Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:40 AM GMT

PDB ID	:	3MKQ
Title	:	Crystal structure of yeast alpha/betaprime-COP subcomplex of the COPI vesicular coat
Authors	:	Lee, C.; Goldberg, J.
Deposited on	:	2010-04-15
Resolution	:	2.50 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:

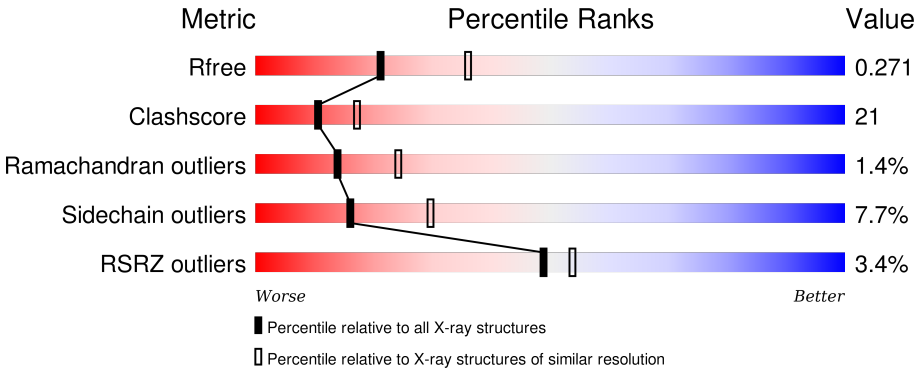
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	814	3% 64% 31% 5%
1	C	814	4% 60% 35% 5%
1	E	814	2% 59% 35% 5%
2	B	177	3% 68% 27% 5%
2	D	177	7% 63% 30% 7%

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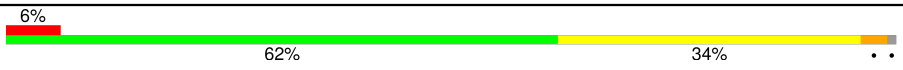
Mol	Chain	Length	Quality of chain
2	F	177	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23730 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 Coatomer beta'-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	811	Total	C	N	O	S	0	0	0
			6438	4110	1063	1252	13			
1	C	811	Total	C	N	O	S	0	0	0
			6437	4109	1063	1252	13			
1	E	810	Total	C	N	O	S	0	0	0
			6430	4107	1061	1248	14			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	701	ILE	VAL	VARIANT	UNP A6ZU46
C	701	ILE	VAL	VARIANT	UNP A6ZU46
E	701	ILE	VAL	VARIANT	UNP A6ZU46

- Molecule 2 is a protein called Coatomer subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	177	Total	C	N	O	S	0	0	0
			1390	877	230	279	4			
2	D	177	Total	C	N	O	S	0	0	0
			1390	877	230	279	4			
2	F	175	Total	C	N	O	S	0	0	0
			1375	869	228	274	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	664	ALA	VAL	VARIANT	UNP P53622
B	676	ILE	SER	VARIANT	UNP P53622
D	664	ALA	VAL	VARIANT	UNP P53622
D	676	ILE	SER	VARIANT	UNP P53622
F	664	ALA	VAL	VARIANT	UNP P53622

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Chain	Residue	Modelled	Actual	Comment	Reference
F	676	ILE	SER	VARIANT	UNP P53622

- Molecule 3 is water.

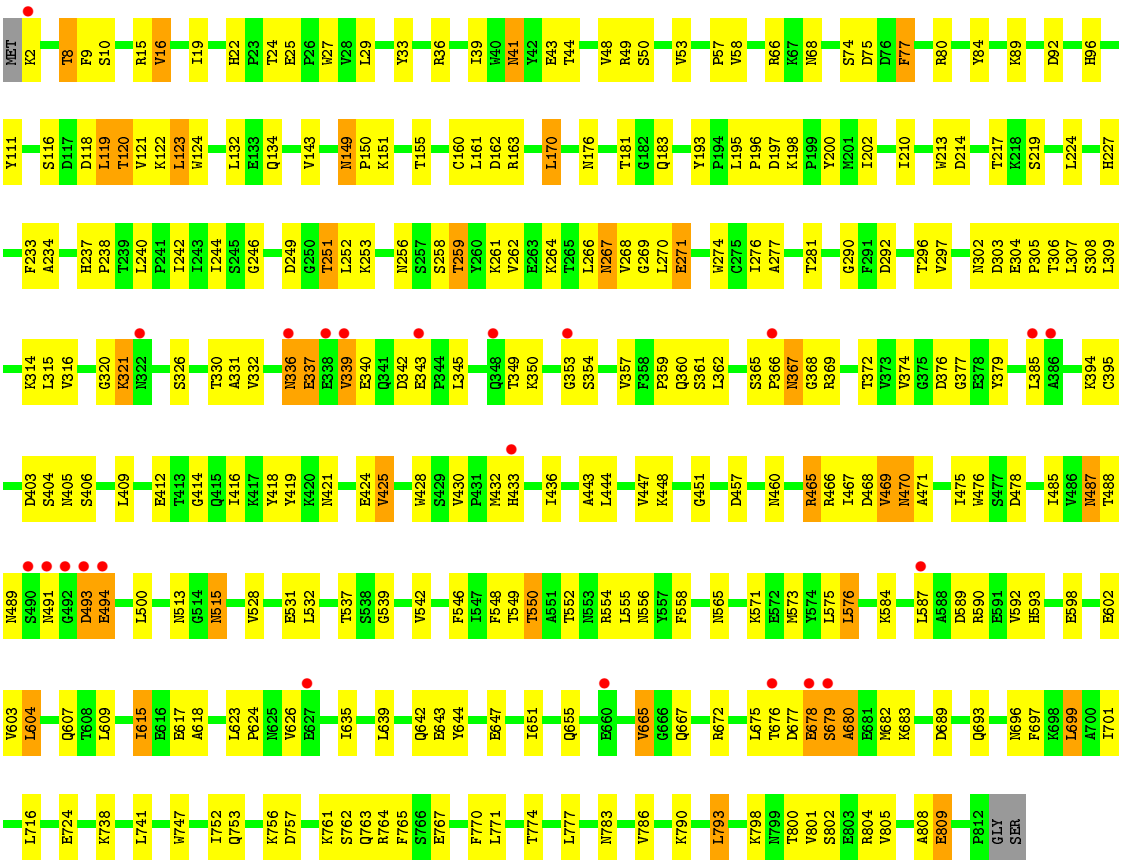
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	100	Total O 100 100	0	0
3	B	17	Total O 17 17	0	0
3	C	76	Total O 76 76	0	0
3	D	5	Total O 5 5	0	0
3	E	66	Total O 66 66	0	0
3	F	6	Total O 6 6	0	0

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.

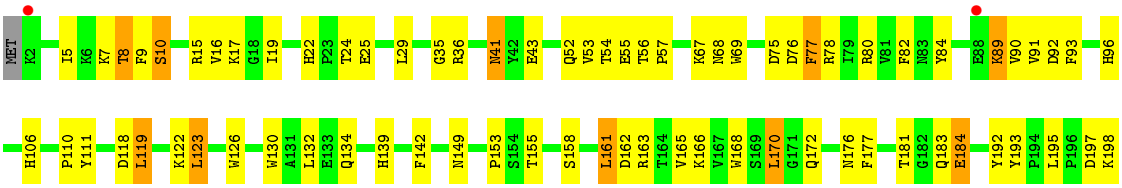
- Molecule 1: Coatomer beta'-subunit

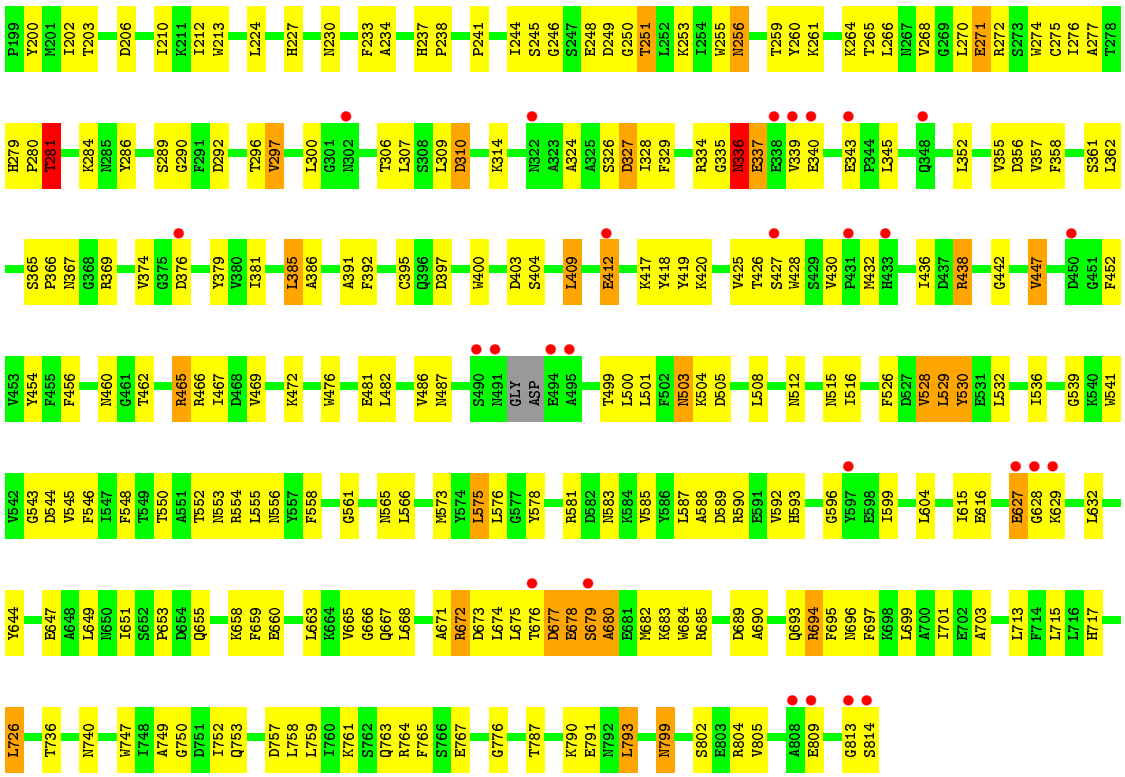
Chain A:



