Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2023 – 06:37 am GMT

PDB ID	:	2VSK
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:

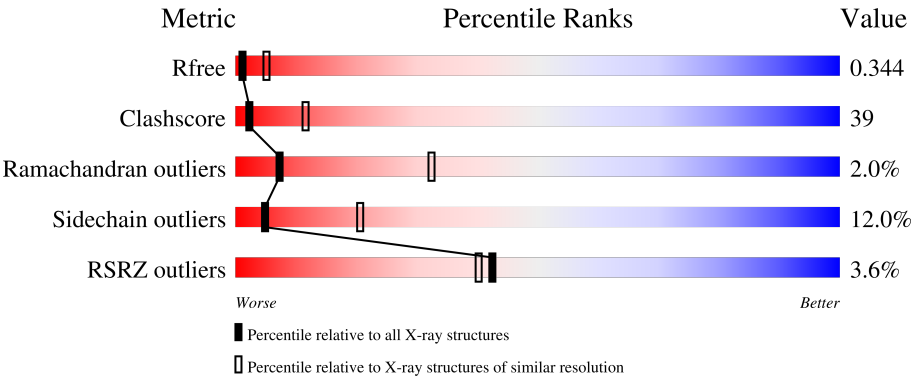
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 <=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	2% 38% 48% 9% ·
1	C	416	3% 43% 45% 8% ·
2	B	138	% 47% 39% 8% · 5%
2	D	138	13% 48% 43% · 5%

2 Entry composition (i)

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.

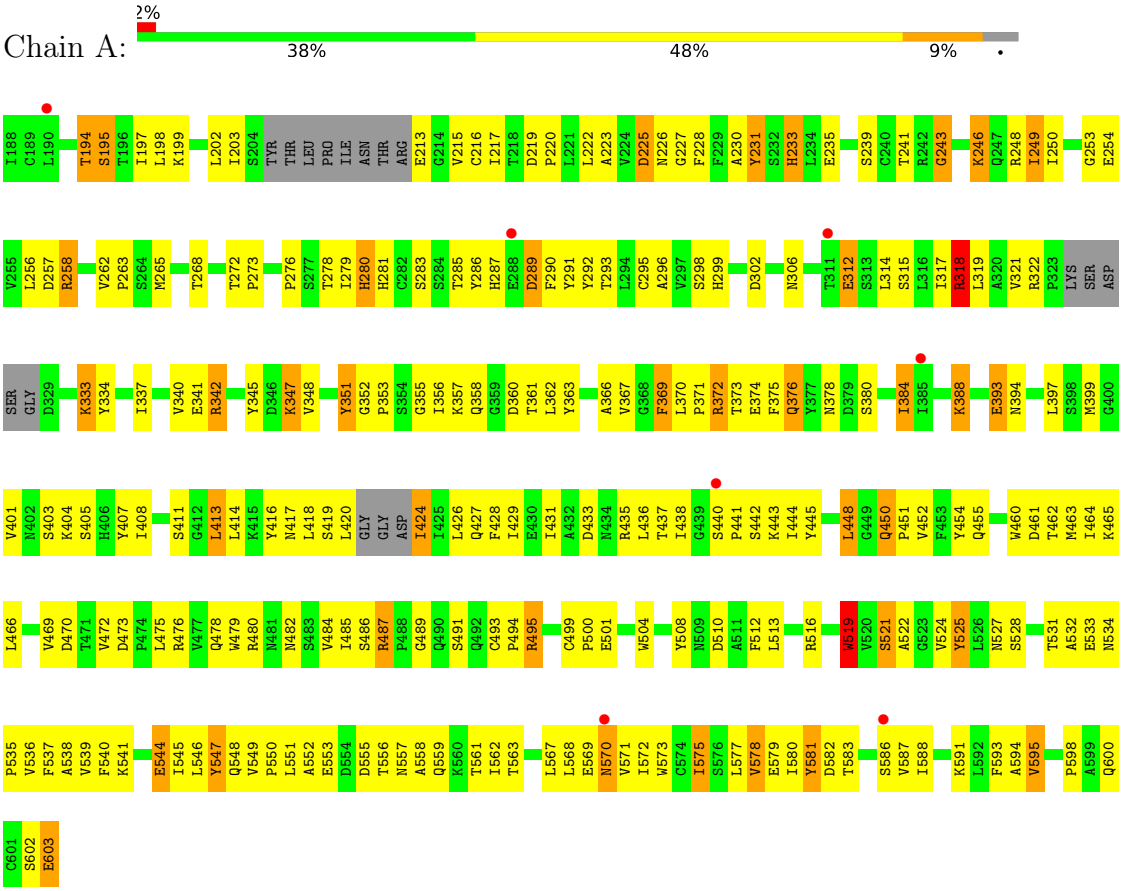
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	131	Total	C	N	O	S	0	0	0
			1056	681	169	199	7			
2	D	131	Total	C	N	O	S	0	0	0
			1056	681	169	199	7			

