Full wwPDB X-ray Structure Validation Report (i)

Jun 11, 2024 – 10:29 PM EDT

PDB ID	:	2D0P
Title	:	Structure of diol dehydratase-reactivating factor in nucleotide free form
Authors	:	Shibata, N.; Mori, K.; Hieda, N.; Higuchi, Y.; Yamanishi, M.; Toraya, T.
Deposited on	:	2005-08-05
Resolution	:	3.00 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 (i) 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 (i)) were used in the production of this report:

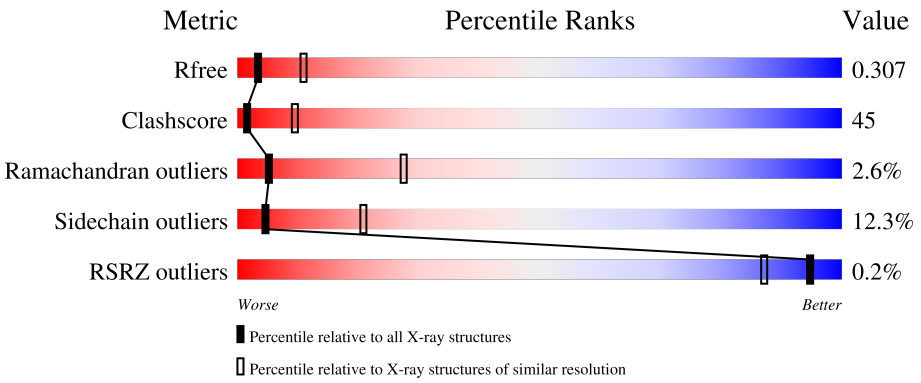
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	610	41% 50% 8% •
1	C	610	34% 55% 10% •
2	B	125	35% 47% 5% • 12%
2	D	125	33% 49% 6% 13%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10689 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.

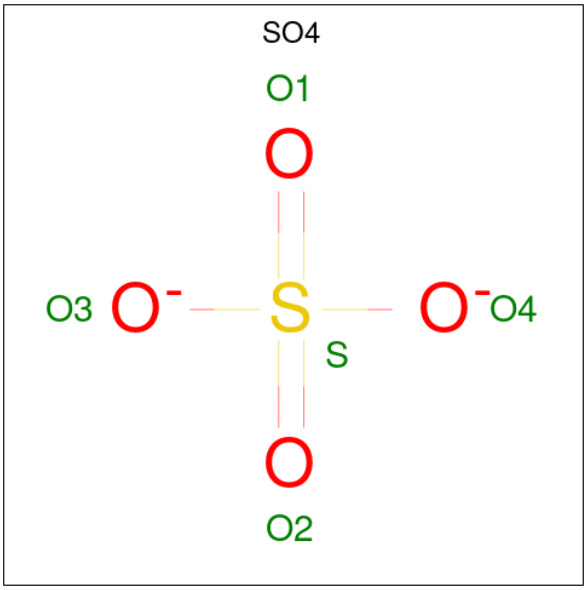
- Molecule 1 is a protein called diol dehydratase-reactivating factor large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	606	4478	2823	778	862	15	0	0	0
1	C	605	4467	2814	777	861	15	0	0	0

- Molecule 2 is a protein called diol dehydratase-reactivating factor small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	110	846	532	160	150	4	0	0	0
2	D	109	838	528	158	148	4	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	A	1	5	4	1	0	0
			Total	O	S		
3	A	1	5	4	1	0	0
			Total	O	S		
3	A	1	5	4	1	0	0
			Total	O	S		
3	C	1	5	4	1	0	0
			Total	O	S		
3	C	1	5	4	1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	1	1	1	0	0
			Total	Ca		
4	C	1	1	1	0	0

- Molecule 5 is water.

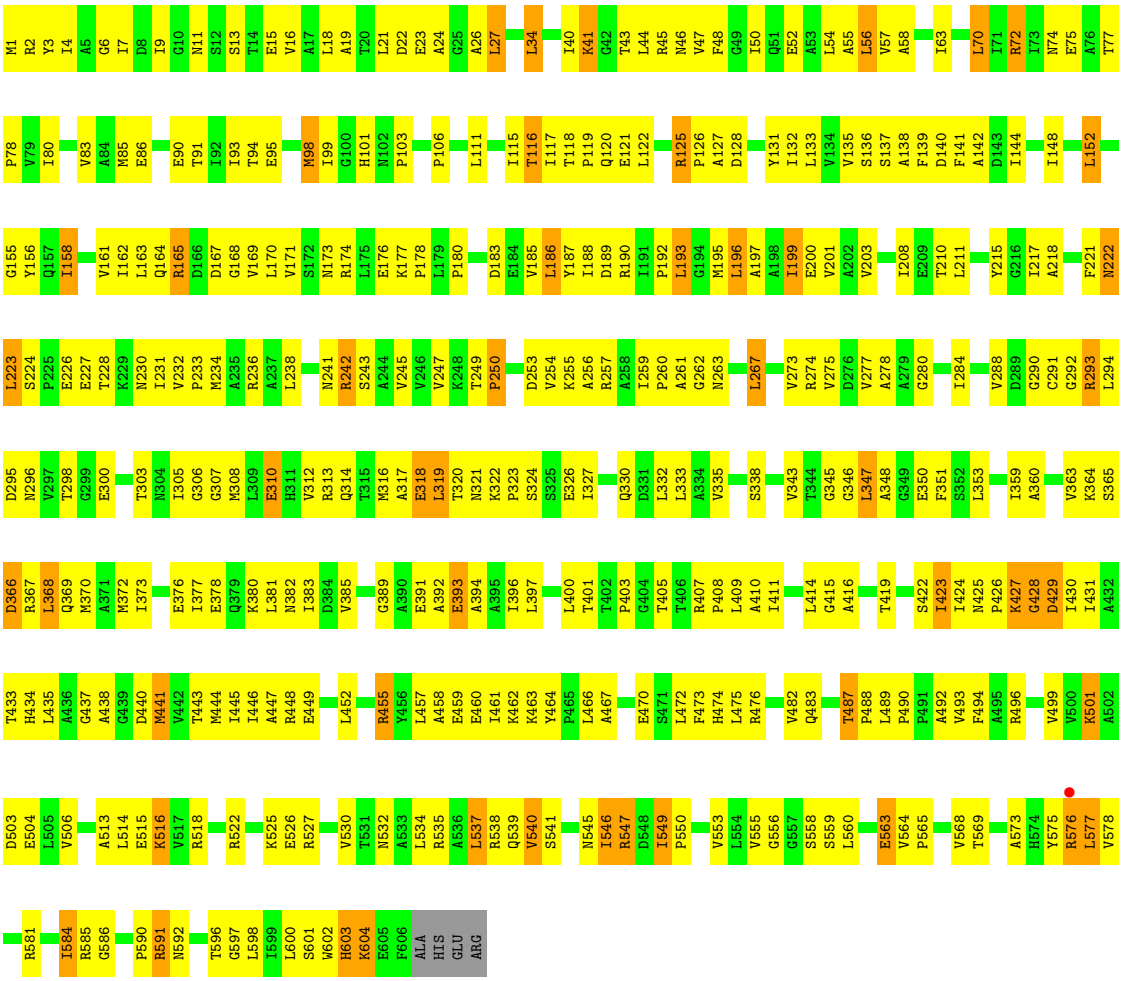
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	13	13	13	0	0
			Total	O		
5	B	10	10	10	0	0
			Total	O		
5	C	4	4	4	0	0
			Total	O		
5	D	6	6	6	0	0

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.

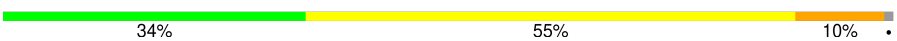
• Molecule 1: diol dehydratase-reactivating factor large subunit

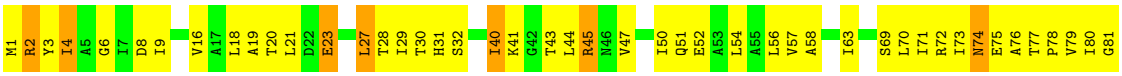
Chain A:

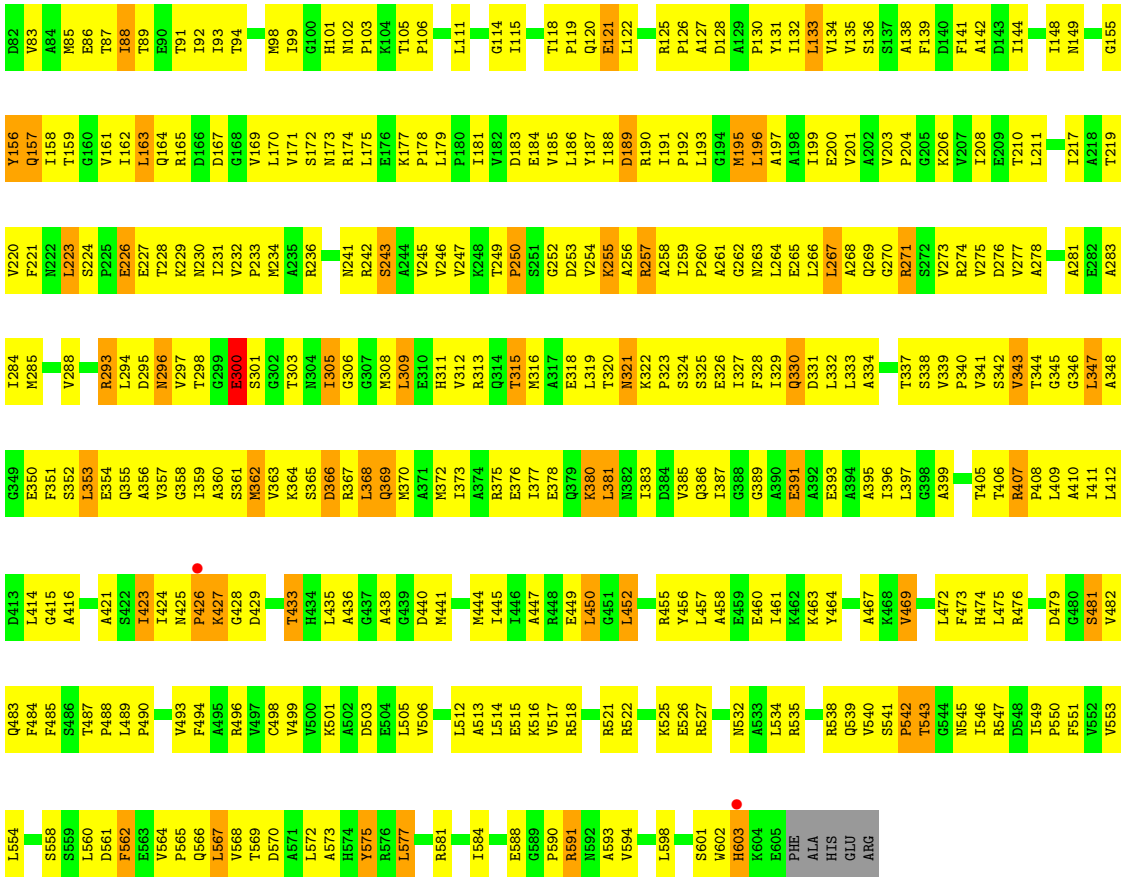


• Molecule 1: diol dehydratase-reactivating factor large subunit

Chain C:

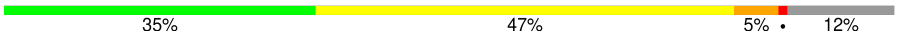


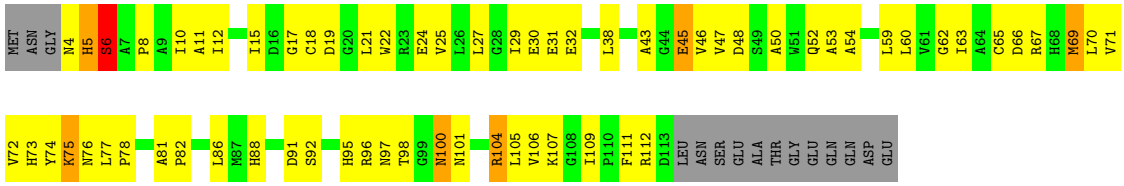




• Molecule 2: diol dehydratase-reactivating factor small subunit

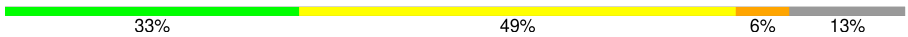
Chain B:

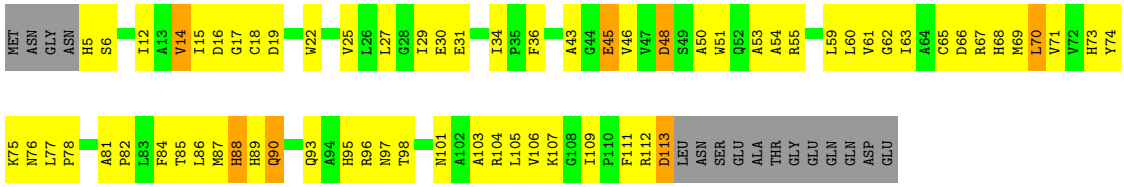




• Molecule 2: diol dehydratase-reactivating factor small subunit

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	81.92Å 85.37Å 296.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.58 – 3.00 41.02 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.8 (40.58-3.00) 92.7 (41.02-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.27 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.238 , 0.313 0.233 , 0.307	Depositor DCC
R_{free} test set	4211 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å^2)	74.4	Xtriage
Anisotropy	0.788	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 72.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.034 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10689	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CA

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	0.38	0/4539	0.60	0/6174
1	C	0.37	0/4527	0.59	0/6158
2	B	0.38	0/868	0.54	0/1182
2	D	0.41	0/860	0.58	0/1171
All	All	0.38	0/10794	0.59	0/14685

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
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	6	SER	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	4478	0	4627	388	0
1	C	4467	0	4618	457	0
2	B	846	0	829	70	0
2	D	838	0	823	77	0
3	A	15	0	0	0	0
3	C	10	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	13	0	0	0	0
5	B	10	0	0	1	0
5	C	4	0	0	0	0
5	D	6	0	0	0	0
All	All	10689	0	10897	973	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 45.

