23	2:B:57:ILE:HG22	1.65	0.76
2:D:119:GLU:HG2	2:D:130:GLN:HE22	1.50	0.76
1:A:347:LYS:CB	1:A:347:LYS:NZ	2.48	0.75
1:C:399:MET:HE1	1:C:436:LEU:HG	1.67	0.75
1:C:452:VAL:HG22	1:C:468:ASP:OD1	1.87	0.75
2:D:31:ILE:HG22	2:D:33:LEU:HD23	1.67	0.75
2:B:52:VAL:HG22	2:B:164:LEU:HB3	1.68	0.74
1:C:594:ALA:O	1:C:595:VAL:HG23	1.88	0.74
1:C:442:SER:HB3	1:C:455:GLN:HA	1.70	0.73
1:A:408:ILE:C	1:A:408:ILE:CD1	2.60	0.73
1:C:198:LEU:CB	1:C:549:VAL:HG21	2.18	0.73
1:C:541:LYS:NZ	1:C:546:LEU:HD21	2.03	0.73
2:D:52:VAL:HG22	2:D:164:LEU:HD23	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:ALA:HB1	1:A:558:ALA:O	1.89	0.73
1:A:366:ALA:CB	1:A:414:LEU:HD12	2.19	0.72
2:D:92:CYS:SG	2:D:157:GLN:HB2	2.29	0.72
2:D:155:VAL:O	2:D:159:ARG:O	2.07	0.72
1:A:393:GLU:HB2	1:A:397:LEU:HD11	1.72	0.72
1:C:536:VAL:HG13	1:C:549:VAL:C	2.15	0.72
1:C:536:VAL:HG22	1:C:550:PRO:HA	1.72	0.72
1:A:533:GLU:OE2	1:A:555:ASP:HA	1.89	0.72
1:C:351:TYR:HB2	1:C:367:VAL:HG12	1.72	0.72
1:A:442:SER:HB2	1:A:454:TYR:O	1.90	0.71
2:B:80:LYS:O	2:B:139:SER:OG	2.05	0.71
1:A:361:THR:HG23	1:A:417:ASN:HA	1.72	0.71
1:C:250:ILE:HG22	1:C:319:LEU:HD11	1.72	0.71
1:A:262:VAL:HG12	1:A:263:PRO:O	1.90	0.71
2:B:91:ARG:NH1	1:C:213:GLU:HG3	2.05	0.71
1:C:462:THR:HG22	1:C:487:ARG:NH2	2.05	0.71
1:A:537:PHE:CE2	1:A:595:VAL:HG11	2.25	0.70
1:C:305:LEU:HD21	1:C:504:TRP:HH2	1.55	0.70
1:C:312:GLU:HB2	1:C:347:LYS:HB2	1.72	0.70
1:C:535:PRO:HG3	1:C:558:ALA:HB2	1.74	0.70
1:C:197:ILE:HD12	1:C:598:PRO:CG	2.22	0.70
1:A:416:TYR:HD1	1:A:426:LEU:HD23	1.56	0.70
1:C:198:LEU:HD11	1:C:539:VAL:CG2	2.22	0.70
1:C:293:THR:H	1:C:316:LEU:HD11	1.54	0.70
1:A:372:ARG:HA	1:A:375:PHE:HB3	1.74	0.69
1:A:367:VAL:HG13	1:A:369:PHE:HE2	1.55	0.69
1:A:463:MET:HE2	1:A:482:ASN:O	1.92	0.69
2:B:80:LYS:HG3	2:B:148:LEU:HD11	1.73	0.69
1:C:287:HIS:CD2	1:C:418:LEU:CD1	2.60	0.69
1:C:577:LEU:O	1:C:578:VAL:HG23	1.92	0.69
2:D:155:VAL:HG23	2:D:161:MET:HB2	1.75	0.69
1:C:265:MET:O	1:C:265:MET:HG3	1.91	0.69
1:A:573:TRP:HZ3	1:A:594:ALA:HB1	1.57	0.68
1:A:577:LEU:HG	1:A:578:VAL:N	2.05	0.68
1:A:254:GLU:HB3	1:A:256:LEU:HD21	1.76	0.68
1:A:257:ASP:HB3	1:A:568:LEU:HD21	1.75	0.68
1:C:203:ILE:HG23	1:C:203:ILE:O	1.92	0.68
1:C:456:ALA:HB1	1:C:458:TYR:CE2	2.29	0.67
1:A:198:LEU:HD11	1:A:539:VAL:HG23	1.75	0.67
1:A:257:ASP:HB3	1:A:568:LEU:HD11	1.77	0.67
2:D:82:TYR:CE2	2:D:94:ILE:HD12	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:TYR:HE2	1:A:249:ILE:HD11	1.58	0.67
1:A:536:VAL:HG13	1:A:549:VAL:C	2.20	0.67
1:A:378:ASN:OD1	1:A:378:ASN:C	2.37	0.67
1:C:548:GLN:C	1:C:549:VAL:HG23	2.18	0.67
2:D:78:TYR:HB3	2:D:148:LEU:HD13	1.75	0.67
1:C:256:LEU:HD12	1:C:266:PHE:CD2	2.30	0.66
1:A:366:ALA:HB2	1:A:414:LEU:HD12	1.76	0.66
1:A:399:MET:CE	1:A:436:LEU:HG	2.24	0.66
1:A:552:ALA:HB1	1:A:556:THR:CG2	2.22	0.66
1:C:310:TRP:CG	1:C:347:LYS:HZ2	2.13	0.66
1:C:401:VAL:HG22	1:C:504:TRP:CE3	2.31	0.66
2:B:63:ILE:HG22	2:B:102:LEU:CD1	2.24	0.66
1:A:220:PRO:HB2	1:A:577:LEU:HD21	1.76	0.66
1:C:562:ILE:HD12	1:C:577:LEU:HD23	1.77	0.66
1:C:437:THR:HG23	1:C:465:LYS:NZ	2.11	0.66
1:A:493:CYS:SG	1:A:501:GLU:HB2	2.36	0.66
1:C:294:LEU:HD12	1:C:316:LEU:HB2	1.78	0.66
1:A:450:GLN:OE1	1:A:469:VAL:O	2.14	0.66
1:C:535:PRO:HG3	1:C:558:ALA:CB	2.26	0.66
1:C:293:THR:O	1:C:293:THR:HG23	1.94	0.65
1:A:581:TYR:HD2	2:B:120:PHE:CE2	2.14	0.65
1:A:545:ILE:HG21	1:A:548:GLN:HG3	1.78	0.65
1:C:463:MET:HE2	1:C:483:SER:HA	1.79	0.65
1:A:213:GLU:O	1:A:587:VAL:CG2	2.45	0.65
2:D:32:VAL:HG22	2:D:60:LYS:CG	2.27	0.65
1:C:226:ASN:N	1:C:226:ASN:ND2	2.44	0.65
1:C:294:LEU:HD11	1:C:337:ILE:HD11	1.78	0.64
1:C:310:TRP:HB3	1:C:347:LYS:HZ3	1.57	0.64
1:C:413:LEU:HD11	1:C:475:LEU:CD2	2.27	0.64
1:A:417:ASN:O	1:A:420:LEU:HD12	1.97	0.64
2:B:78:TYR:CE1	2:B:145:LEU:HD13	2.32	0.64
1:C:547:TYR:N	1:C:547:TYR:CD2	2.66	0.64
