Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:38 AM GMT

PDB ID	:	2HYE
Title	:	Crystal Structure of the DDB1-Cul4A-Rbx1-SV5V Complex
Authors	:	Angers, S.; Li, T.; Yi, X.; MacCoss, M.J.; Moon, R.T.; Zheng, N.
Deposited on	:	2006-08-05
Resolution	:	3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

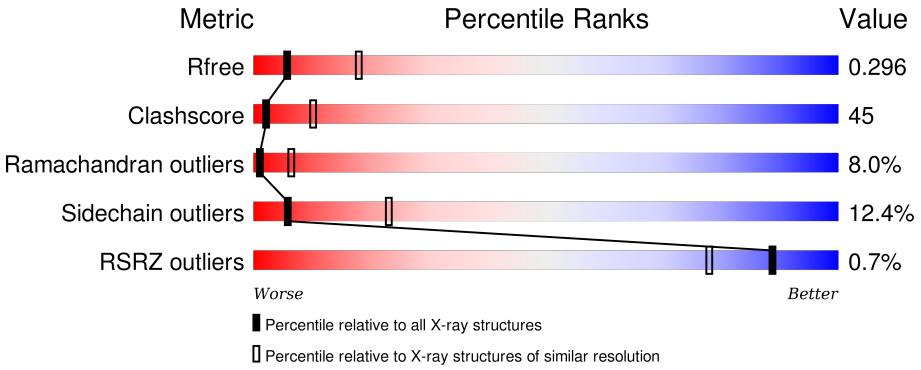
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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

Mol	Chain	Length	Quality of chain
1	A	1140	% 36% 51% 12% •
2	B	222	% 20% 47% 12% • 19%
3	C	759	33% 47% 13% • 5%
4	D	108	31% 27% 19% 6% 17%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16943 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 DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1140	Total	C	N	O	S	0	0	0
			8920	5645	1503	1723	49			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	422	TYR	ASP	CONFLICT	UNP Q16531
A	898	ASP	GLU	CONFLICT	UNP Q16531
A	899	VAL	LEU	CONFLICT	UNP Q16531

- Molecule 2 is a protein called Nonstructural protein V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	180	Total	C	N	O	S	0	0	0
			1373	856	237	272	8			

- Molecule 3 is a protein called Cullin-4A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	719	Total	C	N	O	S	0	0	0
			5899	3753	1023	1089	34			

- Molecule 4 is a protein called RING-box protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	90	Total	C	N	O	S	0	0	0
			746	472	137	128	9			

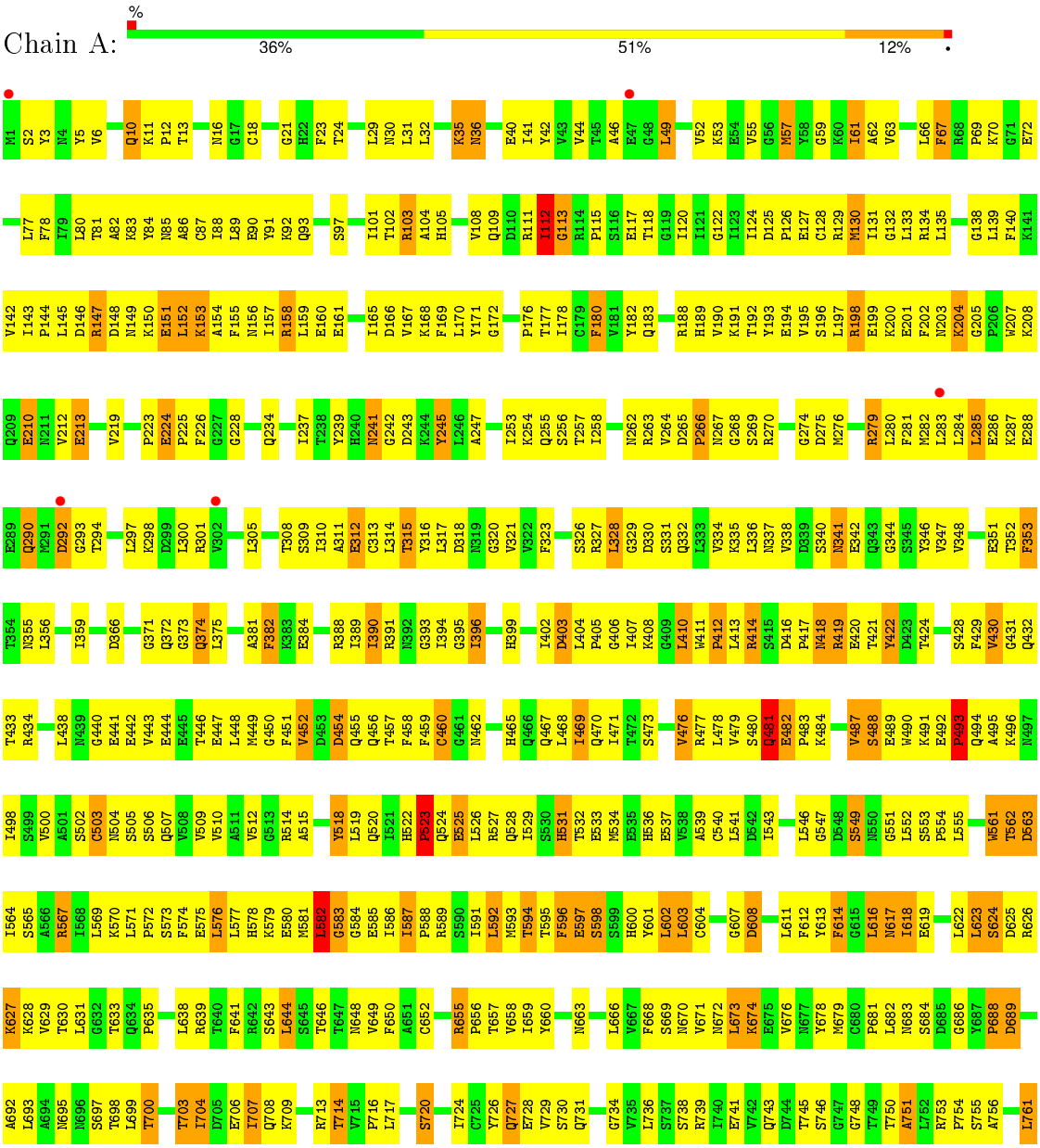
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

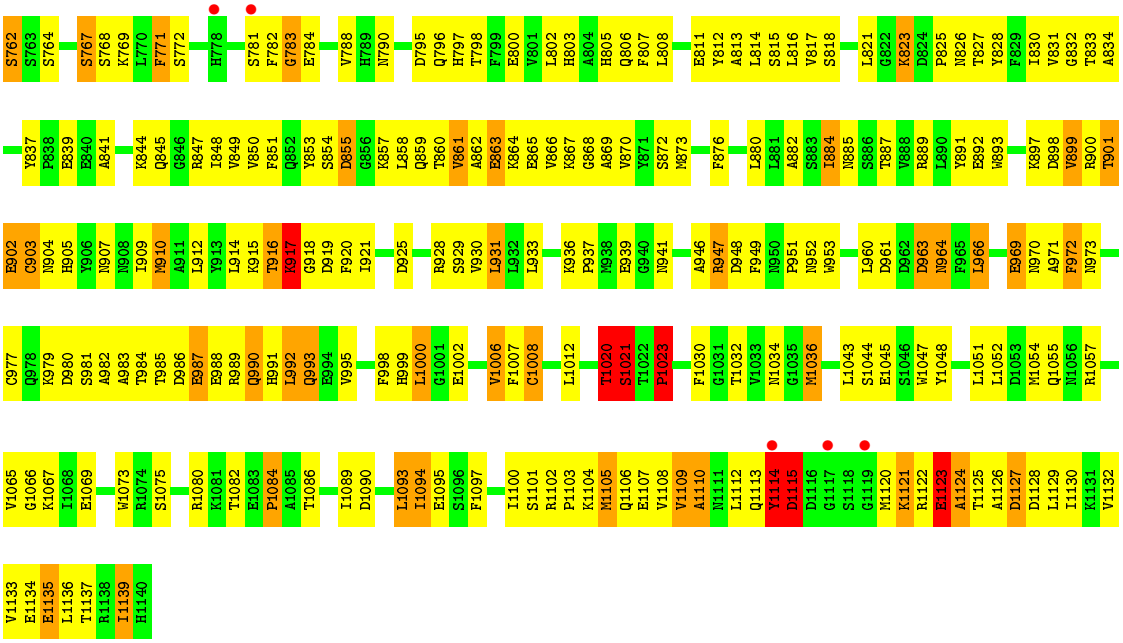
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total Zn 2 2	0	0
5	D	3	Total Zn 3 3	0	0

3 Residue-property plots (i)

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

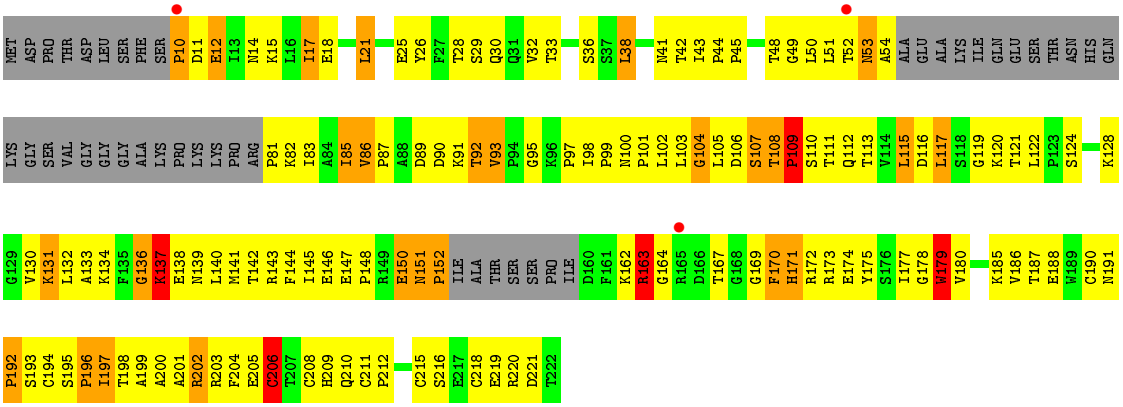
- Molecule 1: DNA damage-binding protein 1





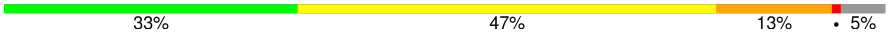
• Molecule 2: Nonstructural protein V

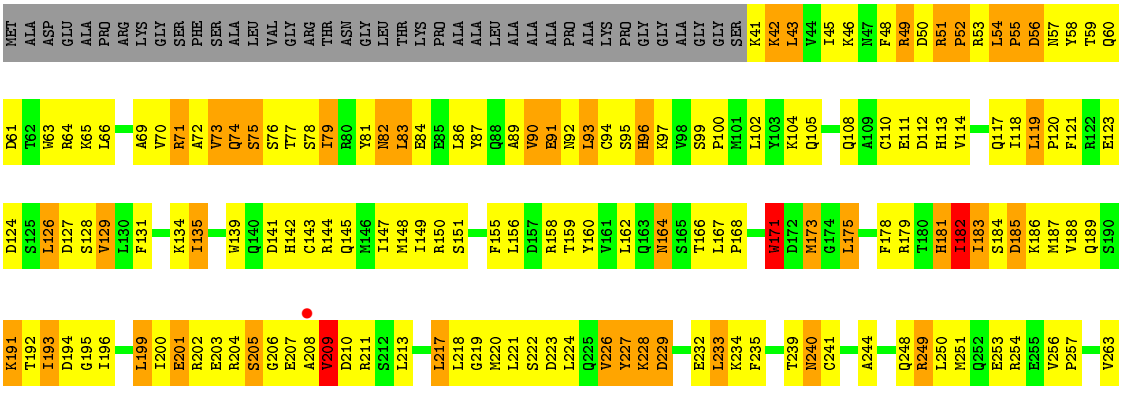
Chain B:

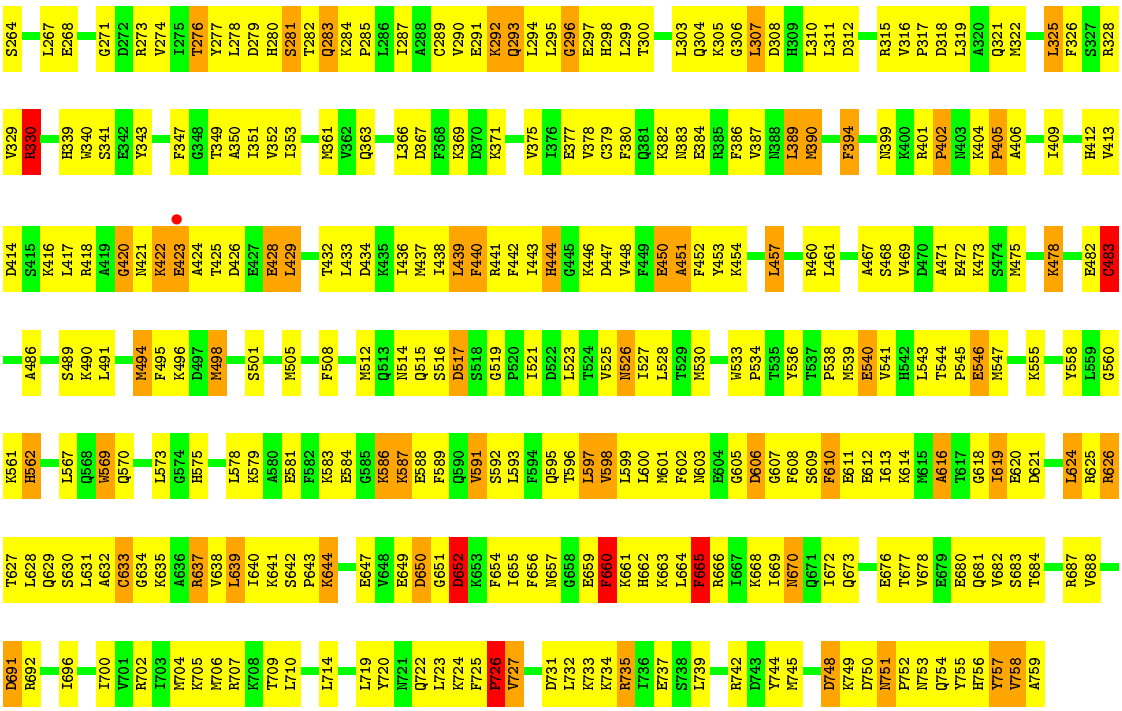


• Molecule 3: Cullin-4A

Chain C:

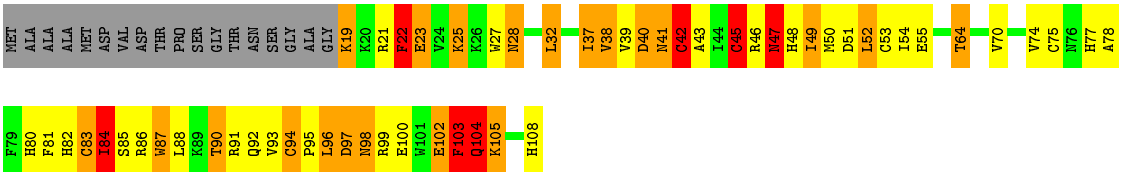






- Molecule 4: RING-box protein 1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	83.45Å 203.16Å 424.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 49.30 – 3.07	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.10) 88.6 (49.30-3.07)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 3.07Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.250 , 0.316 0.244 , 0.296	Depositor DCC
R_{free} test set	3024 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	80.8	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 48.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 62408 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	16943	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.48	1/9086 (0.0%)	0.89	30/12311 (0.2%)
2	B	0.54	1/1401 (0.1%)	1.12	10/1899 (0.5%)
3	C	0.47	0/6007	0.80	16/8068 (0.2%)
4	D	0.62	0/768	1.16	11/1040 (1.1%)
All	All	0.49	2/17262 (0.0%)	0.90	67/23318 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	582	LEU	C-N	6.78	1.45	1.33
2	B	179	TRP	C-N	-5.16	1.22	1.34

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	10	PRO	CA-N-CD	-17.53	86.95	111.50
1	A	151	GLU	N-CA-C	-16.61	66.15	111.00
1	A	561	TRP	N-CA-C	15.57	153.04	111.00
1	A	561	TRP	CB-CA-C	-15.48	79.43	110.40
2	B	109	PRO	CA-N-CD	-15.47	89.85	111.50
4	D	22	PHE	CB-CA-C	-12.89	84.63	110.40
2	B	179	TRP	CB-CA-C	-12.40	85.59	110.40
1	A	767	SER	N-CA-C	-11.97	78.68	111.00
3	C	126	LEU	CB-CA-C	-11.91	87.58	110.20
1	A	767	SER	CB-CA-C	-11.16	88.89	110.10
3	C	298	HIS	CB-CA-C	-10.71	88.98	110.40
1	A	1023	PRO	CA-N-CD	-10.56	96.71	111.50
1	A	1115	ASP	N-CA-C	10.55	139.48	111.00
2	B	107	SER	N-CA-C	-10.21	83.43	111.00
2	B	152	PRO	CA-N-CD	-9.86	97.69	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	916	THR	N-CA-C	9.83	137.54	111.00
3	C	182	ILE	N-CA-C	9.30	136.10	111.00
1	A	266	PRO	CA-N-CD	-9.26	98.53	111.50
1	A	1114	TYR	C-N-CA	9.22	144.76	121.70
1	A	916	THR	CB-CA-C	-8.64	88.27	111.60
1	A	382	PHE	CB-CG-CD2	-8.10	115.13	120.80
1	A	1114	TYR	N-CA-C	7.94	132.44	111.00
4	D	103	PHE	CB-CA-C	-7.73	94.94	110.40
3	C	126	LEU	N-CA-C	7.69	131.75	111.00
4	D	103	PHE	N-CA-C	7.64	131.62	111.00
3	C	420	GLY	C-N-CA	7.54	140.54	121.70
4	D	42	CYS	N-CA-C	-7.29	91.31	111.00
3	C	181	HIS	CB-CA-C	7.08	124.56	110.40
4	D	103	PHE	CB-CG-CD1	-6.98	115.92	120.80
1	A	624	SER	N-CA-C	6.98	129.84	111.00
2	B	150	GLU	CB-CA-C	6.92	124.24	110.40
3	C	206	GLY	N-CA-C	6.91	130.38	113.10
1	A	382	PHE	CB-CG-CD1	6.82	125.57	120.80
4	D	97	ASP	CB-CA-C	6.71	123.82	110.40
4	D	45	CYS	CA-CB-SG	6.62	125.92	114.00
1	A	688	PRO	N-CA-C	6.59	129.22	112.10
4	D	104	GLN	N-CA-C	6.53	128.64	111.00
1	A	689	ASP	N-CA-C	-6.45	93.58	111.00
3	C	616	ALA	N-CA-C	6.44	128.38	111.00
4	D	22	PHE	CB-CG-CD1	-6.33	116.37	120.80
3	C	83	LEU	N-CA-C	6.26	127.91	111.00
4	D	47	ASN	N-CA-C	-6.25	94.12	111.00
1	A	562	THR	N-CA-CB	-6.24	98.44	110.30
1	A	917	LYS	N-CA-CB	-6.13	99.57	110.60
1	A	1020	THR	N-CA-C	6.10	127.46	111.00
3	C	84	GLU	N-CA-CB	-6.08	99.65	110.60
4	D	103	PHE	CB-CG-CD2	6.03	125.02	120.80
1	A	1020	THR	CB-CA-C	-5.99	95.42	111.60
2	B	12	GLU	CB-CA-C	-5.97	98.45	110.40
1	A	709	LYS	CB-CA-C	5.94	122.28	110.40
3	C	182	ILE	N-CA-CB	-5.92	97.19	110.80
1	A	688	PRO	CA-N-CD	-5.91	103.23	111.50
1	A	624	SER	CB-CA-C	-5.86	98.97	110.10
1	A	1114	TYR	CB-CA-C	-5.79	98.81	110.40
1	A	781	SER	N-CA-C	5.75	126.53	111.00
2	B	179	TRP	N-CA-CB	5.71	120.87	110.60
2	B	12	GLU	N-CA-C	5.65	126.26	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	296	GLY	N-CA-C	-5.56	99.19	113.10
3	C	637	ARG	N-CA-C	5.48	125.78	111.00
3	C	665	PHE	N-CA-C	-5.36	96.52	111.00
3	C	74	GLN	N-CA-C	-5.32	96.64	111.00
1	A	523	PRO	CA-N-CD	-5.30	104.08	111.50
3	C	73	VAL	N-CA-C	-5.22	96.91	111.00
1	A	917	LYS	N-CA-C	5.14	124.87	111.00
1	A	1115	ASP	CB-CA-C	-5.06	100.29	110.40
1	A	768	SER	N-CA-C	-5.04	97.38	111.00
2	B	179	TRP	CA-CB-CG	5.00	123.21	113.70

There are no chirality outliers.