All (973) 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:125:ARG:HG3	1:C:126:PRO:HD2	1.18	1.15
2:B:60:LEU:HD22	2:B:75:LYS:HD2	1.37	1.00
1:A:2:ARG:HD3	1:A:21:LEU:HD23	1.40	0.99
1:C:407:ARG:HG2	1:C:407:ARG:HH21	1.28	0.98
2:D:87:MET:O	2:D:90:GLN:HG3	1.64	0.98
1:A:411:ILE:HD11	1:A:422:SER:HB2	1.41	0.98
1:C:322:LYS:HB3	1:C:326:GLU:HG3	1.42	0.97
1:A:242:ARG:HG3	1:A:242:ARG:HH21	1.29	0.96
1:A:125:ARG:HG3	1:A:126:PRO:HD2	1.45	0.96
2:B:8:PRO:HB2	2:B:59:LEU:HD11	1.48	0.95
1:C:83:VAL:HG23	1:C:359:ILE:O	1.66	0.93
1:C:467:ALA:HB1	1:C:475:LEU:HD13	1.52	0.89
1:A:77:THR:HG22	1:A:368:LEU:HD11	1.54	0.89
1:C:157:GLN:H	1:C:157:GLN:HE21	1.19	0.89
1:A:467:ALA:HB1	1:A:475:LEU:HD13	1.53	0.89
1:C:561:ASP:OD2	1:C:564:VAL:HG23	1.74	0.88
1:C:572:LEU:HD22	1:C:577:LEU:HD21	1.53	0.88
1:C:408:PRO:HB3	1:C:426:PRO:HD3	1.56	0.87
1:C:40:ILE:HD12	1:C:40:ILE:H	1.41	0.86
1:C:315:THR:O	1:C:319:LEU:HG	1.75	0.86
1:C:259:ILE:HB	1:C:260:PRO:HD2	1.58	0.85
1:C:572:LEU:HB3	1:C:577:LEU:HD11	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:ILE:HD13	2:B:72:VAL:HA	1.59	0.84
1:A:4:ILE:HG23	1:A:70:LEU:HD23	1.60	0.84
2:B:25:VAL:HG22	2:B:95:HIS:O	1.78	0.84
1:C:293:ARG:HA	1:C:293:ARG:HH11	1.42	0.84
1:C:423:ILE:HG21	1:C:540:VAL:HG21	1.60	0.84
1:A:411:ILE:HG22	1:A:553:VAL:HB	1.59	0.83
2:B:12:ILE:HG12	2:B:63:ILE:HB	1.59	0.83
2:D:65:CYS:HB3	2:D:70:LEU:HB2	1.59	0.83
1:A:394:ALA:HB2	1:A:598:LEU:HD23	1.60	0.82
1:C:88:ILE:HD13	1:C:278:ALA:HB1	1.62	0.82
1:A:411:ILE:O	1:A:411:ILE:HD12	1.80	0.82
1:A:223:LEU:HD13	1:A:227:GLU:HG3	1.62	0.81
1:C:395:ALA:HB1	1:C:411:ILE:HD11	1.61	0.81
1:C:421:ALA:HB3	1:C:433:THR:HG23	1.62	0.81
1:A:85:MET:HG3	1:A:86:GLU:H	1.46	0.81
1:A:487:THR:HG22	1:A:488:PRO:HD2	1.61	0.81
1:A:452:LEU:HD21	1:A:457:LEU:HD23	1.64	0.80
1:C:186:LEU:HG	1:C:187:TYR:HD1	1.47	0.80
1:A:522:ARG:HH22	1:A:563:GLU:HG2	1.47	0.80
2:B:59:LEU:HD23	2:B:106:VAL:HG11	1.63	0.80
1:C:266:LEU:HA	1:C:297:VAL:HG22	1.64	0.80
1:A:515:GLU:HB2	1:A:516:LYS:HE3	1.63	0.80
1:C:268:ALA:HB2	1:C:294:LEU:HD23	1.62	0.80
1:C:441:MET:O	1:C:445:ILE:HG13	1.82	0.79
1:C:232:VAL:HB	1:C:233:PRO:HD3	1.63	0.79
1:A:323:PRO:HD2	1:A:326:GLU:OE1	1.82	0.79
1:A:323:PRO:HG2	1:A:326:GLU:HG3	1.63	0.79
1:A:423:ILE:HG21	1:A:540:VAL:HG21	1.63	0.79
1:C:450:LEU:HB3	1:C:452:LEU:HD13	1.65	0.79
1:A:293:ARG:HH21	1:A:539:GLN:NE2	1.81	0.79
1:A:2:ARG:HB2	1:A:21:LEU:HB3	1.65	0.79
1:C:321:ASN:O	1:C:323:PRO:HD3	1.82	0.78
1:A:503:ASP:OD1	1:A:504:GLU:HG2	1.83	0.78
2:D:59:LEU:HD22	2:D:106:VAL:HG13	1.63	0.78
1:A:78:PRO:HG2	1:A:365:SER:HB3	1.66	0.77
2:D:12:ILE:HG12	2:D:63:ILE:HB	1.67	0.77
2:B:65:CYS:HB3	2:B:70:LEU:HB2	1.67	0.77
2:D:25:VAL:HG22	2:D:95:HIS:O	1.84	0.76
1:A:530:VAL:O	1:A:534:LEU:HD23	1.84	0.76
1:C:102:ASN:HB2	1:C:241:ASN:OD1	1.84	0.76
1:C:407:ARG:HG2	1:C:407:ARG:NH2	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423:ILE:HG21	1:C:540:VAL:CG2	2.15	0.76
1:C:201:VAL:HG22	1:C:243:SER:HB3	1.67	0.76
2:D:16:ASP:HB3	2:D:67:ARG:HE	1.51	0.76
1:A:545:ASN:HB3	1:A:547:ARG:HG3	1.66	0.75
1:A:72:ARG:NE	1:A:602:TRP:HB2	2.00	0.75
1:A:338:SER:O	1:A:449:GLU:HG3	1.86	0.75
1:C:40:ILE:HD13	1:C:43:THR:HG21	1.69	0.75
1:C:118:THR:HB	1:C:119:PRO:HD2	1.68	0.75
1:C:409:LEU:HD23	1:C:410:ALA:N	2.01	0.75
1:C:203:VAL:HG23	1:C:206:LYS:HG3	1.68	0.74
1:C:23:GLU:CD	1:C:23:GLU:H	1.89	0.74
1:A:193:LEU:HD12	1:A:193:LEU:H	1.52	0.74
1:A:515:GLU:HG3	1:C:515:GLU:HG2	1.68	0.74
1:C:285:MET:HE2	1:C:334:ALA:H	1.50	0.74
1:A:490:PRO:O	1:A:493:VAL:HG22	1.87	0.74
1:A:47:VAL:HG21	1:A:376:GLU:HG2	1.69	0.74
1:C:285:MET:HG2	1:C:334:ALA:HB3	1.68	0.74
1:A:223:LEU:HD12	1:A:228:THR:HA	1.69	0.73
1:A:367:ARG:O	1:A:369:GLN:N	2.21	0.73
1:A:152:LEU:CD2	1:A:158:ILE:HG13	2.19	0.73
1:C:347:LEU:HD12	1:C:347:LEU:N	2.04	0.73
2:D:34:ILE:HD11	2:D:107:LYS:HD3	1.70	0.73
1:A:7:ILE:HD13	1:A:50:ILE:HG23	1.70	0.72
1:C:186:LEU:HG	1:C:187:TYR:CD1	2.23	0.72
1:C:267:LEU:HB2	1:C:296:ASN:O	1.88	0.72
1:C:170:LEU:HD11	2:D:96:ARG:HH12	1.54	0.72
1:C:366:ASP:O	1:C:368:LEU:HD22	1.89	0.72
1:A:242:ARG:HG3	1:A:242:ARG:NH2	1.95	0.72
1:A:135:VAL:HG21	1:A:144:ILE:HG21	1.70	0.72
1:A:437:GLY:HA2	1:A:441:MET:HG3	1.71	0.72
1:C:285:MET:CE	1:C:333:LEU:HD12	2.20	0.72
1:A:425:ASN:HB3	1:A:427:LYS:HE3	1.71	0.72
1:C:40:ILE:CD1	1:C:43:THR:HG21	2.19	0.72
2:D:18:CYS:HB3	2:D:67:ARG:HG3	1.69	0.72
1:A:18:LEU:HD12	1:A:19:ALA:H	1.54	0.71
1:A:72:ARG:HH11	1:A:72:ARG:HG2	1.55	0.71
1:C:88:ILE:CD1	1:C:278:ALA:HB1	2.20	0.71
1:C:456:TYR:O	1:C:460:GLU:HG3	1.89	0.71
2:B:59:LEU:HD23	2:B:106:VAL:CG1	2.20	0.71
1:C:322:LYS:CB	1:C:326:GLU:HG3	2.19	0.71
1:C:306:GLY:HA2	1:C:309:LEU:HB2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:572:LEU:HB3	1:C:577:LEU:CD1	2.21	0.71
2:D:70:LEU:HD23	2:D:86:LEU:HB3	1.73	0.71
2:B:8:PRO:HB2	2:B:59:LEU:CD1	2.19	0.70
1:C:435:LEU:HD23	1:C:535:ARG:HH21	1.56	0.70
1:C:91:THR:HB	1:C:343:VAL:HG12	1.72	0.70
1:C:526:GLU:HG2	1:C:567:LEU:CD2	2.21	0.70
1:A:515:GLU:HB2	1:A:516:LYS:CE	2.21	0.70
1:C:157:GLN:H	1:C:157:GLN:NE2	1.89	0.70
1:A:427:LYS:HE3	1:A:427:LYS:H	1.55	0.70
1:C:490:PRO:O	1:C:493:VAL:HG22	1.91	0.70
1:A:249:THR:HB	1:A:250:PRO:HD2	1.74	0.70
1:C:144:ILE:O	1:C:148:ILE:HG13	1.92	0.70
2:B:105:LEU:HD13	2:B:111:PHE:HZ	1.57	0.69
1:C:40:ILE:O	1:C:43:THR:HG23	1.91	0.69
1:C:111:LEU:HD21	1:C:210:THR:HG21	1.74	0.69
1:C:268:ALA:CB	1:C:294:LEU:HD23	2.23	0.69
1:C:341:VAL:HB	1:C:354:GLU:HG3	1.72	0.69
1:A:555:VAL:HA	1:A:590:PRO:HB2	1.75	0.69
1:A:121:GLU:O	1:A:125:ARG:HB2	1.93	0.68
1:A:169:VAL:HG12	1:A:173:ASN:HD21	1.58	0.68
1:A:180:PRO:HB2	1:A:199:ILE:HD13	1.74	0.68
1:A:423:ILE:HD12	1:A:424:ILE:N	2.09	0.68
1:A:545:ASN:C	1:A:547:ARG:H	1.94	0.68
1:C:83:VAL:HB	1:C:360:ALA:HB2	1.75	0.68
1:C:125:ARG:HG3	1:C:126:PRO:CD	2.11	0.68
1:C:170:LEU:HD11	2:D:96:ARG:NH1	2.08	0.68
1:C:170:LEU:HD23	2:D:30:GLU:OE2	1.93	0.68
1:A:189:ASP:OD2	1:A:190:ARG:N	2.26	0.68
2:D:112:ARG:O	2:D:113:ASP:HB2	1.92	0.68
2:D:65:CYS:HB3	2:D:70:LEU:CB	2.22	0.68
1:A:513:ALA:HB3	1:A:516:LYS:HD2	1.76	0.68
2:D:71:VAL:HG13	2:D:84:PHE:O	1.93	0.68
1:A:425:ASN:HD22	1:A:429:ASP:HB3	1.57	0.68
1:A:44:LEU:HD12	1:A:373:ILE:HG12	1.76	0.68
1:A:556:GLY:O	1:A:559:SER:HB2	1.94	0.68
1:C:125:ARG:CG	1:C:126:PRO:HD2	2.11	0.67
1:C:262:GLY:C	1:C:263:ASN:HD22	1.97	0.67
1:C:74:ASN:HD21	1:C:391:GLU:HA	1.59	0.67
1:C:450:LEU:HB3	1:C:452:LEU:CD1	2.25	0.67
1:C:223:LEU:HD12	1:C:231:ILE:HD13	1.75	0.67
1:C:469:VAL:HG23	1:C:496:ARG:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ASN:H	1:A:300:GLU:CG	2.07	0.67
1:C:285:MET:HE1	1:C:333:LEU:HA	1.76	0.67
1:A:170:LEU:HD22	2:B:27:LEU:HD22	1.77	0.67
1:C:526:GLU:HG2	1:C:567:LEU:HD22	1.76	0.67
1:A:427:LYS:HB2	1:A:427:LYS:NZ	2.09	0.66
1:A:91:THR:HB	1:A:343:VAL:HG22	1.77	0.66
1:A:427:LYS:HZ1	1:A:428:GLY:N	1.93	0.66
1:C:114:GLY:O	1:C:196:LEU:HD23	1.96	0.66
1:C:521:ARG:O	1:C:525:LYS:HG3	1.94	0.66
1:C:309:LEU:O	1:C:312:VAL:HG12	1.95	0.66
1:A:221:PHE:HB3	1:A:223:LEU:HD23	1.76	0.66
1:C:424:ILE:HG13	1:C:429:ASP:O	1.95	0.66
1:A:164:GLN:HG3	1:A:188:ILE:HB	1.78	0.66
1:A:230:ASN:O	1:A:233:PRO:HD2	1.95	0.66
1:A:585:ARG:NH1	1:A:596:THR:OG1	2.29	0.66
1:C:135:VAL:HG21	1:C:144:ILE:HG12	1.77	0.66
2:B:70:LEU:HD23	2:B:86:LEU:HB3	1.76	0.66
2:B:74:TYR:HB3	2:B:77:LEU:HD12	1.76	0.66
1:A:201:VAL:HG22	1:A:243:SER:HB3	1.77	0.65
1:C:298:THR:CG2	1:C:313:ARG:NH1	2.59	0.65
1:A:167:ASP:HA	1:A:170:LEU:HD12	1.77	0.65
1:C:316:MET:SD	1:C:365:SER:HB2	2.35	0.65
1:A:425:ASN:HB3	1:A:427:LYS:CE	2.26	0.65
1:C:89:THR:HG22	1:C:258:ALA:HA	1.79	0.65
1:C:285:MET:CE	1:C:334:ALA:H	2.09	0.65
1:C:115:ILE:HB	1:C:131:TYR:HD2	1.61	0.65
1:C:487:THR:HB	1:C:488:PRO:HD2	1.79	0.65
1:A:263:ASN:H	1:A:300:GLU:HG2	1.62	0.64
1:C:257:ARG:HD3	1:C:257:ARG:N	2.11	0.64
1:A:148:ILE:HG23	1:A:158:ILE:HD12	1.79	0.64
1:A:72:ARG:HG2	1:A:72:ARG:NH1	2.12	0.64
1:C:3:TYR:CE1	1:C:20:THR:HG22	2.33	0.64
1:C:161:VAL:HG12	1:C:162:ILE:N	2.13	0.64
1:C:203:VAL:CG2	1:C:206:LYS:HG3	2.28	0.64
1:C:320:THR:HA	1:C:367:ARG:HH21	1.61	0.64
1:A:575:TYR:HB2	1:A:577:LEU:HD21	1.79	0.63
2:B:70:LEU:CD2	2:B:86:LEU:HB3	2.27	0.63
1:C:40:ILE:HD12	1:C:40:ILE:N	2.13	0.63
1:A:262:GLY:HA2	1:A:300:GLU:HG3	1.80	0.63
1:C:203:VAL:HG23	1:C:206:LYS:CG	2.28	0.63
1:C:522:ARG:HG2	1:C:522:ARG:HH21	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:LEU:HD23	1:A:410:ALA:N	2.13	0.63
2:B:65:CYS:HB3	2:B:70:LEU:CB	2.28	0.63
1:C:550:PRO:HG2	1:C:551:PHE:HD2	1.63	0.63
1:A:515:GLU:HB2	1:A:516:LYS:NZ	2.14	0.62
1:C:132:ILE:HD11	1:C:197:ALA:O	1.99	0.62
1:A:274:ARG:HG2	1:A:275:VAL:N	2.13	0.62
1:C:77:THR:HG22	1:C:79:VAL:HG23	1.80	0.62
1:C:263:ASN:O	1:C:264:LEU:HD23	2.00	0.62
1:C:224:SER:OG	1:C:227:GLU:HG2	1.99	0.62
1:A:137:SER:HG	1:A:164:GLN:CD	2.01	0.62
1:C:316:MET:HA	1:C:319:LEU:HD12	1.80	0.62
2:D:59:LEU:HD22	2:D:106:VAL:CG1	2.28	0.62
1:A:425:ASN:HB2	1:A:429:ASP:CB	2.30	0.62
2:B:104:ARG:HG3	2:B:109:ILE:HG13	1.81	0.62
1:A:217:ILE:HB	1:A:231:ILE:HD12	1.82	0.62
1:C:377:ILE:HB	1:C:385:VAL:HG21	1.81	0.61
1:C:435:LEU:HD12	1:C:435:LEU:N	2.15	0.61
1:A:193:LEU:HD12	1:A:193:LEU:N	2.15	0.61
1:A:224:SER:HB3	1:A:227:GLU:HG2	1.82	0.61
1:C:148:ILE:HG23	1:C:158:ILE:HD13	1.82	0.61
1:A:83:VAL:HG12	1:A:360:ALA:HB2	1.82	0.61
1:C:195:MET:HE1	1:C:250:PRO:HD2	1.82	0.61
1:C:467:ALA:CB	1:C:475:LEU:HD13	2.27	0.61
1:C:513:ALA:HB3	1:C:516:LYS:HG3	1.82	0.61
1:C:187:TYR:HB3	1:C:190:ARG:HG3	1.81	0.61
1:C:257:ARG:HH21	1:C:259:ILE:CG2	2.14	0.61
1:A:74:ASN:HD22	1:A:391:GLU:CD	2.04	0.61
1:A:425:ASN:HD22	1:A:429:ASP:CB	2.14	0.61
1:C:298:THR:HG21	1:C:313:ARG:NH1	2.16	0.61
1:A:228:THR:O	1:A:231:ILE:HG12	2.00	0.61
1:C:88:ILE:HD13	1:C:278:ALA:CB	2.30	0.61
1:C:332:LEU:HD23	1:C:332:LEU:H	1.65	0.60
1:C:103:PRO:O	1:C:106:PRO:HD3	2.00	0.60
1:C:167:ASP:HA	1:C:170:LEU:HD12	1.83	0.60
2:D:15:ILE:HD12	2:D:65:CYS:O	2.01	0.60
1:A:115:ILE:HB	1:A:131:TYR:HD2	1.66	0.60
1:A:169:VAL:HB	2:B:31:GLU:OE2	2.01	0.60
1:C:4:ILE:HD13	1:C:4:ILE:N	2.17	0.60
1:C:228:THR:O	1:C:231:ILE:HG12	2.00	0.60
2:B:21:LEU:HB3	2:B:88:HIS:CD2	2.37	0.60
1:A:310:GLU:OE2	1:A:313:ARG:HD2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LEU:HD23	2:B:30:GLU:OE1	2.02	0.60
1:C:161:VAL:HB	1:C:181:ILE:HG12	1.84	0.60
1:A:261:ALA:HB1	1:A:277:VAL:HB	1.83	0.60
1:A:427:LYS:HZ1	1:A:428:GLY:H	1.50	0.60
1:A:180:PRO:HB2	1:A:199:ILE:CD1	2.32	0.60
1:A:482:VAL:HG12	1:A:483:GLN:N	2.16	0.60
1:C:3:TYR:HE1	1:C:20:THR:HG22	1.67	0.60
1:C:200:GLU:OE2	1:C:210:THR:HB	2.02	0.60
1:C:298:THR:CG2	1:C:313:ARG:HH12	2.15	0.60
1:C:380:LYS:HB3	1:C:381:LEU:HD23	1.83	0.60
1:A:164:GLN:HA	1:A:185:VAL:O	2.02	0.59
1:A:293:ARG:HH21	1:A:539:GLN:HE22	1.49	0.59
2:B:18:CYS:O	2:B:21:LEU:HD13	2.02	0.59
1:C:157:GLN:HE21	1:C:157:GLN:N	1.97	0.59