2:D:119:GLU:HG2	2:D:130:GLN:NE2	2.11	0.64
1:C:292:TYR:HB3	1:C:316:LEU:HD21	1.79	0.64
2:D:84:VAL:HG22	2:D:136:TYR:O	1.98	0.64
1:A:198:LEU:HD11	1:A:539:VAL:CG2	2.28	0.63
1:A:318:ARG:HG3	1:A:333:LYS:HB3	1.81	0.63
1:C:198:LEU:HD11	1:C:539:VAL:HG23	1.81	0.63
1:C:370:LEU:HB3	1:C:408:ILE:HD11	1.79	0.63
1:A:223:ALA:HB3	1:A:230:ALA:HB3	1.81	0.62
1:A:416:TYR:HD1	1:A:426:LEU:CD2	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:ALA:O	1:A:595:VAL:HG23	1.99	0.62
1:A:351:TYR:CE1	1:A:441:PRO:HD3	2.35	0.62
1:A:399:MET:HE3	1:A:436:LEU:HG	1.81	0.62
1:A:567:LEU:HD22	1:A:571:VAL:N	2.15	0.62
1:C:197:ILE:CG2	1:C:602:SER:O	2.48	0.62
2:D:82:TYR:CE2	2:D:94:ILE:HD13	2.35	0.62
2:B:94:ILE:HD12	2:B:151:GLN:NE2	2.15	0.62
1:A:256:LEU:O	1:A:258:ARG:NH1	2.33	0.61
2:B:68:VAL:HG13	2:B:68:VAL:O	1.99	0.61
1:C:578:VAL:CG1	1:C:579:GLU:N	2.64	0.61
2:B:96:LYS:HZ3	2:B:97:GLU:HB2	1.65	0.61
1:C:257:ASP:CB	1:C:568:LEU:HD21	2.24	0.61
1:A:280:HIS:NE2	1:A:298:SER:HB3	2.14	0.61
1:A:401:VAL:HG13	1:A:504:TRP:CE3	2.35	0.61
1:A:555:ASP:C	1:A:555:ASP:OD1	2.43	0.61
1:C:490:GLN:HB2	1:C:505:GLU:OE1	2.01	0.61
1:A:370:LEU:CD2	1:A:375:PHE:HB2	2.25	0.60
1:C:221:LEU:HD23	1:C:222:LEU:N	2.16	0.60
1:C:202:LEU:HD11	1:C:591:LYS:HE2	1.82	0.60
2:D:78:TYR:CZ	2:D:145:LEU:HD22	2.36	0.60
1:A:356:ILE:HD11	1:A:444:ILE:HD11	1.82	0.60
1:A:545:ILE:HD13	1:A:548:GLN:OE1	2.00	0.60
1:C:229:PHE:CD1	1:C:229:PHE:C	2.79	0.60
1:C:525:TYR:CE2	1:C:536:VAL:HB	2.37	0.60
1:A:318:ARG:CG	1:A:333:LYS:HB3	2.31	0.60
2:D:51:LEU:HD22	2:D:163:ILE:HG23	1.81	0.60
1:C:525:TYR:HD2	1:C:536:VAL:O	1.84	0.60
1:A:257:ASP:O	1:A:257:ASP:OD2	2.20	0.60
1:A:349:MET:HE3	1:A:350:PRO:O	2.02	0.59
1:C:375:PHE:CE2	1:C:377:TYR:HB2	2.37	0.59
1:C:399:MET:CE	1:C:436:LEU:HG	2.32	0.59
2:D:138:ILE:HG22	2:D:162:LYS:HB2	1.83	0.59
1:A:416:TYR:CD1	1:A:426:LEU:CD2	2.86	0.59
1:C:312:GLU:CB	1:C:347:LYS:HB2	2.32	0.59
1:C:294:LEU:HD11	1:C:337:ILE:CD1	2.32	0.59
1:C:294:LEU:CD1	1:C:316:LEU:HB2	2.33	0.59
1:A:296:ALA:HA	1:A:314:LEU:HD23	1.85	0.59
1:C:188:ILE:HD12	1:C:188:ILE:C	2.28	0.59
1:C:279:ILE:HG23	1:C:295:CYS:HB3	1.83	0.59
1:A:443:LYS:NZ	1:A:563:THR:O	2.35	0.59
1:C:463:MET:HE2	1:C:482:ASN:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:VAL:HG12	1:A:561:THR:HG21	1.85	0.58
2:B:78:TYR:CZ	2:B:145:LEU:HD13	2.38	0.58
1:C:437:THR:HG23	1:C:465:LYS:HZ2	1.68	0.58
1:A:363:TYR:HB3	1:A:413:LEU:HD22	1.85	0.58
2:D:130:GLN:HB2	2:D:133:LYS:HD2	1.84	0.58
1:C:336:ALA:O	1:C:338:THR:HG23	2.04	0.58
1:A:263:PRO:HG3	1:A:568:LEU:HD22	1.84	0.58
1:A:567:LEU:CD2	1:A:570:ASN:C	2.77	0.58
1:C:408:ILE:HD12	1:C:408:ILE:C	2.29	0.58
2:D:138:ILE:HG22	2:D:162:LYS:CB	2.33	0.58
1:A:573:TRP:CE3	1:A:594:ALA:HB1	2.39	0.58
1:A:567:LEU:CD2	1:A:571:VAL:N	2.67	0.57
1:C:420:LEU:CD1	1:C:424:ILE:HG23	2.33	0.57
1:A:213:GLU:C	1:A:587:VAL:HG22	2.29	0.57
1:A:416:TYR:CD1	1:A:426:LEU:HD23	2.38	0.57
1:C:305:LEU:HD21	1:C:504:TRP:CH2	2.38	0.57
1:A:285:THR:HG22	1:A:362:LEU:HD22	1.85	0.57
2:D:85:ASP:OD1	2:D:86:LYS:N	2.38	0.57
1:A:567:LEU:HD23	1:A:571:VAL:C	2.29	0.57
1:A:228:PHE:CD1	1:A:321:VAL:HG21	2.40	0.57
2:B:155:VAL:HG23	2:B:161:MET:CB	2.34	0.57
1:C:369:PHE:N	1:C:369:PHE:CD2	2.73	0.57
2:D:83:MET:CE	2:D:165:MET:HE1	2.35	0.57
1:C:280:HIS:CE1	1:C:298:SER:HB3	2.40	0.57
2:D:44:LYS:HB3	2:D:51:LEU:HD12	1.86	0.57
2:D:32:VAL:HG22	2:D:60:LYS:HG2	1.87	0.56
1:A:231:TYR:CE2	1:A:249:ILE:HD11	2.38	0.56
1:A:241:THR:HB	2:B:126:GLY:CA	2.35	0.56
1:A:536:VAL:HG22	1:A:550:PRO:HA	1.86	0.56
2:D:122:PRO:O	2:D:124:LEU:HD22	2.05	0.56
1:A:462:THR:HG22	1:A:487:ARG:CZ	2.35	0.56
1:A:534:ASN:O	1:A:536:VAL:HG23	2.05	0.56
1:C:456:ALA:HB1	1:C:458:TYR:HE2	1.68	0.56
1:C:546:LEU:HB2	1:C:547:TYR:CD2	2.41	0.56
1:A:524:VAL:HG23	1:A:537:PHE:HD1	1.69	0.56
1:C:397:LEU:HD12	1:C:502:VAL:CG2	2.33	0.56