There are no planarity outliers.

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	8920	0	8880	812	0
2	B	1373	0	1356	176	0
3	C	5899	0	5977	489	1
4	D	746	0	699	82	0
5	B	2	0	0	0	0
5	D	3	0	0	0	0
All	All	16943	0	16912	1515	1

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 45.

All (1515) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1114:TYR:CD1	1:A:1114:TYR:O	1.68	1.47
1:A:381:ALA:O	1:A:720:SER:HB3	1.35	1.23
3:C:422:LYS:NZ	3:C:422:LYS:HB3	1.30	1.22
1:A:381:ALA:O	1:A:720:SER:CB	1.90	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:889:ARG:HD3	1:A:904:ASN:HD21	1.16	1.11
3:C:69:ALA:HA	3:C:79:ILE:HG21	1.33	1.10
4:D:25:LYS:HA	4:D:25:LYS:HE3	1.30	1.10
1:A:189:HIS:ND1	1:A:210:GLU:O	1.85	1.09
3:C:54:LEU:HB2	3:C:55:PRO:HD3	1.40	1.04
1:A:889:ARG:HD2	1:A:901:THR:HG23	1.36	1.03
2:B:151:ASN:OD1	2:B:170:PHE:HZ	1.42	1.03
1:A:1120:MET:HE3	1:A:1122:ARG:CZ	1.90	1.01
3:C:118:ILE:HD11	3:C:181:HIS:HB3	1.38	1.01
1:A:112:ILE:HD13	1:A:112:ILE:H	1.24	1.01
3:C:422:LYS:CB	3:C:422:LYS:NZ	2.20	1.01
3:C:626:ARG:HA	3:C:629:GLN:HB2	1.41	1.00
2:B:85:ILE:HD12	2:B:85:ILE:H	1.28	0.99
1:A:771:PHE:HE2	1:A:845:GLN:HB3	1.24	0.99
3:C:657:ASN:HD21	3:C:659:GLU:HB2	1.28	0.99
1:A:889:ARG:HD3	1:A:904:ASN:ND2	1.79	0.98
1:A:328:LEU:H	1:A:328:LEU:HD12	1.27	0.97
1:A:226:PHE:CE1	1:A:268:GLY:O	2.17	0.97
4:D:41:ASN:ND2	4:D:47:ASN:O	1.98	0.96
3:C:491:LEU:HA	3:C:494:MET:HG3	1.47	0.96
1:A:1120:MET:HE3	1:A:1122:ARG:NH2	1.79	0.96
1:A:1120:MET:CE	1:A:1122:ARG:CZ	2.44	0.96
3:C:638:VAL:HG12	3:C:639:LEU:HD23	1.47	0.95
3:C:642:SER:HB2	3:C:643:PRO:HD3	1.46	0.95
1:A:1114:TYR:CG	1:A:1114:TYR:O	2.20	0.95
2:B:30:GLN:HE21	2:B:36:SER:HB3	1.30	0.94
2:B:170:PHE:O	2:B:193:SER:HB2	1.67	0.94
1:A:465:HIS:ND1	1:A:523:PRO:HD3	1.82	0.93
1:A:985:THR:HG22	1:A:987:GLU:H	1.35	0.92
1:A:866:VAL:HG21	1:A:884:ILE:HG12	1.50	0.91
3:C:422:LYS:HB3	3:C:422:LYS:HZ3	1.09	0.91
1:A:507:GLN:NE2	1:A:552:LEU:HA	1.85	0.91
1:A:444:GLU:HB3	3:C:46:LYS:HB2	1.54	0.90
1:A:335:LYS:HB3	1:A:348:VAL:HG23	1.54	0.90
3:C:99:SER:HB2	3:C:100:PRO:HD3	1.53	0.89
4:D:102:GLU:O	4:D:103:PHE:HB2	1.69	0.89
4:D:94:CYS:SG	4:D:97:ASP:HB2	2.12	0.89
1:A:465:HIS:CE1	1:A:523:PRO:HD3	2.07	0.89
3:C:635:LYS:HD3	3:C:637:ARG:HD2	1.53	0.89
3:C:745:MET:HA	3:C:757:TYR:O	1.71	0.88
4:D:49:ILE:HD12	4:D:70:VAL:HG22	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:THR:H	1:A:30:ASN:ND2	1.71	0.88
1:A:649:VAL:HG12	1:A:650:PHE:H	1.39	0.88
1:A:176:PRO:HB2	1:A:195:VAL:HG22	1.56	0.88
3:C:422:LYS:HB3	3:C:422:LYS:HZ2	1.10	0.87
1:A:578:HIS:CD2	1:A:623:LEU:HD12	2.09	0.87
1:A:1120:MET:HE2	1:A:1122:ARG:NE	1.89	0.87
1:A:1120:MET:HG3	1:A:1122:ARG:HG2	1.55	0.87
4:D:41:ASN:HB3	4:D:42:CYS:O	1.75	0.87
3:C:538:PRO:HA	3:C:570:GLN:HE22	1.40	0.86
1:A:149:ASN:C	1:A:151:GLU:O	2.14	0.86
3:C:274:VAL:HA	3:C:278:LEU:HB2	1.57	0.86
1:A:928:ARG:HH12	1:A:947:ARG:NH2	1.74	0.86
3:C:213:LEU:O	3:C:217:LEU:HD12	1.76	0.85
1:A:771:PHE:CE2	1:A:845:GLN:HB3	2.10	0.85
3:C:605:GLY:O	3:C:606:ASP:HB2	1.75	0.85
1:A:507:GLN:HE22	1:A:553:SER:H	1.25	0.85
2:B:51:LEU:HD22	2:B:141:MET:HA	1.59	0.85
4:D:42:CYS:O	4:D:46:ARG:HA	1.77	0.84
1:A:736:LEU:HD11	1:A:815:SER:O	1.78	0.84
3:C:144:ARG:HA	3:C:147:ILE:HD12	1.57	0.84
2:B:51:LEU:HD11	2:B:143:ARG:H	1.42	0.84
1:A:224:GLU:HB2	1:A:225:PRO:HD3	1.59	0.84
2:B:15:LYS:O	2:B:15:LYS:HG3	1.78	0.84
1:A:520:GLN:HG3	1:A:529:ILE:HG13	1.60	0.84
2:B:177:ILE:HG12	2:B:186:VAL:HG22	1.59	0.83
1:A:1080:ARG:NH1	2:B:120:LYS:H	1.74	0.83
1:A:1032:THR:HG22	1:A:1034:ASN:H	1.42	0.83
1:A:1127:ASP:HA	1:A:1130:ILE:HD12	1.58	0.82
1:A:270:ARG:HG2	1:A:284:LEU:HG	1.60	0.82
3:C:199:LEU:O	3:C:209:VAL:HG11	1.79	0.82
3:C:119:LEU:HB2	3:C:120:PRO:HD3	1.59	0.82
3:C:284:LYS:HB3	3:C:285:PRO:HD3	1.62	0.82
1:A:482:GLU:CD	1:A:483:PRO:HD3	2.00	0.82
2:B:196:PRO:HD2	2:B:204:PHE:HE2	1.45	0.82
2:B:38:LEU:HD22	2:B:131:LYS:HZ2	1.43	0.81
1:A:736:LEU:HG	1:A:816:LEU:HD22	1.62	0.81
3:C:183:ILE:HD11	3:C:220:MET:SD	2.20	0.81
1:A:889:ARG:HG2	1:A:891:TYR:CE1	2.15	0.81
2:B:170:PHE:HA	2:B:212:PRO:CD	2.09	0.81
1:A:446:THR:HG22	1:A:447:GLU:H	1.43	0.81
1:A:534:MET:HE2	1:A:569:LEU:HD11	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:LEU:HB2	1:A:424:THR:HB	1.63	0.81
1:A:262:ASN:ND2	1:A:316:TYR:H	1.78	0.81
3:C:757:TYR:HE1	3:C:759:ALA:HA	1.46	0.80
3:C:366:LEU:HD23	3:C:439:LEU:HD12	1.62	0.80
1:A:381:ALA:O	1:A:720:SER:OG	1.99	0.80
1:A:969:GLU:HG2	1:A:971:ALA:H	1.46	0.80
3:C:678:VAL:O	3:C:682:VAL:HG23	1.81	0.80
1:A:985:THR:HB	1:A:988:GLU:HG3	1.62	0.80
1:A:328:LEU:N	1:A:328:LEU:HD12	1.97	0.80
1:A:808:LEU:HG	1:A:847:ARG:HH21	1.47	0.80
1:A:509:VAL:HG23	1:A:543:ILE:HD13	1.62	0.80
1:A:909:ILE:HG12	1:A:928:ARG:HD2	1.63	0.79
1:A:340:SER:OG	1:A:344:GLY:HA2	1.82	0.79
1:A:1114:TYR:HD1	1:A:1114:TYR:O	1.63	0.79
3:C:680:GLU:O	3:C:684:THR:HG22	1.81	0.79
1:A:176:PRO:HB2	1:A:195:VAL:CG2	2.13	0.78
3:C:593:LEU:HD21	4:D:27:TRP:HE1	1.48	0.78
1:A:166:ASP:HB3	1:A:219:VAL:HG23	1.65	0.78
3:C:599:LEU:HD21	3:C:631:LEU:HD12	1.64	0.78
1:A:963:ASP:C	1:A:964:ASN:HD22	1.86	0.78
1:A:167:VAL:O	1:A:168:LYS:HG2	1.83	0.78
3:C:274:VAL:HG11	3:C:283:GLN:HE21	1.49	0.78
1:A:859:GLN:HE22	3:C:281:SER:HB2	1.47	0.78
1:A:24:THR:H	1:A:30:ASN:HD21	1.30	0.78
3:C:211:ARG:HD2	3:C:276:THR:HG21	1.64	0.78
1:A:889:ARG:HH11	1:A:904:ASN:HD21	1.29	0.78
3:C:329:VAL:HG12	3:C:330:ARG:H	1.49	0.78
1:A:578:HIS:NE2	1:A:623:LEU:HD12	1.99	0.77
1:A:1094:ILE:HG22	1:A:1094:ILE:O	1.82	0.77
3:C:296:GLY:O	3:C:297:GLU:HB2	1.82	0.77
2:B:32:VAL:HG23	2:B:33:THR:HG23	1.66	0.77
1:A:59:GLY:HA2	1:A:1073:TRP:CZ3	2.19	0.77
2:B:52:THR:HG21	2:B:85:ILE:HG13	1.67	0.77
1:A:602:LEU:C	1:A:603:LEU:HD23	2.04	0.77
3:C:461:LEU:HB3	3:C:498:MET:HE1	1.65	0.77
3:C:422:LYS:CB	3:C:422:LYS:HZ2	1.93	0.77
3:C:527:ILE:HD11	3:C:567:LEU:HD22	1.65	0.77
1:A:649:VAL:HG12	1:A:650:PHE:N	2.00	0.76
2:B:87:PRO:HB2	2:B:198:THR:HG22	1.65	0.76
3:C:578:LEU:HD11	3:C:596:THR:HG23	1.67	0.76
1:A:507:GLN:HE22	1:A:552:LEU:HA	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:ASN:OD1	2:B:170:PHE:CZ	2.34	0.76
1:A:300:LEU:HD23	1:A:300:LEU:H	1.50	0.76
3:C:294:LEU:O	3:C:295:LEU:HD23	1.86	0.75
1:A:189:HIS:HD1	1:A:210:GLU:C	1.89	0.75
1:A:1080:ARG:HD2	2:B:119:GLY:HA3	1.68	0.75
3:C:186:LYS:HB3	3:C:188:VAL:HG23	1.68	0.75
1:A:469:ILE:HD11	1:A:476:VAL:HG23	1.69	0.75
3:C:279:ASP:OD1	3:C:281:SER:HB3	1.87	0.75
4:D:25:LYS:HA	4:D:25:LYS:CE	2.15	0.75
3:C:423:GLU:OE1	3:C:467:ALA:HB2	1.87	0.75
1:A:90:GLU:OE2	1:A:92:LYS:HE3	1.87	0.75
1:A:450:GLY:HA3	1:A:479:VAL:CG2	2.17	0.74
1:A:452:VAL:HG12	1:A:454:ASP:OD2	1.86	0.74
1:A:767:SER:O	1:A:767:SER:OG	1.91	0.74
1:A:149:ASN:O	1:A:151:GLU:O	2.04	0.74
1:A:1120:MET:CG	1:A:1122:ARG:HG2	2.17	0.74
4:D:49:ILE:HD12	4:D:70:VAL:CG2	2.16	0.74
1:A:36:ASN:O	1:A:61:ILE:HG12	1.88	0.74
2:B:202:ARG:HB2	2:B:204:PHE:HE1	1.51	0.74
1:A:862:ALA:HB2	1:A:893:TRP:HH2	1.51	0.74
4:D:41:ASN:O	4:D:42:CYS:C	2.19	0.74
1:A:633:THR:HB	3:C:162:LEU:CD2	2.18	0.74
1:A:1120:MET:HG3	1:A:1122:ARG:NH1	2.03	0.74
1:A:451:PHE:CD1	1:A:470:GLN:HB2	2.23	0.73
1:A:743:GLN:HB3	1:A:783:GLY:HA2	1.68	0.73
3:C:630:SER:HB3	3:C:672:ILE:HD11	1.71	0.73
3:C:595:GLN:HE22	3:C:669:ILE:HG22	1.52	0.73
1:A:657:THR:HG22	1:A:658:VAL:H	1.54	0.73
3:C:635:LYS:HG2	3:C:637:ARG:HG3	1.68	0.73
4:D:91:ARG:HG2	4:D:92:GLN:H	1.53	0.73
1:A:1120:MET:CE	1:A:1122:ARG:NH2	2.51	0.73
1:A:964:ASN:HD22	1:A:964:ASN:N	1.87	0.73
1:A:1109:VAL:HG21	1:A:1125:THR:HA	1.71	0.73
3:C:422:LYS:CB	3:C:422:LYS:HZ3	1.89	0.73
2:B:26:TYR:CE1	2:B:38:LEU:HD21	2.23	0.73
2:B:38:LEU:HD22	2:B:131:LYS:NZ	2.03	0.72
1:A:1120:MET:HE2	1:A:1122:ARG:CZ	2.19	0.72
3:C:609:SER:O	3:C:612:GLU:HG2	1.87	0.72
1:A:1082:THR:O	1:A:1082:THR:HG22	1.89	0.72
1:A:465:HIS:HB2	1:A:467:GLN:HE21	1.54	0.72
2:B:117:LEU:HD13	2:B:137:LYS:NZ	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:77:THR:HG22	3:C:78:SER:H	1.53	0.72
1:A:578:HIS:CD2	1:A:623:LEU:H	2.06	0.72
3:C:276:THR:HG22	3:C:277:TYR:N	2.02	0.72
1:A:356:LEU:HB3	1:A:359:ILE:HD11	1.71	0.72
1:A:876:PHE:HD1	1:A:916:THR:HG23	1.51	0.72
1:A:465:HIS:O	1:A:467:GLN:HG3	1.89	0.72
1:A:448:LEU:HB3	1:A:451:PHE:HD2	1.52	0.72
3:C:127:ASP:O	3:C:129:VAL:N	2.22	0.72
3:C:696:ILE:O	3:C:700:ILE:HG12	1.88	0.72
3:C:240:ASN:OD1	3:C:289:CYS:HB3	1.90	0.72
1:A:192:THR:OG1	1:A:205:GLY:HA3	1.90	0.72
3:C:447:ASP:OD2	3:C:725:PHE:HB3	1.90	0.72
1:A:726:TYR:OH	1:A:796:GLN:NE2	2.22	0.72
3:C:602:PHE:HD2	3:C:656:PHE:HB2	1.54	0.72
3:C:49:ARG:HD2	3:C:51:ARG:NH2	2.05	0.72
2:B:195:SER:HB3	2:B:204:PHE:CD2	2.25	0.72
4:D:83:CYS:O	4:D:84:ILE:HB	1.89	0.72
3:C:340:TRP:CH2	3:C:390:MET:HB2	2.25	0.72
4:D:55:GLU:HG3	4:D:86:ARG:NH2	2.06	0.71
2:B:43:ILE:HD12	2:B:44:PRO:HD2	1.72	0.71
3:C:239:THR:C	3:C:241:CYS:H	1.91	0.71
2:B:89:ASP:CG	2:B:90:ASP:H	1.93	0.71
1:A:1002:GLU:HB3	1:A:1032:THR:HG21	1.71	0.71
1:A:971:ALA:O	1:A:972:PHE:HB2	1.89	0.71
3:C:660:PHE:O	3:C:662:HIS:N	2.23	0.71
3:C:316:VAL:HB	3:C:317:PRO:HD3	1.71	0.71
2:B:206:CYS:SG	2:B:211:CYS:HB2	2.30	0.71
4:D:70:VAL:CG1	4:D:78:ALA:HB1	2.20	0.71
1:A:451:PHE:CE1	1:A:470:GLN:HB2	2.26	0.71
1:A:275:ASP:CB	1:A:279:ARG:HB2	2.21	0.71
1:A:633:THR:HB	3:C:162:LEU:HD23	1.72	0.71
1:A:399:HIS:NE2	1:A:703:THR:HG22	2.06	0.71
1:A:652:CYS:HB3	1:A:676:VAL:O	1.91	0.71
1:A:532:THR:HG22	1:A:533:GLU:N	2.06	0.70
1:A:828:TYR:HB3	1:A:851:PHE:O	1.90	0.70
2:B:51:LEU:HB2	2:B:141:MET:HE3	1.73	0.70
1:A:480:SER:O	1:A:484:LYS:HA	1.92	0.70
1:A:864:LYS:HB2	1:A:899:VAL:HG23	1.72	0.70
2:B:92:THR:O	2:B:93:VAL:HG13	1.91	0.70
1:A:81:THR:HG22	1:A:82:ALA:N	2.06	0.70
3:C:587:LYS:H	3:C:587:LYS:HD2	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:ILE:HD13	1:A:470:GLN:N	2.06	0.70
3:C:578:LEU:HD13	3:C:591:VAL:CG2	2.21	0.70
1:A:450:GLY:HA3	1:A:479:VAL:HG21	1.73	0.70
1:A:125:ASP:OD2	1:A:127:GLU:HB2	1.90	0.70
2:B:208:CYS:O	2:B:210:GLN:N	2.24	0.70
1:A:32:LEU:HD22	1:A:41:ILE:HG12	1.74	0.70
1:A:834:ALA:HB2	1:A:869:ALA:HA	1.73	0.69
1:A:862:ALA:HB2	1:A:893:TRP:CH2	2.27	0.69
3:C:602:PHE:O	4:D:21:ARG:HD2	1.91	0.69
1:A:592:LEU:HD23	1:A:593:MET:O	1.92	0.69
1:A:596:PHE:HE2	1:A:648:ASN:HA	1.57	0.69
1:A:704:ILE:HD12	1:A:704:ILE:H	1.57	0.69
3:C:643:PRO:CD	3:C:652:ASP:HA	2.21	0.69
1:A:724:ILE:HA	1:A:734:GLY:O	1.92	0.69
1:A:1115:ASP:CA	1:A:1120:MET:O	2.41	0.69
1:A:889:ARG:HD2	1:A:901:THR:CG2	2.21	0.69
1:A:158:ARG:NH1	1:A:158:ARG:HB3	2.06	0.69
1:A:815:SER:HB2	1:A:832:GLY:HA3	1.75	0.69
3:C:432:THR:O	3:C:436:ILE:HG13	1.91	0.69
2:B:143:ARG:NH2	2:B:145:ILE:HD11	2.08	0.69
1:A:1007:PHE:O	1:A:1008:CYS:HB3	1.93	0.69
3:C:329:VAL:HG12	3:C:330:ARG:N	2.08	0.68
3:C:619:ILE:HG22	3:C:620:GLU:H	1.57	0.68
1:A:739:ARG:NH1	1:A:790:ASN:HD21	1.92	0.68
4:D:41:ASN:C	4:D:42:CYS:O	2.21	0.68
4:D:19:LYS:HE3	4:D:19:LYS:HA	1.76	0.68
1:A:24:THR:HG23	1:A:91:TYR:CE2	2.29	0.68
1:A:762:SER:HB2	1:A:803:HIS:ND1	2.09	0.68
1:A:157:ILE:HG22	1:A:158:ARG:N	2.08	0.68
1:A:864:LYS:HB2	1:A:899:VAL:CG2	2.24	0.68
1:A:876:PHE:CD1	1:A:916:THR:HG23	2.29	0.68
2:B:92:THR:HG22	2:B:92:THR:O	1.94	0.68
1:A:618:ILE:HG13	1:A:619:GLU:N	2.08	0.68
3:C:555:LYS:HD2	3:C:569:TRP:HZ3	1.58	0.68
3:C:630:SER:CB	3:C:672:ILE:HD11	2.24	0.68
3:C:560:GLY:O	3:C:561:LYS:HB2	1.93	0.68
3:C:751:ASN:O	3:C:753:ASN:N	2.27	0.68
1:A:452:VAL:HG23	1:A:470:GLN:OE1	1.93	0.67
1:A:1100:ILE:HG13	1:A:1105:MET:HE1	1.74	0.67
1:A:903:CYS:SG	1:A:941:ASN:HA	2.33	0.67
2:B:111:THR:HB	2:B:188:GLU:HG2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:743:GLN:HE22	1:A:748:GLY:HA2	1.59	0.67
3:C:249:ARG:O	3:C:253:GLU:HB2	1.95	0.67
1:A:440:GLY:O	1:A:686:GLY:HA3	1.94	0.67
2:B:144:PHE:O	2:B:145:ILE:HD12	1.94	0.67
3:C:366:LEU:CD2	3:C:439:LEU:HD12	2.25	0.67
1:A:310:ILE:HG13	1:A:384:GLU:OE2	1.95	0.67
3:C:274:VAL:HG11	3:C:283:GLN:HB2	1.76	0.67
1:A:49:LEU:N	1:A:49:LEU:HD22	2.08	0.67
1:A:105:HIS:CA	1:A:152:LEU:HD12	2.25	0.67
1:A:112:ILE:CD1	1:A:112:ILE:H	2.01	0.67
4:D:94:CYS:SG	4:D:97:ASP:CB	2.81	0.67
2:B:98:ILE:HB	2:B:201:ALA:HB1	1.76	0.67
2:B:198:THR:C	2:B:200:ALA:H	1.98	0.66
3:C:714:LEU:N	3:C:714:LEU:HD12	2.10	0.66
1:A:889:ARG:HH11	1:A:904:ASN:ND2	1.94	0.66
1:A:422:TYR:CE2	1:A:683:ASN:HB3	2.31	0.66
4:D:52:LEU:HD22	4:D:52:LEU:N	2.10	0.66
4:D:104:GLN:O	4:D:105:LYS:HB2	1.93	0.66
2:B:196:PRO:HD2	2:B:204:PHE:CE2	2.28	0.66
1:A:1007:PHE:HD2	1:A:1030:PHE:HB3	1.61	0.66
1:A:394:ILE:HD12	1:A:706:GLU:HA	1.77	0.66
1:A:1130:ILE:O	1:A:1134:GLU:HB3	1.96	0.66
1:A:312:GLU:HG3	1:A:327:ARG:HB2	1.76	0.66
3:C:538:PRO:CA	3:C:570:GLN:HE22	2.08	0.66
1:A:412:PRO:HB2	1:A:422:TYR:CD1	2.30	0.66
3:C:630:SER:O	3:C:631:LEU:HB2	1.95	0.66
1:A:884:ILE:N	1:A:884:ILE:HD12	2.11	0.66
4:D:95:PRO:O	4:D:96:LEU:HG	1.96	0.66
1:A:460:CYS:HA	1:A:469:ILE:O	1.95	0.66
1:A:864:LYS:HG3	1:A:865:GLU:H	1.60	0.66
3:C:409:ILE:HG13	3:C:443:ILE:CD1	2.26	0.66
1:A:841:ALA:HA	2:B:45:PRO:HG2	1.76	0.66
3:C:79:ILE:H	3:C:79:ILE:HD12	1.60	0.65
3:C:635:LYS:CD	3:C:637:ARG:HD2	2.26	0.65
1:A:914:LEU:O	1:A:915:LYS:HG2	1.96	0.65
1:A:1120:MET:HG2	1:A:1121:LYS:H	1.61	0.65
2:B:170:PHE:CD2	2:B:170:PHE:N	2.63	0.65
1:A:507:GLN:HE22	1:A:553:SER:N	1.94	0.65
1:A:828:TYR:CE2	1:A:861:VAL:HG21	2.32	0.65
1:A:1057:ARG:NH2	1:A:1112:LEU:HA	2.11	0.65
1:A:564:ILE:O	1:A:564:ILE:HG22	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1023:PRO:HG2	1:A:1135:GLU:OE2	1.96	0.65