- Molecule 1: Coatomer beta'-subunit

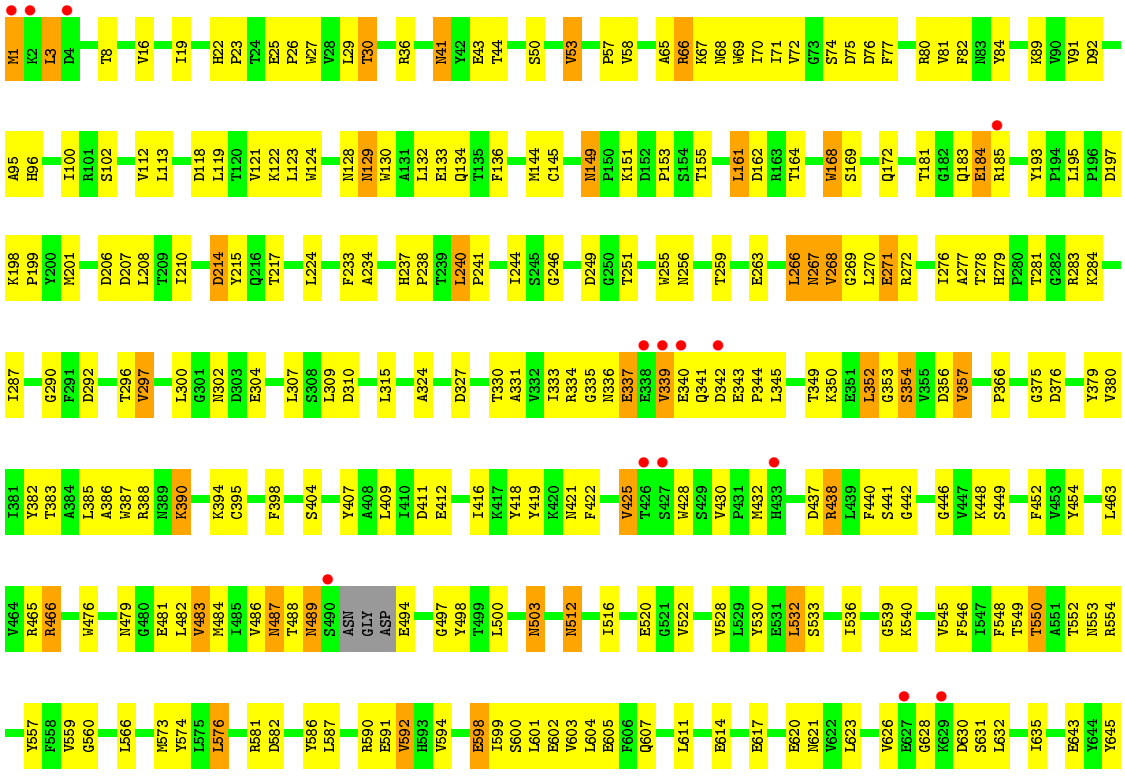
Chain C:

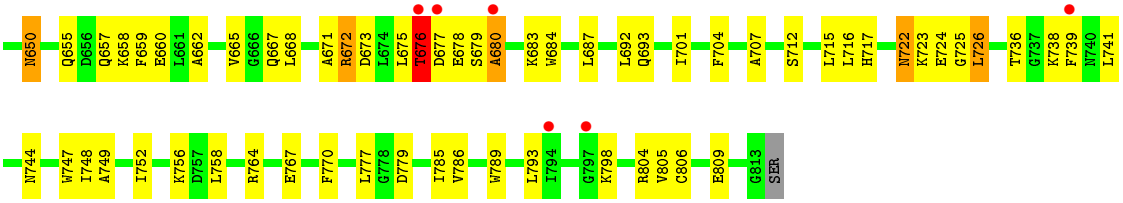




• Molecule 1: Coatomer beta'-subunit

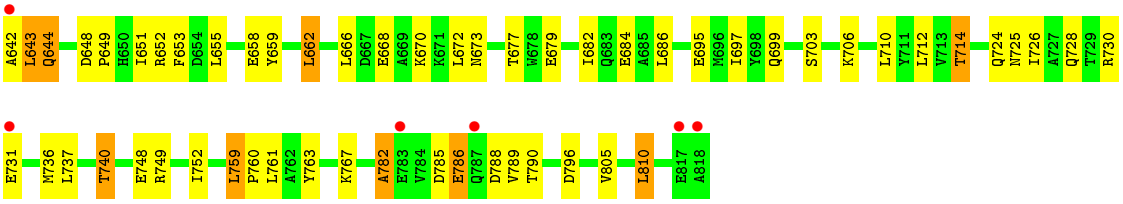
Chain E:





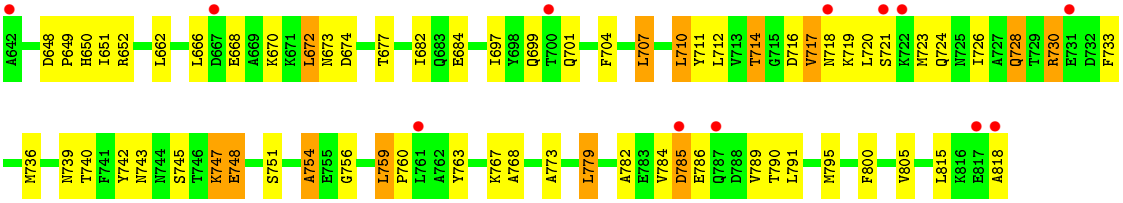
- Molecule 2: Coatomer subunit alpha

Chain B:



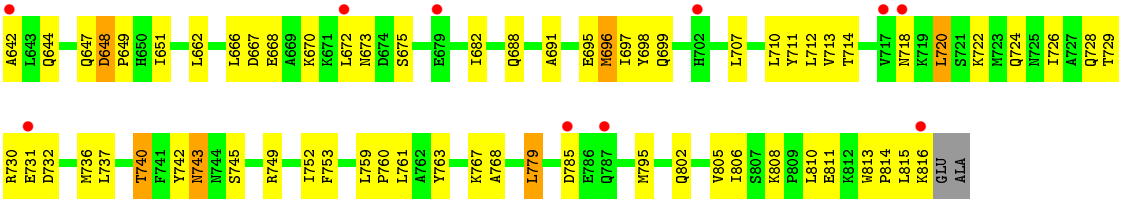
- Molecule 2: Coatomer subunit alpha

Chain D:



- Molecule 2: Coatomer subunit alpha

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	152.64Å 152.64Å 294.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.98 – 2.50 24.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.9 (24.98-2.50) 91.0 (24.98-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.272 0.219 , 0.271	Depositor DCC
R_{free} test set	6381 reflections (5.10%)	DCC
Wilson B-factor (Å^2)	36.3	Xtriage
Anisotropy	0.693	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 57.2	EDS
Estimated twinning fraction	0.012 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 132218 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	23730	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.16% 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

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	0.41	0/6591	0.68	0/8960
1	C	0.39	0/6589	0.66	0/8954
1	E	0.39	0/6582	0.65	0/8945
2	B	0.37	0/1415	0.57	1/1915 (0.1%)
2	D	0.35	0/1415	0.56	0/1915
2	F	0.36	0/1400	0.55	1/1896 (0.1%)
All	All	0.39	0/23992	0.64	2/32585 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	782	ALA	N-CA-C	-5.43	96.33	111.00
2	F	647	GLN	N-CA-C	5.21	125.06	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6438	0	6225	276	0
1	C	6437	0	6225	288	0
1	E	6430	0	6226	273	0
2	B	1390	0	1349	49	0
2	D	1390	0	1349	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1375	0	1338	68	0
3	A	100	0	0	3	0
3	B	17	0	0	0	0
3	C	76	0	0	5	0
3	D	5	0	0	0	0
3	E	66	0	0	2	0
3	F	6	0	0	0	0
All	All	23730	0	22712	985	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 21.