1:C:310:TRP:CE3	1:C:347:LYS:HE3	2.40	0.56
1:C:318:ARG:O	1:C:318:ARG:HG3	2.06	0.56
2:D:101:LEU:HD13	2:D:113:PHE:CD2	2.41	0.56
2:D:119:GLU:CG	2:D:130:GLN:HE22	2.19	0.56
1:A:312:GLU:HB3	1:A:347:LYS:HZ2	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:VAL:HG12	1:A:579:GLU:N	2.21	0.55
1:C:257:ASP:OD1	1:C:568:LEU:HD11	2.06	0.55
1:C:393:GLU:O	1:C:394:ASN:C	2.49	0.55
1:A:595:VAL:O	1:A:595:VAL:HG12	2.06	0.55
1:C:198:LEU:HD11	1:C:539:VAL:HG21	1.88	0.55
1:A:358:GLN:HE22	1:A:472:VAL:HG21	1.70	0.55
1:A:235:GLU:O	1:A:246:LYS:N	2.38	0.55
1:A:361:THR:HG23	1:A:417:ASN:CA	2.36	0.55
1:A:535:PRO:HG3	1:A:558:ALA:HB2	1.89	0.55
1:C:198:LEU:HD23	1:C:598:PRO:HD3	1.89	0.55
1:A:602:SER:O	1:A:603:GLU:C	2.47	0.55
1:C:197:ILE:HD11	1:C:547:TYR:CD1	2.42	0.55
1:C:337:ILE:HD13	1:C:426:LEU:HD11	1.89	0.55
1:C:463:MET:CE	1:C:482:ASN:O	2.54	0.55
1:C:532:ALA:HB1	1:C:558:ALA:O	2.05	0.55
1:C:553:GLU:HB2	1:C:556:THR:CG2	2.36	0.55
1:A:572:ILE:H	1:A:572:ILE:HD12	1.72	0.55
1:A:397:LEU:HD22	1:A:403:SER:HB2	1.88	0.55
1:C:450:GLN:CD	1:C:451:PRO:HD2	2.32	0.55
1:C:512:PHE:O	1:C:521:SER:HA	2.07	0.54
1:C:366:ALA:CB	1:C:414:LEU:HG	2.37	0.54
2:D:68:VAL:HG13	2:D:68:VAL:O	2.08	0.54
1:A:451:PRO:O	1:A:469:VAL:HG22	2.08	0.54
1:C:337:ILE:HD13	1:C:426:LEU:CD1	2.37	0.54
1:C:506:GLY:O	2:D:124:LEU:HD21	2.07	0.54
1:A:249:ILE:O	1:A:250:ILE:HG13	2.08	0.54
1:A:540:PHE:CB	1:A:545:ILE:HA	2.37	0.54
1:A:581:TYR:CD2	1:A:588:ILE:HD13	2.42	0.54
1:A:241:THR:HB	2:B:126:GLY:HA2	1.89	0.54
1:A:420:LEU:CD1	1:A:424:ILE:CG2	2.74	0.54
2:D:36:ILE:HD11	2:D:53:LEU:HD22	1.90	0.54
1:A:463:MET:HE3	1:A:485:ILE:O	2.08	0.54
1:C:226:ASN:N	1:C:226:ASN:HD22	2.05	0.54
1:C:453:PHE:CE1	1:C:475:LEU:HD21	2.42	0.54
2:D:82:TYR:CZ	2:D:94:ILE:CD1	2.85	0.54
1:A:222:LEU:HD21	1:A:575:ILE:HG21	1.90	0.54
1:A:537:PHE:HB3	1:A:549:VAL:HG12	1.90	0.54
1:C:487:ARG:O	1:C:487:ARG:HD3	2.08	0.54
1:C:578:VAL:HG12	1:C:579:GLU:N	2.22	0.54
1:C:462:THR:CG2	1:C:487:ARG:CZ	2.85	0.53
2:D:106:LYS:HD2	2:D:111:ILE:HD11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:GLU:O	1:A:586:SER:O	2.27	0.53
1:A:356:ILE:HD11	1:A:444:ILE:CD1	2.39	0.53
1:C:563:THR:HG22	1:C:576:SER:OG	2.09	0.53
2:D:32:VAL:HG22	2:D:60:LYS:HG3	1.91	0.53
1:A:202:LEU:HD11	1:A:591:LYS:HD3	1.88	0.53
1:A:460:TRP:O	1:A:462:THR:HG23	2.08	0.53
1:A:366:ALA:HB1	1:A:414:LEU:HD12	1.91	0.53
1:C:316:LEU:HG	1:C:317:ILE:N	2.23	0.53
1:A:480:ARG:CG	1:A:519:TRP:CZ3	2.91	0.53
1:C:561:THR:HG22	1:C:578:VAL:HG22	1.91	0.53
1:C:580:ILE:HG21	1:C:591:LYS:HD2	1.88	0.53
2:B:155:VAL:O	2:B:159:ARG:O	2.26	0.53
1:A:213:GLU:N	1:A:587:VAL:CG2	2.72	0.53
1:A:253:GLY:HA2	1:A:268:THR:HG23	1.91	0.52
1:A:394:ASN:HD22	1:A:500:PRO:C	2.17	0.52
2:D:89:ALA:HA	2:D:138:ILE:HD13	1.91	0.52
1:A:317:ILE:N	1:A:317:ILE:HD12	2.24	0.52
1:A:411:SER:O	1:A:431:ILE:CG2	2.51	0.52
2:B:137:ILE:CG1	2:B:165:MET:HE2	2.37	0.52
1:A:348:VAL:HG11	1:A:428:PHE:CG	2.44	0.52
1:A:378:ASN:OD1	1:A:380:SER:N	2.42	0.52
1:C:462:THR:O	1:C:486:SER:OG	2.19	0.52
2:D:51:LEU:C	2:D:51:LEU:HD23	2.34	0.52
1:C:293:THR:O	1:C:293:THR:CG2	2.57	0.52
1:C:444:ILE:HD11	1:C:451:PRO:HB2	1.90	0.52
1:A:287:HIS:HB2	1:A:362:LEU:HD21	1.92	0.52
2:B:164:LEU:CD2	2:B:166:LYS:HZ2	2.21	0.52
1:C:262:VAL:HG12	1:C:263:PRO:O	2.09	0.52
1:C:541:LYS:NZ	1:C:541:LYS:HB2	2.25	0.52
1:A:541:LYS:HB2	1:A:541:LYS:NZ	2.25	0.52
1:C:485:ILE:HG22	1:C:486:SER:N	2.24	0.52
1:C:233:HIS:C	1:C:233:HIS:CD2	2.88	0.52
1:C:523:GLY:HA2	1:C:563:THR:HG21	1.91	0.52
1:A:372:ARG:HA	1:A:375:PHE:CB	2.38	0.52
1:C:196:THR:O	1:C:196:THR:OG1	2.17	0.52
1:C:495:ARG:HD3	1:C:529:ASN:HA	1.92	0.52
1:C:541:LYS:HZ3	1:C:546:LEU:HD21	1.73	0.52
1:C:223:ALA:HB3	1:C:230:ALA:HB3	1.92	0.51
1:A:254:GLU:OE1	1:A:256:LEU:HD21	2.10	0.51
1:A:440:SER:OG	1:A:455:GLN:CG	2.58	0.51