2:D:73:HIS:CD2	2:D:82:PRO:HB3	2.37	0.59
1:A:208:ILE:O	1:A:208:ILE:HG13	2.01	0.59
2:B:4:ASN:O	2:B:5:HIS:HB2	2.02	0.59
1:C:447:ALA:HB2	1:C:458:ALA:HB2	1.83	0.59
1:A:118:THR:HB	1:A:119:PRO:HD2	1.82	0.59
1:C:545:ASN:C	1:C:547:ARG:N	2.55	0.59
1:A:280:GLY:O	1:A:284:ILE:HG13	2.01	0.59
1:C:447:ALA:HB2	1:C:458:ALA:CB	2.33	0.59
1:C:572:LEU:CB	1:C:577:LEU:HD11	2.30	0.59
1:A:259:ILE:HB	1:A:260:PRO:HD2	1.84	0.59
1:A:410:ALA:HB2	1:A:423:ILE:HD13	1.82	0.59
1:A:18:LEU:HD12	1:A:19:ALA:N	2.15	0.59
1:A:22:ASP:OD2	1:A:24:ALA:HB3	2.03	0.59
2:B:78:PRO:HG2	2:B:81:ALA:HB3	1.84	0.59
1:A:425:ASN:HB2	1:A:429:ASP:HB2	1.84	0.59
1:A:596:THR:O	1:A:600:LEU:HD23	2.03	0.59
2:B:46:VAL:HG13	2:B:47:VAL:H	1.68	0.59
1:C:119:PRO:HG2	1:C:139:PHE:CZ	2.38	0.59
1:C:545:ASN:C	1:C:547:ARG:H	2.05	0.59
1:C:550:PRO:HG2	1:C:551:PHE:CD2	2.37	0.59
1:C:572:LEU:HD22	1:C:577:LEU:CD2	2.31	0.59
1:A:267:LEU:N	1:A:267:LEU:HD12	2.17	0.59
1:A:475:LEU:HD12	1:A:476:ARG:N	2.18	0.59
2:B:63:ILE:CD1	2:B:72:VAL:HA	2.32	0.59
1:C:220:VAL:HG23	1:C:221:PHE:CD2	2.38	0.59
1:A:125:ARG:HG2	1:A:131:TYR:CZ	2.38	0.58
1:A:34:LEU:C	1:A:34:LEU:HD12	2.24	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:LYS:HE2	2:B:109:ILE:HD11	1.85	0.58
1:C:378:GLU:HG3	1:C:385:VAL:HG23	1.85	0.58
1:C:489:LEU:HB3	1:C:490:PRO:HD2	1.84	0.58
1:A:99:ILE:HB	1:A:245:VAL:HB	1.85	0.58
1:A:4:ILE:HD12	1:A:70:LEU:HD23	1.85	0.58
1:A:425:ASN:CB	1:A:426:PRO:HD2	2.33	0.58
1:C:115:ILE:HD12	1:C:130:PRO:O	2.03	0.58
1:C:513:ALA:O	1:C:517:VAL:HG23	2.02	0.58
1:C:522:ARG:HG2	1:C:522:ARG:NH2	2.19	0.58
1:A:19:ALA:HB1	1:A:27:LEU:CD1	2.34	0.58
1:A:3:TYR:CZ	1:A:63:ILE:HG21	2.39	0.58
1:A:83:VAL:HG12	1:A:360:ALA:CB	2.33	0.58
2:D:16:ASP:CB	2:D:67:ARG:HE	2.16	0.58
2:D:34:ILE:HD11	2:D:107:LYS:CD	2.34	0.58
1:A:218:ALA:HA	1:A:223:LEU:HB2	1.86	0.58
1:C:99:ILE:HB	1:C:245:VAL:HB	1.85	0.58
1:A:161:VAL:HG12	1:A:162:ILE:N	2.16	0.58
1:C:479:ASP:OD1	1:C:481:SER:HB3	2.03	0.58
2:D:54:ALA:N	2:D:62:GLY:HA3	2.19	0.58
1:A:27:LEU:HD21	1:A:602:TRP:HZ3	1.68	0.58
1:A:314:GLN:HB3	1:A:318:GLU:OE2	2.04	0.58
2:B:8:PRO:CB	2:B:59:LEU:HD11	2.30	0.58
2:B:22:TRP:NE1	2:B:65:CYS:HB2	2.19	0.58
1:C:3:TYR:C	1:C:4:ILE:HD13	2.24	0.58
1:A:103:PRO:O	1:A:106:PRO:HD3	2.04	0.57
1:A:186:LEU:HD13	1:A:187:TYR:CE1	2.39	0.57
1:A:492:ALA:O	1:A:496:ARG:HD2	2.04	0.57
1:C:91:THR:O	1:C:343:VAL:HG12	2.03	0.57
1:C:316:MET:HA	1:C:319:LEU:CG	2.35	0.57
1:C:515:GLU:CD	1:C:515:GLU:H	2.06	0.57
1:A:54:LEU:HD13	1:A:381:LEU:HD11	1.86	0.57
1:C:1:MET:HE3	1:C:2:ARG:N	2.20	0.57
1:A:127:ALA:HA	1:A:156:TYR:CD1	2.39	0.57
2:D:14:VAL:HG11	2:D:19:ASP:HB3	1.85	0.57
1:A:332:LEU:HD12	1:A:359:ILE:CG2	2.35	0.57
1:A:427:LYS:HB2	1:A:427:LYS:HZ2	1.67	0.57
1:C:584:ILE:HG12	1:C:593:ALA:HA	1.86	0.57
2:D:70:LEU:CD2	2:D:86:LEU:HB3	2.34	0.57
1:A:522:ARG:HH21	1:A:522:ARG:HG2	1.70	0.57
1:A:522:ARG:NH2	1:A:563:GLU:HG2	2.17	0.57
1:C:411:ILE:HG22	1:C:553:VAL:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ASP:OD1	1:A:26:ALA:HB3	2.05	0.57
1:C:149:ASN:HD21	1:C:175:LEU:HA	1.69	0.57
1:C:228:THR:HG23	1:C:231:ILE:HD11	1.86	0.57
1:C:351:PHE:HD1	1:C:352:SER:N	2.03	0.57
1:A:564:VAL:O	1:A:568:VAL:HG23	2.04	0.56
1:C:54:LEU:O	1:C:57:VAL:HG12	2.05	0.56
1:C:320:THR:HA	1:C:367:ARG:NH2	2.19	0.56
1:C:83:VAL:HG23	1:C:359:ILE:C	2.25	0.56
1:C:322:LYS:HB3	1:C:326:GLU:CG	2.27	0.56
1:A:405:THR:HB	1:A:409:LEU:HD12	1.86	0.56
2:B:32:GLU:OE2	2:B:104:ARG:NH2	2.38	0.56
1:C:132:ILE:HD12	1:C:197:ALA:HB3	1.87	0.56
1:C:170:LEU:CD1	2:D:96:ARG:HH12	2.18	0.56
1:C:316:MET:HG3	1:C:327:ILE:HD12	1.88	0.56
1:C:415:GLY:O	1:C:438:ALA:HB1	2.05	0.56
2:D:51:TRP:HB2	2:D:73:HIS:CD2	2.40	0.56
1:A:168:GLY:HA3	1:A:183:ASP:OD1	2.05	0.56
2:B:46:VAL:HG13	2:B:47:VAL:N	2.20	0.56
1:C:195:MET:HE3	1:C:249:THR:HG22	1.87	0.56
1:A:394:ALA:O	1:A:597:GLY:HA3	2.06	0.56
1:C:444:MET:HG3	1:C:455:ARG:NH1	2.20	0.56
1:C:569:THR:O	1:C:573:ALA:HB2	2.05	0.56
1:A:52:GLU:O	1:A:56:LEU:HG	2.05	0.56
1:A:119:PRO:HG2	1:A:139:PHE:CZ	2.40	0.56
1:C:490:PRO:HG2	1:C:493:VAL:HG13	1.87	0.56
1:A:296:ASN:HD21	1:A:298:THR:HG23	1.71	0.56
1:C:257:ARG:HE	1:C:259:ILE:CG2	2.19	0.56
1:A:487:THR:CG2	1:A:488:PRO:HD2	2.34	0.55
1:C:135:VAL:CG2	1:C:144:ILE:HG12	2.35	0.55
1:C:545:ASN:HB3	1:C:547:ARG:CG	2.36	0.55
1:A:415:GLY:O	1:A:438:ALA:HB1	2.07	0.55
2:B:100:ASN:OD1	2:B:112:ARG:NH2	2.40	0.55
1:C:377:ILE:HG23	1:C:381:LEU:HD11	1.88	0.55
2:D:93:GLN:HA	2:D:93:GLN:NE2	2.21	0.55
1:A:457:LEU:O	1:A:461:ILE:HG13	2.06	0.55
1:A:578:VAL:HG22	1:C:232:VAL:HG21	1.88	0.55
1:C:164:GLN:HA	1:C:185:VAL:O	2.05	0.55
2:D:69:MET:HB2	2:D:86:LEU:O	2.07	0.55
2:D:104:ARG:NH2	2:D:112:ARG:HB2	2.22	0.55
1:A:199:ILE:HG23	1:A:199:ILE:O	2.06	0.55
1:A:423:ILE:HD12	1:A:424:ILE:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:LEU:HD23	1:C:381:LEU:N	2.21	0.55
1:C:534:LEU:O	1:C:538:ARG:HB2	2.05	0.55
1:A:564:VAL:N	1:A:565:PRO:HD2	2.22	0.55
2:B:50:ALA:CB	2:B:71:VAL:HG23	2.36	0.55
1:A:238:LEU:O	1:A:241:ASN:ND2	2.40	0.55
2:B:104:ARG:HG3	2:B:109:ILE:CD1	2.37	0.55
1:C:78:PRO:HG2	1:C:365:SER:HB3	1.87	0.55
1:A:274:ARG:HG2	1:A:275:VAL:H	1.71	0.55
1:A:584:ILE:N	1:A:584:ILE:CD1	2.70	0.55
1:C:565:PRO:HG2	1:C:581:ARG:HH21	1.72	0.55
1:A:515:GLU:CD	1:A:515:GLU:H	2.10	0.54
1:C:132:ILE:CD1	1:C:197:ALA:HB3	2.36	0.54
1:C:262:GLY:O	1:C:277:VAL:HB	2.07	0.54
1:A:83:VAL:HG11	1:A:441:MET:HG2	1.89	0.54
1:C:223:LEU:CD1	1:C:231:ILE:HD13	2.36	0.54
1:C:111:LEU:CD2	1:C:210:THR:HG21	2.37	0.54
2:D:78:PRO:HG2	2:D:81:ALA:HB3	1.90	0.54
1:A:188:ILE:HG23	1:A:189:ASP:N	2.23	0.54
1:C:409:LEU:HD23	1:C:409:LEU:C	2.27	0.54
1:C:259:ILE:HB	1:C:260:PRO:CD	2.34	0.54
1:C:483:GLN:NE2	1:C:485:PHE:HE2	2.06	0.54
1:C:564:VAL:O	1:C:568:VAL:HG23	2.07	0.54
1:A:115:ILE:H	1:A:131:TYR:HA	1.73	0.54
1:A:195:MET:HE1	1:A:250:PRO:HD3	1.90	0.54
1:A:545:ASN:C	1:A:547:ARG:N	2.61	0.54
1:A:305:ILE:CG2	1:A:359:ILE:HD12	2.38	0.54
1:C:257:ARG:HH21	1:C:259:ILE:HG22	1.71	0.54
1:C:316:MET:HA	1:C:319:LEU:CD1	2.37	0.54
1:A:569:THR:O	1:A:573:ALA:HB2	2.08	0.54
1:C:221:PHE:HB3	1:C:223:LEU:HD23	1.88	0.54
1:C:257:ARG:HE	1:C:259:ILE:HG22	1.72	0.54
1:C:266:LEU:CA	1:C:297:VAL:HG22	2.37	0.54
1:C:269:GLN:HG2	1:C:270:GLY:H	1.72	0.54
1:C:473:PHE:CE2	2:D:76:ASN:HB3	2.43	0.54
1:C:234:MET:SD	1:C:246:VAL:HG22	2.47	0.54
1:A:435:LEU:HD12	1:A:435:LEU:N	2.23	0.53
1:A:474:HIS:HB2	1:A:483:GLN:O	2.08	0.53
2:B:73:HIS:HD2	2:B:74:TYR:H	1.56	0.53
1:C:9:ILE:HD11	1:C:50:ILE:HD11	1.89	0.53
1:A:396:ILE:O	1:A:400:LEU:HD12	2.07	0.53
1:C:323:PRO:O	1:C:326:GLU:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:PRO:O	1:C:325:SER:N	2.41	0.53
1:C:8:ASP:OD2	1:C:594:VAL:HB	2.08	0.53
1:C:217:ILE:HB	1:C:231:ILE:HD12	1.90	0.53
2:B:21:LEU:N	2:B:21:LEU:HD12	2.23	0.53
2:B:107:LYS:HE2	2:B:109:ILE:CD1	2.38	0.53
1:C:165:ARG:O	1:C:183:ASP:HB2	2.08	0.53
1:C:288:VAL:CG1	1:C:332:LEU:HD21	2.39	0.53
1:A:40:ILE:N	1:A:40:ILE:HD12	2.24	0.53
1:C:91:THR:HB	1:C:343:VAL:CG1	2.38	0.53
1:C:253:ASP:OD2	1:C:255:LYS:HE3	2.07	0.53
1:C:320:THR:HG22	1:C:367:ARG:HD2	1.89	0.53
1:C:377:ILE:CG2	1:C:381:LEU:HD11	2.39	0.53
1:C:541:SER:O	1:C:542:PRO:C	2.47	0.53
1:A:545:ASN:O	1:A:547:ARG:N	2.42	0.53
1:C:266:LEU:HD12	1:C:266:LEU:N	2.24	0.53
1:A:425:ASN:HB3	1:A:426:PRO:HD2	1.91	0.53
1:A:482:VAL:CG1	1:A:483:GLN:N	2.71	0.53
1:A:101:HIS:CG	1:A:348:ALA:HB1	2.44	0.53
1:A:261:ALA:CB	1:A:277:VAL:HB	2.39	0.53
1:A:575:TYR:HB2	1:A:577:LEU:CD2	2.38	0.53
1:C:6:GLY:O	1:C:16:VAL:HA	2.09	0.53
1:C:115:ILE:HB	1:C:131:TYR:CD2	2.43	0.52
1:C:118:THR:HG23	1:C:193:LEU:HD13	1.91	0.52
1:C:266:LEU:HB3	1:C:294:LEU:HD22	1.91	0.52
1:C:575:TYR:N	1:C:575:TYR:CD2	2.77	0.52
1:A:560:LEU:HA	1:A:581:ARG:NH1	2.24	0.52
1:A:464:TYR:CE1	1:A:501:LYS:HD2	2.44	0.52
1:A:575:TYR:CB	1:A:577:LEU:HD21	2.39	0.52
2:B:73:HIS:CD2	2:B:74:TYR:H	2.28	0.52
1:C:83:VAL:HB	1:C:360:ALA:CB	2.38	0.52
1:C:255:LYS:H	1:C:255:LYS:HZ2	1.57	0.52
2:D:12:ILE:HA	2:D:63:ILE:O	2.09	0.52
2:B:15:ILE:HD12	2:B:15:ILE:N	2.25	0.52
1:C:157:GLN:HG2	1:C:157:GLN:O	2.09	0.52
1:C:261:ALA:CB	1:C:278:ALA:HB2	2.40	0.52
1:C:369:GLN:HG2	1:C:372:MET:CE	2.39	0.52
1:C:141:PHE:O	1:C:144:ILE:HG22	2.08	0.52
1:C:221:PHE:HB3	1:C:223:LEU:CD2	2.40	0.52
1:C:498:CYS:HB2	1:C:505:LEU:HD22	1.91	0.52
1:A:333:LEU:O	1:A:359:ILE:HA	2.09	0.52
1:A:499:VAL:HB	1:A:506:VAL:HB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:TYR:CD2	1:A:575:TYR:N	2.78	0.52
1:C:295:ASP:O	1:C:296:ASN:HB2	2.10	0.52
2:D:5:HIS:CG	2:D:6:SER:H	2.28	0.52
1:A:263:ASN:H	1:A:300:GLU:HG3	1.75	0.52
1:C:457:LEU:O	1:C:461:ILE:HG13	2.09	0.52
1:C:115:ILE:H	1:C:131:TYR:HA	1.74	0.52
1:C:121:GLU:O	1:C:125:ARG:HB2	2.10	0.52
1:C:191:ILE:O	1:C:193:LEU:HD23	2.10	0.52
1:A:221:PHE:CB	1:A:223:LEU:HD23	2.40	0.51
1:A:261:ALA:HB2	1:A:278:ALA:HB2	1.92	0.51
1:C:334:ALA:HA	1:C:359:ILE:HD13	1.92	0.51
1:C:407:ARG:NH2	1:C:407:ARG:CG	2.70	0.51
1:C:475:LEU:HD12	1:C:476:ARG:N	2.25	0.51
2:D:34:ILE:CG1	2:D:103:ALA:HB1	2.41	0.51
1:A:119:PRO:O	1:A:122:LEU:HB2	2.11	0.51
1:A:444:MET:HG3	1:A:455:ARG:HH21	1.75	0.51
1:C:329:ILE:HG12	1:C:363:VAL:HG12	1.92	0.51
1:C:330:GLN:NE2	1:C:364:LYS:HE2	2.25	0.51
1:A:50:ILE:HD13	1:A:377:ILE:HD11	1.93	0.51
1:A:518:ARG:HH11	1:A:522:ARG:HD2	1.75	0.51
1:C:178:PRO:O	1:C:179:LEU:HD12	2.11	0.51
1:C:518:ARG:HG3	1:C:521:ARG:NH2	2.25	0.51
1:A:373:ILE:O	1:A:376:GLU:N	2.43	0.51
1:A:403:PRO:HG3	1:C:219:THR:OG1	2.11	0.51
1:A:475:LEU:HD12	1:A:475:LEU:C	2.31	0.51
1:C:73:ILE:HD11	1:C:377:ILE:CD1	2.41	0.51
1:C:126:PRO:HB2	1:C:128:ASP:OD1	2.11	0.51
1:C:340:PRO:HA	1:C:352:SER:O	2.10	0.51
1:C:395:ALA:HB1	1:C:411:ILE:CD1	2.38	0.51
1:C:414:LEU:HB2	1:C:558:SER:HB2	1.92	0.51
2:D:101:ASN:HA	2:D:104:ARG:HB2	1.92	0.51
1:A:447:ALA:HB2	1:A:458:ALA:CB	2.41	0.51
2:B:73:HIS:CD2	2:B:82:PRO:HA	2.45	0.51
1:C:27:LEU:HB2	1:C:603:HIS:CD2	2.46	0.51
1:A:381:LEU:HB3	1:A:383:ILE:HD12	1.93	0.51
2:B:22:TRP:HD1	2:B:65:CYS:HG	1.58	0.51
2:B:24:GLU:O	2:B:96:ARG:HD3	2.11	0.51
1:C:288:VAL:HG11	1:C:332:LEU:HD21	1.93	0.51
1:A:9:ILE:O	1:A:41:LYS:HG3	2.10	0.51
1:A:72:ARG:HE	1:A:602:TRP:HB2	1.71	0.51
1:A:152:LEU:HD23	1:A:158:ILE:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:THR:OG1	1:A:322:LYS:HG3	2.11	0.51
1:C:312:VAL:HG13	1:C:313:ARG:N	2.26	0.51
1:C:341:VAL:HG12	1:C:342:SER:O	2.10	0.51
1:A:6:GLY:O	1:A:16:VAL:HA	2.10	0.51
1:A:555:VAL:HG12	1:A:590:PRO:HA	1.92	0.51
1:C:157:GLN:NE2	1:C:157:GLN:N	2.56	0.51
1:C:316:MET:SD	1:C:319:LEU:HD12	2.51	0.51
1:C:407:ARG:H	1:C:407:ARG:HD2	1.74	0.51
1:C:378:GLU:CG	1:C:385:VAL:H	2.24	0.51
1:A:187:TYR:CD1	1:A:187:TYR:N	2.79	0.50
2:B:50:ALA:O	2:B:53:ALA:HB3	2.12	0.50
1:C:361:SER:HA	1:C:436:ALA:CB	2.41	0.50
1:C:526:GLU:HG2	1:C:567:LEU:HD21	1.91	0.50
1:C:539:GLN:HB2	1:C:540:VAL:HG13	1.93	0.50