1:A:520:GLN:HG3	1:A:529:ILE:CG1	2.27	0.65
1:A:1100:ILE:HG13	1:A:1105:MET:CE	2.27	0.65
1:A:23:PHE:H	1:A:30:ASN:HD22	1.45	0.64
1:A:582:LEU:O	1:A:583:GLY:O	2.14	0.64
3:C:312:ASP:HB3	3:C:343:TYR:OH	1.96	0.64
3:C:69:ALA:O	3:C:73:VAL:HG23	1.97	0.64
1:A:601:TYR:CE2	1:A:666:LEU:HD21	2.32	0.64
3:C:49:ARG:HD2	3:C:51:ARG:HH21	1.60	0.64
1:A:280:LEU:HB2	1:A:308:THR:HG23	1.80	0.64
3:C:249:ARG:HB3	3:C:249:ARG:HH11	1.62	0.64
3:C:734:LYS:HA	3:C:737:GLU:CD	2.18	0.64
4:D:49:ILE:CD1	4:D:70:VAL:HG22	2.25	0.64
1:A:5:TYR:CZ	1:A:1136:LEU:HD21	2.31	0.64
3:C:74:GLN:HB3	3:C:113:HIS:CD2	2.32	0.64
3:C:630:SER:C	3:C:632:ALA:H	2.01	0.64
2:B:115:LEU:HD22	2:B:115:LEU:C	2.18	0.64
1:A:727:GLN:OE1	1:A:827:THR:HG22	1.98	0.64
1:A:518:TYR:HD2	1:A:519:LEU:N	1.95	0.64
3:C:642:SER:CB	3:C:643:PRO:HD3	2.24	0.64
2:B:89:ASP:OD2	2:B:90:ASP:N	2.30	0.64
3:C:251:MET:CE	3:C:251:MET:HA	2.27	0.64
1:A:985:THR:HG22	1:A:987:GLU:N	2.10	0.63
1:A:118:THR:HG21	1:A:165:ILE:O	1.99	0.63
3:C:757:TYR:O	3:C:758:VAL:HB	1.99	0.63
3:C:538:PRO:HA	3:C:570:GLN:NE2	2.12	0.63
1:A:808:LEU:HD12	1:A:847:ARG:HE	1.63	0.63
3:C:310:LEU:HD22	3:C:315:ARG:HB2	1.80	0.63
2:B:163:ARG:HA	2:B:167:THR:HB	1.81	0.63
1:A:998:PHE:CZ	1:A:1090:ASP:HB3	2.33	0.63
1:A:408:LYS:HZ1	3:C:92:ASN:HA	1.61	0.63
4:D:37:ILE:CD1	4:D:43:ALA:HB2	2.29	0.63
1:A:81:THR:HG22	1:A:82:ALA:H	1.64	0.63
1:A:993:GLN:O	1:A:995:VAL:HG13	1.98	0.63
2:B:117:LEU:HD13	2:B:137:LYS:HZ2	1.62	0.63
3:C:404:LYS:N	3:C:405:PRO:HD2	2.14	0.63
1:A:285:LEU:HD22	1:A:297:LEU:HD11	1.81	0.63
4:D:87:TRP:CZ2	4:D:95:PRO:HB3	2.34	0.63
1:A:476:VAL:HG13	1:A:490:TRP:HB3	1.81	0.63
3:C:66:LEU:HD23	3:C:86:LEU:HD22	1.81	0.63
1:A:617:ASN:HD21	1:A:619:GLU:HB2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:PHE:CE2	1:A:178:ILE:HD11	2.34	0.62
3:C:164:ASN:OD1	3:C:166:THR:HB	1.99	0.62
1:A:67:PHE:HZ	1:A:88:ILE:HD13	1.62	0.62
1:A:507:GLN:NE2	1:A:553:SER:H	1.94	0.62
1:A:591:ILE:O	1:A:592:LEU:HB2	2.00	0.62
1:A:374:GLN:HG2	1:A:391:ARG:NH1	2.13	0.62
3:C:523:LEU:HD11	3:C:525:VAL:HG22	1.81	0.62
1:A:833:THR:O	1:A:870:VAL:HG23	1.99	0.62
1:A:741:GLU:OE1	1:A:788:VAL:HG21	1.99	0.62
1:A:482:GLU:OE2	1:A:483:PRO:HD3	1.99	0.62
3:C:77:THR:HG22	3:C:78:SER:N	2.13	0.62
3:C:292:LYS:O	3:C:292:LYS:HD2	1.99	0.62
4:D:37:ILE:HD11	4:D:43:ALA:HB2	1.80	0.62
1:A:414:ARG:CB	1:A:462:ASN:HD21	2.12	0.62
3:C:609:SER:H	3:C:612:GLU:CD	2.03	0.62
1:A:536:HIS:CD2	1:A:563:ASP:HB3	2.34	0.62
1:A:582:LEU:HD13	1:A:583:GLY:H	1.65	0.62
3:C:148:MET:O	3:C:151:SER:OG	2.17	0.62
3:C:724:LYS:HA	3:C:724:LYS:HE2	1.82	0.62
1:A:731:GLN:O	1:A:796:GLN:HB2	2.00	0.62
4:D:85:SER:HA	4:D:88:LEU:HD12	1.81	0.62
1:A:1097:PHE:CE1	1:A:1105:MET:HG3	2.35	0.62
1:A:180:PHE:HE2	1:A:191:LYS:HG3	1.65	0.61
1:A:1126:ALA:O	1:A:1128:ASP:N	2.33	0.61
1:A:312:GLU:HG3	1:A:327:ARG:CB	2.29	0.61
3:C:409:ILE:O	3:C:413:VAL:HG23	2.00	0.61
3:C:726:PRO:O	3:C:727:VAL:HB	2.00	0.61
1:A:391:ARG:HG3	1:A:391:ARG:HH11	1.65	0.61
1:A:207:TRP:CD1	1:A:208:LYS:N	2.68	0.61
3:C:108:GLN:HA	3:C:111:GLU:HB3	1.81	0.61
3:C:228:LYS:HD3	3:C:232:GLU:HG2	1.81	0.61
1:A:10:GLN:NE2	1:A:11:LYS:O	2.33	0.61
3:C:282:THR:O	3:C:285:PRO:HD2	2.01	0.61
3:C:183:ILE:CD1	3:C:220:MET:SD	2.89	0.61
2:B:205:GLU:O	2:B:206:CYS:HB2	2.00	0.61
2:B:208:CYS:C	2:B:210:GLN:H	2.02	0.61
1:A:120:ILE:HD12	1:A:135:LEU:HD22	1.83	0.61
1:A:142:VAL:O	1:A:154:ALA:HB1	2.00	0.61
2:B:171:HIS:NE2	2:B:212:PRO:HB2	2.16	0.61
1:A:828:TYR:HE2	1:A:861:VAL:HG21	1.66	0.61
3:C:624:LEU:CD2	3:C:628:LEU:HG	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:527:ILE:HD11	3:C:567:LEU:CD2	2.31	0.61
1:A:564:ILE:HG22	1:A:582:LEU:CD1	2.31	0.61
1:A:86:ALA:O	1:A:87:CYS:HB3	2.01	0.61
4:D:93:VAL:O	4:D:94:CYS:C	2.38	0.60
1:A:446:THR:HG22	1:A:447:GLU:N	2.16	0.60
1:A:341:ASN:ND2	1:A:342:GLU:HG2	2.15	0.60
1:A:589:ARG:HD3	3:C:87:TYR:OH	2.01	0.60
1:A:396:ILE:HD13	1:A:396:ILE:H	1.66	0.60
1:A:81:THR:HB	1:A:85:ASN:HB2	1.82	0.60
1:A:573:SER:OG	1:A:575:GLU:HB2	2.01	0.60
3:C:233:LEU:O	3:C:234:LYS:C	2.39	0.60
1:A:373:GLY:O	1:A:1012:LEU:HD23	2.01	0.60
2:B:15:LYS:HD2	2:B:82:LYS:HB2	1.81	0.60
1:A:657:THR:HG21	1:A:668:PHE:HB3	1.82	0.60
3:C:692:ARG:O	3:C:696:ILE:HG12	2.02	0.60
2:B:215:CYS:HB3	2:B:218:CYS:SG	2.42	0.60
1:A:24:THR:HA	1:A:91:TYR:CD2	2.36	0.60
1:A:18:CYS:N	1:A:313:CYS:SG	2.75	0.60
1:A:492:GLU:HG3	1:A:496:LYS:HB2	1.83	0.60
3:C:204:ARG:CG	3:C:273:ARG:HH12	2.15	0.60
2:B:169:GLY:O	2:B:212:PRO:HD3	2.01	0.60
3:C:296:GLY:O	3:C:297:GLU:CB	2.50	0.60
2:B:170:PHE:HA	2:B:212:PRO:HD3	1.81	0.60
3:C:276:THR:HG22	3:C:277:TYR:H	1.67	0.60
3:C:417:LEU:HD23	3:C:460:ARG:HH12	1.66	0.60
3:C:751:ASN:HD22	3:C:751:ASN:N	2.00	0.60
1:A:741:GLU:HG2	1:A:751:ALA:HA	1.83	0.60
3:C:228:LYS:HA	3:C:232:GLU:HB2	1.84	0.60
1:A:716:PRO:O	1:A:717:LEU:HD23	2.01	0.60
3:C:305:LYS:HG3	3:C:305:LYS:O	2.02	0.60
3:C:490:LYS:HE3	4:D:104:GLN:O	2.01	0.60
3:C:204:ARG:HG3	3:C:273:ARG:HH12	1.65	0.60
1:A:1115:ASP:CB	1:A:1120:MET:O	2.50	0.59
3:C:602:PHE:CD2	3:C:656:PHE:HB2	2.35	0.59
1:A:864:LYS:HG3	1:A:865:GLU:N	2.17	0.59
3:C:587:LYS:CD	3:C:587:LYS:H	2.15	0.59
1:A:441:GLU:HG2	1:A:441:GLU:O	2.02	0.59
3:C:340:TRP:HH2	3:C:390:MET:HB2	1.65	0.59
1:A:53:LYS:HE3	1:A:55:VAL:HG13	1.83	0.59
1:A:280:LEU:HD22	1:A:308:THR:HG21	1.84	0.59
3:C:51:ARG:H	3:C:52:PRO:HD2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:LEU:O	1:A:359:ILE:HD13	2.03	0.59
2:B:108:THR:HB	2:B:109:PRO:HD2	1.84	0.59
3:C:192:THR:O	3:C:196:ILE:HG13	2.03	0.59
3:C:640:ILE:O	3:C:654:PHE:HA	2.01	0.59
2:B:17:ILE:HD13	2:B:17:ILE:N	2.16	0.59
3:C:486:ALA:HA	3:C:489:SER:HB2	1.84	0.59
1:A:443:VAL:CG1	3:C:45:ILE:HG12	2.32	0.59
3:C:725:PHE:HB2	3:C:726:PRO:HD2	1.85	0.59
2:B:100:ASN:OD1	2:B:102:LEU:HB2	2.02	0.59
1:A:498:ILE:N	1:A:498:ILE:HD12	2.18	0.59
1:A:305:LEU:HD13	1:A:336:LEU:HD21	1.84	0.59
1:A:1055:GLN:HE21	1:A:1089:ILE:HG23	1.67	0.59
1:A:889:ARG:CD	1:A:904:ASN:HD21	2.02	0.59
4:D:45:CYS:HB2	4:D:47:ASN:HD21	1.66	0.59
4:D:42:CYS:SG	4:D:45:CYS:N	2.76	0.59
3:C:454:LYS:HD2	3:C:534:PRO:HG3	1.83	0.59
1:A:692:ALA:C	1:A:693:LEU:HD23	2.23	0.59
1:A:1121:LYS:HB2	1:A:1121:LYS:NZ	2.18	0.59
1:A:847:ARG:NH1	1:A:849:VAL:HG22	2.18	0.59
1:A:316:TYR:HE1	1:A:320:GLY:HA2	1.67	0.59
3:C:589:PHE:CD2	3:C:669:ILE:HD11	2.37	0.59
1:A:726:TYR:HE1	1:A:796:GLN:HE21	1.50	0.59
1:A:953:TRP:HB2	1:A:970:ASN:OD1	2.02	0.58
3:C:228:LYS:HE2	3:C:232:GLU:OE2	2.03	0.58
3:C:244:ALA:HA	3:C:293:GLN:OE1	2.03	0.58
1:A:414:ARG:HB3	1:A:462:ASN:HD21	1.68	0.58
3:C:228:LYS:CE	3:C:232:GLU:HG2	2.34	0.58
1:A:588:PRO:HB3	1:A:604:CYS:SG	2.43	0.58
2:B:52:THR:O	2:B:54:ALA:N	2.37	0.58
1:A:553:SER:O	1:A:571:LEU:HD12	2.03	0.58
1:A:1002:GLU:OE1	1:A:1032:THR:HG21	2.04	0.58
3:C:429:LEU:O	3:C:433:LEU:HB2	2.03	0.58
1:A:81:THR:HG22	1:A:83:LYS:H	1.68	0.58
1:A:177:THR:C	1:A:178:ILE:HD12	2.23	0.58
3:C:249:ARG:CB	3:C:249:ARG:HH11	2.16	0.58
1:A:1075:SER:HA	1:A:1084:PRO:O	2.03	0.58
1:A:407:ILE:HG21	1:A:410:LEU:HD23	1.84	0.58
3:C:239:THR:O	3:C:241:CYS:N	2.36	0.58
3:C:369:LYS:HE2	3:C:390:MET:HE3	1.84	0.58
1:A:1000:LEU:HD11	1:A:1030:PHE:CZ	2.38	0.58
3:C:421:ASN:O	3:C:424:ALA:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:521:ILE:HD12	3:C:521:ILE:N	2.18	0.58
3:C:135:ILE:HD11	3:C:188:VAL:CG1	2.34	0.58
1:A:414:ARG:HG2	1:A:414:ARG:HH11	1.69	0.58
3:C:468:SER:HB3	3:C:471:ALA:HB2	1.85	0.58
1:A:753:ARG:HG3	1:A:754:PRO:O	2.03	0.58
2:B:177:ILE:HG22	2:B:179:TRP:CZ3	2.38	0.58
3:C:369:LYS:HE2	3:C:390:MET:CE	2.33	0.58
1:A:5:TYR:OH	1:A:1136:LEU:HD21	2.03	0.58
1:A:806:GLN:HG2	1:A:807:PHE:N	2.18	0.58
1:A:963:ASP:HA	1:A:979:LYS:HE2	1.86	0.58
1:A:125:ASP:HB2	1:A:169:PHE:CD2	2.39	0.58
1:A:481:GLN:HA	1:A:484:LYS:HZ3	1.69	0.58
1:A:143:ILE:HG12	1:A:154:ALA:HB2	1.85	0.58
1:A:155:PHE:HE1	1:A:157:ILE:HG12	1.69	0.58
3:C:405:PRO:O	3:C:409:ILE:HG12	2.02	0.58
1:A:429:PHE:O	1:A:430:VAL:O	2.22	0.58
1:A:477:ARG:HG2	1:A:489:GLU:HG3	1.86	0.58
1:A:859:GLN:NE2	3:C:281:SER:HB2	2.18	0.58
1:A:81:THR:CB	1:A:85:ASN:HB2	2.33	0.58
3:C:240:ASN:ND2	3:C:289:CYS:SG	2.77	0.58
1:A:1007:PHE:CD2	1:A:1030:PHE:HB3	2.37	0.58
1:A:673:LEU:HD23	1:A:674:LYS:H	1.67	0.58
1:A:138:GLY:O	1:A:139:LEU:HD23	2.04	0.58
1:A:57:MET:HE3	1:A:57:MET:HA	1.84	0.57
3:C:700:ILE:HD13	3:C:719:LEU:HD21	1.85	0.57
1:A:330:ASP:OD1	1:A:388:ARG:NH2	2.37	0.57
3:C:155:PHE:O	3:C:159:THR:HB	2.04	0.57
1:A:706:GLU:O	1:A:706:GLU:HG2	2.04	0.57
2:B:107:SER:HB2	2:B:203:ARG:HH22	1.69	0.57
1:A:854:SER:O	1:A:855:ASP:OD1	2.22	0.57
1:A:929:SER:OG	1:A:930:VAL:N	2.36	0.57
3:C:528:LEU:HD22	3:C:533:TRP:CZ2	2.40	0.57
3:C:540:GLU:H	3:C:540:GLU:CD	2.08	0.57
3:C:665:PHE:O	3:C:666:ARG:HB2	2.04	0.57
3:C:621:ASP:O	3:C:625:ARG:HG2	2.03	0.57
2:B:177:ILE:HG22	2:B:179:TRP:HZ3	1.68	0.57
3:C:390:MET:HE2	3:C:390:MET:O	2.05	0.57
1:A:1093:LEU:C	1:A:1095:GLU:H	2.08	0.57
1:A:1002:GLU:OE1	1:A:1034:ASN:HB2	2.03	0.57
1:A:502:SER:O	1:A:503:CYS:HB2	2.04	0.57
1:A:432:GLN:HA	1:A:455:GLN:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ARG:HB3	1:A:158:ARG:HH11	1.68	0.57
1:A:578:HIS:CE1	1:A:623:LEU:HD12	2.39	0.57
1:A:798:THR:OG1	1:A:800:GLU:HG2	2.04	0.57
1:A:200:LYS:O	1:A:201:GLU:HG3	2.04	0.57
3:C:601:MET:HB3	3:C:608:PHE:HE1	1.69	0.57
3:C:159:THR:HG22	3:C:160:TYR:N	2.18	0.57
1:A:157:ILE:HG21	1:A:202:PHE:CD1	2.40	0.57
2:B:108:THR:HG22	2:B:109:PRO:HD3	1.86	0.57
1:A:430:VAL:HG12	1:A:431:GLY:N	2.19	0.57
1:A:443:VAL:HG12	3:C:45:ILE:HG12	1.86	0.57
1:A:152:LEU:O	1:A:153:LYS:C	2.43	0.57
2:B:198:THR:C	2:B:200:ALA:N	2.59	0.57
1:A:671:VAL:O	1:A:673:LEU:N	2.38	0.57
1:A:600:HIS:HB2	1:A:616:LEU:O	2.04	0.57
1:A:695:ASN:OD1	1:A:697:SER:N	2.30	0.57
3:C:57:ASN:O	3:C:59:THR:N	2.28	0.57
1:A:850:VAL:HB	1:A:862:ALA:HB3	1.85	0.57
1:A:12:PRO:HG3	1:A:1036:MET:HB2	1.87	0.57
1:A:228:GLY:HA3	1:A:239:TYR:HE1	1.69	0.56
1:A:761:LEU:HB2	1:A:802:LEU:O	2.05	0.56
1:A:432:GLN:NE2	3:C:52:PRO:HG2	2.19	0.56
3:C:49:ARG:CD	3:C:51:ARG:HH21	2.18	0.56
2:B:86:VAL:CG1	2:B:198:THR:HA	2.35	0.56
1:A:388:ARG:HH11	1:A:714:THR:HB	1.70	0.56
1:A:280:LEU:HG	1:A:305:LEU:HD12	1.85	0.56
3:C:51:ARG:O	3:C:53:ARG:N	2.36	0.56
2:B:87:PRO:HB2	2:B:198:THR:CG2	2.33	0.56
2:B:197:ILE:O	2:B:197:ILE:HG12	2.06	0.56
1:A:255:GLN:HE21	1:A:279:ARG:HH22	1.53	0.56
1:A:127:GLU:HB3	1:A:129:ARG:HH11	1.70	0.56
3:C:251:MET:HE2	3:C:251:MET:HA	1.85	0.56
3:C:643:PRO:HD2	3:C:652:ASP:HA	1.86	0.56
1:A:433:THR:HG22	1:A:434:ARG:H	1.68	0.56
2:B:137:LYS:O	2:B:137:LYS:HD3	2.05	0.56
2:B:172:ARG:NH1	2:B:197:ILE:HG22	2.20	0.56
2:B:197:ILE:N	2:B:197:ILE:HD13	2.19	0.56
1:A:454:ASP:OD2	1:A:454:ASP:N	2.28	0.56
1:A:503:CYS:SG	1:A:504:ASN:N	2.78	0.56
1:A:936:LYS:HB3	1:A:939:GLU:HB2	1.88	0.56
3:C:541:VAL:HG12	3:C:618:GLY:O	2.05	0.56
1:A:335:LYS:HB3	1:A:348:VAL:CG2	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:117:LEU:HD23	2:B:134:LYS:NZ	2.21	0.56
4:D:84:ILE:O	4:D:88:LEU:HG	2.05	0.56
1:A:255:GLN:HG3	1:A:279:ARG:NH2	2.20	0.56
2:B:115:LEU:C	2:B:115:LEU:CD2	2.72	0.56
1:A:806:GLN:HG2	1:A:807:PHE:H	1.69	0.56
1:A:293:GLY:O	1:A:294:THR:HG23	2.05	0.56
3:C:748:ASP:O	3:C:749:LYS:HB2	2.06	0.56
1:A:112:ILE:HD13	1:A:112:ILE:N	2.08	0.56
3:C:657:ASN:ND2	3:C:659:GLU:HB2	2.11	0.56
3:C:420:GLY:O	3:C:423:GLU:HG3	2.06	0.56
2:B:100:ASN:OD1	2:B:102:LEU:N	2.39	0.56
3:C:221:LEU:HD22	3:C:226:VAL:HG23	1.87	0.56
1:A:669:SER:O	1:A:670:ASN:C	2.43	0.56
3:C:65:LYS:HD2	3:C:81:TYR:CD2	2.41	0.56
3:C:390:MET:O	3:C:394:PHE:HB2	2.06	0.56
2:B:11:ASP:HB3	2:B:85:ILE:HD11	1.86	0.56
1:A:300:LEU:H	1:A:300:LEU:CD2	2.19	0.56
1:A:518:TYR:C	1:A:518:TYR:CD2	2.79	0.56
1:A:884:ILE:HG22	1:A:885:ASN:OD1	2.05	0.56
3:C:48:PHE:O	3:C:50:ASP:N	2.39	0.56
3:C:757:TYR:CE1	3:C:759:ALA:HA	2.36	0.56
1:A:813:ALA:HA	1:A:833:THR:HG22	1.88	0.56
1:A:493:PRO:HB2	1:A:494:GLN:HE22	1.70	0.56
1:A:928:ARG:NH1	1:A:947:ARG:NH2	2.50	0.55
1:A:192:THR:O	1:A:193:TYR:CD2	2.59	0.55
3:C:586:LYS:HG2	3:C:586:LYS:O	2.06	0.55
3:C:751:ASN:C	3:C:753:ASN:H	2.10	0.55
1:A:525:GLU:OE1	1:A:527:ARG:NH2	2.39	0.55
1:A:948:ASP:N	1:A:992:LEU:HD11	2.20	0.55
3:C:72:ALA:HB3	3:C:79:ILE:HG23	1.87	0.55
1:A:1002:GLU:HB3	1:A:1032:THR:CG2	2.36	0.55
1:A:633:THR:HB	3:C:162:LEU:HD21	1.88	0.55
3:C:227:TYR:HD2	3:C:228:LYS:N	2.04	0.55
1:A:493:PRO:HB2	1:A:494:GLN:NE2	2.21	0.55
1:A:276:MET:HG2	1:A:276:MET:O	2.06	0.55
3:C:287:ILE:O	3:C:291:GLU:HG3	2.07	0.55
3:C:267:LEU:HD23	3:C:290:VAL:HG11	1.87	0.55
2:B:216:SER:HA	2:B:219:GLU:OE1	2.06	0.55
2:B:21:LEU:N	2:B:21:LEU:HD23	2.22	0.55
1:A:502:SER:OG	1:A:543:ILE:HG12	2.07	0.55
1:A:78:PHE:HD1	1:A:87:CYS:O	1.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:VAL:HG11	1:A:347:VAL:HG13	1.88	0.55
2:B:48:THR:OG1	2:B:81:PRO:HB2	2.06	0.55
1:A:16:ASN:ND2	1:A:36:ASN:HA	2.21	0.55
1:A:84:TYR:CD2	1:A:135:LEU:HD13	2.42	0.55
3:C:94:CYS:SG	3:C:156:LEU:HD13	2.47	0.55
1:A:848:ILE:O	1:A:848:ILE:HG22	2.05	0.55
2:B:52:THR:HB	2:B:85:ILE:HG23	1.88	0.55
1:A:442:GLU:HG2	3:C:46:LYS:HE2	1.89	0.55
4:D:93:VAL:HG12	4:D:100:GLU:HA	1.89	0.55
1:A:59:GLY:HA2	1:A:1073:TRP:CE3	2.41	0.55
3:C:89:ALA:O	3:C:93:LEU:HB2	2.07	0.55
3:C:193:ILE:HG22	3:C:194:ASP:N	2.21	0.55
1:A:90:GLU:CD	1:A:92:LYS:HE3	2.27	0.55
1:A:105:HIS:C	1:A:152:LEU:HD12	2.27	0.55
1:A:226:PHE:CZ	1:A:268:GLY:O	2.59	0.55
1:A:522:HIS:HB3	1:A:523:PRO:HD2	1.89	0.55
1:A:987:GLU:HA	1:A:990:GLN:NE2	2.22	0.55
1:A:928:ARG:HH12	1:A:947:ARG:CZ	2.19	0.55