1:C:248:ARG:H	1:C:276:PRO:HB3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:456:ALA:CB	1:C:458:TYR:CE2	2.93	0.51
1:A:340:VAL:HG12	1:A:342:ARG:HD2	1.91	0.51
1:A:440:SER:OG	1:A:455:GLN:HG2	2.09	0.51
1:C:257:ASP:HB3	1:C:568:LEU:CD2	2.25	0.51
1:C:548:GLN:O	1:C:549:VAL:HG22	2.09	0.51
1:A:249:ILE:C	1:A:250:ILE:HG13	2.35	0.51
1:A:455:GLN:OE1	1:A:465:LYS:NZ	2.23	0.51
1:C:437:THR:CG2	1:C:465:LYS:HZ3	2.23	0.51
1:C:286:TYR:C	1:C:286:TYR:CD2	2.88	0.51
1:C:466:LEU:HD11	1:C:519:TRP:HZ3	1.75	0.51
1:C:510:ASP:OD1	1:C:510:ASP:C	2.54	0.51
1:A:399:MET:HE1	1:A:436:LEU:HG	1.93	0.51
1:C:228:PHE:CD1	1:C:321:VAL:HB	2.46	0.51
2:D:140:THR:OG1	2:D:150:ASN:O	2.28	0.51
1:A:286:TYR:HA	1:A:291:TYR:HA	1.92	0.51
1:A:478:GLN:HG3	1:A:478:GLN:O	2.10	0.51
1:A:215:VAL:CG1	1:A:216:CYS:N	2.73	0.51
1:A:372:ARG:HH12	1:A:397:LEU:HA	1.76	0.51
1:C:188:ILE:HD13	1:C:597:ILE:HG21	1.92	0.51
2:D:137:ILE:HD11	2:D:165:MET:CE	2.41	0.51
1:A:312:GLU:HB3	1:A:347:LYS:NZ	2.26	0.50
2:B:157:GLN:C	2:B:158:THR:HG23	2.37	0.50
1:C:215:VAL:CG1	1:C:216:CYS:N	2.71	0.50
1:C:413:LEU:HD11	1:C:475:LEU:HD13	1.93	0.50
1:A:553:GLU:HB2	1:A:556:THR:CG2	2.38	0.50
1:A:366:ALA:CB	1:A:414:LEU:CD1	2.88	0.50
1:A:466:LEU:H	1:A:466:LEU:HD23	1.77	0.50
1:C:352:GLY:HA3	1:C:442:SER:O	2.11	0.50
1:C:450:GLN:NE2	1:C:469:VAL:O	2.45	0.50
1:C:372:ARG:HA	1:C:375:PHE:CB	2.42	0.50
1:A:524:VAL:HG21	1:A:551:LEU:CD1	2.42	0.49
1:C:437:THR:OG1	1:C:455:GLN:OE1	2.30	0.49
2:D:139:SER:OG	2:D:141:SER:HB2	2.12	0.49
1:C:312:GLU:CG	1:C:312:GLU:O	2.60	0.49
1:A:228:PHE:CE1	1:A:321:VAL:HG21	2.48	0.49
2:B:118:GLN:NE2	2:B:120:PHE:O	2.46	0.49
1:C:437:THR:CG2	1:C:465:LYS:NZ	2.75	0.49
1:C:562:ILE:HG22	1:C:563:THR:N	2.28	0.49
1:A:372:ARG:C	1:A:374:GLU:N	2.70	0.49
1:C:213:GLU:CG	1:C:214:GLY:N	2.76	0.49
2:D:83:MET:HE1	2:D:165:MET:HE1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:MET:O	1:A:438:ILE:HG13	2.13	0.49
1:A:484:VAL:HG11	1:A:544:GLU:N	2.28	0.49
2:B:95:LYS:O	2:B:98:ASN:HB2	2.12	0.49
1:C:221:LEU:C	1:C:221:LEU:CD2	2.80	0.49
1:C:494:PRO:O	1:C:495:ARG:C	2.56	0.49
1:A:233:HIS:C	1:A:233:HIS:CD2	2.91	0.49
1:A:279:ILE:HG23	1:A:295:CYS:HB3	1.93	0.49
1:C:256:LEU:HD12	1:C:266:PHE:CG	2.48	0.49
1:A:235:GLU:OE2	1:A:246:LYS:NZ	2.45	0.48
1:A:369:PHE:N	1:A:369:PHE:CD2	2.81	0.48
1:A:525:TYR:CE2	1:A:536:VAL:HB	2.47	0.48
1:C:340:VAL:HG12	1:C:342:ARG:HD2	1.95	0.48
1:C:372:ARG:C	1:C:374:GLU:N	2.71	0.48
1:C:394:ASN:HD22	1:C:500:PRO:C	2.20	0.48
1:A:573:TRP:HZ3	1:A:594:ALA:CB	2.24	0.48
1:A:494:PRO:O	1:A:495:ARG:C	2.56	0.48
2:D:44:LYS:CB	2:D:51:LEU:HD12	2.43	0.48
1:A:202:LEU:HD13	1:A:593:PHE:CZ	2.47	0.48
1:A:512:PHE:O	1:A:521:SER:HA	2.12	0.48
2:B:63:ILE:CG2	2:B:102:LEU:HD12	2.38	0.48
1:C:198:LEU:CD1	1:C:539:VAL:HG23	2.44	0.48
1:A:352:GLY:HA3	1:A:442:SER:O	2.13	0.48
1:A:487:ARG:HH12	1:A:489:GLY:HA3	1.79	0.48
2:B:101:LEU:HD13	2:B:113:PHE:CD2	2.49	0.48
1:C:545:ILE:HD13	1:C:548:GLN:OE1	2.13	0.48
2:D:52:VAL:CG2	2:D:164:LEU:HD23	2.39	0.48
1:A:194:THR:O	1:A:195:SER:C	2.57	0.48
1:A:547:TYR:N	1:A:547:TYR:CD2	2.81	0.48
1:A:578:VAL:CG1	1:A:579:GLU:N	2.77	0.48
2:B:38:TRP:NE1	2:B:161:MET:SD	2.87	0.48
1:C:436:LEU:HD12	1:C:436:LEU:HA	1.56	0.48
1:A:525:TYR:OH	1:A:527:ASN:ND2	2.46	0.48
1:A:581:TYR:CE2	1:A:588:ILE:HD13	2.49	0.48
2:B:76:TYR:CD1	2:B:107:PRO:HA	2.48	0.48
2:B:106:LYS:O	2:B:107:PRO:C	2.54	0.48
1:C:242:ARG:HH12	2:D:127:LEU:HD23	1.79	0.48
2:B:80:LYS:O	2:B:139:SER:CB	2.62	0.47
1:C:408:ILE:C	1:C:408:ILE:CD1	2.87	0.47
2:D:122:PRO:O	2:D:124:LEU:HD23	2.12	0.47
2:B:86:LYS:HG2	2:B:90:ASP:OD2	2.14	0.47
1:A:281:HIS:NE2	1:A:302:ASP:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:PHE:HB2	1:A:292:TYR:CE2	2.50	0.47
1:A:545:ILE:CG2	1:A:548:GLN:HG3	2.44	0.47
1:C:493:CYS:SG	1:C:501:GLU:HB2	2.55	0.47
1:C:193:THR:HG23	1:C:193:THR:O	2.14	0.47
1:C:293:THR:N	1:C:316:LEU:CD1	2.69	0.47