1:C:591:ARG:HH11	1:C:591:ARG:HB3	1.76	0.50
2:D:15:ILE:HG23	2:D:43:ALA:HA	1.93	0.50
1:A:7:ILE:HD13	1:A:50:ILE:CG2	2.39	0.50
1:A:347:LEU:N	1:A:347:LEU:HD23	2.26	0.50
1:C:316:MET:HB2	1:C:363:VAL:HG21	1.91	0.50
1:C:93:ILE:O	1:C:345:GLY:HA3	2.11	0.50
1:C:396:ILE:HD13	1:C:424:ILE:HB	1.93	0.50
1:C:514:LEU:HD23	1:C:514:LEU:O	2.11	0.50
1:C:588:GLU:OE1	1:C:588:GLU:HA	2.10	0.50
2:D:105:LEU:HD13	2:D:111:PHE:HZ	1.77	0.50
1:A:164:GLN:CG	1:A:188:ILE:HB	2.41	0.50
1:A:405:THR:HB	1:A:409:LEU:CD1	2.42	0.50
1:A:546:ILE:HG13	1:A:546:ILE:O	2.11	0.50
1:C:1:MET:HE3	1:C:2:ARG:H	1.76	0.50
1:C:73:ILE:HG22	1:C:74:ASN:N	2.26	0.50
1:C:92:ILE:HD11	1:C:257:ARG:NH1	2.27	0.50
1:C:277:VAL:HG21	1:C:305:ILE:HD13	1.93	0.50
1:C:329:ILE:HG23	1:C:362:MET:O	2.12	0.50
1:A:192:PRO:HG2	1:A:247:VAL:HG11	1.93	0.50
1:A:549:ILE:N	1:A:549:ILE:HD12	2.25	0.50
1:A:573:ALA:HB1	1:C:236:ARG:NH1	2.26	0.50
1:C:424:ILE:HG12	1:C:425:ASN:O	2.12	0.50
1:A:293:ARG:HE	1:A:539:GLN:HE22	1.59	0.50
1:A:584:ILE:N	1:A:584:ILE:HD12	2.25	0.50
2:B:91:ASP:O	2:B:95:HIS:HD2	1.94	0.50
1:A:7:ILE:HD11	1:A:54:LEU:HG	1.93	0.50
1:A:327:ILE:CG2	1:A:363:VAL:HG21	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:GLY:O	1:A:347:LEU:HD23	2.11	0.50
1:C:73:ILE:HB	1:C:387:ILE:CD1	2.42	0.50
1:C:393:GLU:OE1	1:C:601:SER:HB2	2.11	0.50
1:A:54:LEU:HD13	1:A:381:LEU:CD1	2.41	0.50
1:A:411:ILE:CD1	1:A:422:SER:HB2	2.29	0.50
1:A:467:ALA:CB	1:A:475:LEU:HD13	2.34	0.50
1:A:534:LEU:O	1:A:538:ARG:HB2	2.12	0.49
1:A:604:LYS:NZ	1:A:604:LYS:HB3	2.27	0.49
2:B:54:ALA:N	2:B:62:GLY:HA3	2.27	0.49
1:C:285:MET:HE2	1:C:333:LEU:HD12	1.93	0.49
1:A:288:VAL:C	1:A:290:GLY:H	2.15	0.49
1:A:414:LEU:CB	1:A:558:SER:HB2	2.42	0.49
1:C:73:ILE:HB	1:C:387:ILE:HD13	1.93	0.49
1:A:85:MET:HG3	1:A:86:GLU:N	2.21	0.49
1:A:441:MET:O	1:A:445:ILE:HG13	2.13	0.49
1:C:120:GLN:C	1:C:122:LEU:H	2.14	0.49
1:C:482:VAL:HG12	1:C:483:GLN:N	2.27	0.49
2:B:97:ASN:N	2:B:97:ASN:HD22	2.08	0.49
1:C:86:GLU:OE2	1:C:305:ILE:HG13	2.12	0.49
1:C:351:PHE:CD1	1:C:352:SER:N	2.79	0.49
1:C:397:LEU:HD12	1:C:601:SER:HB3	1.93	0.49
1:A:19:ALA:HB1	1:A:27:LEU:HD11	1.94	0.49
1:A:41:LYS:O	1:A:78:PRO:HA	2.12	0.49
1:A:446:ILE:HD12	1:A:462:LYS:HB2	1.94	0.49
1:A:515:GLU:CD	1:A:515:GLU:N	2.64	0.49
1:A:515:GLU:CG	1:A:516:LYS:NZ	2.75	0.49
1:A:335:VAL:HG11	1:A:527:ARG:HB3	1.95	0.49
1:A:365:SER:OG	1:A:366:ASP:N	2.44	0.49
2:B:104:ARG:CG	2:B:109:ILE:HG13	2.41	0.49
1:C:18:LEU:HB2	1:C:57:VAL:HG21	1.95	0.49
1:A:93:ILE:HD12	1:A:346:GLY:CA	2.42	0.49
1:A:234:MET:O	1:A:238:LEU:HG	2.12	0.49
1:A:319:LEU:HD22	1:A:319:LEU:O	2.12	0.49
1:A:460:GLU:HG2	1:A:501:LYS:HE3	1.95	0.49
2:D:55:ARG:HG2	2:D:75:LYS:HG3	1.94	0.49
1:A:416:ALA:HB1	1:A:440:ASP:OD2	2.12	0.49
1:C:266:LEU:HB3	1:C:294:LEU:CD2	2.43	0.49
1:C:308:MET:HE3	1:C:309:LEU:N	2.28	0.49
1:C:561:ASP:OD1	1:C:562:PHE:N	2.46	0.49
1:A:111:LEU:HD22	1:A:210:THR:HG21	1.93	0.49
1:C:94:THR:HG23	1:C:255:LYS:NZ	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:88:HIS:CG	2:D:89:HIS:N	2.81	0.49
1:A:177:LYS:HG2	1:A:178:PRO:HD2	1.95	0.48
1:C:342:SER:HA	1:C:351:PHE:HA	1.94	0.48
1:C:393:GLU:O	1:C:397:LEU:HG	2.13	0.48
1:A:1:MET:HA	1:A:1:MET:HE2	1.94	0.48
1:A:118:THR:HG23	1:A:193:LEU:HD23	1.95	0.48
1:A:447:ALA:HB2	1:A:458:ALA:HB2	1.94	0.48
2:B:78:PRO:HA	5:B:134:HOH:O	2.13	0.48
1:C:195:MET:CE	1:C:249:THR:HG22	2.43	0.48
1:C:300:GLU:O	1:C:306:GLY:HA3	2.12	0.48
1:A:101:HIS:CE1	1:A:103:PRO:HD3	2.47	0.48
1:A:470:GLU:HB2	1:A:474:HIS:NE2	2.27	0.48
1:C:161:VAL:CG1	1:C:162:ILE:N	2.77	0.48
1:A:27:LEU:HD23	1:A:603:HIS:CD2	2.48	0.48
2:B:63:ILE:HD11	2:B:72:VAL:HG13	1.94	0.48
1:C:249:THR:HB	1:C:250:PRO:HD2	1.95	0.48
1:C:288:VAL:CG2	1:C:332:LEU:HD21	2.43	0.48
1:C:332:LEU:HD23	1:C:332:LEU:N	2.27	0.48
1:C:408:PRO:CB	1:C:426:PRO:HD3	2.38	0.48
2:D:22:TRP:NE1	2:D:65:CYS:HB2	2.28	0.48
2:D:107:LYS:HE3	2:D:109:ILE:HD13	1.95	0.48
1:A:394:ALA:CB	1:A:598:LEU:HD23	2.39	0.48
1:A:522:ARG:HG2	1:A:522:ARG:NH2	2.28	0.48
2:B:12:ILE:HA	2:B:63:ILE:O	2.14	0.48
1:C:472:LEU:HD12	2:D:74:TYR:CD1	2.47	0.48
1:A:195:MET:CE	1:A:250:PRO:HD3	2.44	0.48
1:A:472:LEU:O	1:A:489:LEU:HG	2.14	0.48
2:B:92:SER:O	2:B:95:HIS:HB2	2.13	0.48
1:C:183:ASP:OD2	1:C:184:GLU:HG3	2.14	0.48
1:C:472:LEU:C	1:C:473:PHE:HD1	2.17	0.48
2:D:97:ASN:O	2:D:98:THR:C	2.52	0.48
1:A:50:ILE:O	1:A:54:LEU:HD12	2.13	0.48
1:A:101:HIS:CD2	1:A:348:ALA:HB1	2.49	0.48
1:A:224:SER:O	1:A:226:GLU:N	2.47	0.48
1:C:378:GLU:HG3	1:C:385:VAL:CG2	2.43	0.48
1:A:169:VAL:HG12	1:A:173:ASN:ND2	2.25	0.48
1:A:434:HIS:C	1:A:435:LEU:HD12	2.34	0.48
1:A:581:ARG:HD3	1:A:590:PRO:HG3	1.95	0.48
1:C:75:GLU:OE2	1:C:368:LEU:HB2	2.14	0.48
1:C:572:LEU:HD22	1:C:577:LEU:HD11	1.96	0.48
1:A:161:VAL:CG1	1:A:162:ILE:N	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:ARG:HH11	1:A:591:ARG:CG	2.27	0.47
1:C:301:SER:C	1:C:303:THR:H	2.18	0.47
1:C:331:ASP:CG	1:C:535:ARG:HH22	2.18	0.47
1:C:373:ILE:O	1:C:376:GLU:N	2.47	0.47
2:D:5:HIS:CD2	2:D:6:SER:H	2.32	0.47
1:A:72:ARG:HH11	1:A:72:ARG:CG	2.23	0.47
1:A:267:LEU:HD12	1:A:267:LEU:H	1.79	0.47
2:B:73:HIS:ND1	2:B:82:PRO:HB3	2.29	0.47
1:C:28:THR:O	1:C:30:THR:HG23	2.13	0.47
1:C:366:ASP:N	1:C:366:ASP:OD2	2.46	0.47
1:C:423:ILE:HG13	1:C:549:ILE:HD13	1.96	0.47
1:A:141:PHE:C	1:A:141:PHE:CD2	2.88	0.47
1:A:392:ALA:O	1:A:396:ILE:HG13	2.15	0.47
1:C:120:GLN:C	1:C:122:LEU:N	2.68	0.47
1:C:268:ALA:HB2	1:C:294:LEU:HA	1.96	0.47
1:C:338:SER:OG	1:C:353:LEU:HD13	2.14	0.47
1:C:584:ILE:HG12	1:C:593:ALA:CA	2.44	0.47
1:A:232:VAL:HB	1:A:233:PRO:HD3	1.96	0.47
1:C:257:ARG:NH2	1:C:259:ILE:HG22	2.29	0.47
1:C:474:HIS:HB2	1:C:483:GLN:O	2.15	0.47
1:C:532:ASN:HA	1:C:535:ARG:HB2	1.96	0.47
1:A:414:LEU:HB2	1:A:558:SER:HB2	1.95	0.47
1:A:549:ILE:HD12	1:A:549:ILE:H	1.79	0.47
1:C:232:VAL:CB	1:C:233:PRO:HD3	2.41	0.47
1:C:296:ASN:HB2	1:C:328:PHE:HB3	1.97	0.47
1:A:115:ILE:HB	1:A:131:TYR:CD2	2.49	0.47
1:A:144:ILE:O	1:A:148:ILE:HG13	2.14	0.47
1:A:332:LEU:HD12	1:A:359:ILE:HG23	1.97	0.47
1:A:526:GLU:HA	1:A:530:VAL:HG23	1.96	0.47
1:A:539:GLN:C	1:A:541:SER:H	2.17	0.47
2:B:10:ILE:HG22	2:B:11:ALA:N	2.29	0.47
1:C:19:ALA:HB2	1:C:29:ILE:HG12	1.96	0.47
1:C:575:TYR:N	1:C:575:TYR:HD2	2.12	0.47
1:C:204:PRO:HD3	1:C:242:ARG:NH1	2.30	0.47
1:C:281:ALA:HB1	1:C:334:ALA:HB1	1.96	0.47
1:C:320:THR:O	1:C:322:LYS:N	2.47	0.47
2:D:69:MET:SD	2:D:87:MET:HE1	2.54	0.47
1:A:120:GLN:C	1:A:122:LEU:H	2.18	0.47
1:A:165:ARG:O	1:A:183:ASP:HB2	2.14	0.47
1:A:516:LYS:HE3	1:A:516:LYS:N	2.30	0.47
2:B:97:ASN:O	2:B:98:THR:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LEU:O	1:A:58:ALA:N	2.48	0.47
2:B:59:LEU:N	2:B:59:LEU:HD12	2.30	0.47
1:C:265:GLU:C	1:C:297:VAL:HG13	2.36	0.47
1:C:351:PHE:CD1	1:C:351:PHE:C	2.87	0.47
1:A:91:THR:HG23	1:A:256:ALA:HB2	1.97	0.46
1:C:85:MET:HB2	1:C:357:VAL:O	2.15	0.46
1:C:337:THR:OG1	1:C:356:ALA:HB3	2.15	0.46
1:C:378:GLU:HG2	1:C:383:ILE:O	2.14	0.46
1:C:416:ALA:HB1	1:C:440:ASP:CG	2.35	0.46
1:A:127:ALA:HA	1:A:156:TYR:CE1	2.51	0.46
1:A:262:GLY:CA	1:A:300:GLU:HG3	2.45	0.46
2:B:104:ARG:HG3	2:B:109:ILE:CG1	2.43	0.46
1:A:515:GLU:HG2	1:A:516:LYS:HZ2	1.79	0.46
1:C:208:ILE:O	1:C:208:ILE:HG13	2.13	0.46
1:C:249:THR:O	1:C:250:PRO:C	2.53	0.46
1:C:316:MET:HA	1:C:319:LEU:HG	1.96	0.46
1:C:514:LEU:HD23	1:C:514:LEU:C	2.35	0.46
2:D:34:ILE:HD11	2:D:107:LYS:CG	2.45	0.46
1:C:163:LEU:HD21	1:C:171:VAL:HG21	1.98	0.46
1:C:200:GLU:OE2	1:C:211:LEU:HG	2.15	0.46
1:C:268:ALA:O	1:C:271:ARG:O	2.33	0.46
1:C:30:THR:OG1	1:C:31:HIS:ND1	2.38	0.46
1:C:167:ASP:OD1	2:D:96:ARG:NH2	2.49	0.46
1:A:91:THR:O	1:A:343:VAL:HG13	2.16	0.46
1:A:234:MET:HG3	1:A:254:VAL:HG23	1.98	0.46
1:A:242:ARG:HH21	1:A:242:ARG:CG	2.11	0.46
1:A:367:ARG:O	1:A:367:ARG:HG3	2.15	0.46
1:C:283:ALA:O	1:C:284:ILE:C	2.54	0.46
1:C:318:GLU:HG2	1:C:318:GLU:O	2.16	0.46
1:C:416:ALA:HB1	1:C:440:ASP:OD2	2.15	0.46
1:A:125:ARG:HG2	1:A:131:TYR:OH	2.16	0.46
1:A:267:LEU:H	1:A:267:LEU:CD1	2.28	0.46
1:A:425:ASN:CG	1:A:426:PRO:HD2	2.36	0.46
1:A:501:LYS:HB2	1:A:504:GLU:HG3	1.97	0.46
1:C:223:LEU:HD12	1:C:228:THR:HA	1.98	0.46
1:A:223:LEU:HD12	1:A:228:THR:CA	2.41	0.46
2:D:5:HIS:CG	2:D:6:SER:N	2.83	0.46
1:A:80:ILE:HD11	1:A:316:MET:HB2	1.98	0.46
1:A:98:MET:SD	1:A:254:VAL:HG21	2.56	0.46
1:A:136:SER:HA	1:A:188:ILE:HG12	1.98	0.46
2:B:8:PRO:C	2:B:59:LEU:HD11	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:ARG:HB2	1:C:69:SER:OG	2.16	0.46
2:D:45:GLU:OE2	2:D:46:VAL:N	2.49	0.46
1:A:262:GLY:HA3	1:A:303:THR:HG21	1.97	0.45
1:A:537:LEU:HD23	1:A:549:ILE:HD13	1.97	0.45
1:C:320:THR:C	1:C:322:LYS:H	2.19	0.45
1:A:46:ASN:O	1:A:50:ILE:HG13	2.17	0.45
1:A:382:ASN:OD1	1:A:382:ASN:O	2.33	0.45
1:A:584:ILE:C	1:A:586:GLY:N	2.68	0.45
1:C:532:ASN:OD1	1:C:535:ARG:HD3	2.16	0.45
1:C:564:VAL:N	1:C:565:PRO:CD	2.79	0.45
1:C:581:ARG:HD3	1:C:590:PRO:HG3	1.97	0.45
1:A:106:PRO:HD2	1:A:242:ARG:NH1	2.32	0.45
1:C:309:LEU:HD22	1:C:309:LEU:HA	1.72	0.45
1:C:512:LEU:HD12	1:C:512:LEU:HA	1.68	0.45
1:A:45:ARG:O	1:A:48:PHE:HD1	1.99	0.45
1:A:313:ARG:HG3	1:A:327:ILE:HB	1.99	0.45
1:A:575:TYR:C	1:A:577:LEU:H	2.19	0.45
1:C:196:LEU:HD23	1:C:196:LEU:HA	1.81	0.45
1:C:224:SER:O	1:C:226:GLU:N	2.50	0.45
1:A:136:SER:C	1:A:138:ALA:N	2.70	0.45
1:C:91:THR:HG23	1:C:256:ALA:HB2	1.99	0.45
1:A:316:MET:HG3	1:A:327:ILE:HD12	1.98	0.45
1:A:332:LEU:HB2	1:A:360:ALA:O	2.17	0.45
1:A:397:LEU:CD1	1:A:601:SER:HB2	2.46	0.45
1:A:473:PHE:CE2	2:B:76:ASN:HB3	2.51	0.45
2:B:50:ALA:HB2	2:B:71:VAL:HG23	1.98	0.45
1:C:28:THR:HG22	1:C:30:THR:HG22	1.97	0.45
1:C:545:ASN:HB3	1:C:547:ARG:HG3	1.98	0.45
1:C:76:ALA:HB3	1:C:370:MET:SD	2.57	0.45
1:C:333:LEU:HD22	1:C:436:ALA:O	2.15	0.45
1:C:414:LEU:CB	1:C:558:SER:HB2	2.47	0.45
1:A:515:GLU:CG	1:A:516:LYS:HZ2	2.30	0.45
1:C:134:VAL:HG12	1:C:134:VAL:O	2.15	0.45
1:C:406:THR:OG1	1:C:407:ARG:N	2.49	0.45
2:D:34:ILE:HG12	2:D:103:ALA:HB1	1.97	0.45
1:A:115:ILE:HA	1:A:195:MET:O	2.17	0.45
1:C:405:THR:HB	1:C:409:LEU:HD12	1.98	0.45
1:A:314:GLN:O	1:A:317:ALA:N	2.50	0.45
1:A:343:VAL:HB	1:A:350:GLU:O	2.17	0.45
1:C:257:ARG:NE	1:C:259:ILE:HG22	2.32	0.45
2:D:66:ASP:OD1	2:D:66:ASP:C	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:GLU:CD	1:A:23:GLU:H	2.20	0.44
1:A:378:GLU:HG2	1:A:385:VAL:H	1.82	0.44
1:A:411:ILE:HD11	1:A:422:SER:CB	2.29	0.44
2:B:15:ILE:HD12	2:B:15:ILE:H	1.81	0.44
1:C:54:LEU:HD11	1:C:71:ILE:HD13	1.99	0.44
1:C:85:MET:HA	1:C:358:GLY:HA2	1.99	0.44
1:C:127:ALA:HA	1:C:156:TYR:CD1	2.51	0.44
1:C:407:ARG:HD2	1:C:407:ARG:N	2.32	0.44
1:A:120:GLN:C	1:A:122:LEU:N	2.70	0.44
1:A:308:MET:O	1:A:312:VAL:HG12	2.17	0.44
1:C:114:GLY:HA3	1:C:132:ILE:HG13	2.00	0.44
1:C:341:VAL:HB	1:C:354:GLU:CG	2.44	0.44
1:C:522:ARG:O	1:C:526:GLU:HG3	2.18	0.44
2:D:25:VAL:O	2:D:29:ILE:HG13	2.17	0.44