1:A:946:ALA:O	1:A:947:ARG:HB3	2.06	0.55
2:B:136:GLY:O	2:B:139:ASN:O	2.25	0.55
3:C:733:LYS:O	3:C:737:GLU:HG3	2.07	0.55
1:A:402:ILE:HD13	3:C:43:LEU:HB3	1.87	0.55
2:B:164:GLY:HA2	2:B:194:CYS:O	2.06	0.55
3:C:643:PRO:HG2	3:C:652:ASP:HA	1.88	0.55
2:B:198:THR:O	2:B:200:ALA:N	2.40	0.55
3:C:676:GLU:HA	3:C:680:GLU:OE1	2.06	0.55
3:C:292:LYS:HG3	3:C:330:ARG:NH2	2.22	0.55
1:A:170:LEU:HB2	1:A:177:THR:OG1	2.06	0.55
3:C:732:LEU:O	3:C:733:LYS:C	2.45	0.55
1:A:434:ARG:NH2	3:C:50:ASP:HA	2.22	0.54
1:A:659:ILE:HG22	1:A:660:TYR:N	2.21	0.54
1:A:448:LEU:HD23	1:A:451:PHE:CE2	2.42	0.54
1:A:1109:VAL:HB	1:A:1124:ALA:O	2.07	0.54
1:A:532:THR:CG2	1:A:533:GLU:N	2.69	0.54
3:C:448:VAL:O	3:C:452:PHE:HD1	1.90	0.54
3:C:597:LEU:O	3:C:598:VAL:C	2.45	0.54
1:A:614:PHE:N	1:A:614:PHE:CD1	2.75	0.54
2:B:171:HIS:CD2	2:B:171:HIS:H	2.23	0.54
1:A:142:VAL:HB	1:A:155:PHE:CE1	2.42	0.54
1:A:977:CYS:HB3	1:A:992:LEU:HD13	1.89	0.54
1:A:29:LEU:HD23	1:A:44:VAL:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:ILE:H	2:B:85:ILE:CD1	2.02	0.54
3:C:267:LEU:HD13	3:C:328:ARG:NH1	2.22	0.54
3:C:657:ASN:HD21	3:C:659:GLU:CB	2.10	0.54
4:D:41:ASN:CG	4:D:47:ASN:O	2.46	0.54
1:A:433:THR:HG22	1:A:434:ARG:N	2.22	0.54
3:C:472:GLU:HG2	3:C:495:PHE:HZ	1.72	0.54
1:A:1101:SER:O	1:A:1105:MET:HE3	2.08	0.54
1:A:1066:GLY:O	1:A:1067:LYS:HB2	2.07	0.54
1:A:138:GLY:HA2	1:A:159:LEU:HB2	1.88	0.54
1:A:182:TYR:CE1	1:A:189:HIS:HB2	2.43	0.54
3:C:630:SER:OG	3:C:672:ILE:HD11	2.08	0.54
3:C:183:ILE:HD11	3:C:220:MET:CE	2.37	0.54
1:A:518:TYR:CD2	1:A:519:LEU:N	2.75	0.54
3:C:42:LYS:O	3:C:43:LEU:HD23	2.07	0.54
1:A:402:ILE:CD1	3:C:43:LEU:HB3	2.38	0.54
1:A:1114:TYR:CE1	1:A:1114:TYR:O	2.48	0.54
1:A:182:TYR:CZ	1:A:189:HIS:HB2	2.43	0.54
1:A:909:ILE:HD11	2:B:124:SER:HA	1.89	0.54
2:B:21:LEU:HD12	2:B:25:GLU:HB3	1.90	0.54
1:A:864:LYS:HD3	1:A:899:VAL:O	2.08	0.54
1:A:1120:MET:HG2	1:A:1121:LYS:N	2.22	0.54
4:D:70:VAL:HG13	4:D:78:ALA:HB1	1.90	0.54
3:C:655:ILE:N	3:C:655:ILE:HD12	2.23	0.54
1:A:198:ARG:HH11	1:A:198:ARG:CA	2.21	0.54
1:A:728:GLU:O	1:A:728:GLU:HG3	2.08	0.54
3:C:581:GLU:HB2	4:D:21:ARG:HA	1.89	0.54
2:B:111:THR:HB	2:B:188:GLU:CG	2.38	0.54
2:B:119:GLY:C	2:B:121:THR:H	2.11	0.54
1:A:1126:ALA:C	1:A:1128:ASP:H	2.10	0.54
1:A:532:THR:OG1	1:A:574:PHE:HD1	1.90	0.54
1:A:42:TYR:HB3	1:A:49:LEU:HB3	1.89	0.54
3:C:642:SER:C	3:C:644:LYS:H	2.11	0.54
1:A:596:PHE:CZ	1:A:649:VAL:HG23	2.43	0.54
2:B:139:ASN:O	2:B:141:MET:N	2.41	0.54
1:A:808:LEU:HG	1:A:847:ARG:NH2	2.21	0.54
1:A:128:CYS:O	1:A:145:LEU:HD23	2.08	0.54
1:A:403:ASP:HA	1:A:698:THR:HG22	1.88	0.54
1:A:837:TYR:HB3	1:A:839:GLU:OE1	2.08	0.54
3:C:347:PHE:CE2	3:C:351:ILE:HD11	2.43	0.53
1:A:1120:MET:HG2	1:A:1122:ARG:H	1.73	0.53
3:C:628:LEU:O	3:C:630:SER:O	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:GLY:O	1:A:432:GLN:HB3	2.07	0.53
3:C:316:VAL:CB	3:C:317:PRO:HD3	2.38	0.53
1:A:582:LEU:CD1	1:A:583:GLY:H	2.19	0.53
1:A:388:ARG:HD3	1:A:714:THR:HB	1.90	0.53
1:A:525:GLU:OE1	1:A:527:ARG:NE	2.41	0.53
1:A:321:VAL:HA	1:A:334:VAL:O	2.09	0.53
4:D:53:CYS:HB3	4:D:80:HIS:ND1	2.22	0.53
1:A:77:LEU:HD23	1:A:89:LEU:HD12	1.91	0.53
3:C:100:PRO:HG3	3:C:160:TYR:CZ	2.43	0.53
3:C:704:MET:HG3	3:C:745:MET:HE2	1.89	0.53
1:A:479:VAL:HG12	1:A:480:SER:N	2.22	0.53
1:A:602:LEU:O	1:A:603:LEU:HD23	2.07	0.53
1:A:203:ASN:O	1:A:204:LYS:HB2	2.08	0.53
1:A:539:ALA:HB2	1:A:561:TRP:CD1	2.44	0.53
3:C:54:LEU:HB2	3:C:55:PRO:CD	2.25	0.53
1:A:112:ILE:HG12	1:A:113:GLY:N	2.23	0.53
2:B:10:PRO:N	2:B:85:ILE:HD13	2.23	0.53
3:C:239:THR:C	3:C:241:CYS:N	2.60	0.53
1:A:265:ASP:C	1:A:267:ASN:H	2.10	0.53
1:A:987:GLU:C	1:A:989:ARG:H	2.11	0.53
4:D:102:GLU:O	4:D:103:PHE:CB	2.47	0.53
1:A:375:LEU:O	1:A:389:ILE:HA	2.09	0.53
3:C:363:GLN:NE2	3:C:367:ASP:OD1	2.42	0.53
2:B:21:LEU:HG	2:B:26:TYR:CE2	2.43	0.53
1:A:658:VAL:HG12	1:A:658:VAL:O	2.09	0.53
3:C:539:MET:HE3	3:C:619:ILE:HA	1.91	0.53
4:D:104:GLN:O	4:D:105:LYS:CB	2.55	0.53
3:C:406:ALA:HB2	3:C:443:ILE:HG21	1.91	0.53
3:C:731:ASP:O	3:C:734:LYS:HB3	2.08	0.53
3:C:468:SER:HB3	3:C:471:ALA:CB	2.39	0.53
3:C:139:TRP:HD1	3:C:178:PHE:CE2	2.27	0.53
1:A:487:VAL:O	1:A:488:SER:HB2	2.09	0.53
1:A:985:THR:HB	1:A:988:GLU:CG	2.36	0.53
1:A:408:LYS:NZ	3:C:92:ASN:ND2	2.57	0.53
1:A:902:GLU:O	1:A:903:CYS:HB2	2.08	0.53
4:D:37:ILE:HG12	4:D:37:ILE:O	2.08	0.53
1:A:866:VAL:CG2	1:A:884:ILE:HG12	2.32	0.53
1:A:821:LEU:HD11	1:A:830:ILE:HD11	1.91	0.53
1:A:1123:GLU:HG2	1:A:1124:ALA:N	2.24	0.53
1:A:910:MET:CE	1:A:912:LEU:HD21	2.38	0.53
3:C:544:THR:O	3:C:547:MET:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:643:PRO:CG	3:C:652:ASP:HA	2.39	0.52
2:B:136:GLY:O	2:B:139:ASN:N	2.38	0.52
1:A:1126:ALA:O	1:A:1130:ILE:HG13	2.10	0.52
4:D:90:THR:OG1	4:D:91:ARG:N	2.42	0.52
4:D:54:ILE:HG22	4:D:55:GLU:N	2.24	0.52
1:A:188:ARG:O	1:A:212:VAL:HG22	2.09	0.52
1:A:196:SER:OG	1:A:199:GLU:HB2	2.09	0.52
3:C:579:LYS:O	4:D:22:PHE:HA	2.09	0.52
3:C:100:PRO:O	3:C:104:LYS:HG3	2.08	0.52
3:C:735:ARG:NE	3:C:735:ARG:HA	2.24	0.52
2:B:18:GLU:HB2	2:B:42:THR:HG22	1.90	0.52
3:C:119:LEU:HB2	3:C:120:PRO:CD	2.37	0.52
1:A:127:GLU:HB3	1:A:129:ARG:NH1	2.24	0.52
4:D:47:ASN:HD22	4:D:47:ASN:H	1.57	0.52
1:A:24:THR:HG23	1:A:91:TYR:HE2	1.73	0.52
2:B:97:PRO:HA	2:B:202:ARG:HA	1.91	0.52
3:C:182:ILE:HG22	3:C:183:ILE:HG13	1.89	0.52
3:C:587:LYS:HE3	3:C:664:LEU:O	2.09	0.52
2:B:128:LYS:HE2	2:B:146:GLU:OE1	2.09	0.52
3:C:299:LEU:HD23	3:C:326:PHE:CE2	2.45	0.52
2:B:50:LEU:CD1	2:B:145:ILE:HD13	2.40	0.52
2:B:202:ARG:CB	2:B:204:PHE:HE1	2.22	0.52
2:B:43:ILE:HD12	2:B:44:PRO:CD	2.39	0.52
3:C:41:LYS:O	3:C:42:LYS:O	2.26	0.52
2:B:219:GLU:O	2:B:220:ARG:HB2	2.09	0.52
2:B:117:LEU:HD13	2:B:137:LYS:HZ3	1.75	0.52
1:A:631:LEU:O	1:A:655:ARG:HB2	2.10	0.52
1:A:594:THR:CG2	1:A:595:THR:N	2.73	0.52
1:A:23:PHE:N	1:A:30:ASN:HD22	2.08	0.52
1:A:150:LYS:N	1:A:151:GLU:O	2.42	0.52
1:A:450:GLY:HA3	1:A:479:VAL:HG22	1.91	0.52
1:A:953:TRP:O	1:A:969:GLU:HB2	2.09	0.52
2:B:102:LEU:C	2:B:104:GLY:H	2.13	0.52
3:C:227:TYR:O	3:C:229:ASP:N	2.37	0.52
1:A:622:LEU:HD12	1:A:622:LEU:C	2.29	0.52
1:A:57:MET:HE3	1:A:1065:VAL:HB	1.91	0.52
1:A:262:ASN:HD22	1:A:316:TYR:H	1.57	0.52
4:D:84:ILE:O	4:D:84:ILE:HD13	2.10	0.52
3:C:63:TRP:HZ3	3:C:105:GLN:HG3	1.75	0.52
1:A:982:ALA:C	1:A:984:THR:H	2.13	0.52
1:A:167:VAL:C	1:A:168:LYS:HG2	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:GLU:CB	3:C:46:LYS:HB2	2.33	0.52
1:A:585:GLU:OE2	3:C:147:ILE:HG23	2.09	0.52
1:A:422:TYR:CD2	1:A:422:TYR:N	2.77	0.52
1:A:256:SER:HB3	1:A:275:ASP:OD1	2.10	0.52
3:C:228:LYS:NZ	3:C:232:GLU:HG2	2.24	0.52
1:A:62:ALA:HB3	1:A:80:LEU:O	2.10	0.52
1:A:180:PHE:N	1:A:180:PHE:CD2	2.77	0.52
3:C:121:PHE:HE2	3:C:134:LYS:HB3	1.74	0.52
1:A:225:PRO:HG2	1:A:267:ASN:CB	2.40	0.51
1:A:578:HIS:CE1	1:A:623:LEU:CD1	2.93	0.51
2:B:179:TRP:CE3	2:B:179:TRP:N	2.78	0.51
3:C:676:GLU:HG3	3:C:676:GLU:O	2.09	0.51
2:B:102:LEU:HD13	2:B:180:VAL:HG23	1.92	0.51
1:A:1093:LEU:O	1:A:1095:GLU:N	2.42	0.51
1:A:402:ILE:O	1:A:698:THR:HB	2.10	0.51
3:C:583:LYS:O	3:C:584:GLU:HB2	2.10	0.51
3:C:702:ARG:HD2	3:C:722:GLN:HE22	1.75	0.51
3:C:625:ARG:O	3:C:629:GLN:N	2.43	0.51
3:C:99:SER:HB2	3:C:100:PRO:CD	2.35	0.51
2:B:174:GLU:O	2:B:188:GLU:HA	2.10	0.51
1:A:1112:LEU:O	1:A:1123:GLU:HA	2.10	0.51
1:A:1135:GLU:OE1	1:A:1135:GLU:O	2.27	0.51
1:A:1051:LEU:CD2	1:A:1094:ILE:HG21	2.40	0.51
3:C:609:SER:H	3:C:612:GLU:CG	2.23	0.51
2:B:48:THR:O	2:B:144:PHE:HA	2.10	0.51
2:B:89:ASP:CG	2:B:90:ASP:N	2.63	0.51
1:A:471:ILE:HA	1:A:476:VAL:HA	1.92	0.51
3:C:439:LEU:O	3:C:440:PHE:C	2.49	0.51
3:C:227:TYR:CD2	3:C:227:TYR:C	2.83	0.51
3:C:501:SER:O	3:C:505:MET:HB2	2.11	0.51
1:A:285:LEU:O	1:A:285:LEU:HD12	2.10	0.51
1:A:866:VAL:HG22	1:A:867:LYS:N	2.25	0.51
1:A:659:ILE:HD12	1:A:659:ILE:H	1.75	0.51
1:A:490:TRP:CG	1:A:491:LYS:N	2.79	0.51
1:A:81:THR:CG2	1:A:82:ALA:N	2.73	0.51
1:A:1020:THR:O	1:A:1021:SER:C	2.46	0.51
2:B:145:ILE:HG23	2:B:172:ARG:HD3	1.92	0.51
4:D:82:HIS:O	4:D:84:ILE:N	2.43	0.51
3:C:228:LYS:CD	3:C:232:GLU:HG2	2.41	0.51
3:C:352:VAL:HG12	3:C:361:MET:SD	2.50	0.51
3:C:55:PRO:O	3:C:56:ASP:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:LEU:O	2:B:51:LEU:HG	2.11	0.51
1:A:451:PHE:HD1	1:A:470:GLN:HB2	1.73	0.51
4:D:86:ARG:C	4:D:88:LEU:H	2.14	0.51
3:C:660:PHE:C	3:C:662:HIS:H	2.14	0.51
2:B:170:PHE:HA	2:B:212:PRO:CG	2.41	0.51
1:A:282:MET:HG3	1:A:284:LEU:CD1	2.41	0.51
1:A:155:PHE:CE1	1:A:157:ILE:HG12	2.46	0.51
1:A:897:LYS:O	1:A:898:ASP:OD2	2.29	0.51
3:C:742:ARG:HD3	4:D:64:THR:HG21	1.92	0.51
1:A:769:LYS:HB3	1:A:772:SER:OG	2.10	0.51
1:A:180:PHE:N	1:A:180:PHE:HD2	2.08	0.51
1:A:224:GLU:HB2	1:A:225:PRO:CD	2.37	0.51
1:A:270:ARG:HG2	1:A:284:LEU:CG	2.34	0.51
2:B:30:GLN:HE21	2:B:36:SER:CB	2.13	0.51
1:A:157:ILE:CG2	1:A:158:ARG:N	2.73	0.51
1:A:831:VAL:HG12	1:A:832:GLY:N	2.26	0.51
3:C:257:PRO:HB3	3:C:318:ASP:OD1	2.10	0.51
3:C:757:TYR:HD1	3:C:758:VAL:N	2.09	0.51
2:B:172:ARG:O	2:B:190:CYS:HA	2.11	0.51
1:A:815:SER:O	1:A:816:LEU:HB2	2.11	0.51
1:A:459:PHE:CD2	1:A:460:CYS:N	2.79	0.51
1:A:805:HIS:HB2	1:A:858:LEU:HD12	1.93	0.51
3:C:602:PHE:N	3:C:602:PHE:CD1	2.79	0.50
1:A:404:LEU:HD21	3:C:45:ILE:HD11	1.93	0.50
1:A:408:LYS:HA	1:A:678:TYR:CE1	2.45	0.50
1:A:448:LEU:HD23	1:A:451:PHE:HE2	1.75	0.50
3:C:696:ILE:HD11	3:C:727:VAL:HG22	1.92	0.50
1:A:570:LYS:O	1:A:574:PHE:N	2.41	0.50
3:C:202:ARG:O	3:C:207:GLU:HB2	2.11	0.50
3:C:688:VAL:O	3:C:692:ARG:HG3	2.11	0.50
1:A:795:ASP:OD1	1:A:798:THR:HG23	2.11	0.50
1:A:771:PHE:CD1	1:A:771:PHE:N	2.79	0.50
1:A:844:LYS:O	1:A:867:LYS:HA	2.11	0.50
1:A:408:LYS:NZ	3:C:92:ASN:HA	2.25	0.50
1:A:578:HIS:HD2	1:A:623:LEU:H	1.56	0.50
1:A:893:TRP:CE3	1:A:899:VAL:HG13	2.46	0.50
1:A:280:LEU:HD22	1:A:308:THR:CG2	2.41	0.50
3:C:638:VAL:HG12	3:C:639:LEU:CD2	2.31	0.50
1:A:408:LYS:HZ1	3:C:92:ASN:ND2	2.09	0.50
3:C:437:MET:HE2	3:C:475:MET:HE1	1.94	0.50
1:A:782:PHE:O	1:A:783:GLY:C	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:696:ILE:CD1	3:C:727:VAL:HG22	2.42	0.50
1:A:275:ASP:HB2	1:A:279:ARG:HB2	1.92	0.50
1:A:279:ARG:HB3	1:A:281:PHE:CE1	2.46	0.50
1:A:573:SER:O	1:A:574:PHE:HB2	2.10	0.50
1:A:388:ARG:NH1	1:A:714:THR:HB	2.26	0.50
2:B:52:THR:HG21	2:B:85:ILE:CG1	2.38	0.50
1:A:969:GLU:CD	1:A:971:ALA:HB3	2.32	0.50
1:A:422:TYR:CE1	1:A:682:LEU:HA	2.46	0.50
1:A:1108:VAL:C	1:A:1110:ALA:H	2.13	0.50
1:A:52:VAL:HG23	1:A:53:LYS:N	2.27	0.50
3:C:516:SER:O	3:C:517:ASP:O	2.29	0.50
1:A:109:GLN:HE22	1:A:111:ARG:HH11	1.59	0.50
1:A:267:ASN:O	1:A:268:GLY:C	2.50	0.50
3:C:457:LEU:HD22	3:C:461:LEU:HD12	1.94	0.50
3:C:417:LEU:HD23	3:C:460:ARG:NH1	2.26	0.50
1:A:416:ASP:OD1	1:A:418:ASN:HB2	2.11	0.50
1:A:328:LEU:N	1:A:328:LEU:CD1	2.67	0.50
3:C:726:PRO:O	3:C:727:VAL:CB	2.60	0.50
1:A:279:ARG:HB3	1:A:281:PHE:HE1	1.76	0.50
1:A:198:ARG:HH11	1:A:198:ARG:N	2.10	0.50
1:A:257:THR:HG22	1:A:258:ILE:O	2.12	0.50
2:B:162:LYS:O	2:B:162:LYS:HG3	2.12	0.50
3:C:347:PHE:O	3:C:351:ILE:HG13	2.12	0.50
1:A:869:ALA:O	1:A:884:ILE:HA	2.12	0.49
3:C:141:ASP:C	3:C:143:CYS:N	2.64	0.49
1:A:81:THR:OG1	1:A:85:ASN:HB2	2.12	0.49
4:D:51:ASP:OD1	4:D:52:LEU:HD23	2.12	0.49
1:A:579:LYS:HG2	1:A:581:MET:HE3	1.92	0.49
3:C:380:PHE:CD1	3:C:386:PHE:CD2	3.00	0.49
3:C:696:ILE:HD11	3:C:725:PHE:HE1	1.78	0.49
1:A:66:LEU:HD23	1:A:77:LEU:HA	1.93	0.49
1:A:612:PHE:CE2	1:A:628:LYS:HD2	2.46	0.49
1:A:226:PHE:CE2	1:A:287:LYS:HB3	2.48	0.49
1:A:1097:PHE:HD2	1:A:1133:VAL:HG21	1.77	0.49
1:A:40:GLU:HB3	1:A:42:TYR:CE1	2.47	0.49
3:C:173:MET:HG2	3:C:173:MET:O	2.11	0.49
3:C:440:PHE:CE2	3:C:446:LYS:HD3	2.47	0.49
3:C:57:ASN:C	3:C:59:THR:H	2.14	0.49
1:A:180:PHE:CE2	1:A:191:LYS:HG3	2.47	0.49
2:B:52:THR:OG1	2:B:85:ILE:HA	2.13	0.49
2:B:143:ARG:HH22	2:B:145:ILE:HD11	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:LEU:HD11	2:B:145:ILE:HD13	1.94	0.49
1:A:736:LEU:HD11	1:A:816:LEU:HB2	1.93	0.49
2:B:91:LYS:O	2:B:93:VAL:N	2.45	0.49
1:A:178:ILE:N	1:A:178:ILE:HD12	2.27	0.49
3:C:404:LYS:O	3:C:405:PRO:C	2.49	0.49
1:A:960:LEU:HD21	1:A:966:LEU:HB2	1.93	0.49
1:A:168:LYS:HG3	1:A:219:VAL:O	2.12	0.49
1:A:161:GLU:HG2	1:A:182:TYR:CE2	2.48	0.49
3:C:49:ARG:CD	3:C:51:ARG:NH2	2.75	0.49
1:A:649:VAL:CG1	1:A:650:PHE:H	2.17	0.49
1:A:971:ALA:O	1:A:972:PHE:CB	2.60	0.49
3:C:732:LEU:O	3:C:735:ARG:N	2.45	0.49
1:A:194:GLU:HB2	1:A:203:ASN:HB2	1.95	0.49
1:A:194:GLU:HG3	1:A:204:LYS:O	2.13	0.49
3:C:469:VAL:HG12	3:C:473:LYS:HE3	1.94	0.49
1:A:613:TYR:CE1	1:A:627:LYS:HB2	2.46	0.49
1:A:13:THR:OG1	1:A:355:ASN:HA	2.12	0.49
2:B:174:GLU:HG3	2:B:191:ASN:HB2	1.93	0.49
1:A:668:PHE:CD1	1:A:668:PHE:N	2.80	0.49
1:A:514:ARG:HG3	1:A:514:ARG:HH11	1.78	0.49
2:B:38:LEU:CD2	2:B:131:LYS:NZ	2.75	0.49
1:A:490:TRP:CD2	1:A:491:LYS:N	2.81	0.49
1:A:512:VAL:HB	1:A:515:ALA:HB3	1.94	0.49
1:A:630:THR:HG21	1:A:797:HIS:HB3	1.94	0.49
3:C:73:VAL:C	3:C:74:GLN:O	2.45	0.49
1:A:641:PHE:CE2	1:A:650:PHE:HB2	2.48	0.49
1:A:1129:LEU:N	1:A:1129:LEU:HD22	2.28	0.49
1:A:657:THR:HG22	1:A:658:VAL:N	2.24	0.49
1:A:399:HIS:CE1	1:A:703:THR:HG22	2.47	0.49
1:A:394:ILE:HG22	1:A:395:GLY:N	2.27	0.49
1:A:492:GLU:CG	1:A:496:LYS:HB2	2.42	0.49
3:C:437:MET:HE3	3:C:478:LYS:HD2	1.95	0.49
3:C:601:MET:HE3	3:C:616:ALA:HB3	1.95	0.49
3:C:300:THR:O	3:C:304:GLN:HB2	2.13	0.49
1:A:103:ARG:NH1	1:A:103:ARG:HG3	2.28	0.49
1:A:587:ILE:HD12	1:A:587:ILE:H	1.77	0.49
1:A:873:MET:HA	1:A:882:ALA:HA	1.95	0.49
4:D:47:ASN:ND2	4:D:47:ASN:N	2.61	0.48