1:C:487:ARG:HH12	1:C:489:GLY:HA3	1.79	0.47
1:A:197:ILE:CG2	1:A:602:SER:O	2.50	0.47
1:A:228:PHE:N	1:A:228:PHE:CD2	2.82	0.47
1:A:466:LEU:HG	1:A:519:TRP:HH2	1.80	0.47
1:A:472:VAL:O	1:A:473:ASP:OD1	2.33	0.47
2:B:93:THR:HG22	2:B:152:GLU:OE2	2.14	0.47
1:C:203:ILE:O	1:C:203:ILE:CG2	2.63	0.47
1:C:450:GLN:OE1	1:C:451:PRO:HD2	2.15	0.47
1:C:513:LEU:HD21	1:C:516:ARG:HA	1.96	0.47
1:A:341:GLU:O	1:A:427:GLN:HA	2.15	0.47
1:A:355:GLY:HA3	1:A:363:TYR:O	2.14	0.47
1:C:460:TRP:CD2	1:C:500:PRO:HA	2.49	0.47
2:D:89:ALA:HB2	2:D:136:TYR:HB3	1.96	0.47
1:A:317:ILE:HG13	1:A:334:TYR:CD2	2.49	0.47
1:C:349:MET:HG2	1:C:350:PRO:HD2	1.97	0.47
1:C:535:PRO:HD3	1:C:558:ALA:CB	2.42	0.47
2:D:101:LEU:HD13	2:D:113:PHE:CE2	2.50	0.47
1:A:445:TYR:CD1	1:A:512:PHE:CE1	3.02	0.47
1:A:443:LYS:NZ	1:A:510:ASP:OD2	2.25	0.46
1:A:538:ALA:HA	1:A:548:GLN:HG2	1.97	0.46
1:A:450:GLN:HG3	1:A:451:PRO:N	2.29	0.46
1:A:536:VAL:HG13	1:A:549:VAL:O	2.15	0.46
2:B:68:VAL:O	2:B:68:VAL:CG1	2.63	0.46
1:C:454:TYR:CD2	1:C:454:TYR:C	2.92	0.46
1:C:552:ALA:HB1	1:C:556:THR:CG2	2.36	0.46
2:D:36:ILE:HG21	2:D:163:ILE:CD1	2.46	0.46
1:C:578:VAL:HG12	1:C:579:GLU:C	2.40	0.46
1:A:268:THR:HG21	1:A:321:VAL:O	2.15	0.46
1:A:287:HIS:N	1:A:290:PHE:O	2.35	0.46
2:B:38:TRP:CE2	2:B:161:MET:SD	3.09	0.46
1:C:469:VAL:HG13	1:C:476:ARG:O	2.15	0.46
1:C:580:ILE:CG2	1:C:591:LYS:HD2	2.46	0.46
1:C:378:ASN:HB3	1:C:381:ASN:ND2	2.29	0.46
1:C:221:LEU:HD23	1:C:222:LEU:CA	2.45	0.46
1:A:254:GLU:HB3	1:A:256:LEU:CD2	2.45	0.46
1:A:262:VAL:CG1	1:A:263:PRO:O	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:TYR:N	1:A:366:ALA:HA	2.29	0.46
1:C:307:SER:O	1:C:347:LYS:NZ	2.44	0.46
1:A:248:ARG:H	1:A:276:PRO:HB3	1.80	0.46
2:D:115:ILE:HG23	2:D:129:PHE:HE2	1.81	0.46
1:A:508:TYR:C	1:A:508:TYR:CD2	2.93	0.46
2:B:140:THR:O	2:B:154:GLY:HA3	2.16	0.46
1:C:287:HIS:HB3	1:C:292:TYR:HE2	1.81	0.46
1:C:397:LEU:HD13	1:C:403:SER:HB2	1.97	0.46
1:C:485:ILE:HD11	1:C:540:PHE:CD2	2.51	0.46
1:C:546:LEU:HB2	1:C:547:TYR:CE2	2.51	0.46
1:A:525:TYR:HE2	1:A:536:VAL:HB	1.80	0.45
2:B:84:VAL:HG11	2:B:138:ILE:CD1	2.46	0.45
1:C:189:CYS:HB3	1:C:547:TYR:CZ	2.51	0.45
2:D:83:MET:CE	2:D:165:MET:CE	2.94	0.45
2:D:83:MET:HE1	2:D:129:PHE:CZ	2.51	0.45
2:D:95:LYS:O	2:D:98:ASN:HB2	2.16	0.45
1:A:393:GLU:HB2	1:A:397:LEU:CD1	2.43	0.45
1:A:272:THR:HG22	1:A:273:PRO:O	2.15	0.45
1:A:348:VAL:HG11	1:A:428:PHE:HB2	1.99	0.45
1:A:413:LEU:HG	1:A:475:LEU:HD22	1.99	0.45
2:D:81:VAL:O	2:D:101:LEU:HG	2.16	0.45
1:A:371:PRO:HA	1:A:407:TYR:HA	1.98	0.45
2:B:82:TYR:CD1	2:B:98:ASN:HB3	2.51	0.45
1:C:456:ALA:HB1	1:C:458:TYR:CD2	2.51	0.45
1:A:366:ALA:HB1	1:A:414:LEU:CD1	2.47	0.45
1:C:569:GLU:C	1:C:570:ASN:CG	2.84	0.45
1:C:401:VAL:HG22	1:C:504:TRP:CZ3	2.52	0.45
1:C:546:LEU:C	1:C:547:TYR:HD2	2.25	0.45
1:A:283:SER:HA	1:A:353:PRO:O	2.17	0.45
1:A:577:LEU:CG	1:A:578:VAL:H	2.09	0.45
1:C:442:SER:CB	1:C:454:TYR:O	2.65	0.45
1:A:370:LEU:HD22	1:A:375:PHE:CB	2.33	0.45
1:C:456:ALA:CB	1:C:458:TYR:HE2	2.30	0.45
1:C:573:TRP:CZ3	1:C:594:ALA:HB1	2.52	0.45
1:A:437:THR:HG21	1:A:465:LYS:HD2	1.98	0.45
1:C:200:PRO:HA	1:C:595:VAL:HG22	1.99	0.45
1:C:462:THR:HG22	1:C:487:ARG:NE	2.30	0.45
2:D:115:ILE:HG23	2:D:129:PHE:CE2	2.52	0.45
1:A:197:ILE:HG13	1:A:598:PRO:HG2	1.99	0.45
1:A:358:GLN:NE2	1:A:472:VAL:HG21	2.30	0.45
2:B:137:ILE:HD11	2:B:165:MET:HE1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:ASN:ND2	1:C:500:PRO:O	2.46	0.45
1:A:512:PHE:O	1:A:522:ALA:N	2.50	0.44
1:C:440:SER:HB2	1:C:456:ALA:HB3	1.99	0.44
1:C:597:ILE:N	1:C:597:ILE:CD1	2.80	0.44
1:A:531:THR:HG21	2:B:114:THR:HG22	1.99	0.44
2:B:157:GLN:O	2:B:158:THR:CG2	2.65	0.44
1:C:231:TYR:C	1:C:231:TYR:CD2	2.94	0.44
1:C:577:LEU:HG	1:C:578:VAL:H	1.83	0.44
1:C:585:ASP:OD1	1:C:585:ASP:N	2.49	0.44
1:A:466:LEU:HD11	1:A:519:TRP:CZ3	2.52	0.44