1:A:141:PHE:CG	1:A:142:ALA:N	2.85	0.44
1:A:316:MET:CE	1:A:365:SER:HB2	2.47	0.44
1:C:288:VAL:HG21	1:C:332:LEU:HD21	1.98	0.44
1:C:572:LEU:O	1:C:577:LEU:CD1	2.66	0.44
1:A:15:GLU:OE1	1:A:592:ASN:HA	2.18	0.44
1:A:433:THR:C	1:A:434:HIS:ND1	2.71	0.44
2:B:65:CYS:CB	2:B:70:LEU:CB	2.96	0.44
1:C:51:GLN:NE2	1:C:380:LYS:HD3	2.33	0.44
1:C:498:CYS:CB	1:C:505:LEU:HD22	2.48	0.44
2:D:112:ARG:O	2:D:113:ASP:CB	2.63	0.44
1:A:187:TYR:HB2	1:A:347:LEU:HB3	2.00	0.44
1:A:267:LEU:N	1:A:267:LEU:CD1	2.80	0.44
1:A:293:ARG:HA	1:A:293:ARG:HD3	1.66	0.44
1:A:295:ASP:O	1:A:296:ASN:HB2	2.18	0.44
1:C:188:ILE:HG23	1:C:189:ASP:N	2.33	0.44
1:C:257:ARG:HD3	1:C:257:ARG:H	1.83	0.44
1:C:534:LEU:HD22	1:C:546:ILE:HD13	1.98	0.44
1:A:50:ILE:CD1	1:A:377:ILE:HD11	2.48	0.44
1:A:196:LEU:HD13	1:A:221:PHE:CD2	2.53	0.44
1:A:316:MET:O	1:A:319:LEU:HB3	2.18	0.44
1:A:460:GLU:OE1	1:A:501:LYS:HE3	2.18	0.44
1:A:575:TYR:O	1:A:577:LEU:N	2.50	0.44
2:B:15:ILE:HG23	2:B:43:ALA:HA	1.99	0.44
1:C:475:LEU:HD23	1:C:485:PHE:CE1	2.53	0.44
1:C:483:GLN:NE2	1:C:485:PHE:CE2	2.85	0.44
2:D:15:ILE:O	2:D:16:ASP:HB2	2.18	0.44
1:A:312:VAL:HG22	1:A:363:VAL:HG11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ILE:HG13	1:A:430:ILE:HD13	1.99	0.44
1:C:87:THR:HG22	1:C:339:VAL:HG21	2.00	0.44
1:C:479:ASP:OD1	1:C:479:ASP:C	2.56	0.44
1:C:490:PRO:HG2	1:C:493:VAL:CG1	2.46	0.44
1:A:54:LEU:O	1:A:57:VAL:HG12	2.17	0.44
1:A:56:LEU:O	1:A:57:VAL:C	2.56	0.44
1:A:306:GLY:O	1:A:307:GLY:C	2.54	0.44
1:C:234:MET:HG3	1:C:254:VAL:CG2	2.48	0.44
1:A:55:ALA:O	1:A:58:ALA:HB3	2.18	0.43
1:A:111:LEU:HD13	1:A:200:GLU:HB2	2.00	0.43
1:A:313:ARG:CG	1:A:327:ILE:HB	2.49	0.43
1:A:343:VAL:H	1:A:351:PHE:HA	1.83	0.43
1:A:525:LYS:NZ	1:A:563:GLU:OE1	2.50	0.43
2:B:66:ASP:OD2	2:B:67:ARG:N	2.51	0.43
1:C:265:GLU:O	1:C:297:VAL:HG13	2.17	0.43
1:C:301:SER:C	1:C:303:THR:N	2.71	0.43
1:C:346:GLY:C	1:C:347:LEU:HD12	2.38	0.43
1:C:423:ILE:HG13	1:C:549:ILE:CD1	2.47	0.43
1:C:512:LEU:HD11	1:C:516:LYS:HD2	1.98	0.43
1:C:562:PHE:H	1:C:562:PHE:HD2	1.66	0.43
2:D:16:ASP:O	2:D:17:GLY:C	2.57	0.43
2:D:73:HIS:CE1	2:D:82:PRO:HA	2.53	0.43
2:B:46:VAL:HG11	2:B:69:MET:CE	2.48	0.43
1:C:3:TYR:CE2	1:C:63:ILE:HG21	2.53	0.43
1:C:377:ILE:O	1:C:381:LEU:HG	2.17	0.43
1:C:391:GLU:H	1:C:391:GLU:HG2	1.48	0.43
1:C:399:ALA:CB	1:C:411:ILE:HG21	2.48	0.43
1:A:133:LEU:HD23	1:A:133:LEU:HA	1.60	0.43
2:B:15:ILE:CD1	2:B:65:CYS:O	2.66	0.43
1:C:316:MET:HE2	1:C:363:VAL:HG23	2.00	0.43
1:C:54:LEU:HD23	1:C:54:LEU:HA	1.80	0.43
2:D:61:VAL:HG22	2:D:105:LEU:HD23	2.00	0.43
1:A:141:PHE:HE2	1:A:174:ARG:NE	2.16	0.43
1:A:305:ILE:HG21	1:A:359:ILE:HD12	2.00	0.43
1:A:316:MET:CG	1:A:327:ILE:HD12	2.48	0.43
1:C:267:LEU:HD22	1:C:296:ASN:O	2.18	0.43
2:D:16:ASP:HB3	2:D:67:ARG:NE	2.27	0.43
1:C:57:VAL:HG13	1:C:58:ALA:N	2.32	0.43
1:C:81:GLY:CA	1:C:362:MET:HA	2.49	0.43
1:A:90:GLU:HG2	1:A:259:ILE:HG21	2.01	0.43
1:A:224:SER:C	1:A:226:GLU:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:ILE:HA	1:C:344:THR:OG1	2.19	0.43
1:C:316:MET:HG3	1:C:316:MET:O	2.17	0.43
1:C:474:HIS:HB3	1:C:484:PHE:CD1	2.54	0.43
1:C:545:ASN:HB3	1:C:547:ARG:CB	2.48	0.43
2:D:18:CYS:SG	2:D:66:ASP:HA	2.59	0.43
2:D:36:PHE:C	2:D:36:PHE:CD2	2.92	0.43
1:A:224:SER:H	1:A:227:GLU:CG	2.32	0.43
1:A:234:MET:HG3	1:A:254:VAL:CG2	2.49	0.43
2:B:101:ASN:HA	2:B:104:ARG:HB2	2.00	0.43
1:C:369:GLN:HG2	1:C:372:MET:HE1	2.00	0.43
1:C:542:PRO:O	1:C:543:THR:C	2.56	0.43
2:D:60:LEU:HB3	2:D:74:TYR:CE2	2.54	0.43
1:A:330:GLN:HG3	1:A:364:LYS:H	1.84	0.43
1:A:393:GLU:O	1:A:397:LEU:HG	2.19	0.43
1:C:161:VAL:HG12	1:C:163:LEU:HD13	2.01	0.43
1:C:226:GLU:OE2	1:C:226:GLU:HA	2.17	0.43
1:C:341:VAL:CB	1:C:354:GLU:HG3	2.44	0.43
1:C:350:GLU:OE1	1:C:350:GLU:N	2.44	0.43
1:A:537:LEU:HB3	1:A:546:ILE:CD1	2.48	0.43
1:C:133:LEU:HD22	1:C:135:VAL:HG22	2.00	0.43
1:C:352:SER:OG	1:C:353:LEU:N	2.51	0.43
2:D:22:TRP:CZ3	2:D:95:HIS:HE1	2.36	0.43
1:A:332:LEU:HD12	1:A:359:ILE:HG21	1.99	0.42
1:A:401:THR:OG1	1:A:584:ILE:HG23	2.18	0.42
1:A:487:THR:CB	1:A:488:PRO:HD2	2.49	0.42
1:C:81:GLY:HA3	1:C:362:MET:HA	2.01	0.42
1:C:332:LEU:N	1:C:332:LEU:CD2	2.82	0.42
1:A:369:GLN:O	1:A:369:GLN:OE1	2.37	0.42
1:A:522:ARG:NH2	1:A:563:GLU:OE2	2.52	0.42
1:C:130:PRO:HA	1:C:157:GLN:HG2	2.02	0.42
1:C:378:GLU:CG	1:C:385:VAL:HG23	2.47	0.42
1:C:380:LYS:HA	1:C:380:LYS:NZ	2.34	0.42
2:D:27:LEU:HB3	2:D:96:ARG:NH1	2.34	0.42
2:D:68:HIS:O	2:D:88:HIS:HB3	2.19	0.42
1:A:522:ARG:HH22	1:A:563:GLU:CG	2.26	0.42
1:C:111:LEU:HD13	1:C:200:GLU:HB2	2.00	0.42
1:C:120:GLN:O	1:C:122:LEU:N	2.52	0.42
1:C:321:ASN:O	1:C:323:PRO:CD	2.60	0.42
1:C:499:VAL:HB	1:C:506:VAL:HB	2.00	0.42
2:D:59:LEU:O	2:D:60:LEU:HB2	2.19	0.42
1:A:94:THR:O	1:A:95:GLU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:PHE:CD2	1:A:142:ALA:N	2.88	0.42
1:A:338:SER:OG	1:A:353:LEU:HD13	2.18	0.42
1:A:514:LEU:C	1:A:514:LEU:HD23	2.39	0.42
1:C:115:ILE:HA	1:C:195:MET:O	2.19	0.42
1:C:231:ILE:HG22	1:C:234:MET:CE	2.48	0.42
1:A:83:VAL:HG12	1:A:360:ALA:HA	2.01	0.42
1:A:121:GLU:OE2	1:A:125:ARG:NH2	2.53	0.42
1:C:298:THR:HG22	1:C:313:ARG:NH1	2.34	0.42
1:C:494:PHE:HE2	2:D:109:ILE:O	2.03	0.42
1:A:34:LEU:HD12	1:A:34:LEU:O	2.18	0.42
1:A:222:ASN:O	1:A:222:ASN:ND2	2.52	0.42
1:C:1:MET:HE3	1:C:21:LEU:O	2.20	0.42
1:C:119:PRO:CG	1:C:139:PHE:CZ	3.02	0.42
1:C:361:SER:CA	1:C:436:ALA:CB	2.98	0.42
1:A:111:LEU:CD2	1:A:210:THR:HG21	2.50	0.42
1:C:4:ILE:HD11	1:C:21:LEU:HB2	2.01	0.42
1:C:101:HIS:CG	1:C:348:ALA:HB1	2.55	0.42
1:C:332:LEU:HA	1:C:360:ALA:O	2.19	0.42
1:A:137:SER:HA	1:A:165:ARG:HE	1.85	0.42
1:A:263:ASN:N	1:A:300:GLU:HG3	2.35	0.42
1:A:409:LEU:HD23	1:A:409:LEU:C	2.39	0.42
1:C:1:MET:HE1	1:C:20:THR:HB	2.02	0.42
1:C:347:LEU:N	1:C:347:LEU:CD1	2.75	0.42
2:D:16:ASP:O	2:D:18:CYS:N	2.53	0.42
2:D:67:ARG:HG2	2:D:67:ARG:HH21	1.84	0.42
2:D:74:TYR:HB3	2:D:77:LEU:HD12	2.01	0.42
1:A:187:TYR:N	1:A:187:TYR:HD1	2.16	0.42
1:A:515:GLU:CB	1:A:516:LYS:NZ	2.82	0.42
1:C:192:PRO:HG2	1:C:247:VAL:HG11	2.02	0.42
1:C:255:LYS:HZ2	1:C:255:LYS:N	2.17	0.42
1:C:275:VAL:HG22	1:C:276:ASP:N	2.35	0.42
1:C:330:GLN:CD	1:C:364:LYS:HE2	2.39	0.42
1:C:341:VAL:CG2	1:C:354:GLU:HG3	2.50	0.42
2:D:27:LEU:HB3	2:D:96:ARG:HH11	1.84	0.42
2:D:48:ASP:OD2	2:D:48:ASP:C	2.59	0.42
2:D:87:MET:HB3	2:D:89:HIS:NE2	2.35	0.42
1:A:408:PRO:HG2	1:A:550:PRO:HD2	2.02	0.41
2:B:74:TYR:CB	2:B:77:LEU:HD12	2.49	0.41
1:C:72:ARG:NE	1:C:602:TRP:HB2	2.35	0.41
1:C:80:ILE:O	1:C:363:VAL:HG22	2.21	0.41
1:C:101:HIS:CD2	1:C:348:ALA:HB1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:VAL:HG12	1:C:173:ASN:ND2	2.34	0.41
1:A:136:SER:C	1:A:138:ALA:H	2.22	0.41
1:A:360:ALA:HB2	1:A:441:MET:CG	2.50	0.41
1:A:394:ALA:CA	1:A:597:GLY:HA3	2.50	0.41
1:A:555:VAL:HG12	1:A:590:PRO:CA	2.49	0.41
2:B:17:GLY:C	2:B:19:ASP:H	2.23	0.41
2:B:70:LEU:CD2	2:B:86:LEU:HD23	2.49	0.41
1:C:118:THR:HG23	1:C:193:LEU:CD1	2.50	0.41
1:C:285:MET:CE	1:C:333:LEU:HA	2.46	0.41
1:A:564:VAL:N	1:A:565:PRO:CD	2.83	0.41
1:C:40:ILE:HD12	1:C:43:THR:HG21	1.99	0.41
1:A:443:THR:OG1	1:A:462:LYS:HE2	2.20	0.41
1:A:532:ASN:HA	1:A:535:ARG:HB2	2.02	0.41
1:C:435:LEU:HD23	1:C:535:ARG:HD3	2.02	0.41
2:D:51:TRP:HD1	2:D:73:HIS:CE1	2.38	0.41
2:D:67:ARG:HG2	2:D:67:ARG:NH2	2.34	0.41
1:A:40:ILE:O	1:A:43:THR:HG23	2.21	0.41
1:C:136:SER:C	1:C:138:ALA:N	2.72	0.41
1:C:252:GLY:O	1:C:253:ASP:HB2	2.20	0.41
1:C:285:MET:HE2	1:C:334:ALA:N	2.24	0.41
1:C:331:ASP:O	1:C:361:SER:HA	2.21	0.41
1:A:132:ILE:HD12	1:A:197:ALA:HB3	2.02	0.41
1:A:137:SER:OG	1:A:164:GLN:CD	2.59	0.41
1:A:140:ASP:OD1	1:A:142:ALA:N	2.48	0.41
1:A:293:ARG:NH2	1:A:539:GLN:HE22	2.16	0.41
1:C:247:VAL:HG12	1:C:249:THR:HG23	2.03	0.41
1:C:273:VAL:HG12	1:C:274:ARG:N	2.36	0.41
1:C:380:LYS:CB	1:C:381:LEU:HD23	2.50	0.41
1:A:75:GLU:HA	1:A:370:MET:HG3	2.03	0.41
1:A:140:ASP:OD1	1:A:142:ALA:HB3	2.20	0.41
1:A:163:LEU:HD11	1:A:171:VAL:HG21	2.03	0.41
1:A:368:LEU:HD22	1:A:368:LEU:H	1.85	0.41
2:B:10:ILE:CG2	2:B:11:ALA:N	2.84	0.41
1:C:45:ARG:O	1:C:45:ARG:HG3	2.20	0.41
1:C:141:PHE:HE2	1:C:174:ARG:CZ	2.33	0.41
1:A:227:GLU:HA	1:A:230:ASN:HD22	1.86	0.41
1:A:515:GLU:HB2	1:A:516:LYS:HZ1	1.82	0.41
1:A:576:ARG:HD3	1:A:576:ARG:O	2.21	0.41
2:B:45:GLU:OE2	2:B:46:VAL:HG12	2.20	0.41
1:C:217:ILE:HA	1:C:220:VAL:HG22	2.02	0.41
1:C:226:GLU:O	1:C:229:LYS:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:MET:SD	1:C:246:VAL:CG2	3.09	0.41
1:C:464:TYR:CD1	1:C:501:LYS:HA	2.56	0.41
1:C:569:THR:HG22	1:C:570:ASP:N	2.34	0.41
1:A:116:THR:HB	1:A:193:LEU:HA	2.03	0.41
1:A:117:ILE:HG12	1:A:131:TYR:HB3	2.03	0.41
1:A:136:SER:O	1:A:138:ALA:N	2.54	0.41
1:A:215:TYR:CE2	1:C:405:THR:HG22	2.56	0.41
1:A:425:ASN:CB	1:A:426:PRO:CD	2.98	0.41
1:A:493:VAL:O	1:A:494:PHE:C	2.58	0.41
1:C:74:ASN:ND2	1:C:391:GLU:HA	2.33	0.41
1:C:101:HIS:HB3	1:C:348:ALA:HB3	2.02	0.41
1:C:545:ASN:HB3	1:C:547:ARG:HB2	2.03	0.41
1:C:569:THR:O	1:C:573:ALA:CB	2.68	0.41
1:A:18:LEU:HD21	1:A:63:ILE:HD11	2.02	0.41
1:A:217:ILE:O	1:A:218:ALA:C	2.59	0.41
1:A:305:ILE:HD13	1:A:359:ILE:HD12	2.02	0.41
1:A:473:PHE:HE2	2:B:76:ASN:HB3	1.85	0.41
1:C:70:LEU:HD11	1:C:386:GLN:HB2	2.02	0.41
1:C:234:MET:HG3	1:C:254:VAL:HG23	2.02	0.41
1:C:288:VAL:HG11	1:C:332:LEU:CD2	2.52	0.41
1:A:459:GLU:O	1:A:463:LYS:HG3	2.21	0.40
1:C:18:LEU:HD21	1:C:63:ILE:HD11	2.03	0.40
1:C:122:LEU:HA	1:C:122:LEU:HD12	1.80	0.40
1:C:125:ARG:HG2	1:C:131:TYR:CZ	2.56	0.40
1:C:141:PHE:CG	1:C:142:ALA:N	2.88	0.40
1:C:312:VAL:CG1	1:C:313:ARG:N	2.83	0.40
1:C:320:THR:O	1:C:322:LYS:HG3	2.21	0.40
1:C:412:LEU:HD12	1:C:554:LEU:HD22	2.03	0.40
1:C:449:GLU:CD	1:C:527:ARG:HH12	2.25	0.40
2:D:61:VAL:CG2	2:D:105:LEU:HD23	2.51	0.40
1:A:449:GLU:OE1	1:A:527:ARG:NH1	2.46	0.40
1:C:118:THR:HB	1:C:119:PRO:CD	2.43	0.40
1:C:348:ALA:HB3	1:C:350:GLU:OE1	2.21	0.40
1:C:518:ARG:NH2	1:C:522:ARG:HD2	2.37	0.40
1:C:167:ASP:CA	1:C:170:LEU:HD12	2.49	0.40
1:C:169:VAL:HB	2:D:31:GLU:OE2	2.21	0.40
1:C:224:SER:C	1:C:226:GLU:N	2.74	0.40
1:C:308:MET:HA	1:C:311:HIS:HB3	2.03	0.40
2:D:50:ALA:O	2:D:53:ALA:HB3	2.21	0.40
1:A:430:ILE:O	1:A:431:ILE:HD13	2.21	0.40
1:C:261:ALA:HB1	1:C:277:VAL:CG1	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ILE:CG2	1:A:70:LEU:HD23	2.43	0.40
1:A:211:LEU:HD23	1:A:211:LEU:HA	1.87	0.40
1:A:381:LEU:HD23	1:A:381:LEU:HA	1.89	0.40
1:A:464:TYR:CD1	1:A:501:LYS:HA	2.57	0.40
1:A:591:ARG:NH1	1:A:591:ARG:HG2	2.37	0.40
1:C:228:THR:C	1:C:230:ASN:H	2.24	0.40
1:C:463:LYS:C	1:C:464:TYR:CD2	2.95	0.40
2:D:54:ALA:CA	2:D:62:GLY:HA3	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	604/610 (99%)	519 (86%)	71 (12%)	14 (2%)	6	30
1	C	603/610 (99%)	522 (87%)	62 (10%)	19 (3%)	4	22
2	B	108/125 (86%)	96 (89%)	8 (7%)	4 (4%)	3	19
2	D	107/125 (86%)	93 (87%)	14 (13%)	0	100	100
All	All	1422/1470 (97%)	1230 (86%)	155 (11%)	37 (3%)	5	27