3 Residue-property plots (i)

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.

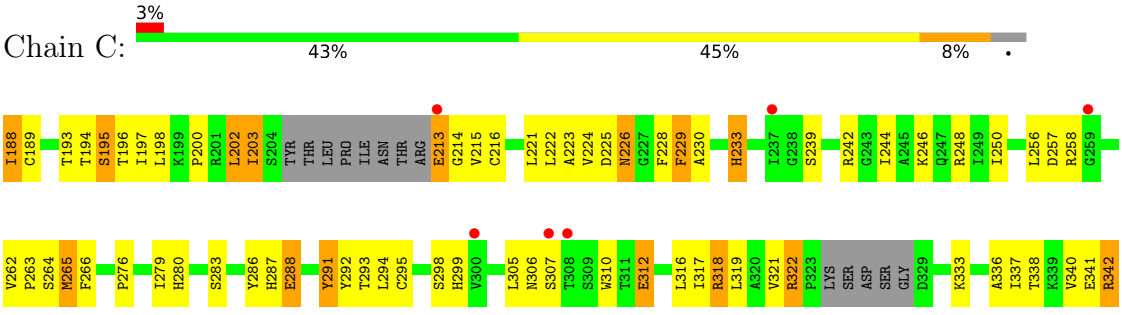
• Molecule 1: HEMAGGLUTININ-NEURAMINIDASE

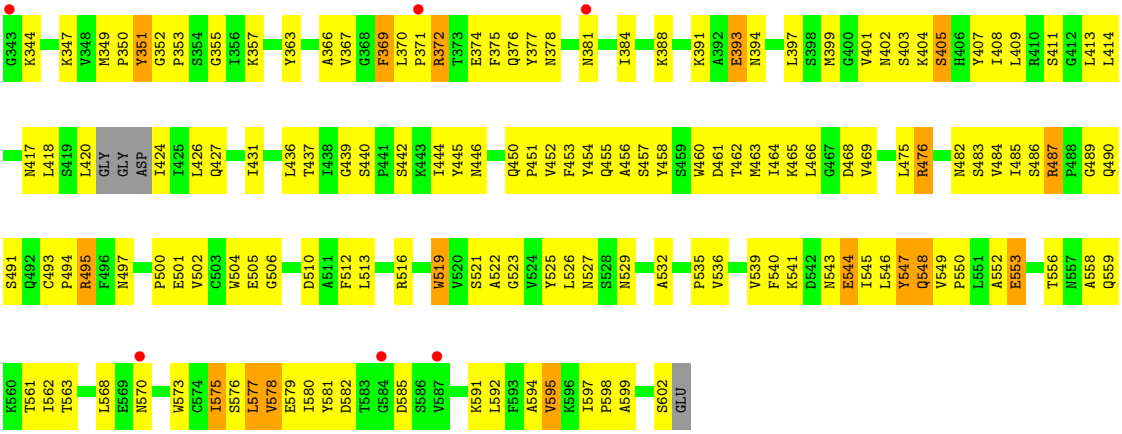
Chain A:



• Molecule 1: HEMAGGLUTININ-NEURAMINIDASE

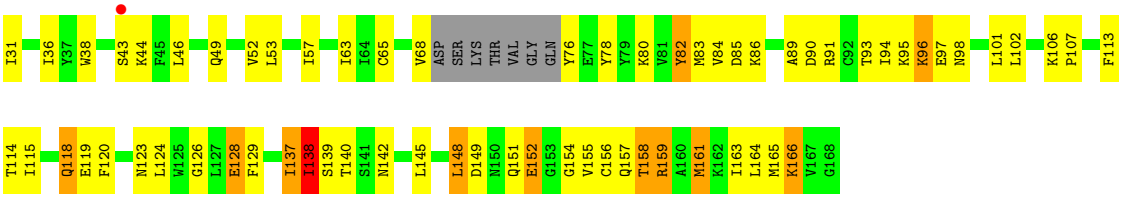
Chain C:





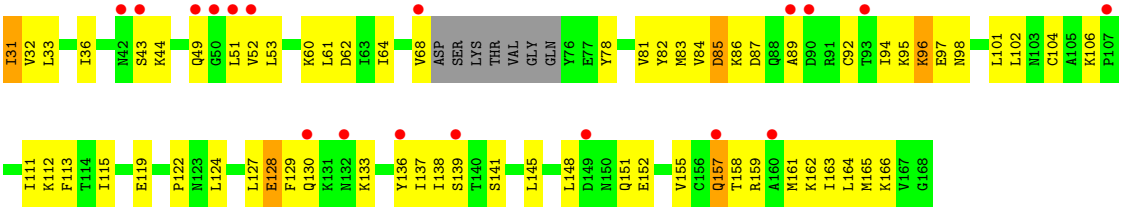
• Molecule 2: EPHRIN-B2

Chain B:



• Molecule 2: EPHRIN-B2

Chain D:



4 Data and refinement statistics (i)

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 29.61 – 3.30	Depositor EDS
% Data completeness (in resolution range)	82.7 (20.00-3.30) 93.6 (29.61-3.30)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 3.31Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.300 , 0.350 0.287 , 0.344	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)	0.26 , 25.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.27$, $< L^2 > = 0.11$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.69	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.87	1/3245 (0.0%)	0.91	2/4415 (0.0%)
1	C	0.79	0/3236	0.86	2/4403 (0.0%)
2	B	0.87	1/1078 (0.1%)	0.88	1/1454 (0.1%)
2	D	0.79	0/1078	0.83	1/1454 (0.1%)
All	All	0.83	2/8637 (0.0%)	0.88	6/11726 (0.1%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	65	CYS	CB-SG	-5.70	1.72	1.81
1	A	569	GLU	CG-CD	5.10	1.59	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	202	LEU	CA-CB-CG	5.72	128.45	115.30
1	A	413	LEU	CA-CB-CG	5.68	128.36	115.30
1	A	318	ARG	NE-CZ-NH1	5.46	123.03	120.30
2	D	104	CYS	CA-CB-SG	-5.38	104.31	114.00
1	C	577	LEU	N-CA-C	-5.24	96.87	111.00
2	B	156	CYS	CA-CB-SG	5.05	123.08	114.00

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 (i)

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	279	2
1	C	3161	0	3111	263	3
2	B	1056	0	1053	60	0
2	D	1056	0	1053	66	0
All	All	8443	0	8334	651	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 39.