2:B:36:ILE:HD11	2:B:53:LEU:HD22	1.99	0.44
1:C:283:SER:HA	1:C:353:PRO:O	2.18	0.44
1:C:316:LEU:HD12	1:C:317:ILE:H	1.81	0.44
1:C:318:ARG:CG	1:C:333:LYS:HB3	2.48	0.44
1:A:285:THR:CG2	1:A:362:LEU:HD22	2.46	0.44
1:A:287:HIS:CE1	1:A:418:LEU:CD1	2.92	0.44
1:A:524:VAL:CG2	1:A:551:LEU:CD1	2.95	0.44
1:C:526:LEU:HD11	1:C:559:GLN:O	2.18	0.44
2:D:85:ASP:OD1	2:D:87:ASP:N	2.47	0.44
1:A:286:TYR:HB2	1:A:291:TYR:CE1	2.53	0.44
1:A:575:ILE:HD13	1:A:594:ALA:HA	1.99	0.44
1:C:263:PRO:O	1:C:264:SER:OG	2.30	0.44
1:A:370:LEU:HD23	1:A:371:PRO:C	2.42	0.44
1:A:393:GLU:C	1:A:397:LEU:HD12	2.43	0.44
2:D:83:MET:HE1	2:D:129:PHE:CE1	2.53	0.44
1:C:198:LEU:CD2	1:C:598:PRO:HD3	2.48	0.43
1:C:287:HIS:O	1:C:288:GLU:C	2.61	0.43
1:C:341:GLU:O	1:C:427:GLN:HA	2.17	0.43
1:A:219:ASP:N	1:A:220:PRO:HD3	2.34	0.43
1:A:460:TRP:CE3	1:A:461:ASP:N	2.86	0.43
1:C:355:GLY:HA3	1:C:363:TYR:O	2.18	0.43
1:C:525:TYR:HE2	1:C:536:VAL:HB	1.82	0.43
1:A:435:ARG:HD3	1:A:479:TRP:HB2	2.00	0.43
2:B:86:LYS:O	2:B:89:ALA:HB3	2.18	0.43
2:B:115:ILE:HG23	2:B:129:PHE:HE2	1.83	0.43
1:C:411:SER:O	1:C:431:ILE:HG22	2.18	0.43
1:C:545:ILE:O	1:C:545:ILE:HG22	2.17	0.43
1:C:552:ALA:HB3	1:C:556:THR:OG1	2.18	0.43
1:A:372:ARG:NH1	1:A:397:LEU:HA	2.33	0.43
1:A:499:CYS:O	1:A:501:GLU:HG2	2.19	0.43
1:C:394:ASN:O	1:C:395:CYS:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:MET:HE1	2:B:129:PHE:CE1	2.53	0.43
1:C:188:ILE:N	1:C:599:ALA:O	2.51	0.43
1:A:315:SER:N	1:A:337:ILE:HD12	2.34	0.43
1:A:452:VAL:HG22	1:A:516:ARG:NH2	2.34	0.43
1:C:569:GLU:O	1:C:570:ASN:CG	2.62	0.43
2:D:113:PHE:CE2	2:D:115:ILE:HG13	2.54	0.43
1:A:367:VAL:CG1	1:A:369:PHE:CE2	2.93	0.43
1:A:557:ASN:HB3	2:B:118:GLN:OE1	2.18	0.43
1:A:360:ASP:C	1:A:361:THR:OG1	2.61	0.43
1:A:463:MET:CE	1:A:485:ILE:O	2.67	0.43
1:A:525:TYR:HD2	1:A:536:VAL:O	2.02	0.43
1:C:222:LEU:HD12	1:C:223:ALA:N	2.34	0.43
1:C:371:PRO:HA	1:C:407:TYR:HA	2.01	0.43
1:A:312:GLU:CG	1:A:312:GLU:O	2.67	0.43
1:A:370:LEU:CD2	1:A:371:PRO:O	2.61	0.43
1:A:544:GLU:HG2	1:A:546:LEU:HD23	2.01	0.43
2:B:44:LYS:O	2:B:46:LEU:HG	2.19	0.43
2:B:84:VAL:HG11	2:B:138:ILE:HD13	2.00	0.43
1:C:251:GLY:C	1:C:252:VAL:HG13	2.44	0.43
1:C:257:ASP:HB3	1:C:568:LEU:HD11	2.01	0.43
1:C:414:LEU:HA	1:C:414:LEU:HD23	1.81	0.43
1:C:575:ILE:HD13	1:C:593:PHE:C	2.44	0.43
2:D:137:ILE:HD11	2:D:165:MET:HE2	2.01	0.43
1:A:437:THR:O	1:A:438:ILE:C	2.61	0.42
1:A:194:THR:C	1:A:195:SER:O	2.62	0.42
1:A:257:ASP:CB	1:A:568:LEU:HD11	2.45	0.42
1:A:394:ASN:HA	1:A:397:LEU:HD12	2.01	0.42
1:A:448:LEU:N	1:A:448:LEU:CD2	2.64	0.42
1:C:404:LYS:O	1:C:405:SER:C	2.63	0.42
1:C:464:ILE:HB	1:C:485:ILE:CG2	2.49	0.42
1:A:317:ILE:HD11	1:A:334:TYR:CE2	2.55	0.42
1:A:387:CYS:O	1:A:388:LYS:C	2.62	0.42
1:A:393:GLU:H	1:A:393:GLU:HG3	1.75	0.42
1:A:581:TYR:CD2	2:B:120:PHE:CE2	3.03	0.42
1:C:491:SER:O	1:C:494:PRO:HD3	2.19	0.42
1:A:239:SER:HB2	2:B:128:GLU:OE1	2.19	0.42
1:C:431:ILE:HA	1:C:475:LEU:HB3	2.00	0.42
1:C:463:MET:HE1	1:C:483:SER:C	2.44	0.42
1:C:543:ASN:O	1:C:544:GLU:HB2	2.20	0.42
1:A:567:LEU:HD22	1:A:570:ASN:CA	2.49	0.42
2:B:91:ARG:HD3	1:C:213:GLU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:399:MET:C	1:C:408:ILE:HG22	2.45	0.42
1:C:401:VAL:HG12	1:C:402:ASN:N	2.33	0.42
1:C:485:ILE:CG2	1:C:486:SER:N	2.82	0.42
1:C:546:LEU:CB	1:C:547:TYR:CD2	3.02	0.42
1:A:345:TYR:OH	1:A:430:GLU:OE1	2.27	0.42
1:A:388:LYS:NZ	1:A:388:LYS:CB	2.82	0.42
1:A:491:SER:HB3	2:B:113:PHE:HB2	2.02	0.42
1:C:194:THR:O	1:C:195:SER:C	2.61	0.42
1:C:387:CYS:O	1:C:388:LYS:C	2.62	0.42
2:D:102:LEU:HD23	2:D:102:LEU:HA	1.73	0.42
1:A:289:ASP:N	1:A:289:ASP:OD1	2.52	0.42
1:C:286:TYR:HA	1:C:291:TYR:HA	2.02	0.42
1:C:445:TYR:CD1	1:C:512:PHE:CE1	3.08	0.42
1:A:393:GLU:O	1:A:394:ASN:C	2.63	0.42
1:A:528:SER:OG	1:A:531:THR:O	2.37	0.42
2:D:36:ILE:HG13	2:D:61:LEU:HD11	2.02	0.42