1:A:596:PHE:CE1	1:A:659:ILE:HG22	2.48	0.48
1:A:951:PRO:HD2	1:A:1080:ARG:NH1	2.27	0.48
3:C:330:ARG:H	3:C:330:ARG:CD	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:992:LEU:O	1:A:992:LEU:HD12	2.13	0.48
3:C:74:GLN:O	3:C:75:SER:C	2.50	0.48
3:C:649:GLU:HB2	3:C:652:ASP:OD2	2.13	0.48
1:A:868:GLY:O	1:A:884:ILE:HG23	2.13	0.48
1:A:459:PHE:O	1:A:460:CYS:HB3	2.13	0.48
1:A:808:LEU:CG	1:A:847:ARG:HH21	2.24	0.48
1:A:743:GLN:NE2	1:A:748:GLY:HA2	2.26	0.48
1:A:1106:GLN:C	1:A:1108:VAL:H	2.14	0.48
4:D:51:ASP:O	4:D:52:LEU:C	2.50	0.48
1:A:117:GLU:O	1:A:118:THR:HB	2.13	0.48
1:A:594:THR:HG23	1:A:595:THR:N	2.28	0.48
1:A:823:LYS:HD2	1:A:823:LYS:N	2.28	0.48
1:A:917:LYS:O	1:A:920:PHE:HB2	2.13	0.48
3:C:71:ARG:NH2	3:C:74:GLN:OE1	2.45	0.48
3:C:704:MET:HG3	3:C:745:MET:CE	2.43	0.48
3:C:382:LYS:O	3:C:383:ASN:C	2.50	0.48
1:A:157:ILE:HG21	1:A:202:PHE:CE1	2.48	0.48
1:A:1129:LEU:H	1:A:1129:LEU:HD22	1.77	0.48
1:A:81:THR:CG2	1:A:82:ALA:H	2.25	0.48
1:A:104:ALA:O	1:A:105:HIS:HB3	2.13	0.48
1:A:1136:LEU:O	1:A:1139:ILE:HD12	2.13	0.48
3:C:634:GLY:O	3:C:635:LYS:HB3	2.14	0.48
1:A:36:ASN:ND2	1:A:1002:GLU:OE2	2.46	0.48
1:A:876:PHE:HD1	1:A:916:THR:CG2	2.23	0.48
3:C:751:ASN:ND2	3:C:751:ASN:O	2.46	0.48
3:C:541:VAL:HG23	3:C:543:LEU:CD2	2.44	0.48
1:A:587:ILE:N	1:A:587:ILE:HD12	2.28	0.48
1:A:3:TYR:CE2	1:A:1045:GLU:HG3	2.48	0.48
1:A:161:GLU:OE1	1:A:161:GLU:N	2.47	0.48
1:A:985:THR:HG22	1:A:986:ASP:N	2.27	0.48
1:A:596:PHE:HZ	1:A:649:VAL:HG23	1.78	0.48
2:B:91:LYS:C	2:B:93:VAL:H	2.15	0.48
1:A:1100:ILE:O	1:A:1105:MET:HE3	2.14	0.48
2:B:147:GLU:OE1	2:B:163:ARG:HD3	2.13	0.48
2:B:85:ILE:HD12	2:B:85:ILE:N	2.12	0.48
3:C:587:LYS:N	3:C:587:LYS:HD2	2.26	0.48
1:A:910:MET:HE2	1:A:912:LEU:HD21	1.96	0.48
3:C:515:GLN:O	3:C:515:GLN:HG2	2.14	0.48
1:A:659:ILE:O	1:A:660:TYR:HB3	2.13	0.48
1:A:931:LEU:HG	1:A:947:ARG:NH2	2.29	0.48
2:B:143:ARG:NH2	2:B:174:GLU:OE1	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:VAL:HG13	2:B:87:PRO:HD2	1.96	0.48
1:A:808:LEU:CD1	1:A:847:ARG:HE	2.25	0.48
1:A:340:SER:HB2	1:A:346:TYR:CE1	2.48	0.48
3:C:248:GLN:O	3:C:249:ARG:C	2.52	0.48
3:C:315:ARG:O	3:C:319:LEU:HG	2.14	0.48
3:C:601:MET:HB3	3:C:608:PHE:CE1	2.49	0.48
1:A:900:ARG:O	1:A:901:THR:C	2.51	0.48
3:C:751:ASN:ND2	3:C:751:ASN:N	2.61	0.48
4:D:39:VAL:O	4:D:40:ASP:C	2.51	0.48
2:B:103:LEU:O	2:B:105:LEU:HG	2.13	0.48
3:C:599:LEU:HB3	4:D:22:PHE:CE1	2.49	0.48
1:A:433:THR:O	1:A:434:ARG:HG3	2.14	0.48
1:A:641:PHE:HB2	1:A:681:PRO:HG3	1.95	0.48
1:A:847:ARG:HH11	1:A:849:VAL:HG22	1.79	0.48
3:C:193:ILE:C	3:C:195:GLY:N	2.68	0.48
1:A:288:GLU:CD	1:A:298:LYS:HG2	2.34	0.48
3:C:705:LYS:HD3	3:C:705:LYS:C	2.35	0.47
2:B:144:PHE:C	2:B:145:ILE:HD12	2.35	0.47
1:A:16:ASN:ND2	1:A:35:LYS:O	2.47	0.47
1:A:602:LEU:HD13	1:A:602:LEU:C	2.33	0.47
3:C:719:LEU:HD22	3:C:723:LEU:HD21	1.96	0.47
3:C:450:GLU:OE2	3:C:454:LYS:HE3	2.14	0.47
1:A:198:ARG:NH1	1:A:198:ARG:N	2.61	0.47
1:A:286:GLU:CG	1:A:301:ARG:HH12	2.26	0.47
4:D:47:ASN:HD22	4:D:47:ASN:N	2.11	0.47
1:A:443:VAL:HG12	1:A:443:VAL:O	2.13	0.47
2:B:89:ASP:O	2:B:198:THR:HG21	2.14	0.47
4:D:91:ARG:NH1	4:D:91:ARG:HB2	2.30	0.47
3:C:588:GLU:O	3:C:666:ARG:HA	2.14	0.47
2:B:164:GLY:O	2:B:194:CYS:HB3	2.13	0.47
3:C:482:GLU:O	3:C:483:CYS:HB2	2.14	0.47
3:C:642:SER:HB2	3:C:643:PRO:CD	2.32	0.47
1:A:479:VAL:CG1	1:A:480:SER:N	2.77	0.47
1:A:316:TYR:HE1	1:A:320:GLY:CA	2.27	0.47
3:C:412:HIS:HE1	3:C:416:LYS:HE3	1.77	0.47
1:A:679:MET:C	1:A:679:MET:SD	2.92	0.47
1:A:459:PHE:CG	1:A:460:CYS:N	2.82	0.47
3:C:592:SER:HB2	3:C:673:GLN:NE2	2.29	0.47
1:A:929:SER:HB2	1:A:952:ASN:HB2	1.97	0.47
1:A:579:LYS:HE3	1:A:581:MET:CE	2.45	0.47
1:A:182:TYR:HE2	1:A:191:LYS:HG2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:178:GLY:C	2:B:179:TRP:HE3	2.18	0.47
1:A:1082:THR:O	1:A:1082:THR:CG2	2.61	0.47
1:A:731:GLN:O	1:A:796:GLN:CB	2.61	0.47
3:C:641:LYS:HE2	3:C:647:GLU:O	2.14	0.47
3:C:629:GLN:O	3:C:633:CYS:HB2	2.15	0.47
1:A:282:MET:CB	1:A:305:LEU:HD21	2.45	0.47
1:A:884:ILE:CD1	1:A:884:ILE:N	2.77	0.47
3:C:417:LEU:CD2	3:C:460:ARG:HH12	2.27	0.47
2:B:102:LEU:CD1	2:B:180:VAL:HG23	2.44	0.47
1:A:207:TRP:CE3	1:A:242:GLY:HA2	2.48	0.47
1:A:396:ILE:O	1:A:396:ILE:HD13	2.15	0.47
2:B:107:SER:HB2	2:B:203:ARG:NH2	2.30	0.47
1:A:403:ASP:O	1:A:405:PRO:HD3	2.15	0.47
1:A:729:VAL:HG23	1:A:730:SER:N	2.28	0.47
3:C:624:LEU:HD22	3:C:628:LEU:CD1	2.44	0.47
1:A:571:LEU:O	1:A:572:PRO:C	2.50	0.47
1:A:925:ASP:CB	1:A:928:ARG:HB3	2.45	0.47
2:B:86:VAL:HG13	2:B:197:ILE:O	2.15	0.47
1:A:457:THR:HG22	1:A:458:PHE:N	2.29	0.47
1:A:264:VAL:HG13	1:A:316:TYR:CG	2.49	0.47
1:A:847:ARG:NH1	1:A:849:VAL:CG2	2.78	0.47
3:C:263:VAL:HG11	3:C:295:LEU:HD21	1.97	0.47
1:A:1107:GLU:O	1:A:1107:GLU:HG2	2.14	0.47
1:A:812:TYR:O	1:A:833:THR:HB	2.14	0.47
1:A:407:ILE:CD1	1:A:699:LEU:HB2	2.45	0.47
1:A:148:ASP:OD2	1:A:148:ASP:N	2.46	0.47
2:B:113:THR:O	2:B:185:LYS:HA	2.15	0.47
3:C:341:SER:HB3	3:C:389:LEU:HD12	1.97	0.47
3:C:329:VAL:CG1	3:C:330:ARG:H	2.23	0.47
3:C:457:LEU:O	3:C:460:ARG:N	2.47	0.47
3:C:401:ARG:NH2	3:C:404:LYS:HG3	2.30	0.47
1:A:589:ARG:NH1	3:C:87:TYR:HE2	2.13	0.47
1:A:374:GLN:HG2	1:A:391:ARG:HH11	1.79	0.47
1:A:589:ARG:HD3	3:C:87:TYR:CZ	2.50	0.47
3:C:748:ASP:C	3:C:750:ASP:H	2.16	0.47
3:C:544:THR:HG23	3:C:545:PRO:HD2	1.96	0.47
1:A:183:GLN:HB2	1:A:188:ARG:HG2	1.96	0.47
1:A:366:ASP:OD1	1:A:371:GLY:N	2.48	0.47
1:A:311:ALA:HB1	1:A:314:LEU:HD13	1.97	0.47
3:C:329:VAL:CG1	3:C:330:ARG:N	2.78	0.47
2:B:92:THR:CG2	2:B:92:THR:O	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:PHE:HE2	1:A:178:ILE:HG12	1.80	0.47
4:D:50:MET:SD	4:D:108:HIS:CE1	3.08	0.47
3:C:627:THR:O	3:C:631:LEU:HD23	2.14	0.46
1:A:225:PRO:HG2	1:A:267:ASN:HB2	1.97	0.46
3:C:705:LYS:HB2	3:C:757:TYR:HE2	1.79	0.46
3:C:276:THR:CG2	3:C:277:TYR:N	2.71	0.46
1:A:356:LEU:HD11	1:A:390:ILE:HD12	1.98	0.46
1:A:656:PRO:HG2	1:A:676:VAL:HG23	1.97	0.46
1:A:207:TRP:HD1	1:A:208:LYS:N	2.13	0.46
1:A:189:HIS:HD1	1:A:210:GLU:HA	1.81	0.46
1:A:450:GLY:O	1:A:477:ARG:NH2	2.46	0.46
3:C:308:ASP:OD1	3:C:343:TYR:HD1	1.97	0.46
3:C:91:GLU:HA	3:C:155:PHE:CD2	2.50	0.46
4:D:74:VAL:CG2	4:D:102:GLU:HB3	2.46	0.46
3:C:203:GLU:OE1	3:C:277:TYR:OH	2.29	0.46
1:A:808:LEU:O	1:A:811:GLU:HB3	2.15	0.46
1:A:169:PHE:CD2	1:A:178:ILE:HD11	2.51	0.46
1:A:2:SER:HB3	1:A:995:VAL:HG23	1.97	0.46
1:A:512:VAL:O	1:A:515:ALA:HB3	2.15	0.46
1:A:353:PHE:N	1:A:353:PHE:CD1	2.84	0.46
1:A:31:LEU:HD13	1:A:317:LEU:HD21	1.97	0.46
1:A:189:HIS:HD1	1:A:210:GLU:CA	2.28	0.46
3:C:705:LYS:HA	3:C:757:TYR:CD2	2.50	0.46
1:A:596:PHE:CZ	1:A:659:ILE:HG22	2.51	0.46
3:C:714:LEU:N	3:C:714:LEU:CD1	2.77	0.46
3:C:448:VAL:O	3:C:451:ALA:HB3	2.14	0.46
1:A:1136:LEU:C	1:A:1136:LEU:HD23	2.35	0.46
3:C:702:ARG:NH1	3:C:722:GLN:NE2	2.64	0.46
3:C:702:ARG:NH1	3:C:722:GLN:HE21	2.14	0.46
1:A:638:LEU:O	1:A:639:ARG:HG2	2.14	0.46
1:A:93:GLN:HG3	1:A:97:SER:O	2.16	0.46
1:A:949:PHE:C	2:B:122:LEU:HD21	2.35	0.46
1:A:985:THR:CB	1:A:988:GLU:HG3	2.41	0.46
1:A:931:LEU:HD23	1:A:946:ALA:O	2.16	0.46
1:A:490:TRP:O	1:A:491:LYS:HB2	2.15	0.46
1:A:633:THR:O	3:C:158:ARG:NH1	2.47	0.46
4:D:91:ARG:CG	4:D:92:GLN:H	2.25	0.46
3:C:587:LYS:HB2	3:C:660:PHE:CE1	2.51	0.46
1:A:998:PHE:HZ	1:A:1090:ASP:HB3	1.77	0.46
1:A:402:ILE:HG22	1:A:403:ASP:H	1.80	0.46
1:A:438:LEU:CD1	1:A:684:SER:HB2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:ASP:OD2	2:B:116:ASP:C	2.53	0.46
3:C:757:TYR:CD1	3:C:758:VAL:N	2.83	0.46
1:A:964:ASN:ND2	1:A:964:ASN:N	2.59	0.46
1:A:1057:ARG:CB	1:A:1108:VAL:HG13	2.45	0.46
2:B:92:THR:C	2:B:93:VAL:HG22	2.36	0.46
1:A:414:ARG:HB3	1:A:462:ASN:ND2	2.29	0.46
1:A:802:LEU:HD13	1:A:853:TYR:OH	2.16	0.46
1:A:764:SER:O	1:A:805:HIS:HA	2.15	0.46
3:C:341:SER:CB	3:C:389:LEU:HD12	2.46	0.46
1:A:283:LEU:C	1:A:283:LEU:HD23	2.36	0.46
1:A:315:THR:HG22	1:A:323:PHE:HB3	1.98	0.46
2:B:83:ILE:CD1	2:B:141:MET:HE1	2.45	0.46
1:A:815:SER:HB2	1:A:832:GLY:CA	2.45	0.46
3:C:440:PHE:CZ	3:C:446:LYS:HD3	2.51	0.46
3:C:433:LEU:HD23	3:C:478:LYS:HE3	1.97	0.46
3:C:587:LYS:HD3	3:C:660:PHE:CE1	2.51	0.46
1:A:531:HIS:ND1	1:A:532:THR:N	2.63	0.46
1:A:32:LEU:CD2	1:A:41:ILE:HG23	2.46	0.46
1:A:1101:SER:OG	1:A:1104:LYS:HD2	2.15	0.46
4:D:52:LEU:N	4:D:52:LEU:CD2	2.78	0.46
1:A:936:LYS:CB	1:A:939:GLU:HB2	2.46	0.46
3:C:141:ASP:OD2	3:C:144:ARG:NH2	2.46	0.46
3:C:321:GLN:O	3:C:325:LEU:HD12	2.16	0.46
1:A:443:VAL:O	3:C:45:ILE:HA	2.15	0.46
1:A:411:TRP:HB2	1:A:460:CYS:SG	2.56	0.46
1:A:1102:ARG:N	1:A:1103:PRO:CD	2.79	0.46
1:A:197:LEU:HB2	1:A:198:ARG:HH12	1.81	0.46
1:A:332:GLN:HE21	1:A:352:THR:HG22	1.81	0.46
2:B:171:HIS:HD1	2:B:215:CYS:HB3	1.81	0.46
1:A:143:ILE:HG12	1:A:154:ALA:CB	2.46	0.46
2:B:208:CYS:C	2:B:210:GLN:N	2.66	0.46
1:A:52:VAL:HG23	1:A:53:LYS:H	1.81	0.46
3:C:375:VAL:HG13	3:C:379:CYS:HB2	1.98	0.46
3:C:114:VAL:O	3:C:117:GLN:N	2.50	0.45
1:A:1115:ASP:HA	1:A:1120:MET:O	2.14	0.45
3:C:630:SER:C	3:C:632:ALA:N	2.67	0.45
1:A:442:GLU:HG3	1:A:443:VAL:H	1.81	0.45
1:A:334:VAL:HG12	1:A:335:LYS:N	2.31	0.45
1:A:1133:VAL:O	1:A:1137:THR:HG23	2.16	0.45
3:C:55:PRO:O	3:C:56:ASP:CB	2.64	0.45
2:B:171:HIS:CD2	2:B:171:HIS:N	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:ASN:HD21	2:B:139:ASN:HD21	1.63	0.45
3:C:578:LEU:HD13	3:C:591:VAL:HG21	1.99	0.45
1:A:1108:VAL:C	1:A:1110:ALA:N	2.69	0.45
1:A:5:TYR:CE2	1:A:1136:LEU:HD21	2.51	0.45
1:A:407:ILE:HD11	1:A:699:LEU:HB2	1.98	0.45
1:A:629:VAL:HG23	1:A:630:THR:N	2.31	0.45
3:C:303:LEU:HD23	3:C:322:MET:CE	2.46	0.45
3:C:208:ALA:O	3:C:209:VAL:HG13	2.16	0.45
3:C:241:CYS:O	3:C:244:ALA:HB3	2.15	0.45
3:C:460:ARG:NH1	3:C:472:GLU:OE2	2.49	0.45
3:C:227:TYR:CD2	3:C:228:LYS:N	2.83	0.45
3:C:271:GLY:C	3:C:273:ARG:H	2.20	0.45
4:D:98:ASN:HA	4:D:98:ASN:HD22	1.52	0.45
3:C:79:ILE:H	3:C:79:ILE:CD1	2.23	0.45
3:C:632:ALA:O	3:C:633:CYS:C	2.54	0.45
1:A:155:PHE:C	1:A:155:PHE:CD1	2.89	0.45
3:C:274:VAL:CG1	3:C:283:GLN:HE21	2.23	0.45
2:B:141:MET:O	2:B:179:TRP:HH2	1.99	0.45
3:C:696:ILE:HD11	3:C:725:PHE:CE1	2.50	0.45
2:B:110:SER:N	2:B:221:ASP:HB3	2.30	0.45
1:A:982:ALA:O	1:A:984:THR:N	2.44	0.45
1:A:880:LEU:O	1:A:880:LEU:HG	2.17	0.45
2:B:52:THR:CG2	2:B:85:ILE:HG13	2.42	0.45
3:C:757:TYR:O	3:C:758:VAL:CB	2.64	0.45
3:C:595:GLN:HE22	3:C:669:ILE:CG2	2.27	0.45
1:A:1112:LEU:HD12	1:A:1113:GLN:H	1.81	0.45
1:A:108:VAL:HG21	1:A:133:LEU:HD23	1.99	0.45
4:D:75:CYS:CB	4:D:97:ASP:OD2	2.64	0.45
1:A:893:TRP:CZ3	1:A:899:VAL:HG13	2.52	0.45
1:A:32:LEU:CD2	1:A:41:ILE:HG12	2.45	0.45
3:C:534:PRO:HB2	3:C:536:TYR:CE1	2.51	0.45
2:B:28:THR:HG22	2:B:29:SER:N	2.30	0.45
1:A:528:GLN:O	1:A:528:GLN:HG2	2.17	0.45
3:C:54:LEU:CB	3:C:55:PRO:HD3	2.27	0.45
1:A:476:VAL:HG22	1:A:526:LEU:CD1	2.47	0.45
3:C:610:PHE:CE2	3:C:614:LYS:HE3	2.52	0.45
4:D:37:ILE:O	4:D:38:VAL:C	2.55	0.45
3:C:200:ILE:O	3:C:202:ARG:N	2.50	0.45
1:A:659:ILE:CG2	1:A:660:TYR:N	2.79	0.45
2:B:50:LEU:C	2:B:51:LEU:HD12	2.37	0.45
2:B:205:GLU:O	2:B:206:CYS:CB	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ILE:N	1:A:396:ILE:CD1	2.79	0.45
3:C:149:ILE:O	3:C:150:ARG:C	2.55	0.45
1:A:597:GLU:O	1:A:598:SER:HB3	2.16	0.45
1:A:263:ARG:CG	1:A:265:ASP:O	2.65	0.45
3:C:725:PHE:HB2	3:C:726:PRO:CD	2.47	0.45
1:A:1104:LYS:HA	1:A:1107:GLU:HB3	1.98	0.45
1:A:102:THR:HG23	1:A:104:ALA:O	2.17	0.45
1:A:755:SER:O	1:A:756:ALA:C	2.55	0.45
1:A:695:ASN:OD1	1:A:698:THR:N	2.42	0.45
3:C:267:LEU:CD2	3:C:290:VAL:HG11	2.47	0.45
1:A:478:LEU:HB3	1:A:488:SER:HB3	1.99	0.45
1:A:103:ARG:HH11	1:A:103:ARG:CG	2.30	0.45
3:C:303:LEU:HD13	3:C:339:HIS:CD2	2.51	0.45
4:D:45:CYS:C	4:D:46:ARG:HG2	2.36	0.45
3:C:758:VAL:HG12	3:C:758:VAL:O	2.17	0.45
2:B:195:SER:CB	2:B:204:PHE:CD2	2.97	0.45
1:A:66:LEU:HD21	1:A:77:LEU:HD13	1.99	0.45
1:A:258:ILE:HA	1:A:274:GLY:O	2.17	0.45
1:A:1044:SER:O	1:A:1045:GLU:C	2.56	0.45
1:A:546:LEU:O	1:A:549:SER:HB3	2.17	0.45
1:A:245:TYR:HD2	1:A:245:TYR:C	2.21	0.45
1:A:889:ARG:NH1	1:A:904:ASN:HD21	2.04	0.44
4:D:41:ASN:CB	4:D:42:CYS:O	2.57	0.44
2:B:142:THR:HG22	2:B:179:TRP:CH2	2.52	0.44
4:D:52:LEU:H	4:D:52:LEU:HD22	1.83	0.44
1:A:63:VAL:HB	1:A:80:LEU:HB3	1.98	0.44
1:A:138:GLY:HA2	1:A:159:LEU:CB	2.47	0.44
1:A:586:ILE:HG22	1:A:607:GLY:H	1.82	0.44
3:C:264:SER:O	3:C:268:GLU:HG2	2.17	0.44
1:A:263:ARG:HG2	1:A:265:ASP:O	2.18	0.44
1:A:265:ASP:C	1:A:267:ASN:N	2.71	0.44
3:C:48:PHE:O	3:C:49:ARG:C	2.55	0.44
2:B:83:ILE:HD12	2:B:141:MET:HE1	1.98	0.44
1:A:830:ILE:HG12	1:A:850:VAL:HG22	1.98	0.44
1:A:396:ILE:HD13	1:A:396:ILE:N	2.29	0.44
3:C:496:LYS:HD3	3:C:496:LYS:HA	1.84	0.44
3:C:491:LEU:HA	3:C:494:MET:CG	2.33	0.44
1:A:987:GLU:HA	1:A:990:GLN:HE21	1.81	0.44
1:A:16:ASN:HD22	1:A:36:ASN:HA	1.81	0.44
3:C:203:GLU:C	3:C:205:SER:H	2.20	0.44
1:A:587:ILE:CD1	1:A:587:ILE:H	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ASP:C	1:A:148:ASP:H	2.20	0.44
3:C:579:LYS:HE3	4:D:23:GLU:OE2	2.18	0.44
3:C:51:ARG:N	3:C:52:PRO:HD2	2.32	0.44
3:C:218:LEU:HD12	3:C:277:TYR:HB2	2.00	0.44
3:C:179:ARG:O	3:C:184:SER:HB3	2.16	0.44
3:C:307:LEU:O	3:C:308:ASP:C	2.56	0.44
1:A:673:LEU:HD23	1:A:674:LYS:N	2.33	0.44
1:A:72:GLU:CD	1:A:103:ARG:HH22	2.21	0.44
3:C:70:VAL:O	3:C:72:ALA:N	2.50	0.44
1:A:429:PHE:O	1:A:456:GLN:HG3	2.18	0.44
3:C:143:CYS:O	3:C:147:ILE:HG13	2.18	0.44
1:A:821:LEU:HD11	1:A:830:ILE:CD1	2.48	0.44
4:D:53:CYS:HB2	4:D:83:CYS:SG	2.57	0.44
1:A:532:THR:CG2	1:A:533:GLU:H	2.31	0.44
1:A:117:GLU:O	1:A:118:THR:CB	2.65	0.44