All (985) 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:550:THR:HG22	1:A:554:ARG:H	1.11	1.12
1:C:334:ARG:HA	1:C:581:ARG:HH22	1.06	1.10
1:A:615:ILE:H	1:A:615:ILE:HD12	1.22	1.04
1:A:111:TYR:HB3	1:A:123:LEU:HD11	1.41	1.03
2:B:810:LEU:H	2:B:810:LEU:HD23	1.23	1.03
1:C:550:THR:HG22	1:C:554:ARG:H	1.25	1.01
1:A:550:THR:HG23	1:A:552:THR:H	1.27	0.99
1:A:675:LEU:HA	1:A:678:GLU:HG3	1.40	0.98
1:C:556:ASN:HD21	1:C:565:ASN:HD22	1.08	0.97
1:C:799:ASN:HD22	1:C:799:ASN:H	1.03	0.97
1:A:366:PRO:HD2	1:A:404:SER:HA	1.49	0.95
1:E:96:HIS:CE1	1:E:122:LYS:HD2	2.02	0.94
1:E:390:LYS:HA	1:E:390:LYS:HE2	1.49	0.94
1:A:256:ASN:HD22	1:A:259:THR:H	1.05	0.94
1:E:550:THR:HG22	1:E:554:ARG:H	1.33	0.93
1:A:537:THR:HB	1:A:549:THR:HG22	1.48	0.93
1:E:22:HIS:HD2	1:E:25:GLU:H	1.05	0.93
1:E:550:THR:HG23	1:E:552:THR:H	1.33	0.92
2:F:682:ILE:HD11	2:F:697:ILE:HB	1.51	0.92
1:E:256:ASN:HD22	1:E:259:THR:H	0.98	0.92
2:D:759:LEU:HD23	2:D:782:ALA:HB2	1.52	0.91
1:C:334:ARG:HA	1:C:581:ARG:NH2	1.86	0.91
1:C:556:ASN:ND2	1:C:565:ASN:HD22	1.70	0.90
1:E:267:ASN:HD22	1:E:269:GLY:H	1.19	0.89
1:C:253:LYS:HG2	1:C:265:THR:HG22	1.56	0.88
2:F:740:THR:CG2	2:F:749:ARG:HE	1.86	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:22:HIS:CD2	1:E:25:GLU:H	1.92	0.87
1:E:16:VAL:HG22	1:E:290:GLY:HA3	1.56	0.87
1:C:328:ILE:HG22	1:C:352:LEU:HB3	1.56	0.87
2:F:740:THR:HG23	2:F:749:ARG:HE	1.38	0.85
1:A:303:ASP:OD1	1:A:590:ARG:HD3	1.74	0.85
1:E:197:ASP:OD1	1:E:198:LYS:HD3	1.76	0.85
1:E:256:ASN:ND2	1:E:259:THR:H	1.74	0.85
1:A:256:ASN:ND2	1:A:259:THR:H	1.73	0.85
1:A:783:ASN:ND2	1:A:808:ALA:H	1.75	0.84
1:E:89:LYS:HD3	1:E:92:ASP:HB2	1.57	0.84
2:B:740:THR:CG2	2:B:749:ARG:HE	1.91	0.83
1:C:799:ASN:HD22	1:C:799:ASN:N	1.78	0.81
1:C:467:ILE:HG22	1:C:469:VAL:HG13	1.61	0.81
1:E:717:HIS:HB3	1:E:726:LEU:HD13	1.63	0.81
1:C:334:ARG:CA	1:C:581:ARG:HH22	1.90	0.81
1:E:454:TYR:CZ	1:E:466:ARG:HD2	2.15	0.80
1:C:16:VAL:HG22	1:C:290:GLY:HA3	1.64	0.80
1:A:281:THR:HG22	1:A:590:ARG:HH12	1.45	0.80
1:A:149:ASN:ND2	1:A:151:LYS:H	1.80	0.80
1:C:689:ASP:O	1:C:693:GLN:HG3	1.82	0.80
2:D:710:LEU:O	2:D:714:THR:HB	1.82	0.79
1:A:302:ASN:OD1	1:A:304:GLU:HG2	1.83	0.79
1:A:550:THR:HG23	1:A:552:THR:N	1.98	0.78
1:E:41:ASN:ND2	1:E:44:THR:H	1.80	0.78
1:A:2:LYS:NZ	1:A:360:GLN:HE22	1.81	0.78
2:B:740:THR:HG23	2:B:749:ARG:HE	1.49	0.78
1:E:659:PHE:CE1	1:E:675:LEU:HG	2.18	0.78
1:E:809:GLU:H	1:E:809:GLU:CD	1.84	0.78
2:F:649:PRO:HB3	2:F:672:LEU:HD21	1.65	0.78
1:C:90:VAL:HG12	1:C:91:VAL:HG13	1.67	0.77
2:D:747:LYS:HD3	2:D:747:LYS:H	1.50	0.77
1:C:36:ARG:HG2	1:C:52:GLN:HE22	1.50	0.76
2:D:747:LYS:HD3	2:D:747:LYS:N	2.00	0.76
2:B:810:LEU:H	2:B:810:LEU:CD2	1.99	0.76
1:A:487:ASN:HD22	1:A:488:THR:H	1.34	0.75
1:A:432:MET:HG2	1:A:436:ILE:CD1	2.17	0.75
1:A:2:LYS:HZ1	1:A:360:GLN:HE22	1.35	0.75
1:C:799:ASN:ND2	1:C:799:ASN:H	1.81	0.75
1:A:111:TYR:HB3	1:A:123:LEU:CD1	2.15	0.75
1:A:550:THR:CG2	1:A:554:ARG:H	1.96	0.74
1:A:57:PRO:HG2	1:A:75:ASP:OD2	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:ASN:HD21	1:A:565:ASN:HD22	1.32	0.74
1:A:451:GLY:HA2	1:A:470:ASN:HB3	1.69	0.74
1:C:676:THR:C	1:C:678:GLU:H	1.90	0.74
1:A:467:ILE:HG22	1:A:469:VAL:HG12	1.68	0.74
1:C:550:THR:HG23	1:C:552:THR:H	1.51	0.74
1:A:118:ASP:OD1	1:A:120:THR:HB	1.87	0.74
1:E:675:LEU:HD23	1:E:678:GLU:HG3	1.69	0.73
1:A:15:ARG:HD3	1:A:292:ASP:OD1	1.89	0.73
1:A:256:ASN:HB3	1:A:259:THR:HG22	1.71	0.72
1:A:432:MET:HG2	1:A:436:ILE:HD11	1.71	0.72
1:E:155:THR:HG22	1:E:169:SER:HB3	1.70	0.72
1:A:493:ASP:CG	1:A:494:GLU:H	1.91	0.71
1:C:550:THR:HG22	1:C:554:ARG:N	2.04	0.71
1:C:337:GLU:HG2	1:C:345:LEU:HD23	1.70	0.71
1:A:470:ASN:H	1:A:470:ASN:HD22	1.38	0.71
1:A:680:ALA:HB3	1:A:683:LYS:HG3	1.72	0.71
1:A:149:ASN:C	1:A:149:ASN:HD22	1.93	0.71
1:E:549:THR:HG21	1:E:573:MET:O	1.90	0.71
1:E:438:ARG:HB2	1:E:438:ARG:HH11	1.55	0.70
1:E:601:LEU:O	1:E:605:GLU:HG3	1.91	0.70
1:A:405:ASN:ND2	1:A:421:ASN:HA	2.06	0.70
1:A:487:ASN:HD22	1:A:488:THR:N	1.89	0.70
1:C:253:LYS:HZ3	1:C:265:THR:HG21	1.57	0.70
1:C:695:PHE:CE1	2:D:784:VAL:HG21	2.27	0.69
1:E:267:ASN:ND2	1:E:269:GLY:H	1.91	0.69
1:A:701:ILE:HD13	1:A:716:LEU:HD13	1.74	0.69
1:C:556:ASN:ND2	1:C:565:ASN:HA	2.08	0.69
1:A:675:LEU:HA	1:A:678:GLU:CG	2.20	0.69
1:E:675:LEU:HA	1:E:678:GLU:CG	2.23	0.69
1:C:550:THR:CG2	1:C:554:ARG:H	2.05	0.69
1:E:256:ASN:HD22	1:E:259:THR:N	1.83	0.69
1:E:756:LYS:HD2	1:E:785:ILE:HD11	1.72	0.69
1:C:499:THR:HG22	1:C:529:LEU:HB2	1.73	0.69
1:A:550:THR:HG22	1:A:554:ARG:N	1.96	0.68
1:C:764:ARG:HD2	1:C:767:GLU:OE2	1.91	0.68
2:F:644:GLN:H	2:F:644:GLN:CD	1.97	0.68
1:C:91:VAL:HG11	1:C:130:TRP:CD1	2.28	0.68
1:E:123:LEU:HD12	1:E:133:GLU:HB3	1.76	0.68
1:A:89:LYS:HD3	1:A:92:ASP:HB2	1.75	0.68