All (651) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:A:408:ILE:HD12	1:A:408:ILE:C	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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:C:293:THR:C	1:C:316:LEU:HD12	2.02	0.79
1:A:337:ILE:HG21	1:A:426:LEU:HD12	1.62	0.79
1:C:293:THR:C	1:C:316:LEU:CD1	2.50	0.79
1:C:420:LEU:HD13	1:C:424:ILE:HG23	1.65	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: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:137:ILE:HG13	2:B:165:MET:HE2	1.66	0.77
1:C:399:MET:HE1	1:C:436:LEU:HG	1.65	0.76
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:452:VAL:HG22	1:C:468:ASP:OD1	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:567:LEU:HD22	1:A:570:ASN:C	2.07	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: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
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:C:221:LEU:C	1:C:221:LEU:HD23	2.09	0.72
1:A:393:GLU:HB2	1:A:397:LEU:HD11	1.72	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:437:THR:HG23	1:C:465:LYS:HZ2	1.56	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:408:ILE:C	1:A:408:ILE:CD1	2.60	0.69
1:A:367:VAL:HG13	1:A:369:PHE:HE2	1.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:463:MET:HE2	1:A:482:ASN:O	1.94	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
1:A:231:TYR:HE2	1:A:249:ILE:HD11	1.58	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:C:536:VAL:HG13	1:C:549:VAL:C	2.15	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: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:C:463:MET:HE2	1:C:482:ASN:O	1.96	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:84:VAL:HG22	2:D:136:TYR:O	1.98	0.64
2:D:137:ILE:HD11	2:D:165:MET:HE1	1.78	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:399:MET:HE1	1:A:436:LEU:HG	1.81	0.62
1:A:416:TYR:HD1	1:A:426:LEU:CD2	2.12	0.62
1:A:594:ALA:O	1:A:595:VAL:HG23	1.99	0.62
1:A:443:LYS:NZ	1:A:510:ASP:OD2	2.25	0.62
1:A:351:TYR:CE1	1:A:441:PRO:HD3	2.35	0.62
1:A:536:VAL:HG13	1:A:549:VAL:C	2.20	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
1:A:378:ASN:OD1	1:A:378:ASN:C	2.37	0.62
1:C:548:GLN:C	1:C:549:VAL:HG23	2.18	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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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: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: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
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:A:555:ASP:C	1:A:555:ASP:OD1	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:GLU:HB3	1:A:347:LYS:HZ2	1.70	0.55
1:C:229:PHE:CD1	1:C:229:PHE:C	2.79	0.55
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: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: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
2:B:137:ILE:CG1	2:B:165:MET:HE2	2.36	0.54
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:C:188:ILE:HD12	1:C:188:ILE:C	2.28	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: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:C:215:VAL:CG1	1:C:216:CYS:N	2.71	0.53
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:A:567:LEU:CD2	1:A:570:ASN:C	2.77	0.53
1:C:408:ILE:HD12	1:C:408:ILE:C	2.29	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:C	1:A:587:VAL:HG22	2.29	0.53
1:A:213:GLU:N	1:A:587:VAL:CG2	2.72	0.53
1:A:528:SER:HG	1:A:531:THR:H	1.57	0.53
1:A:253:GLY:HA2	1:A:268:THR:HG23	1.91	0.52
1:C:462:THR:O	1:C:486:SER:OG	2.19	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
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:A:567:LEU:HD23	1:A:571:VAL:C	2.29	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: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:223:ALA:HB3	1:C:230:ALA:HB3	1.92	0.51
1:C:463:MET:HE2	1:C:483:SER:HA	1.91	0.51
1:A:254:GLU:OE1	1:A:256:LEU:HD21	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:541:LYS:HZ3	1:C:546:LEU:HD21	1.73	0.51
1:C:548:GLN:O	1:C:549:VAL:HG22	2.09	0.51
1:A:455:GLN:OE1	1:A:465:LYS:NZ	2.23	0.51
1:C:466:LEU:HD11	1:C:519:TRP:HZ3	1.75	0.51
2:D:83:MET:CE	2:D:165:MET:HE1	2.41	0.51
1:C:228:PHE:CD1	1:C:321:VAL:HB	2.46	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