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	368	LEU
1	C	250	PRO
1	C	324	SER
1	A	292	GLY
1	A	294	LEU
1	A	319	LEU
1	A	546	ILE

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Mol	Chain	Res	Type
2	B	5	HIS
1	C	300	GLU
1	C	427	LYS
1	A	56	LEU
1	C	56	LEU
1	C	121	GLU
1	C	156	TYR
1	C	296	ASN
1	C	321	ASN
1	C	355	GLN
1	C	368	LEU
1	C	543	THR
1	A	291	CYS
1	A	540	VAL
1	C	41	LYS
1	C	305	ILE
1	C	426	PRO
1	C	428	GLY
1	A	41	LYS
1	A	155	GLY
2	B	6	SER
2	B	100	ASN
1	C	155	GLY
1	C	542	PRO
1	A	318	GLU
1	A	428	GLY
1	A	389	GLY
1	C	389	GLY
1	A	250	PRO
2	B	29	ILE

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	478/481 (99%)	419 (88%)	59 (12%)	4 21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	477/481 (99%)	413 (87%)	64 (13%)	4 17
2	B	88/100 (88%)	80 (91%)	8 (9%)	9 34
2	D	87/100 (87%)	79 (91%)	8 (9%)	9 34
All	All	1130/1162 (97%)	991 (88%)	139 (12%)	4 21