1:E:722:ASN:ND2	1:E:725:GLY:H	1.91	0.68
1:A:315:LEU:O	1:A:330:THR:HG23	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:783:ASN:HD21	1:A:808:ALA:H	1.42	0.68
1:C:253:LYS:NZ	1:C:265:THR:HG21	2.08	0.67
2:B:668:GLU:O	2:B:672:LEU:HD13	1.94	0.67
1:A:66:ARG:HD3	3:A:823:HOH:O	1.94	0.67
1:A:16:VAL:HG22	1:A:290:GLY:HA3	1.77	0.67
2:D:707:LEU:HD22	2:D:711:TYR:CZ	2.29	0.67
1:E:77:PHE:HB3	1:E:96:HIS:O	1.94	0.67
1:C:409:LEU:HD21	1:C:417:LYS:HB2	1.76	0.67
1:A:697:PHE:O	1:A:701:ILE:HG12	1.94	0.67
1:C:89:LYS:HE3	1:C:92:ASP:HB2	1.76	0.67
1:A:134:GLN:NE2	1:A:170:LEU:O	2.23	0.67
1:E:770:PHE:HB2	2:F:713:VAL:HG12	1.77	0.67
1:C:281:THR:HG23	1:C:590:ARG:HH22	1.59	0.67
1:E:675:LEU:O	1:E:677:ASP:N	2.28	0.66
1:E:675:LEU:HD12	1:E:687:LEU:HD12	1.77	0.66
1:C:5:ILE:HD12	1:C:300:LEU:CD2	2.25	0.66
1:A:256:ASN:HD22	1:A:259:THR:N	1.88	0.66
1:A:774:THR:O	2:B:805:VAL:HG12	1.95	0.66
1:E:41:ASN:C	1:E:41:ASN:HD22	1.99	0.66
1:E:256:ASN:ND2	1:E:259:THR:HG23	2.10	0.66
2:F:718:ASN:OD1	2:F:722:LYS:HE3	1.96	0.66
1:C:41:ASN:HD22	1:C:43:GLU:H	1.44	0.66
1:C:139:HIS:HE1	1:C:158:SER:OG	1.78	0.66
2:F:698:TYR:HB2	2:F:707:LEU:HD13	1.77	0.66
1:C:336:ASN:HD22	1:C:336:ASN:N	1.91	0.66
1:A:281:THR:HG22	1:A:590:ARG:NH1	2.11	0.65
1:A:555:LEU:HD22	1:A:587:LEU:HD11	1.78	0.65
1:A:68:ASN:HA	1:A:84:TYR:CZ	2.31	0.65
2:D:747:LYS:H	2:D:747:LYS:CD	2.08	0.65
1:A:556:ASN:ND2	1:A:565:ASN:HD22	1.94	0.65
1:C:420:LYS:HG3	1:C:425:VAL:HG21	1.78	0.65
2:F:743:ASN:ND2	2:F:745:SER:HB2	2.11	0.65
1:E:770:PHE:CB	2:F:713:VAL:HG12	2.26	0.65
1:A:214:ASP:CG	1:A:217:THR:HG22	2.17	0.65
1:A:592:VAL:O	1:A:592:VAL:HG12	1.97	0.65
1:E:550:THR:HG23	1:E:552:THR:N	2.09	0.65
1:E:394:LYS:HE2	1:E:412:GLU:OE2	1.95	0.65
1:E:599:ILE:HG21	1:E:604:LEU:HD11	1.78	0.65
1:A:647:GLU:O	1:A:651:ILE:HG12	1.96	0.65
1:A:271:GLU:HB2	1:A:292:ASP:HB2	1.79	0.65
1:E:650:ASN:N	1:E:650:ASN:HD22	1.93	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:757:ASP:O	1:A:761:LYS:HG3	1.96	0.64
1:A:149:ASN:HD22	1:A:151:LYS:H	1.45	0.64
1:A:489:ASN:OD1	1:A:494:GLU:HB2	1.98	0.64
1:C:54:THR:HG21	1:C:76:ASP:OD2	1.97	0.64
1:E:752:ILE:CG1	2:F:802:GLN:HG3	2.28	0.64
1:E:786:VAL:O	1:E:789:TRP:HB3	1.98	0.64
1:E:249:ASP:OD1	1:E:251:THR:HB	1.98	0.64
1:C:68:ASN:HA	1:C:84:TYR:CZ	2.33	0.64
1:A:465:ARG:HG3	1:A:466:ARG:N	2.13	0.63
1:C:736:THR:HG22	1:C:736:THR:O	1.96	0.63
1:E:267:ASN:C	1:E:267:ASN:HD22	2.01	0.63
1:A:22:HIS:HD2	1:A:25:GLU:H	1.45	0.63
1:C:647:GLU:CD	1:C:647:GLU:H	2.01	0.63
2:D:779:LEU:HD23	2:D:786:GLU:HG3	1.79	0.63
1:E:8:THR:HB	1:E:297:VAL:HG22	1.79	0.63
1:C:438:ARG:HH11	1:C:438:ARG:HB2	1.64	0.63
1:C:501:LEU:HB2	1:C:529:LEU:HD21	1.80	0.63
2:B:736:MET:HB3	2:B:752:ILE:HD12	1.80	0.63
1:A:111:TYR:CB	1:A:123:LEU:HD11	2.24	0.63
1:A:470:ASN:HD22	1:A:470:ASN:N	1.93	0.63
2:F:642:ALA:HA	2:F:644:GLN:HE22	1.63	0.63
1:E:723:LYS:HE2	1:E:749:ALA:O	1.99	0.63
1:A:267:ASN:HD22	1:A:269:GLY:H	1.47	0.63
1:A:314:LYS:HG2	1:A:332:VAL:HG22	1.81	0.62
1:E:25:GLU:HG3	1:E:26:PRO:HD2	1.81	0.62
1:A:515:ASN:H	1:A:515:ASN:HD22	1.45	0.62
1:A:584:LYS:HG2	1:A:598:GLU:HA	1.80	0.62
1:C:629:LYS:HD3	1:C:653:PRO:HB2	1.80	0.62
1:A:679:SER:O	1:A:680:ALA:C	2.35	0.62
1:A:339:VAL:HG21	1:A:345:LEU:HA	1.80	0.62
1:E:484:MET:HE1	1:E:498:TYR:N	2.15	0.62
1:E:675:LEU:HA	1:E:678:GLU:HG3	1.82	0.62
1:C:676:THR:H	1:C:678:GLU:HG3	1.64	0.62
1:C:339:VAL:HG12	1:C:340:GLU:H	1.65	0.62
1:C:385:LEU:HD22	1:C:386:ALA:N	2.15	0.62
1:E:339:VAL:HG21	1:E:345:LEU:HA	1.82	0.62
1:C:668:LEU:HD11	1:C:694:ARG:HG3	1.81	0.62
1:C:809:GLU:H	1:C:809:GLU:CD	2.03	0.62
1:E:747:TRP:CZ2	2:F:712:LEU:HD11	2.34	0.62
1:C:412:GLU:CD	1:C:412:GLU:H	2.03	0.62
1:C:666:GLY:HA3	1:C:694:ARG:HH11	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:ASP:O	1:C:404:SER:HB2	1.97	0.62
1:A:256:ASN:HD22	1:A:258:SER:H	1.47	0.61
2:B:728:GLN:HG2	2:B:736:MET:CE	2.29	0.61
1:A:116:SER:O	1:A:143:VAL:HG22	1.99	0.61
1:C:757:ASP:O	1:C:761:LYS:HG3	2.01	0.61
2:B:695:GLU:O	2:B:699:GLN:HG3	2.00	0.61
1:A:556:ASN:ND2	1:A:565:ASN:HA	2.15	0.61
1:A:360:GLN:HG2	1:A:374:VAL:O	1.99	0.61
2:B:728:GLN:HG2	2:B:736:MET:HE2	1.82	0.61
2:B:662:LEU:HD11	2:B:684:GLU:HG3	1.83	0.61
1:A:309:LEU:HD22	1:A:576:LEU:HB3	1.83	0.61
1:C:22:HIS:HD2	1:C:24:THR:H	1.47	0.61
1:C:644:TYR:HB3	1:C:647:GLU:HG2	1.83	0.61
1:A:251:THR:HG21	1:A:253:LYS:HE2	1.83	0.61
1:A:770:PHE:HD2	2:B:810:LEU:HD11	1.66	0.61
1:A:267:ASN:C	1:A:267:ASN:HD22	2.04	0.61
2:D:785:ASP:O	2:D:786:GLU:HB2	2.00	0.61
1:A:689:ASP:O	1:A:693:GLN:HG3	2.00	0.61
1:C:627:GLU:CD	1:C:627:GLU:H	2.02	0.61
1:E:70:ILE:HG13	1:E:70:ILE:O	2.00	0.60
2:D:648:ASP:HB3	2:D:651:ILE:HG12	1.83	0.60
1:C:717:HIS:HB3	1:C:726:LEU:HD13	1.82	0.60
1:E:1:MET:HB2	1:E:263:GLU:OE2	2.00	0.60