1:A:2:SER:HB3	1:A:995:VAL:CG2	2.48	0.44
1:A:580:GLU:OE2	1:A:626:ARG:HD2	2.17	0.44
1:A:905:HIS:CD2	1:A:933:LEU:HD21	2.52	0.44
1:A:130:MET:HB2	1:A:143:ILE:O	2.17	0.44
3:C:292:LYS:O	3:C:293:GLN:HG2	2.17	0.44
3:C:65:LYS:HD2	3:C:81:TYR:HD2	1.79	0.44
3:C:61:ASP:O	3:C:65:LYS:HG3	2.17	0.44
1:A:607:GLY:HA2	1:A:635:PRO:HB3	1.99	0.44
1:A:419:ARG:HD3	1:A:421:THR:O	2.18	0.44
3:C:707:ARG:HD2	3:C:710:LEU:HD13	2.00	0.44
3:C:113:HIS:O	3:C:117:GLN:HG2	2.16	0.44
1:A:157:ILE:HG22	1:A:158:ARG:H	1.78	0.44
2:B:51:LEU:HD13	2:B:141:MET:HE2	2.00	0.44
3:C:527:ILE:O	3:C:527:ILE:CG2	2.65	0.44
3:C:428:GLU:O	3:C:432:THR:HG23	2.18	0.44
1:A:257:THR:HG22	1:A:258:ILE:N	2.33	0.44
3:C:545:PRO:O	3:C:546:GLU:C	2.56	0.44
3:C:434:ASP:O	3:C:438:ILE:HG13	2.18	0.44
1:A:171:TYR:CZ	1:A:223:PRO:HG3	2.53	0.44
3:C:668:LYS:NZ	3:C:670:ASN:HB3	2.32	0.44
3:C:390:MET:HE2	3:C:390:MET:C	2.38	0.44
3:C:555:LYS:HD2	3:C:569:TRP:CZ3	2.47	0.44
3:C:409:ILE:HG13	3:C:443:ILE:HD11	1.98	0.44
1:A:855:ASP:C	1:A:857:LYS:H	2.21	0.44
2:B:162:LYS:O	2:B:164:GLY:N	2.51	0.44
3:C:512:MET:HE2	3:C:512:MET:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:GLU:O	1:A:448:LEU:HD12	2.18	0.44
3:C:578:LEU:HD13	3:C:591:VAL:HG23	2.00	0.44
3:C:184:SER:O	3:C:186:LYS:N	2.50	0.44
1:A:657:THR:CG2	1:A:668:PHE:HB3	2.48	0.44
1:A:876:PHE:HZ	1:A:919:ASP:HA	1.82	0.44
1:A:67:PHE:CE1	1:A:145:LEU:HD21	2.53	0.44
1:A:239:TYR:CZ	1:A:241:ASN:HB2	2.53	0.43
2:B:119:GLY:O	2:B:121:THR:N	2.46	0.43
3:C:311:LEU:HD11	3:C:340:TRP:HD1	1.83	0.43
3:C:555:LYS:HB2	3:C:569:TRP:HH2	1.83	0.43
3:C:412:HIS:CE1	3:C:416:LYS:HE3	2.53	0.43
1:A:146:ASP:O	1:A:148:ASP:N	2.45	0.43
1:A:643:SER:OG	1:A:644:LEU:N	2.46	0.43
1:A:430:VAL:O	1:A:456:GLN:HB2	2.18	0.43
4:D:81:PHE:O	4:D:84:ILE:HG22	2.18	0.43
3:C:523:LEU:HD11	3:C:525:VAL:CG2	2.48	0.43
3:C:349:THR:C	3:C:351:ILE:H	2.21	0.43
1:A:823:LYS:O	1:A:825:PRO:HD3	2.18	0.43
1:A:973:ASN:OD1	1:A:999:HIS:ND1	2.43	0.43
4:D:21:ARG:O	4:D:22:PHE:CD2	2.71	0.43
2:B:143:ARG:HA	2:B:175:TYR:O	2.17	0.43
2:B:51:LEU:HD11	2:B:143:ARG:N	2.22	0.43
1:A:1126:ALA:C	1:A:1128:ASP:N	2.72	0.43
3:C:539:MET:HE1	3:C:619:ILE:HG23	2.00	0.43
3:C:171:TRP:CZ3	3:C:175:LEU:HD11	2.52	0.43
1:A:112:ILE:HG12	1:A:113:GLY:H	1.83	0.43
1:A:268:GLY:C	1:A:285:LEU:HD11	2.39	0.43
1:A:534:MET:HE1	1:A:569:LEU:HD21	1.99	0.43
1:A:1057:ARG:HB3	1:A:1108:VAL:HG13	2.00	0.43
1:A:726:TYR:CE1	1:A:796:GLN:NE2	2.86	0.43
4:D:47:ASN:HB2	4:D:48:HIS:H	1.65	0.43
3:C:609:SER:O	3:C:610:PHE:C	2.57	0.43
1:A:582:LEU:CD1	1:A:583:GLY:N	2.81	0.43
3:C:530:MET:HG2	4:D:32:LEU:HB3	2.01	0.43
3:C:702:ARG:HD2	3:C:722:GLN:NE2	2.33	0.43
1:A:245:TYR:CD2	1:A:245:TYR:C	2.91	0.43
1:A:134:ARG:HH11	1:A:134:ARG:HG3	1.82	0.43
1:A:500:VAL:HG12	1:A:541:LEU:HD12	2.01	0.43
1:A:446:THR:CG2	1:A:447:GLU:H	2.05	0.43
3:C:440:PHE:O	3:C:442:PHE:N	2.51	0.43
3:C:295:LEU:HD11	3:C:325:LEU:HD22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:750:THR:HG22	1:A:751:ALA:N	2.33	0.43
3:C:204:ARG:NE	3:C:273:ARG:HH12	2.17	0.43
1:A:138:GLY:C	1:A:159:LEU:HB2	2.38	0.43
1:A:567:ARG:HB3	1:A:579:LYS:HA	2.01	0.43
1:A:351:GLU:HG2	1:A:352:THR:N	2.34	0.43
1:A:869:ALA:O	1:A:884:ILE:HG23	2.17	0.43
1:A:951:PRO:HG2	2:B:119:GLY:HA2	2.00	0.43
1:A:1034:ASN:HD22	1:A:1034:ASN:HA	1.55	0.43
3:C:437:MET:O	3:C:440:PHE:HB3	2.19	0.43
2:B:98:ILE:N	2:B:201:ALA:O	2.32	0.43
1:A:692:ALA:O	1:A:693:LEU:HD23	2.17	0.43
1:A:655:ARG:CG	1:A:655:ARG:HH11	2.31	0.43
1:A:1047:TRP:HZ3	1:A:1132:VAL:HG13	1.83	0.43
3:C:453:TYR:C	3:C:453:TYR:CD1	2.91	0.43
1:A:326:SER:HB3	1:A:329:GLY:O	2.19	0.43
4:D:77:HIS:CE1	4:D:97:ASP:OD1	2.72	0.43
1:A:451:PHE:HE1	1:A:470:GLN:HB2	1.79	0.43
1:A:602:LEU:HD22	1:A:603:LEU:N	2.34	0.43
1:A:1102:ARG:O	1:A:1105:MET:HB2	2.18	0.43
1:A:564:ILE:O	1:A:582:LEU:HD12	2.18	0.43
1:A:407:ILE:HD13	1:A:699:LEU:HD23	2.01	0.43
3:C:222:SER:O	3:C:224:LEU:N	2.51	0.43
1:A:393:GLY:O	1:A:708:GLN:HA	2.19	0.43
3:C:651:GLY:O	3:C:652:ASP:C	2.57	0.43
1:A:641:PHE:HB3	1:A:679:MET:HE1	2.01	0.43
2:B:112:GLN:NE2	2:B:187:THR:HG23	2.34	0.43
3:C:193:ILE:C	3:C:195:GLY:H	2.22	0.43
3:C:583:LYS:O	3:C:584:GLU:CB	2.66	0.43
1:A:109:GLN:HE22	1:A:111:ARG:NH1	2.16	0.43
3:C:399:ASN:ND2	3:C:444:HIS:CE1	2.87	0.43
1:A:553:SER:HA	1:A:554:PRO:HD3	1.80	0.43
3:C:90:VAL:O	3:C:92:ASN:N	2.51	0.43
3:C:141:ASP:O	3:C:145:GLN:HG2	2.19	0.43
3:C:203:GLU:HB2	3:C:209:VAL:HG21	2.00	0.43
3:C:186:LYS:CB	3:C:188:VAL:HG23	2.44	0.43
3:C:709:THR:HA	3:C:755:TYR:O	2.19	0.43
3:C:709:THR:HG23	3:C:756:HIS:CD2	2.53	0.43
1:A:611:LEU:HD23	1:A:611:LEU:C	2.40	0.43
3:C:592:SER:OG	3:C:595:GLN:HG3	2.19	0.42
1:A:494:GLN:O	1:A:495:ALA:HB3	2.19	0.42
3:C:123:GLU:HB3	3:C:124:ASP:H	1.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1020:THR:OG1	1:A:1020:THR:O	2.24	0.42
1:A:70:LYS:O	1:A:147:ARG:NH2	2.49	0.42
1:A:190:VAL:HG13	1:A:190:VAL:O	2.19	0.42
1:A:505:SER:OG	1:A:506:SER:N	2.52	0.42
2:B:170:PHE:HD2	2:B:170:PHE:N	2.13	0.42
3:C:624:LEU:HD22	3:C:628:LEU:HG	2.01	0.42
1:A:239:TYR:CE2	1:A:297:LEU:HD13	2.54	0.42
1:A:428:SER:OG	1:A:456:GLN:HG2	2.18	0.42
2:B:204:PHE:CD1	2:B:204:PHE:N	2.87	0.42
3:C:692:ARG:HG2	3:C:725:PHE:CE2	2.54	0.42
3:C:450:GLU:HG3	3:C:451:ALA:N	2.34	0.42
1:A:586:ILE:HG21	1:A:608:ASP:N	2.34	0.42
1:A:6:VAL:HG13	1:A:6:VAL:O	2.19	0.42
3:C:72:ALA:HB1	3:C:77:THR:HB	2.01	0.42
3:C:603:ASN:OD1	4:D:22:PHE:HB2	2.19	0.42
1:A:507:GLN:HE22	1:A:552:LEU:CA	2.27	0.42
2:B:119:GLY:O	2:B:120:LYS:HB2	2.18	0.42
1:A:1006:VAL:CG2	1:A:1007:PHE:N	2.81	0.42
1:A:80:LEU:HD11	1:A:84:TYR:HA	2.01	0.42
3:C:597:LEU:HA	3:C:600:LEU:HD12	2.02	0.42
1:A:335:LYS:O	1:A:348:VAL:HG22	2.18	0.42
2:B:172:ARG:HG2	2:B:173:ARG:N	2.34	0.42
1:A:105:HIS:HA	1:A:152:LEU:HD12	1.98	0.42
1:A:537:GLU:OE1	3:C:82:ASN:HB2	2.20	0.42
3:C:74:GLN:HB3	3:C:113:HIS:NE2	2.34	0.42
2:B:49:GLY:HA3	2:B:141:MET:HE1	2.01	0.42
1:A:255:GLN:HE21	1:A:279:ARG:NH2	2.16	0.42
3:C:42:LYS:O	3:C:43:LEU:CD2	2.67	0.42
1:A:124:ILE:HG12	1:A:131:ILE:HG23	2.01	0.42
1:A:1121:LYS:HB2	1:A:1121:LYS:HZ2	1.83	0.42
1:A:961:ASP:OD2	1:A:964:ASN:N	2.51	0.42
1:A:859:GLN:HA	1:A:859:GLN:OE1	2.19	0.42
3:C:279:ASP:O	3:C:281:SER:N	2.52	0.42
3:C:184:SER:O	3:C:185:ASP:C	2.58	0.42
3:C:735:ARG:HE	3:C:735:ARG:HA	1.84	0.42
3:C:640:ILE:O	3:C:655:ILE:HD12	2.20	0.42
1:A:699:LEU:HD13	1:A:700:THR:N	2.35	0.42
3:C:59:THR:O	3:C:63:TRP:HD1	2.02	0.42
3:C:541:VAL:HG23	3:C:543:LEU:HD21	2.02	0.42
1:A:1047:TRP:CZ3	1:A:1132:VAL:HG13	2.55	0.42
2:B:52:THR:O	2:B:53:ASN:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:TYR:CE1	1:A:683:ASN:N	2.84	0.42
1:A:1101:SER:CB	1:A:1103:PRO:HD2	2.49	0.42
3:C:536:TYR:CD2	3:C:573:LEU:HD11	2.54	0.42
1:A:197:LEU:O	1:A:200:LYS:HG3	2.19	0.42
1:A:707:ILE:O	1:A:708:GLN:C	2.58	0.42
1:A:1048:TYR:CZ	1:A:1052:LEU:HD22	2.54	0.42
3:C:75:SER:O	3:C:77:THR:N	2.53	0.42
4:D:75:CYS:HB2	4:D:97:ASP:OD2	2.19	0.42
2:B:179:TRP:HE3	2:B:179:TRP:N	2.18	0.42
3:C:182:ILE:CG2	3:C:183:ILE:HG13	2.50	0.42
1:A:1055:GLN:NE2	1:A:1089:ILE:HA	2.34	0.42
2:B:136:GLY:O	2:B:138:GLU:N	2.53	0.42
2:B:86:VAL:HG11	2:B:198:THR:HA	1.99	0.42
1:A:963:ASP:N	1:A:963:ASP:OD2	2.53	0.42
3:C:425:THR:HG22	3:C:426:ASP:N	2.35	0.42
3:C:250:LEU:HD22	3:C:254:ARG:HD3	2.01	0.42
3:C:575:HIS:CE1	4:D:28:ASN:HB2	2.55	0.42
1:A:265:ASP:O	1:A:267:ASN:N	2.53	0.42
1:A:270:ARG:HG2	1:A:284:LEU:CD2	2.50	0.42
1:A:59:GLY:HA3	1:A:81:THR:HG23	2.02	0.42
4:D:37:ILE:HG23	4:D:40:ASP:HA	2.02	0.42
1:A:754:PRO:O	1:A:755:SER:HB3	2.20	0.42
3:C:650:ASP:N	3:C:650:ASP:OD2	2.53	0.42
1:A:92:LYS:HD2	1:A:101:ILE:HD13	2.02	0.41
3:C:200:ILE:O	3:C:201:GLU:C	2.59	0.41
1:A:565:SER:CB	1:A:567:ARG:HH11	2.33	0.41
4:D:87:TRP:CH2	4:D:93:VAL:O	2.74	0.41
2:B:175:TYR:HE2	2:B:188:GLU:OE1	2.03	0.41
1:A:1065:VAL:HG12	1:A:1065:VAL:O	2.20	0.41
3:C:284:LYS:HB2	3:C:284:LYS:HE3	1.88	0.41
1:A:41:ILE:O	1:A:52:VAL:HG22	2.19	0.41
3:C:543:LEU:HD22	3:C:543:LEU:N	2.36	0.41
3:C:707:ARG:O	3:C:707:ARG:HG3	2.19	0.41
3:C:95:SER:O	3:C:96:HIS:O	2.38	0.41
1:A:228:GLY:HA3	1:A:239:TYR:CE1	2.54	0.41
3:C:90:VAL:O	3:C:91:GLU:C	2.58	0.41
1:A:1129:LEU:O	1:A:1130:ILE:C	2.58	0.41
1:A:892:GLU:O	1:A:899:VAL:HA	2.20	0.41
1:A:132:GLY:O	1:A:133:LEU:HD12	2.19	0.41
1:A:980:ASP:OD1	1:A:981:SER:N	2.53	0.41
1:A:404:LEU:HD12	1:A:429:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:PHE:CD1	1:A:641:PHE:C	2.93	0.41
1:A:130:MET:HE3	1:A:195:VAL:HG21	2.03	0.41
3:C:141:ASP:O	3:C:142:HIS:C	2.58	0.41
3:C:751:ASN:HD21	3:C:754:GLN:HB2	1.86	0.41
1:A:565:SER:OG	1:A:567:ARG:NH1	2.54	0.41
1:A:1136:LEU:O	1:A:1136:LEU:HD23	2.21	0.41
1:A:138:GLY:CA	1:A:159:LEU:HB2	2.50	0.41
1:A:728:GLU:O	1:A:728:GLU:CG	2.68	0.41
3:C:131:PHE:O	3:C:134:LYS:HB2	2.21	0.41
4:D:45:CYS:CB	4:D:47:ASN:HD21	2.31	0.41
1:A:523:PRO:HB3	1:A:524:GLN:NE2	2.35	0.41
1:A:844:LYS:O	1:A:867:LYS:CA	2.69	0.41
2:B:204:PHE:HD1	2:B:204:PHE:N	2.19	0.41
1:A:448:LEU:HA	1:A:448:LEU:HD12	1.81	0.41
2:B:100:ASN:HA	2:B:101:PRO:HD3	1.91	0.41
2:B:115:LEU:HG	2:B:130:VAL:HG13	2.03	0.41
3:C:110:CYS:O	3:C:111:GLU:C	2.58	0.41
3:C:256:VAL:O	3:C:257:PRO:C	2.56	0.41
1:A:331:SER:O	1:A:332:GLN:HB3	2.20	0.41
1:A:234:GLN:O	1:A:253:ILE:HG22	2.20	0.41
3:C:739:LEU:HA	3:C:739:LEU:HD23	1.91	0.41
3:C:526:ASN:HD22	3:C:526:ASN:HA	1.61	0.41
3:C:587:LYS:HB2	3:C:660:PHE:CZ	2.55	0.41
1:A:32:LEU:CD1	1:A:77:LEU:HD13	2.50	0.41
2:B:98:ILE:HA	2:B:99:PRO:HD3	1.85	0.41
3:C:734:LYS:HD3	3:C:737:GLU:OE2	2.20	0.41
3:C:232:GLU:O	3:C:235:PHE:HB3	2.20	0.41
1:A:1093:LEU:C	1:A:1095:GLU:N	2.74	0.41
3:C:601:MET:HE3	3:C:613:ILE:HA	2.02	0.41
1:A:487:VAL:HG23	1:A:487:VAL:O	2.20	0.41
1:A:253:ILE:O	1:A:254:LYS:C	2.58	0.41
2:B:132:LEU:O	2:B:133:ALA:C	2.59	0.41
1:A:263:ARG:HD2	1:A:265:ASP:O	2.21	0.41
2:B:44:PRO:HA	2:B:45:PRO:HD2	1.77	0.41
1:A:414:ARG:CG	1:A:414:ARG:HH11	2.32	0.41
1:A:63:VAL:HG11	1:A:122:GLY:HA3	2.02	0.41
1:A:388:ARG:NH1	1:A:714:THR:CB	2.84	0.41
3:C:508:PHE:O	3:C:512:MET:HB2	2.21	0.41
1:A:237:ILE:O	1:A:247:ALA:HA	2.20	0.41
1:A:921:ILE:N	1:A:921:ILE:HD12	2.36	0.41
1:A:265:ASP:OD2	1:A:270:ARG:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:LEU:HA	1:A:404:LEU:HD13	1.89	0.41
3:C:744:TYR:O	3:C:757:TYR:O	2.38	0.41
1:A:21:GLY:O	1:A:30:ASN:HB2	2.20	0.41
1:A:144:PRO:HD2	1:A:149:ASN:ND2	2.36	0.41
2:B:111:THR:O	2:B:187:THR:HA	2.21	0.41
2:B:86:VAL:CG1	2:B:197:ILE:O	2.69	0.41
3:C:219:GLY:O	3:C:220:MET:C	2.57	0.41
1:A:413:LEU:HD13	1:A:468:LEU:HD23	2.03	0.41
1:A:340:SER:HG	1:A:344:GLY:HA2	1.82	0.41
3:C:329:VAL:O	3:C:330:ARG:O	2.39	0.41
1:A:876:PHE:CE1	1:A:918:GLY:O	2.74	0.41
1:A:532:THR:HG22	1:A:533:GLU:H	1.80	0.41
1:A:102:THR:HG21	1:A:1067:LYS:HG3	2.03	0.41
3:C:536:TYR:CD2	3:C:573:LEU:HD21	2.56	0.41
1:A:498:ILE:CD1	1:A:498:ILE:N	2.84	0.41
1:A:949:PHE:CD1	1:A:991:HIS:CE1	3.08	0.41
3:C:707:ARG:CD	3:C:710:LEU:HD13	2.50	0.41
3:C:96:HIS:O	3:C:97:LYS:HB3	2.21	0.41
3:C:167:LEU:HA	3:C:168:PRO:HD3	1.49	0.41
3:C:390:MET:HE2	3:C:394:PHE:HB2	2.02	0.41
1:A:1100:ILE:O	1:A:1105:MET:CE	2.69	0.41
3:C:528:LEU:HB2	4:D:32:LEU:HD23	2.03	0.41
3:C:63:TRP:CZ3	3:C:105:GLN:HG3	2.55	0.41
1:A:452:VAL:HG22	1:A:477:ARG:NH1	2.36	0.40
4:D:39:VAL:O	4:D:39:VAL:HG12	2.21	0.40
1:A:382:PHE:CD1	1:A:382:PHE:N	2.88	0.40
3:C:45:ILE:HG21	3:C:48:PHE:HD1	1.87	0.40
3:C:49:ARG:HA	3:C:49:ARG:NE	2.37	0.40
2:B:137:LYS:CD	2:B:137:LYS:C	2.90	0.40
2:B:177:ILE:HG12	2:B:186:VAL:CG2	2.41	0.40
1:A:451:PHE:HD1	1:A:470:GLN:CB	2.34	0.40
1:A:300:LEU:N	1:A:300:LEU:CD2	2.84	0.40
3:C:311:LEU:HA	3:C:311:LEU:HD23	1.79	0.40
3:C:734:LYS:HA	3:C:737:GLU:OE1	2.20	0.40
1:A:257:THR:O	1:A:276:MET:N	2.54	0.40
1:A:910:MET:HE3	1:A:912:LEU:HD21	2.03	0.40
1:A:301:ARG:HH11	1:A:301:ARG:HG2	1.86	0.40
3:C:187:MET:O	3:C:191:LYS:HB2	2.21	0.40
1:A:167:VAL:HG13	1:A:180:PHE:HB3	2.04	0.40
2:B:169:GLY:C	2:B:212:PRO:HD3	2.41	0.40
4:D:45:CYS:O	4:D:46:ARG:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:GLY:O	2:B:137:LYS:C	2.59	0.40
3:C:209:VAL:O	3:C:210:ASP:HB3	2.21	0.40
3:C:457:LEU:CD2	3:C:461:LEU:HG	2.52	0.40
1:A:40:GLU:HB3	1:A:42:TYR:HE1	1.85	0.40
3:C:454:LYS:HE2	3:C:490:LYS:HD2	2.02	0.40
1:A:67:PHE:N	1:A:67:PHE:CD2	2.90	0.40
1:A:290:GLN:HG3	1:A:294:THR:O	2.21	0.40
3:C:267:LEU:HD21	3:C:290:VAL:HG12	2.03	0.40
1:A:1044:SER:O	1:A:1047:TRP:N	2.54	0.40
1:A:576:LEU:C	1:A:577:LEU:HD23	2.41	0.40
3:C:558:TYR:O	3:C:562:HIS:HB2	2.21	0.40
1:A:412:PRO:HG2	1:A:412:PRO:O	2.22	0.40
1:A:457:THR:CG2	1:A:459:PHE:O	2.69	0.40
1:A:125:ASP:HA	1:A:126:PRO:HD3	2.00	0.40
2:B:99:PRO:O	2:B:100:ASN:C	2.60	0.40
3:C:121:PHE:C	3:C:123:GLU:H	2.25	0.40
3:C:414:ASP:O	3:C:418:ARG:HG3	2.21	0.40
1:A:1043:LEU:HA	1:A:1043:LEU:HD23	1.88	0.40
3:C:384:GLU:HA	3:C:387:VAL:HG23	2.04	0.40
1:A:990:GLN:HB2	1:A:990:GLN:HE21	1.65	0.40
1:A:337:ASN:ND2	1:A:348:VAL:HG11	2.36	0.40
4:D:94:CYS:HA	4:D:95:PRO:HD2	1.91	0.40
3:C:274:VAL:HG21	3:C:283:GLN:HB2	2.04	0.40
1:A:57:MET:HG3	1:A:61:ILE:HD11	2.02	0.40
1:A:411:TRP:HA	1:A:412:PRO:HD3	1.90	0.40
1:A:413:LEU:HA	1:A:413:LEU:HD23	1.83	0.40
1:A:603:LEU:N	1:A:603:LEU:HD23	2.34	0.40
3:C:527:ILE:O	3:C:527:ILE:HG23	2.21	0.40
3:C:591:VAL:CG1	3:C:669:ILE:HD12	2.52	0.40
1:A:105:HIS:HA	1:A:152:LEU:CD1	2.52	0.40
1:A:67:PHE:O	1:A:69:PRO:HD3	2.21	0.40
2:B:219:GLU:C	2:B:221:ASP:H	2.25	0.40
1:A:111:ARG:HA	1:A:111:ARG:HD2	1.63	0.40
1:A:416:ASP:HA	1:A:417:PRO:HD3	1.88	0.40
2:B:148:PRO:C	2:B:150:GLU:H	2.23	0.40