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	13	SER
1	A	27	LEU
1	A	34	LEU
1	A	70	LEU
1	A	72	ARG
1	A	98	MET
1	A	116	THR
1	A	125	ARG
1	A	128	ASP
1	A	152	LEU
1	A	158	ILE
1	A	165	ARG
1	A	176	GLU
1	A	186	LEU
1	A	193	LEU
1	A	196	LEU
1	A	199	ILE
1	A	203	VAL
1	A	222	ASN
1	A	223	LEU
1	A	236	ARG
1	A	242	ARG
1	A	253	ASP
1	A	255	LYS
1	A	257	ARG
1	A	267	LEU
1	A	273	VAL
1	A	293	ARG
1	A	310	GLU
1	A	321	ASN
1	A	324	SER
1	A	347	LEU

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Mol	Chain	Res	Type
1	A	366	ASP
1	A	372	MET
1	A	380	LYS
1	A	393	GLU
1	A	407	ARG
1	A	419	THR
1	A	423	ILE
1	A	427	LYS
1	A	429	ASP
1	A	441	MET
1	A	448	ARG
1	A	455	ARG
1	A	466	LEU
1	A	487	THR
1	A	501	LYS
1	A	516	LYS
1	A	537	LEU
1	A	547	ARG
1	A	549	ILE
1	A	563	GLU
1	A	576	ARG
1	A	577	LEU
1	A	584	ILE
1	A	591	ARG
1	A	603	HIS
1	A	604	LYS
2	B	6	SER
2	B	38	LEU
2	B	45	GLU
2	B	48	ASP
2	B	52	GLN
2	B	69	MET
2	B	75	LYS
2	B	104	ARG
1	C	2	ARG
1	C	4	ILE
1	C	23	GLU
1	C	27	LEU
1	C	32	SER
1	C	40	ILE
1	C	44	LEU
1	C	45	ARG