1:C:198:LYS:HD2	1:C:200:TYR:CE2	2.36	0.60
1:C:804:ARG:CD	2:D:818:ALA:OXT	2.49	0.60
2:D:716:ASP:OD1	2:D:719:LYS:HD3	2.01	0.60
1:C:15:ARG:HD2	1:C:274:TRP:NE1	2.16	0.60
1:E:672:ARG:O	1:E:672:ARG:HD3	1.99	0.60
1:E:121:VAL:HB	1:E:136:PHE:HB2	1.83	0.60
1:C:447:VAL:HG13	1:C:454:TYR:HB2	1.82	0.60
2:B:759:LEU:N	2:B:760:PRO:CD	2.64	0.60
2:D:662:LEU:HD21	2:D:684:GLU:HG3	1.84	0.60
1:C:272:ARG:HB2	1:C:292:ASP:OD2	2.01	0.60
1:E:466:ARG:NH1	1:E:520:GLU:HG2	2.17	0.60
1:E:268:VAL:HG11	1:E:296:THR:HG21	1.83	0.60
1:E:722:ASN:HD22	1:E:722:ASN:C	2.05	0.60
2:B:759:LEU:HD23	2:B:782:ALA:HB2	1.84	0.60
1:A:623:LEU:HD21	1:A:651:ILE:HD12	1.83	0.60
1:C:41:ASN:HD22	1:C:41:ASN:C	2.05	0.59
1:E:592:VAL:O	1:E:592:VAL:HG12	2.02	0.59
1:E:112:VAL:CG1	1:E:124:TRP:HB2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:ASN:HD22	1:A:336:ASN:C	2.05	0.59
1:A:677:ASP:C	1:A:679:SER:H	2.05	0.59
1:C:249:ASP:OD1	1:C:251:THR:HB	2.01	0.59
1:C:430:VAL:HG23	1:C:430:VAL:O	2.03	0.59
1:C:336:ASN:H	1:C:336:ASN:ND2	2.00	0.59
2:B:649:PRO:HB3	2:B:652:ARG:HH21	1.67	0.59
1:C:339:VAL:CG1	1:C:343:GLU:HB2	2.33	0.59
1:E:550:THR:HG22	1:E:554:ARG:N	2.14	0.59
2:B:810:LEU:N	2:B:810:LEU:HD23	2.06	0.59
1:E:352:LEU:HD22	1:E:387:TRP:HB2	1.84	0.59
2:D:728:GLN:HG3	2:D:736:MET:HE3	1.84	0.59
1:C:5:ILE:HD12	1:C:300:LEU:HD22	1.84	0.59
1:A:267:ASN:ND2	1:A:269:GLY:H	2.00	0.59
1:E:770:PHE:HB2	2:F:713:VAL:CG1	2.33	0.59
1:C:310:ASP:OD1	1:C:314:LYS:HD2	2.03	0.59
1:E:271:GLU:HB2	1:E:292:ASP:HB2	1.84	0.59
1:E:352:LEU:CD2	1:E:387:TRP:HB2	2.33	0.58
1:E:144:MET:HG3	1:E:161:LEU:HD13	1.84	0.58
1:E:438:ARG:HB2	1:E:438:ARG:NH1	2.17	0.58
2:B:649:PRO:HA	2:B:652:ARG:HE	1.68	0.58
1:A:77:PHE:HB3	1:A:96:HIS:O	2.02	0.58
1:A:256:ASN:HD21	1:A:258:SER:HB2	1.69	0.58
1:C:676:THR:HG22	1:C:677:ASP:OD1	2.03	0.58
1:E:672:ARG:HD3	1:E:672:ARG:C	2.24	0.58
1:E:386:ALA:HB3	1:E:388:ARG:HG3	1.84	0.58
1:C:552:THR:O	1:C:553:ASN:HB2	2.03	0.58
1:A:532:LEU:HD11	1:A:558:PHE:CD1	2.39	0.58
1:E:798:LYS:NZ	1:E:798:LYS:HB3	2.18	0.58
1:C:776:GLY:HA3	2:D:805:VAL:HG21	1.85	0.58
2:B:710:LEU:O	2:B:714:THR:HB	2.03	0.58
1:A:575:LEU:HA	1:A:587:LEU:HD23	1.85	0.58
1:E:425:VAL:O	1:E:425:VAL:HG22	2.02	0.58
1:C:339:VAL:HG12	1:C:340:GLU:N	2.19	0.58
2:F:724:GLN:HE22	2:F:736:MET:HA	1.69	0.58
2:F:688:GLN:HB3	2:F:815:LEU:HD11	1.87	0.57
2:F:726:ILE:O	2:F:730:ARG:HB2	2.04	0.57
1:C:306:THR:HG22	1:C:362:LEU:HB2	1.86	0.57
1:C:659:PHE:O	1:C:663:LEU:HD13	2.04	0.57
2:F:753:PHE:CE1	2:F:761:LEU:HD23	2.39	0.57
1:C:573:MET:HE2	1:C:589:ASP:HB3	1.86	0.57
2:F:759:LEU:N	2:F:760:PRO:CD	2.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:TYR:HA	1:A:213:TRP:O	2.03	0.57
1:C:499:THR:O	1:C:500:LEU:HD23	2.04	0.57
1:E:193:TYR:CZ	1:E:195:LEU:HB2	2.40	0.57
1:C:550:THR:HG23	1:C:552:THR:N	2.18	0.57
1:C:672:ARG:C	1:C:674:LEU:H	2.08	0.57
1:A:123:LEU:HD12	1:A:124:TRP:N	2.19	0.57
1:E:201:MET:HG3	1:E:215:TYR:HD1	1.69	0.57
1:A:763:GLN:HA	1:A:765:PHE:CE1	2.40	0.57
1:A:367:ASN:HD22	1:A:368:GLY:N	2.03	0.57
1:E:210:ILE:HB	1:E:224:LEU:HB2	1.87	0.57
2:D:763:TYR:CD1	2:D:779:LEU:HD13	2.40	0.56
1:C:573:MET:CE	1:C:589:ASP:HB3	2.34	0.56
1:A:124:TRP:CZ3	1:A:132:LEU:HB2	2.40	0.56
1:C:77:PHE:HB3	1:C:96:HIS:O	2.05	0.56
2:D:745:SER:HA	2:D:747:LYS:HE2	1.88	0.56
1:C:481:GLU:O	1:C:501:LEU:HD12	2.05	0.56
1:A:804:ARG:HH11	1:A:804:ARG:HG3	1.71	0.56
1:C:8:THR:HG23	1:C:297:VAL:O	2.05	0.56
1:E:36:ARG:HD3	1:E:50:SER:OG	2.04	0.56
1:A:36:ARG:HD3	1:A:50:SER:OG	2.05	0.56
2:B:724:GLN:O	2:B:728:GLN:HG3	2.05	0.56
1:C:666:GLY:CA	1:C:694:ARG:HH11	2.18	0.56
1:E:41:ASN:ND2	1:E:43:GLU:H	2.02	0.56
1:C:500:LEU:HD22	1:C:528:VAL:HG12	1.88	0.56
2:D:728:GLN:HG3	2:D:736:MET:CE	2.36	0.56
1:C:210:ILE:HB	1:C:224:LEU:HB2	1.86	0.56
1:A:8:THR:HG23	1:A:297:VAL:O	2.05	0.56
2:F:711:TYR:HA	2:F:714:THR:HG22	1.88	0.56
1:E:71:ILE:HD13	1:E:112:VAL:HG21	1.87	0.56
1:E:418:TYR:HB2	1:E:428:TRP:CD2	2.41	0.56
1:A:615:ILE:N	1:A:615:ILE:HD12	2.07	0.56
1:C:432:MET:HG2	1:C:436:ILE:CD1	2.36	0.56
2:F:768:ALA:HA	2:F:795:MET:CE	2.36	0.56
1:C:592:VAL:HG12	1:C:592:VAL:O	2.06	0.56
1:A:214:ASP:HB3	1:A:217:THR:HG22	1.86	0.56
1:C:339:VAL:HG12	1:C:343:GLU:HB2	1.87	0.56
1:C:165:VAL:HG21	1:C:203:THR:HG21	1.88	0.55
1:A:210:ILE:HB	1:A:224:LEU:HB2	1.88	0.55
1:C:336:ASN:N	1:C:336:ASN:ND2	2.54	0.55
2:D:763:TYR:CE2	2:D:789:VAL:HG11	2.41	0.55
2:D:751:SER:O	2:D:754:ALA:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:THR:O	1:A:281:THR:HG22	2.06	0.55
1:E:675:LEU:O	1:E:676:THR:C	2.44	0.55
1:A:118:ASP:O	1:A:119:LEU:HB2	2.06	0.55
1:C:799:ASN:ND2	1:C:799:ASN:N	2.46	0.55
2:F:720:LEU:HD11	2:F:742:TYR:HB3	1.88	0.55
1:A:602:GLU:HB3	1:A:626:VAL:HG22	1.89	0.55
1:C:587:LEU:HD12	1:C:587:LEU:N	2.22	0.55