1:C:393:GLU:O	1:C:394:ASN:C	2.49	0.51
1:A:312:GLU:HB3	1:A:347:LYS:NZ	2.26	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:A:602:SER:O	1:A:603:GLU:C	2.47	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:312:GLU:CG	1:C:312:GLU:O	2.60	0.50
1:C:450:GLN:CD	1:C:451:PRO:HD2	2.32	0.50
2:D:137:ILE:HD11	2:D:165:MET:CE	2.41	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:A:463:MET:HE3	1:A:485:ILE:O	2.12	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: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:399:MET:HE3	1:A:436:LEU:HG	1.93	0.49
1:C:213:GLU:CG	1:C:214:GLY:N	2.76	0.49
1:A:399:MET:O	1:A:438:ILE:HG13	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:463:MET:HE1	1:C:483:SER:C	2.34	0.49
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:A:573:TRP:HZ3	1:A:594:ALA:CB	2.24	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: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:394:ASN:HD22	1:A:500:PRO:C	2.17	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
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
2:D:51:LEU:C	2:D:51:LEU:HD23	2.34	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
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:233:HIS:C	1:C:233:HIS:CD2	2.88	0.47
1:A:249:ILE:C	1:A:250:ILE:HG13	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:286:TYR:C	1:C:286:TYR:CD2	2.88	0.46
1:C:510:ASP:OD1	1:C:510:ASP:C	2.54	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: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
1:A:351:TYR:N	1:A:366:ALA:HA	2.29	0.46
2:B:157:GLN:C	2:B:158:THR:HG23	2.37	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:83:MET:CE	2:D:165:MET:CE	2.94	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: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:401:VAL:HG22	1:C:504:TRP:CZ3	2.52	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
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:C:221:LEU:C	1:C:221:LEU:CD2	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: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:372:ARG:C	1:A:374:GLU:N	2.70	0.44
1:A:466:LEU:HD11	1:A:519:TRP:CZ3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:494:PRO:O	1:C:495:ARG:C	2.56	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:233:HIS:C	1:A:233:HIS:CD2	2.91	0.44
1:A:524:VAL:CG2	1:A:551:LEU:CD1	2.95	0.44
1:C:372:ARG:C	1:C:374:GLU:N	2.71	0.44
1:C:394:ASN:HD22	1:C:500:PRO:C	2.20	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
2:B:106:LYS:O	2:B:107:PRO:C	2.54	0.44
1:C:263:PRO:O	1:C:264:SER:OG	2.30	0.44
1:A:494:PRO:O	1:A:495:ARG:C	2.56	0.43
1:C:198:LEU:CD2	1:C:598:PRO:HD3	2.48	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:194:THR:O	1:A:195:SER:C	2.57	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: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:408:ILE:C	1:C:408:ILE:CD1	2.87	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:463:MET:CE	1:A:485:ILE:O	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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: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
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: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
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
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:454:TYR:CD2	1:C:454:TYR:C	2.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:578:VAL:HG12	1:C:579:GLU:C	2.40	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:215:VAL:HG13	1:C:216:CYS:N	2.36	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
1:A:545:ILE:HG21	1:A:548:GLN:CG	2.48	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:558:ALA:HA	1:A:579:GLU:O	2.21	0.41
2:D:84:VAL:HG23	2:D:85:ASP:O	2.20	0.41
1:A:278:THR:O	1:A:298:SER:N	2.49	0.41
1:A:508:TYR:C	1:A:508:TYR:CD2	2.93	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
1:C:546:LEU:C	1:C:547:TYR:HD2	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:536:VAL:HG13	1:A:550:PRO:N	2.36	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
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