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Mol	Chain	Res	Type
1	C	47	VAL
1	C	52	GLU
1	C	74	ASN
1	C	88	ILE
1	C	98	MET
1	C	105	THR
1	C	133	LEU
1	C	157	GLN
1	C	159	THR
1	C	163	LEU
1	C	172	SER
1	C	177	LYS
1	C	189	ASP
1	C	195	MET
1	C	196	LEU
1	C	199	ILE
1	C	223	LEU
1	C	226	GLU
1	C	243	SER
1	C	255	LYS
1	C	257	ARG
1	C	267	LEU
1	C	271	ARG
1	C	293	ARG
1	C	300	GLU
1	C	309	LEU
1	C	315	THR
1	C	330	GLN
1	C	343	VAL
1	C	347	LEU
1	C	353	LEU
1	C	362	MET
1	C	366	ASP
1	C	369	GLN
1	C	375	ARG
1	C	380	LYS
1	C	381	LEU
1	C	391	GLU
1	C	407	ARG
1	C	423	ILE
1	C	427	LYS
1	C	433	THR

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Mol	Chain	Res	Type
1	C	450	LEU
1	C	452	LEU
1	C	469	VAL
1	C	481	SER
1	C	503	ASP
1	C	560	LEU
1	C	562	PHE
1	C	566	GLN
1	C	567	LEU
1	C	575	TYR
1	C	577	LEU
1	C	591	ARG
1	C	598	LEU
1	C	603	HIS
2	D	14	VAL
2	D	45	GLU
2	D	48	ASP
2	D	70	LEU
2	D	85	THR
2	D	88	HIS
2	D	90	GLN
2	D	113	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	173	ASN
1	A	222	ASN
1	A	230	ASN
1	A	263	ASN
1	A	296	ASN
1	A	369	GLN
1	A	386	GLN
1	A	425	ASN
1	A	539	GLN
2	B	4	ASN
2	B	52	GLN
2	B	73	HIS
2	B	97	ASN
1	C	51	GLN
1	C	74	ASN

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Mol	Chain	Res	Type
1	C	157	GLN
1	C	173	ASN
1	C	230	ASN
1	C	263	ASN
1	C	603	HIS
2	D	93	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	A	613	-	4,4,4	0.38	0	6,6,6	0.06	0
3	SO4	C	612	-	4,4,4	0.38	0	6,6,6	0.12	0
3	SO4	A	611	-	4,4,4	0.39	0	6,6,6	0.09	0
3	SO4	A	612	-	4,4,4	0.39	0	6,6,6	0.08	0
3	SO4	C	611	-	4,4,4	0.37	0	6,6,6	0.11	0

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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	606/610 (99%)	-0.40	1 (0%)	95	87	36, 78, 124, 164	0
1	C	605/610 (99%)	-0.35	2 (0%)	94	84	36, 84, 136, 166	0
2	B	110/125 (88%)	-0.52	0	100	100	51, 81, 118, 179	0
2	D	109/125 (87%)	-0.46	0	100	100	44, 80, 111, 125	0
All	All	1430/1470 (97%)	-0.39	3 (0%)	95	87	36, 81, 128, 179	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	426	PRO	2.7
1	A	576	ARG	2.3
1	C	603	HIS	2.1

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)

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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å^2)	Q<0.9
3	SO4	A	613	5/5	0.80	0.16	141,144,146,147	0
3	SO4	C	611	5/5	0.86	0.24	174,174,176,176	0
3	SO4	C	612	5/5	0.88	0.33	135,136,139,140	0
3	SO4	A	611	5/5	0.90	0.24	154,156,160,161	0
3	SO4	A	612	5/5	0.92	0.28	107,108,119,122	0
4	CA	C	1006	1/1	0.94	0.21	72,72,72,72	0
4	CA	A	1005	1/1	0.98	0.17	66,66,66,66	0

6.5 Other polymers (i)

There are no such residues in this entry.