1:A:798:LYS:HB3	1:A:801:VAL:HG22	1.87	0.55
1:E:41:ASN:HD22	1:E:43:GLU:H	1.55	0.55
1:A:22:HIS:CD2	1:A:25:GLU:H	2.24	0.55
1:C:181:THR:HB	1:C:183:GLN:HE21	1.71	0.55
1:A:330:THR:HG22	1:A:331:ALA:N	2.22	0.55
1:E:805:VAL:HA	2:F:815:LEU:HD23	1.88	0.55
1:C:678:GLU:O	1:C:679:SER:C	2.45	0.55
1:E:339:VAL:HG12	1:E:340:GLU:O	2.07	0.55
1:A:143:VAL:O	1:A:143:VAL:HG23	2.05	0.55
1:C:41:ASN:ND2	1:C:43:GLU:H	2.03	0.55
1:A:793:LEU:HD23	1:A:802:SER:HA	1.88	0.55
2:F:743:ASN:HD21	2:F:745:SER:HB2	1.71	0.55
1:C:674:LEU:O	1:C:675:LEU:HD12	2.07	0.55
1:A:753:GLN:NE2	1:A:756:LYS:NZ	2.55	0.55
1:E:181:THR:HB	1:E:183:GLN:HE21	1.72	0.55
2:F:740:THR:HG21	2:F:749:ARG:HE	1.70	0.54
1:A:15:ARG:HD2	1:A:274:TRP:NE1	2.22	0.54
1:A:25:GLU:HG2	1:A:27:TRP:CE2	2.42	0.54
2:B:763:TYR:CZ	2:B:767:LYS:HG3	2.42	0.54
2:B:658:GLU:HG2	2:B:659:TYR:CD2	2.42	0.54
1:C:747:TRP:CZ2	2:D:712:LEU:HD11	2.43	0.54
2:D:724:GLN:NE2	2:D:739:ASN:HB2	2.23	0.54
1:C:335:GLY:N	1:C:581:ARG:NH2	2.56	0.54
1:C:550:THR:HG21	1:C:552:THR:OG1	2.08	0.54
1:C:193:TYR:CE1	1:C:195:LEU:HB2	2.43	0.54
1:E:603:VAL:O	1:E:607:GLN:HG3	2.06	0.54
1:C:335:GLY:H	1:C:581:ARG:NH2	2.05	0.54
2:F:732:ASP:O	2:F:736:MET:HG3	2.08	0.54
1:C:787:THR:O	1:C:791:GLU:HG3	2.08	0.54
1:A:336:ASN:HD22	1:A:337:GLU:N	2.05	0.54
1:A:281:THR:O	1:A:281:THR:CG2	2.56	0.54
1:C:409:LEU:CD2	1:C:417:LYS:HB2	2.38	0.54
1:A:162:ASP:O	1:A:163:ARG:HB2	2.07	0.54
1:A:41:ASN:ND2	1:A:44:THR:H	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:670:LYS:O	2:B:673:ASN:HB2	2.07	0.54
2:D:739:ASN:O	2:D:743:ASN:HB2	2.08	0.53
1:E:409:LEU:O	1:E:416:ILE:HA	2.08	0.53
1:C:233:PHE:CE1	1:C:276:ILE:HB	2.43	0.53
1:E:276:ILE:HG13	1:E:277:ALA:N	2.23	0.53
1:A:532:LEU:N	1:A:532:LEU:HD22	2.24	0.53
1:E:744:ASN:O	1:E:748:ILE:HG12	2.08	0.53
1:C:7:LYS:HE2	1:C:10:SER:OG	2.08	0.53
2:F:740:THR:HG23	2:F:749:ARG:NE	2.17	0.53
1:C:409:LEU:HD21	1:C:419:TYR:HE2	1.71	0.53
1:A:22:HIS:HD2	1:A:24:THR:H	1.54	0.53
1:E:304:GLU:HG2	1:E:574:TYR:CE1	2.43	0.53
1:C:790:LYS:HE3	1:C:802:SER:O	2.08	0.53
1:A:412:GLU:CD	1:A:412:GLU:H	2.11	0.53
1:A:242:ILE:HD12	1:A:244:ILE:HD11	1.90	0.53
1:E:279:HIS:HD2	1:E:281:THR:H	1.56	0.53
1:E:81:VAL:HB	1:E:91:VAL:HG12	1.89	0.53
1:C:676:THR:C	1:C:678:GLU:N	2.59	0.53
1:A:493:ASP:CG	1:A:494:GLU:N	2.61	0.53
1:E:337:GLU:HG3	1:E:345:LEU:HD22	1.90	0.53
1:C:176:ASN:ND2	3:C:815:HOH:O	2.42	0.53
1:E:162:ASP:OD2	1:E:164:THR:HB	2.07	0.53
1:A:249:ASP:OD2	1:A:251:THR:HB	2.08	0.53
1:A:349:THR:HG22	1:A:350:LYS:N	2.23	0.53
1:A:276:ILE:HG13	1:A:277:ALA:N	2.22	0.53
1:C:361:SER:OG	1:C:374:VAL:HB	2.08	0.53
1:E:587:LEU:HD12	1:E:587:LEU:N	2.24	0.53
1:A:786:VAL:O	1:A:790:LYS:HG3	2.09	0.53
1:E:476:TRP:CE3	1:E:483:VAL:HG22	2.44	0.53
1:C:550:THR:CG2	1:C:552:THR:OG1	2.57	0.53
1:C:695:PHE:CZ	2:D:784:VAL:HG21	2.44	0.53
1:A:116:SER:N	1:A:143:VAL:CG2	2.72	0.53
1:E:487:ASN:ND2	1:E:488:THR:H	2.06	0.53
1:A:256:ASN:ND2	1:A:258:SER:H	2.07	0.53
1:A:214:ASP:CB	1:A:217:THR:HG22	2.39	0.53
1:E:586:TYR:C	1:E:587:LEU:HD12	2.29	0.53
1:C:500:LEU:CD2	1:C:528:VAL:HG12	2.39	0.53
1:C:336:ASN:H	1:C:336:ASN:HD22	1.53	0.52
1:C:281:THR:HG23	1:C:281:THR:O	2.08	0.52
1:A:515:ASN:H	1:A:515:ASN:ND2	2.06	0.52
1:E:214:ASP:OD2	1:E:217:THR:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:489:ASN:HD22	1:E:494:GLU:HB2	1.74	0.52
1:C:750:GLY:HA3	2:D:800:PHE:O	2.09	0.52
1:C:465:ARG:HD3	1:C:466:ARG:N	2.24	0.52
1:A:542:VAL:HG11	1:A:604:LEU:HD23	1.90	0.52
1:C:53:VAL:O	1:C:54:THR:HG23	2.08	0.52
1:E:270:LEU:O	1:E:271:GLU:HB2	2.07	0.52
1:E:16:VAL:CG2	1:E:290:GLY:HA3	2.34	0.52
1:A:96:HIS:CE1	1:A:122:LYS:HD2	2.44	0.52
1:A:149:ASN:HD22	1:A:150:PRO:N	2.06	0.52
1:E:324:ALA:HB3	1:E:327:ASP:OD2	2.10	0.52
1:E:3:LEU:HD12	1:E:3:LEU:O	2.10	0.52
1:C:82:PHE:CE2	1:C:89:LYS:HG2	2.44	0.52
2:B:740:THR:HG21	2:B:749:ARG:HE	1.74	0.52
1:A:233:PHE:CE1	1:A:276:ILE:HB	2.45	0.52
1:A:160:CYS:HB3	1:A:162:ASP:OD1	2.10	0.52
1:A:58:VAL:HG22	1:A:74:SER:HB3	1.92	0.52
2:B:648:ASP:HB3	2:B:651:ILE:HG13	1.92	0.52
1:E:599:ILE:CG2	1:E:604:LEU:HD11	2.40	0.52
1:E:149:ASN:HD22	1:E:149:ASN:C	2.14	0.52
1:A:361:SER:HB3	1:A:374:VAL:HB	1.92	0.51
2:F:644:GLN:H	2:F:644:GLN:NE2	2.08	0.51
1:C:644:TYR:HB3	1:C:647:GLU:CG	2.41	0.51
2:F:711:TYR:O	2:F:714:THR:HG22	2.09	0.51
2:F:768:ALA:HA	2:F:795:MET:HE3	1.92	0.51
1:E:704:PHE:CE1	1:E:712:SER:HB3	2.45	0.51
1:A:251:THR:CG2	1:A:253:LYS:HG3	2.40	0.51
2:F:806:ILE:HD12	2:F:808:LYS:O	2.09	0.51
1:C:696:ASN:OD1	2:D:790:THR:HB	2.11	0.51
1:E:437:ASP:HB2	1:E:448:LYS:HB3	1.93	0.51
1:A:367:ASN:CG	1:A:404:SER:OG	2.48	0.51
2:F:759:LEU:H	2:F:759:LEU:HD22	1.74	0.51
1:E:65:ALA:C	1:E:67:LYS:H	2.14	0.51
1:A:214:ASP:HB3	1:A:217:THR:CG2	2.41	0.51
1:C:35:GLY:HA3	1:C:54:THR:O	2.11	0.51