All (1) 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)
3:C:60:GLN:NE2	3:C:60:GLN:NE2[3_554]	2.09	0.11

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	1138/1140 (100%)	869 (76%)	201 (18%)	68 (6%)	2 11
2	B	174/222 (78%)	119 (68%)	37 (21%)	18 (10%)	1 4
3	C	717/759 (94%)	516 (72%)	132 (18%)	69 (10%)	1 4
4	D	88/108 (82%)	47 (53%)	27 (31%)	14 (16%)	0 0
All	All	2117/2229 (95%)	1551 (73%)	397 (19%)	169 (8%)	1 6

All (169) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	ILE
1	A	290	GLN
1	A	292	ASP
1	A	430	VAL
1	A	583	GLY
1	A	598	SER
1	A	672	ASN
1	A	746	SER
1	A	761	LEU
1	A	826	ASN
1	A	1020	THR
1	A	1094	ILE
1	A	1110	ALA
1	A	1115	ASP
1	A	1127	ASP
2	B	53	ASN
2	B	92	THR
2	B	163	ARG
2	B	206	CYS
2	B	209	HIS
3	C	42	LYS
3	C	49	ARG

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Mol	Chain	Res	Type
3	C	56	ASP
3	C	58	TYR
3	C	76	SER
3	C	82	ASN
3	C	83	LEU
3	C	96	HIS
3	C	126	LEU
3	C	128	SER
3	C	185	ASP
3	C	191	LYS
3	C	276	THR
3	C	330	ARG
3	C	483	CYS
3	C	517	ASP
3	C	587	LYS
3	C	606	ASP
3	C	633	CYS
3	C	644	LYS
3	C	660	PHE
3	C	661	LYS
3	C	752	PRO
4	D	22	PHE
4	D	38	VAL
4	D	84	ILE
4	D	104	GLN
1	A	46	ALA
1	A	147	ARG
1	A	172	GLY
1	A	279	ARG
1	A	549	SER
1	A	584	GLY
1	A	674	LYS
1	A	860	THR
1	A	863	GLU
1	A	983	ALA
1	A	1084	PRO
1	A	1121	LYS
1	A	1123	GLU
2	B	38	LEU
2	B	104	GLY
2	B	137	LYS
2	B	171	HIS