1:A:351:TYR:CZ	1:A:441:PRO:HD3	2.55	0.42
1:A:394:ASN:ND2	1:A:500:PRO:O	2.52	0.42
1:C:536:VAL:HG22	1:C:550:PRO:CA	2.44	0.42
2:D:81:VAL:HB	2:D:102:LEU:HB2	2.02	0.42
1:A:356:ILE:CD1	1:A:451:PRO:HB3	2.50	0.41
1:A:562:ILE:HG22	1:A:563:THR:N	2.35	0.41
1:C:318:ARG:HG2	1:C:333:LYS:HB3	2.02	0.41
1:C:372:ARG:HA	1:C:375:PHE:HB2	2.02	0.41
1:C:597:ILE:N	1:C:597:ILE:HD12	2.34	0.41
2:D:94:ILE:O	2:D:151:GLN:OE1	2.37	0.41
1:A:466:LEU:HD23	1:A:466:LEU:N	2.34	0.41
1:C:349:MET:CG	1:C:350:PRO:HD2	2.50	0.41
1:A:466:LEU:HD11	1:A:519:TRP:HZ3	1.85	0.41
1:C:188:ILE:HD12	1:C:189:CYS:N	2.35	0.41
1:C:213:GLU:CD	1:C:214:GLY:N	2.78	0.41
1:C:215:VAL:HG13	1:C:216:CYS:N	2.36	0.41
1:C:463:MET:HE3	1:C:463:MET:HB3	1.86	0.41
2:D:113:PHE:CZ	2:D:115:ILE:HG13	2.54	0.41
1:A:433:ASP:HB2	1:A:436:LEU:HD22	2.02	0.41
1:A:450:GLN:OE1	1:A:451:PRO:HD2	2.21	0.41
1:A:583:THR:CG2	2:B:57:ILE:HG22	2.43	0.41
1:C:198:LEU:HB2	1:C:549:VAL:HG23	2.00	0.41
1:C:239:SER:HB3	2:D:128:GLU:OE2	2.21	0.41
1:C:409:LEU:O	1:C:439:GLY:N	2.46	0.41
1:A:491:SER:CB	2:B:102:LEU:HD23	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:ILE:HG21	1:A:548:GLN:CG	2.48	0.41
1:C:562:ILE:C	1:C:563:THR:HG23	2.45	0.41
1:A:217:ILE:HG23	1:A:233:HIS:CG	2.56	0.41
1:A:578:VAL:CG1	1:A:580:ILE:HB	2.50	0.41
1:A:581:TYR:CE1	1:A:588:ILE:HD11	2.56	0.41
1:C:202:LEU:HD11	1:C:591:LYS:CE	2.50	0.41
1:C:446:ASN:HA	1:C:451:PRO:HA	2.02	0.41
1:C:536:VAL:HG13	1:C:549:VAL:O	2.20	0.41
2:D:96:LYS:HZ2	2:D:97:GLU:HB2	1.86	0.41
1:A:225:ASP:CG	1:A:286:TYR:HB3	2.46	0.41
1:A:558:ALA:HA	1:A:579:GLU:O	2.21	0.41
2:B:83:MET:HE1	2:B:129:PHE:CZ	2.56	0.41
2:D:84:VAL:HG23	2:D:85:ASP:O	2.20	0.41
1:A:232:SER:OG	1:A:249:ILE:O	2.37	0.41
1:A:278:THR:O	1:A:298:SER:N	2.49	0.41
2:B:80:LYS:CG	2:B:148:LEU:HD11	2.47	0.41
1:C:372:ARG:NH2	1:C:405:SER:OG	2.54	0.41
1:C:484:VAL:HG23	1:C:485:ILE:N	2.35	0.41
1:A:215:VAL:HG13	1:A:216:CYS:N	2.36	0.41
1:A:455:GLN:HB3	1:A:465:LYS:HD3	2.02	0.41
2:B:115:ILE:HG23	2:B:129:PHE:CE2	2.56	0.41
1:C:351:TYR:N	1:C:366:ALA:HA	2.36	0.41
1:C:456:ALA:CB	1:C:458:TYR:CD2	3.03	0.41
2:D:36:ILE:HG21	2:D:163:ILE:HD13	2.01	0.41
1:A:345:TYR:CD1	1:A:428:PHE:CD2	3.09	0.41
1:C:262:VAL:HG22	1:C:573:TRP:CH2	2.56	0.41
1:A:217:ILE:HD12	1:A:233:HIS:CE1	2.56	0.40
1:A:239:SER:OG	1:A:243:GLY:N	2.53	0.40
1:A:347:LYS:HZ3	1:A:347:LYS:HG2	1.48	0.40
1:C:286:TYR:CD2	1:C:287:HIS:N	2.89	0.40
1:A:397:LEU:CD2	1:A:403:SER:HB2	2.52	0.40
1:A:485:ILE:HG22	1:A:486:SER:N	2.37	0.40
1:C:287:HIS:HD2	1:C:418:LEU:HD11	1.72	0.40
1:A:225:ASP:O	1:A:227:GLY:N	2.54	0.40
1:A:317:ILE:HG21	1:A:319:LEU:HD21	2.03	0.40
1:A:531:THR:CG2	2:B:114:THR:HG22	2.51	0.40
1:A:540:PHE:HB3	1:A:545:ILE:HA	2.03	0.40
2:B:96:LYS:NZ	2:B:97:GLU:HB2	2.36	0.40
1:C:372:ARG:HA	1:C:375:PHE:HB3	2.02	0.40
1:C:457:SER:HB3	1:C:461:ASP:O	2.22	0.40
1:C:512:PHE:N	1:C:522:ALA:O	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:GLU:O	1:A:376:GLN:NE2	2.55	0.40
1:A:416:TYR:CD1	1:A:426:LEU:HD21	2.57	0.40
1:A:513:LEU:HD12	1:A:513:LEU:HA	1.94	0.40
1:C:224:VAL:O	1:C:224:VAL:HG12	2.22	0.40
1:C:464:ILE:HG22	1:C:482:ASN:OD1	2.21	0.40
2:D:78:TYR:CE2	2:D:145:LEU:HB2	2.55	0.40
2:D:102:LEU:HD22	2:D:111:ILE:HG22	2.02	0.40
2:D:123:ASN:C	2:D:124:LEU:HD22	2.46	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:THR:OG1	1:C:391:LYS:CA[4_544]	2.07	0.13
1:A:419:SER:OG	1:C:288:GLU:OE1[3_544]	2.10	0.10
1:A:419:SER:CB	1:C:288:GLU:OE1[3_544]	2.13	0.07

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	392/416 (94%)	342 (87%)	39 (10%)	11 (3%)	4	21
1	C	391/416 (94%)	343 (88%)	40 (10%)	8 (2%)	6	27
2	B	127/138 (92%)	113 (89%)	13 (10%)	1 (1%)	16	45
2	D	127/138 (92%)	113 (89%)	13 (10%)	1 (1%)	16	45
All	All	1037/1108 (94%)	911 (88%)	105 (10%)	21 (2%)	6	27

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	43	SER