1:C:752:ILE:HG23	1:C:753:GLN:N	2.25	0.51
1:A:430:VAL:O	1:A:430:VAL:HG12	2.10	0.51
1:C:677:ASP:O	1:C:679:SER:N	2.43	0.51
1:A:217:THR:HG23	1:A:219:SER:H	1.74	0.51
1:A:198:LYS:HD2	1:A:200:TYR:CE2	2.44	0.51
1:C:233:PHE:CZ	1:C:246:GLY:HA3	2.46	0.51
1:E:479:ASN:HD21	1:E:481:GLU:HB2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:HIS:CD2	1:C:281:THR:HG22	2.45	0.51
1:C:366:PRO:HG2	1:C:404:SER:OG	2.10	0.51
1:C:671:ALA:O	1:C:674:LEU:HB3	2.11	0.51
1:C:193:TYR:HE1	1:C:195:LEU:HB2	1.75	0.51
1:C:503:ASN:HD21	1:C:505:ASP:HB2	1.75	0.51
1:C:253:LYS:HG2	1:C:265:THR:CG2	2.35	0.51
1:A:149:ASN:ND2	1:A:149:ASN:C	2.64	0.51
1:C:764:ARG:CD	1:C:767:GLU:OE2	2.58	0.51
1:A:22:HIS:CD2	1:A:24:THR:H	2.27	0.51
1:A:418:TYR:HB2	1:A:428:TRP:CD2	2.46	0.51
1:A:365:SER:OG	1:A:367:ASN:ND2	2.44	0.51
1:C:134:GLN:NE2	1:C:170:LEU:O	2.34	0.51
1:A:696:ASN:OD1	1:A:699:LEU:HB2	2.11	0.51
2:B:651:ILE:O	2:B:655:LEU:HG	2.10	0.51
1:A:783:ASN:HD21	1:A:808:ALA:N	2.05	0.50
1:C:250:GLY:HA2	1:C:271:GLU:O	2.11	0.50
1:E:233:PHE:CE1	1:E:276:ILE:HB	2.46	0.50
1:E:736:THR:O	1:E:736:THR:HG22	2.11	0.50
1:A:701:ILE:CD1	1:A:716:LEU:HB3	2.41	0.50
2:B:672:LEU:HD12	2:B:672:LEU:N	2.26	0.50
1:C:53:VAL:HG13	1:C:80:ARG:HD2	1.93	0.50
1:A:39:ILE:HG22	1:A:48:VAL:HG13	1.94	0.50
1:C:259:THR:HG22	1:C:261:LYS:HG3	1.93	0.50
1:C:482:LEU:HD23	1:C:541:TRP:CZ3	2.47	0.50
1:A:677:ASP:O	1:A:677:ASP:CG	2.48	0.50
1:C:15:ARG:HG2	1:C:17:LYS:HD2	1.93	0.50
1:E:701:ILE:HG13	1:E:716:LEU:HD13	1.93	0.50
1:C:504:LYS:O	1:C:508:LEU:HG	2.10	0.50
1:A:409:LEU:O	1:A:416:ILE:HA	2.11	0.50
1:A:770:PHE:CD2	2:B:810:LEU:HD11	2.46	0.50
1:A:256:ASN:ND2	1:A:259:THR:N	2.52	0.50
2:F:740:THR:CG2	2:F:749:ARG:NE	2.66	0.50
1:E:770:PHE:CD2	2:F:810:LEU:HD23	2.46	0.50
1:C:57:PRO:HG2	1:C:75:ASP:OD2	2.12	0.50
2:D:789:VAL:HG12	2:D:791:LEU:CD1	2.41	0.50
1:A:237:HIS:HB2	1:A:242:ILE:HG13	1.93	0.50
1:E:149:ASN:ND2	1:E:151:LYS:H	2.09	0.50
1:C:227:HIS:HE1	1:C:245:SER:OG	1.94	0.50
1:A:642:GLN:O	1:A:643:GLU:HB2	2.11	0.50
1:E:234:ALA:HA	1:E:244:ILE:O	2.11	0.50
2:F:695:GLU:O	2:F:699:GLN:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:VAL:HG12	1:A:432:MET:HE1	1.94	0.50
1:A:584:LYS:HG2	1:A:598:GLU:CA	2.41	0.50
1:C:432:MET:HG2	1:C:436:ILE:HD13	1.93	0.50
2:F:666:LEU:HG	2:F:670:LYS:HE3	1.92	0.50
2:B:785:ASP:HB3	2:B:788:ASP:OD1	2.11	0.50
1:C:539:GLY:HA2	1:C:575:LEU:HD12	1.94	0.50
2:D:674:ASP:HB3	2:D:677:THR:HB	1.94	0.50
1:C:442:GLY:HA3	1:C:476:TRP:CD1	2.46	0.50
1:E:553:ASN:HD22	1:E:553:ASN:N	2.10	0.50
1:C:418:TYR:HB2	1:C:428:TRP:CE3	2.47	0.50
1:C:804:ARG:NE	2:D:818:ALA:OXT	2.45	0.49
1:E:717:HIS:CB	1:E:726:LEU:HD13	2.40	0.49
1:C:36:ARG:HG2	1:C:52:GLN:NE2	2.24	0.49
1:C:19:ILE:HA	1:C:29:LEU:O	2.12	0.49
1:A:589:ASP:OD2	1:A:593:HIS:HB2	2.12	0.49
1:C:447:VAL:HG11	1:C:456:PHE:HE1	1.76	0.49
1:A:793:LEU:HG	1:A:801:VAL:HG23	1.94	0.49
1:E:379:TYR:CE2	1:E:409:LEU:HD21	2.47	0.49
1:C:259:THR:O	1:C:260:TYR:HB2	2.13	0.49
1:A:677:ASP:C	1:A:679:SER:N	2.64	0.49
1:C:224:LEU:N	1:C:224:LEU:HD12	2.27	0.49
1:E:479:ASN:ND2	1:E:481:GLU:HB2	2.27	0.49
1:E:344:PRO:HA	1:E:594:VAL:O	2.12	0.49
1:C:578:TYR:CE1	1:C:599:ILE:HD11	2.47	0.49
1:A:767:GLU:HG3	3:A:869:HOH:O	2.12	0.49
1:E:113:LEU:CD2	1:E:123:LEU:HD23	2.43	0.49
1:E:484:MET:CE	1:E:498:TYR:N	2.76	0.49
1:C:15:ARG:HG2	1:C:17:LYS:CD	2.42	0.49
1:A:532:LEU:N	1:A:532:LEU:CD2	2.76	0.49
1:E:798:LYS:HZ2	1:E:798:LYS:HB3	1.78	0.49
1:E:19:ILE:HA	1:E:29:LEU:O	2.12	0.49
1:C:324:ALA:O	1:C:327:ASP:HB2	2.13	0.49
2:D:704:PHE:CE2	2:D:726:ILE:HG21	2.47	0.49
1:A:418:TYR:HB2	1:A:428:TRP:CE3	2.47	0.49
1:A:19:ILE:HA	1:A:29:LEU:O	2.11	0.49
1:E:550:THR:CG2	1:E:554:ARG:HB3	2.43	0.49
1:E:770:PHE:CE2	2:F:810:LEU:HD23	2.47	0.49
1:A:41:ASN:HD22	1:A:41:ASN:C	2.16	0.49
1:E:617:GLU:OE1	1:E:621:ASN:ND2	2.46	0.49
1:C:5:ILE:HD12	1:C:300:LEU:HD23	1.94	0.49
1:C:367:ASN:HB3	1:C:369:ARG:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:747:LYS:N	2:D:747:LYS:CD	2.70	0.49
1:A:264:LYS:HD3	1:A:266:LEU:HD21	1.95	0.49
1:A:181:THR:HB	1:A:183:GLN:HE21	1.78	0.49
1:C:682:MET:HG2	1:C:682:MET:O	2.12	0.49
1:A:767:GLU:HA	1:A:770:PHE:HD1	1.78	0.49
2:B:649:PRO:HB3	2:B:652:ARG:NH2	2.28	0.49
1:E:600:SER:OG	1:E:603:VAL:HG23	2.13	0.49
1:E:185:ARG:HD2	1:E:206:ASP:HB3	1.95	0.49
1:A:615:ILE:HG12	1:A:644:TYR:CE2	2.48	0.48
1:A:451:GLY:CA	1:A:470:ASN:HB3	2.42	0.48
1:E:330:THR:OG1	1:E:352:LEU:HD12	2.13	0.48
1:C:503:ASN:HD22	1:C:503:ASN:C	2.16	0.48
1:A:176:ASN:ND2	3:A:830:HOH:O	2.45	0.48
1:E:614:GLU:HA	3:E:849:HOH:O	2.13	0.48
1:A:532:LEU:H	1:A:532:LEU:CD2	2.26	0.48
1:A:197:ASP:OD1	1:A:198:LYS:HG3	2.13	0.48
1:E:398:PHE:CD1	1:E:409:LEU:HD11	2.48	0.48
1:C:426:THR:O	1:C:427:SER:CB	2.61	0.48