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 (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	392/416 (94%)	342 (87%)	39 (10%)	11 (3%)	5 25
1	C	391/416 (94%)	343 (88%)	40 (10%)	8 (2%)	7 32
2	B	127/138 (92%)	113 (89%)	13 (10%)	1 (1%)	19 51
2	D	127/138 (92%)	113 (89%)	13 (10%)	1 (1%)	19 51
All	All	1037/1108 (94%)	911 (88%)	105 (10%)	21 (2%)	7 32

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	360/373 (96%)	313 (87%)	47 (13%)	4 17
1	C	359/373 (96%)	319 (89%)	40 (11%)	6 23
2	B	119/125 (95%)	100 (84%)	19 (16%)	2 11
2	D	119/125 (95%)	110 (92%)	9 (8%)	13 39
All	All	957/996 (96%)	842 (88%)	115 (12%)	5 20

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	194	THR
1	A	199	LYS
1	A	225	ASP
1	A	231	TYR
1	A	233	HIS
1	A	246	LYS
1	A	249	ILE
1	A	258	ARG
1	A	265	MET
1	A	280	HIS
1	A	289	ASP
1	A	293	THR
1	A	299	HIS
1	A	306	ASN
1	A	312	GLU
1	A	318	ARG
1	A	322	ARG
1	A	333	LYS
1	A	342	ARG
1	A	347	LYS
1	A	351	TYR
1	A	357	LYS
1	A	360	ASP
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	448	LEU
1	A	450	GLN

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Mol	Chain	Res	Type
1	A	464	ILE
1	A	470	ASP
1	A	476	ARG
1	A	487	ARG
1	A	519	TRP
1	A	521	SER
1	A	525	TYR
1	A	547	TYR
1	A	570	ASN
1	A	575	ILE
1	A	581	TYR
1	A	582	ASP
1	A	600	GLN
1	A	603	GLU
2	B	31	ILE
2	B	49	GLN
2	B	82	TYR
2	B	83	MET
2	B	96	LYS
2	B	118	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	159	ARG
2	B	161	MET
2	B	166	LYS
1	C	188	ILE
1	C	195	SER
1	C	203	ILE
1	C	213	GLU
1	C	225	ASP
1	C	226	ASN
1	C	229	PHE
1	C	233	HIS
1	C	244	ILE

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Mol	Chain	Res	Type
1	C	246	LYS
1	C	258	ARG
1	C	265	MET
1	C	291	TYR
1	C	299	HIS
1	C	306	ASN
1	C	312	GLU
1	C	318	ARG
1	C	322	ARG
1	C	342	ARG
1	C	344	LYS
1	C	351	TYR
1	C	357	LYS
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	476	ARG
1	C	487	ARG
1	C	497	ASN
1	C	519	TRP
1	C	527	ASN
1	C	547	TYR
1	C	548	GLN
1	C	570	ASN
1	C	575	ILE
1	C	581	TYR
1	C	582	ASP
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	152	GLU
2	D	157	GLN
2	D	166	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	358	GLN
1	A	376	GLN
2	B	88	GLN
2	B	98	ASN
2	B	151	GLN
1	C	287	HIS
1	C	434	ASN
1	C	527	ASN
2	D	130	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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%)	0.28	7 (1%) 68 67	22, 29, 48, 64	0
1	C	399/416 (95%)	0.38	12 (3%) 50 49	24, 30, 52, 85	0
2	B	131/138 (94%)	0.36	1 (0%) 86 86	26, 28, 51, 69	0
2	D	131/138 (94%)	1.05	18 (13%) 3 2	30, 44, 80, 94	0
All	All	1061/1108 (95%)	0.42	38 (3%) 42 40	22, 30, 59, 94	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	130	GLN	3.8
2	D	149	ASP	3.7
2	D	139	SER	3.7
2	D	52	VAL	3.6
2	D	51	LEU	3.6
2	D	49	GLN	3.4
1	C	343	GLY	3.4
2	D	42	ASN	3.2
1	C	587	VAL	3.2
1	C	307	SER	3.2
2	D	50	GLY	3.0
2	D	90	ASP	2.9
1	A	586	SER	2.8
2	D	43	SER	2.7
1	C	308	THR	2.7
2	D	93	THR	2.7
1	C	237	ILE	2.5
2	D	157	GLN	2.5
1	C	300	VAL	2.5
2	D	68	VAL	2.4
2	D	107	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	213	GLU	2.3
1	C	371	PRO	2.3
1	C	584	GLY	2.3
2	B	43	SER	2.2
1	A	570	ASN	2.2
2	D	160	ALA	2.2
2	D	89	ALA	2.2
1	A	440	SER	2.1
1	A	288	GLU	2.1
1	C	381	ASN	2.1
1	A	190	LEU	2.1
2	D	136	TYR	2.1
1	A	311	THR	2.1
2	D	132	ASN	2.1
1	A	385	ILE	2.0
1	C	259	GLY	2.0
1	C	570	ASN	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 monosaccharides 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.