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Mol	Chain	Res	Type
3	C	129	VAL
3	C	209	VAL
3	C	229	ASP
3	C	240	ASN
3	C	280	HIS
3	C	441	ARG
3	C	598	VAL
3	C	607	GLY
3	C	652	ASP
3	C	670	ASN
3	C	691	ASP
4	D	90	THR
4	D	96	LEU
4	D	105	LYS
1	A	36	ASN
1	A	113	GLY
1	A	115	PRO
1	A	213	GLU
1	A	418	ASN
1	A	449	MET
1	A	481	GLN
1	A	547	GLY
1	A	624	SER
1	A	644	LEU
1	A	738	SER
1	A	861	VAL
1	A	901	THR
1	A	910	MET
1	A	917	LYS
1	A	947	ARG
1	A	1021	SER
1	A	1124	ALA
2	B	140	LEU
2	B	199	ALA
3	C	55	PRO
3	C	71	ARG
3	C	75	SER
3	C	119	LEU
3	C	223	ASP
3	C	293	GLN
3	C	350	ALA
3	C	402	PRO

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Mol	Chain	Res	Type
3	C	451	ALA
3	C	586	LYS
3	C	727	VAL
3	C	757	TYR
3	C	758	VAL
4	D	52	LEU
4	D	83	CYS
4	D	87	TRP
1	A	153	LYS
1	A	204	LYS
1	A	488	SER
1	A	503	CYS
1	A	751	ALA
1	A	783	GLY
1	A	1008	CYS
1	A	1114	TYR
3	C	54	LEU
3	C	91	GLU
3	C	189	GLN
3	C	201	GLU
3	C	205	SER
3	C	228	LYS
3	C	325	LEU
3	C	377	GLU
3	C	514	ASN
3	C	610	PHE
3	C	726	PRO
4	D	102	GLU
1	A	224	GLU
1	A	592	LEU
1	A	745	THR
1	A	884	ILE
1	A	972	PHE
2	B	12	GLU
2	B	108	THR
2	B	192	PRO
3	C	171	TRP
3	C	233	LEU
3	C	378	VAL
3	C	440	PHE
3	C	597	LEU
4	D	40	ASP

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Mol	Chain	Res	Type
4	D	103	PHE
1	A	460	CYS
1	A	903	CYS
1	A	937	PRO
2	B	95	GLY
2	B	136	GLY
2	B	196	PRO
3	C	51	ARG
1	A	61	ILE
1	A	493	PRO
1	A	551	GLY
3	C	52	PRO
3	C	619	ILE
4	D	94	CYS
3	C	306	GLY
1	A	406	GLY
1	A	523	PRO
1	A	707	ILE
2	B	151	ASN
3	C	405	PRO
3	C	519	GLY

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	999/999 (100%)	871 (87%)	128 (13%)	5 21
2	B	157/191 (82%)	137 (87%)	20 (13%)	5 22
3	C	656/679 (97%)	586 (89%)	70 (11%)	8 31
4	D	79/90 (88%)	62 (78%)	17 (22%)	1 5
All	All	1891/1959 (96%)	1656 (88%)	235 (12%)	6 23

All (235) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	35	LYS
1	A	49	LEU
1	A	57	MET
1	A	67	PHE
1	A	103	ARG
1	A	112	ILE
1	A	130	MET
1	A	152	LEU
1	A	156	ASN
1	A	158	ARG
1	A	160	GLU
1	A	180	PHE
1	A	198	ARG
1	A	210	GLU
1	A	213	GLU
1	A	241	ASN
1	A	243	ASP
1	A	245	TYR
1	A	266	PRO
1	A	269	SER
1	A	285	LEU
1	A	292	ASP
1	A	309	SER
1	A	312	GLU
1	A	315	THR
1	A	318	ASP
1	A	328	LEU
1	A	338	VAL
1	A	341	ASN
1	A	353	PHE
1	A	372	GLN
1	A	374	GLN
1	A	390	ILE
1	A	396	ILE
1	A	403	ASP
1	A	410	LEU
1	A	412	PRO
1	A	414	ARG
1	A	419	ARG
1	A	420	GLU
1	A	422	TYR
1	A	452	VAL

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Mol	Chain	Res	Type
1	A	454	ASP
1	A	469	ILE
1	A	473	SER
1	A	476	VAL
1	A	481	GLN
1	A	482	GLU
1	A	487	VAL
1	A	493	PRO
1	A	510	VAL
1	A	518	TYR
1	A	523	PRO
1	A	525	GLU
1	A	531	HIS
1	A	540	CYS
1	A	555	LEU
1	A	562	THR
1	A	563	ASP
1	A	567	ARG
1	A	576	LEU
1	A	582	LEU
1	A	587	ILE
1	A	594	THR
1	A	596	PHE
1	A	597	GLU
1	A	602	LEU
1	A	603	LEU
1	A	608	ASP
1	A	614	PHE
1	A	616	LEU
1	A	617	ASN
1	A	618	ILE
1	A	623	LEU
1	A	625	ASP
1	A	627	LYS
1	A	646	THR
1	A	655	ARG
1	A	663	ASN
1	A	673	LEU
1	A	688	PRO
1	A	689	ASP
1	A	700	THR
1	A	703	THR

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Mol	Chain	Res	Type
1	A	704	ILE
1	A	713	ARG
1	A	714	THR
1	A	720	SER
1	A	727	GLN
1	A	762	SER
1	A	771	PHE
1	A	784	GLU
1	A	814	LEU
1	A	817	VAL
1	A	818	SER
1	A	823	LYS
1	A	855	ASP
1	A	863	GLU
1	A	872	SER
1	A	887	THR
1	A	899	VAL
1	A	902	GLU
1	A	907	ASN
1	A	931	LEU
1	A	963	ASP
1	A	964	ASN
1	A	966	LEU
1	A	969	GLU
1	A	987	GLU
1	A	990	GLN
1	A	992	LEU
1	A	993	GLN
1	A	1000	LEU
1	A	1006	VAL
1	A	1021	SER
1	A	1023	PRO
1	A	1036	MET
1	A	1054	MET
1	A	1069	GLU
1	A	1086	THR
1	A	1093	LEU
1	A	1105	MET
1	A	1109	VAL
1	A	1115	ASP
1	A	1123	GLU
1	A	1135	GLU

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Mol	Chain	Res	Type
1	A	1139	ILE
2	B	14	ASN
2	B	17	ILE
2	B	21	LEU
2	B	85	ILE
2	B	86	VAL
2	B	93	VAL
2	B	106	ASP
2	B	109	PRO
2	B	115	LEU
2	B	117	LEU
2	B	131	LYS
2	B	137	LYS
2	B	152	PRO
2	B	163	ARG
2	B	170	PHE
2	B	179	TRP
2	B	192	PRO
2	B	197	ILE
2	B	202	ARG
2	B	206	CYS
3	C	43	LEU
3	C	64	ARG
3	C	79	ILE
3	C	90	VAL
3	C	93	LEU
3	C	102	LEU
3	C	112	ASP
3	C	135	ILE
3	C	164	ASN
3	C	171	TRP
3	C	173	MET
3	C	175	LEU
3	C	182	ILE
3	C	183	ILE
3	C	193	ILE
3	C	199	LEU
3	C	209	VAL
3	C	217	LEU
3	C	226	VAL
3	C	227	TYR
3	C	249	ARG

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Mol	Chain	Res	Type
3	C	281	SER
3	C	283	GLN
3	C	292	LYS
3	C	307	LEU
3	C	330	ARG
3	C	353	ILE
3	C	371	LYS
3	C	389	LEU
3	C	390	MET
3	C	394	PHE
3	C	402	PRO
3	C	422	LYS
3	C	423	GLU
3	C	428	GLU
3	C	429	LEU
3	C	439	LEU
3	C	444	HIS
3	C	450	GLU
3	C	457	LEU
3	C	478	LYS
3	C	483	CYS
3	C	494	MET
3	C	498	MET
3	C	526	ASN
3	C	540	GLU
3	C	546	GLU
3	C	562	HIS
3	C	569	TRP
3	C	591	VAL
3	C	611	GLU
3	C	624	LEU
3	C	626	ARG
3	C	639	LEU
3	C	650	ASP
3	C	652	ASP
3	C	660	PHE
3	C	663	LYS
3	C	665	PHE
3	C	677	THR
3	C	681	GLN
3	C	683	SER
3	C	687	ARG

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Mol	Chain	Res	Type
3	C	691	ASP
3	C	706	MET
3	C	720	TYR
3	C	726	PRO
3	C	735	ARG
3	C	748	ASP
3	C	751	ASN
4	D	19	LYS
4	D	22	PHE
4	D	23	GLU
4	D	25	LYS
4	D	28	ASN
4	D	32	LEU
4	D	37	ILE
4	D	41	ASN
4	D	42	CYS
4	D	45	CYS
4	D	47	ASN
4	D	49	ILE
4	D	64	THR
4	D	84	ILE
4	D	98	ASN
4	D	99	ARG
4	D	103	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	16	ASN
1	A	30	ASN
1	A	85	ASN
1	A	93	GLN
1	A	109	GLN
1	A	156	ASN
1	A	240	HIS
1	A	241	ASN
1	A	255	GLN
1	A	262	ASN
1	A	319	ASN
1	A	332	GLN
1	A	343	GLN

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Mol	Chain	Res	Type
1	A	372	GLN
1	A	374	GLN
1	A	432	GLN
1	A	455	GLN
1	A	462	ASN
1	A	467	GLN
1	A	481	GLN
1	A	494	GLN
1	A	507	GLN
1	A	524	GLN
1	A	578	HIS
1	A	634	GLN
1	A	648	ASN
1	A	708	GLN
1	A	727	GLN
1	A	743	GLN
1	A	790	ASN
1	A	796	GLN
1	A	809	GLN
1	A	810	ASN
1	A	859	GLN
1	A	904	ASN
1	A	907	ASN
1	A	964	ASN
1	A	990	GLN
1	A	1016	ASN
1	A	1034	ASN
1	A	1055	GLN
1	A	1056	ASN
1	A	1140	HIS
2	B	30	GLN
2	B	41	ASN
2	B	112	GLN
3	C	92	ASN
3	C	283	GLN
3	C	309	HIS
3	C	321	GLN
3	C	333	GLN
3	C	339	HIS
3	C	363	GLN
3	C	399	ASN
3	C	412	HIS

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Mol	Chain	Res	Type
3	C	421	ASN
3	C	526	ASN
3	C	551	GLN
3	C	570	GLN
3	C	575	HIS
3	C	595	GLN
3	C	657	ASN
3	C	673	GLN
3	C	681	GLN
3	C	690	GLN
3	C	712	HIS
3	C	722	GLN
3	C	751	ASN
3	C	754	GLN
3	C	756	HIS
4	D	28	ASN
4	D	41	ASN
4	D	47	ASN
4	D	48	HIS
4	D	98	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	1140/1140 (100%)	-0.28	10 (0%) 85 72	22, 68, 125, 202	0
2	B	180/222 (81%)	-0.03	3 (1%) 73 52	32, 86, 135, 167	0
3	C	719/759 (94%)	-0.40	2 (0%) 94 88	23, 71, 126, 173	0
4	D	90/108 (83%)	-0.35	0 100 100	44, 75, 117, 140	0
All	All	2129/2229 (95%)	-0.30	15 (0%) 89 78	22, 71, 126, 202	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1117	GLY	4.8
1	A	778	HIS	4.2
2	B	10	PRO	3.4
3	C	423	GLU	3.1
2	B	165	ARG	2.9
1	A	1114	TYR	2.8
3	C	208	ALA	2.7
1	A	781	SER	2.5
1	A	283	LEU	2.5
2	B	52	THR	2.5
1	A	1119	GLY	2.4
1	A	292	ASP	2.2
1	A	47	GLU	2.1
1	A	302	VAL	2.1
1	A	1	MET	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	ZN	D	4003	1/1	0.96	0.20	0.02	84,84,84,84	0
5	ZN	D	4002	1/1	0.98	0.15	-0.67	99,99,99,99	0
5	ZN	B	3002	1/1	0.99	0.10	-0.80	91,91,91,91	0
5	ZN	D	4001	1/1	0.97	0.16	-1.18	77,77,77,77	0
5	ZN	B	3001	1/1	0.96	0.09	-1.34	114,114,114,114	0

6.5 Other polymers (i)

There are no such residues in this entry.