2	D	43	SER
1	A	405	SER
1	A	519	TRP
1	A	578	VAL
1	C	195	SER
1	C	405	SER
1	A	195	SER
1	A	495	ARG
1	A	373	THR
1	A	544	GLU
1	C	288	GLU
1	C	544	GLU
1	A	226	ASN
1	C	553	GLU
1	C	578	VAL
1	A	243	GLY
1	A	559	GLN
1	C	495	ARG
1	C	595	VAL
1	A	595	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	360/373 (96%)	308 (86%)	52 (14%)	3	14
1	C	359/373 (96%)	316 (88%)	43 (12%)	5	20
2	B	119/125 (95%)	98 (82%)	21 (18%)	2	9
2	D	119/125 (95%)	111 (93%)	8 (7%)	15	42
All	All	957/996 (96%)	833 (87%)	124 (13%)	4	17

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	194	THR

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Mol	Chain	Res	Type
1	A	199	LYS
1	A	215	VAL
1	A	246	LYS
1	A	249	ILE
1	A	258	ARG
1	A	260	ASP
1	A	262	VAL
1	A	265	MET
1	A	280	HIS
1	A	293	THR
1	A	299	HIS
1	A	306	ASN
1	A	308	THR
1	A	312	GLU
1	A	318	ARG
1	A	322	ARG
1	A	344	LYS
1	A	347	LYS
1	A	357	LYS
1	A	360	ASP
1	A	361	THR
1	A	369	PHE
1	A	372	ARG
1	A	376	GLN
1	A	384	ILE
1	A	388	LYS
1	A	393	GLU
1	A	404	LYS
1	A	424	ILE
1	A	425	ILE
1	A	429	ILE
1	A	436	LEU
1	A	444	ILE
1	A	448	LEU
1	A	450	GLN
1	A	452	VAL
1	A	464	ILE
1	A	470	ASP
1	A	476	ARG
1	A	484	VAL
1	A	519	TRP
1	A	521	SER

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Mol	Chain	Res	Type
1	A	525	TYR
1	A	541	LYS
1	A	547	TYR
1	A	570	ASN
1	A	575	ILE
1	A	582	ASP
1	A	595	VAL
1	A	597	ILE
1	A	603	GLU
2	B	31	ILE
2	B	49	GLN
2	B	64	ILE
2	B	82	TYR
2	B	83	MET
2	B	94	ILE
2	B	96	LYS
2	B	109	GLN
2	B	119	GLU
2	B	123	ASN
2	B	124	LEU
2	B	128	GLU
2	B	137	ILE
2	B	138	ILE
2	B	142	ASN
2	B	148	LEU
2	B	149	ASP
2	B	152	GLU
2	B	161	MET
2	B	166	LYS
2	B	167	VAL
1	C	188	ILE
1	C	195	SER
1	C	203	ILE
1	C	213	GLU
1	C	215	VAL
1	C	225	ASP
1	C	226	ASN
1	C	229	PHE
1	C	244	ILE
1	C	246	LYS
1	C	258	ARG
1	C	262	VAL

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Mol	Chain	Res	Type
1	C	265	MET
1	C	270	VAL
1	C	279	ILE
1	C	299	HIS
1	C	318	ARG
1	C	322	ARG
1	C	344	LYS
1	C	351	TYR
1	C	367	VAL
1	C	369	PHE
1	C	372	ARG
1	C	376	GLN
1	C	384	ILE
1	C	388	LYS
1	C	393	GLU
1	C	404	LYS
1	C	413	LEU
1	C	429	ILE
1	C	442	SER
1	C	476	ARG
1	C	519	TRP
1	C	520	VAL
1	C	541	LYS
1	C	547	TYR
1	C	548	GLN
1	C	551	LEU
1	C	570	ASN
1	C	575	ILE
1	C	580	ILE
1	C	582	ASP
1	C	597	ILE
2	D	31	ILE
2	D	49	GLN
2	D	85	ASP
2	D	96	LYS
2	D	112	LYS
2	D	128	GLU
2	D	145	LEU
2	D	152	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	358	GLN
1	A	481	ASN
2	B	88	GLN
2	B	98	ASN
2	B	151	GLN
1	C	287	HIS
1	C	306	ASN
1	C	394	ASN
1	C	427	GLN
1	C	434	ASN
1	C	527	ASN
1	C	529	ASN
2	D	130	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	400/416 (96%)	0.56	12 (3%) 52 35	22, 29, 48, 64	0
1	C	399/416 (95%)	0.61	11 (2%) 55 36	24, 30, 52, 85	0
2	B	131/138 (94%)	0.55	2 (1%) 72 53	26, 28, 51, 69	0
2	D	131/138 (94%)	1.20	21 (16%) 5 4	30, 44, 80, 94	0
All	All	1061/1108 (95%)	0.66	46 (4%) 40 25	22, 30, 59, 94	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	139	SER	6.2
2	D	160	ALA	4.0
1	A	440	SER	3.8
2	D	93	THR	3.6
2	B	154	GLY	3.5
2	D	130	GLN	3.5
2	D	157	GLN	3.4
1	A	311	THR	3.2
2	D	136	TYR	3.1
1	A	568	LEU	3.1
2	D	40	SER	3.1
1	C	189	CYS	3.0
1	C	300	VAL	2.9
2	D	128	GLU	2.9
1	A	392	ALA	2.9
2	D	84	VAL	2.9
2	B	126	GLY	2.9
1	A	394	ASN	2.7
2	D	52	VAL	2.7
2	D	49	GLN	2.7
1	A	411	SER	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	162	LYS	2.6
1	C	307	SER	2.6
2	D	159	ARG	2.6
1	A	288	GLU	2.5
1	A	250	ILE	2.5
2	D	95	LYS	2.4
1	C	194	THR	2.3
2	D	41	SER	2.3
2	D	134	ASP	2.3
1	A	534	ASN	2.3
2	D	105	ALA	2.3
1	C	360	ASP	2.3
1	C	299	HIS	2.2
2	D	138	ILE	2.2
1	C	502	VAL	2.2
2	D	149	ASP	2.2
1	A	336	ALA	2.1
1	C	532	ALA	2.1
1	C	587	VAL	2.1
1	A	190	LEU	2.0
2	D	111	ILE	2.0
1	C	538	ALA	2.0
2	D	89	ALA	2.0
1	C	424	ILE	2.0
1	A	203	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.