1:C:460:ASN:OD1	1:C:462:THR:HG23	2.13	0.48
1:A:339:VAL:HG12	1:A:340:GLU:N	2.29	0.48
1:A:41:ASN:HD22	1:A:43:GLU:H	1.60	0.48
1:C:696:ASN:ND2	1:C:699:LEU:HD12	2.28	0.48
1:A:430:VAL:CG1	1:A:432:MET:HE1	2.44	0.48
1:A:337:GLU:HG3	1:A:345:LEU:CD2	2.43	0.48
1:E:333:ILE:HG21	1:E:586:TYR:CZ	2.47	0.48
2:D:668:GLU:O	2:D:672:LEU:HB2	2.14	0.48
1:E:530:TYR:CE1	1:E:560:GLY:HA2	2.48	0.48
1:E:112:VAL:HG12	1:E:124:TRP:HB2	1.96	0.48
1:C:465:ARG:HD2	1:C:467:ILE:HD13	1.95	0.48
1:E:199:PRO:HG2	1:E:214:ASP:OD1	2.13	0.48
1:A:193:TYR:CZ	1:A:195:LEU:HB2	2.48	0.48
1:C:628:GLY:O	1:C:632:LEU:HD13	2.14	0.48
1:E:380:VAL:HG23	1:E:382:TYR:HE1	1.77	0.48
1:C:452:PHE:CD2	1:C:466:ARG:HD3	2.48	0.48
2:F:668:GLU:O	2:F:672:LEU:HG	2.14	0.48
2:F:710:LEU:O	2:F:714:THR:HB	2.13	0.48
1:A:406:SER:HB2	1:A:419:TYR:O	2.13	0.48
1:A:665:VAL:CG1	1:A:667:GLN:HG3	2.44	0.48
1:E:484:MET:HG2	1:E:546:PHE:CZ	2.48	0.48
1:E:149:ASN:HD22	1:E:151:LYS:H	1.62	0.48
1:A:268:VAL:HG11	1:A:296:THR:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:516:ILE:HG21	3:C:889:HOH:O	2.13	0.48
1:C:256:ASN:C	1:C:256:ASN:HD22	2.16	0.48
1:C:655:GLN:NE2	1:C:658:LYS:HE2	2.29	0.48
1:C:447:VAL:HG11	1:C:456:PHE:CE1	2.48	0.48
2:F:691:ALA:HB3	2:F:811:GLU:O	2.14	0.48
1:A:403:ASP:O	1:A:404:SER:HB3	2.13	0.48
2:F:743:ASN:HD21	2:F:745:SER:CB	2.27	0.48
1:C:9:PHE:HB3	1:C:297:VAL:CG1	2.44	0.48
1:A:367:ASN:ND2	1:A:369:ARG:H	2.12	0.47
1:E:122:LYS:HD3	1:E:124:TRP:CZ2	2.48	0.47
1:E:81:VAL:HG21	1:E:130:TRP:CZ2	2.49	0.47
2:F:743:ASN:HD22	2:F:743:ASN:C	2.16	0.47
1:E:598:GLU:O	1:E:599:ILE:HD13	2.13	0.47
1:E:546:PHE:O	1:E:557:TYR:HA	2.14	0.47
1:E:224:LEU:HD13	1:E:255:TRP:CD2	2.49	0.47
1:A:405:ASN:HD21	1:A:421:ASN:HA	1.75	0.47
1:C:616:GLU:CD	1:C:616:GLU:H	2.16	0.47
1:A:549:THR:HG21	1:A:573:MET:O	2.15	0.47
1:E:722:ASN:HD22	1:E:725:GLY:H	1.60	0.47
1:E:503:ASN:HD22	1:E:503:ASN:C	2.17	0.47
1:E:466:ARG:HH11	1:E:466:ARG:CG	2.27	0.47
1:C:397:ASP:OD2	1:C:438:ARG:HB2	2.14	0.47
1:E:516:ILE:HG12	1:E:522:VAL:HG22	1.96	0.47
1:A:752:ILE:HD13	1:A:777:LEU:HD21	1.96	0.47
1:A:262:VAL:HG13	1:A:262:VAL:O	2.15	0.47
1:E:539:GLY:O	1:E:540:LYS:HD2	2.14	0.47
1:C:647:GLU:O	1:C:651:ILE:HG12	2.14	0.47
1:A:281:THR:HG22	1:A:590:ARG:HH22	1.79	0.47
1:A:337:GLU:HG3	1:A:345:LEU:HD23	1.95	0.47
1:C:684:TRP:O	1:C:703:ALA:HB1	2.13	0.47
1:C:326:SER:HB3	1:C:355:VAL:O	2.14	0.47
2:F:737:LEU:O	2:F:740:THR:HG22	2.14	0.47
1:E:687:LEU:O	1:E:687:LEU:HD23	2.15	0.47
1:C:52:GLN:HA	1:C:52:GLN:NE2	2.30	0.47
1:A:432:MET:CG	1:A:436:ILE:HD11	2.42	0.47
1:A:489:ASN:OD1	1:A:493:ASP:O	2.32	0.47
1:E:484:MET:HE1	1:E:497:GLY:C	2.34	0.47
1:C:310:ASP:C	1:C:310:ASP:OD2	2.52	0.47
1:E:272:ARG:CD	1:E:292:ASP:OD2	2.62	0.47
1:E:30:THR:HG21	3:E:838:HOH:O	2.15	0.47
1:C:91:VAL:HG11	1:C:130:TRP:NE1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:335:GLY:HA3	1:E:582:ASP:OD1	2.15	0.47
1:E:449:SER:O	1:E:452:PHE:HB2	2.15	0.47
1:E:144:MET:CG	1:E:161:LEU:HD13	2.44	0.47
1:E:603:VAL:CG2	1:E:631:SER:HB3	2.45	0.47
1:E:736:THR:O	1:E:736:THR:CG2	2.63	0.47
2:D:666:LEU:O	2:D:670:LYS:HG3	2.15	0.47
1:C:142:PHE:HB2	1:C:161:LEU:HD22	1.96	0.47
1:E:440:PHE:HB2	1:E:446:GLY:HA3	1.95	0.47
1:A:678:GLU:HB3	1:A:683:LYS:HE3	1.97	0.47
1:C:615:ILE:HD11	1:C:647:GLU:HG3	1.97	0.47
1:E:357:VAL:HG13	1:E:375:GLY:HA3	1.97	0.47
1:C:381:ILE:HD12	1:C:391:ALA:HB3	1.96	0.47
1:C:251:THR:HG21	1:C:253:LYS:HE2	1.97	0.46
1:E:58:VAL:HG22	1:E:74:SER:HB3	1.97	0.46
1:E:118:ASP:O	1:E:119:LEU:HB2	2.15	0.46
2:B:643:LEU:O	2:B:643:LEU:HD13	2.14	0.46
1:C:695:PHE:CE1	2:D:760:PRO:HG3	2.50	0.46
2:B:748:GLU:O	2:B:752:ILE:HG12	2.14	0.46
2:D:721:SER:O	2:D:724:GLN:HB3	2.15	0.46
1:E:736:THR:HG22	1:E:738:LYS:HG3	1.96	0.46
1:A:677:ASP:O	1:A:679:SER:N	2.48	0.46
1:E:390:LYS:CA	1:E:390:LYS:HE2	2.35	0.46
1:A:25:GLU:HG2	1:A:27:TRP:CZ2	2.50	0.46
1:A:515:ASN:N	1:A:515:ASN:ND2	2.63	0.46
1:A:793:LEU:HG	1:A:801:VAL:CG2	2.46	0.46
1:C:454:TYR:CE2	1:C:466:ARG:HG3	2.50	0.46
2:F:743:ASN:ND2	2:F:745:SER:H	2.12	0.46
1:C:96:HIS:CE1	1:C:122:LYS:HD2	2.50	0.46
1:A:457:ASP:HB3	1:A:460:ASN:OD1	2.15	0.46
1:E:770:PHE:HB3	2:F:713:VAL:HG12	1.95	0.46
1:E:237:HIS:CG	1:E:238:PRO:HD2	2.50	0.46
1:E:266:LEU:N	1:E:266:LEU:HD23	2.30	0.46
1:E:752:ILE:HG12	2:F:802:GLN:HG3	1.97	0.46
1:A:626:VAL:O	1:A:626:VAL:HG12	2.15	0.46
1:E:532:LEU:HD11	1:E:548:PHE:CZ	2.51	0.46
1:A:77:PHE:CD1	1:A:77:PHE:N	2.79	0.46
2:F:698:TYR:CB	2:F:707:LEU:HD13	2.45	0.46
1:C:425:VAL:HG12	1:C:425:VAL:O	2.14	0.46
1:C:726:LEU:HB3	1:C:749:ALA:HB2	1.98	0.46
1:A:357:VAL:HB	1:A:376:ASP:OD2	2.16	0.46
1:A:615:ILE:H	1:A:615:ILE:CD1	2.00	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:LEU:O	1:A:271:GLU:HB2	2.15	0.46
1:E:337:GLU:HG3	1:E:345:LEU:HD13	1.97	0.46
1:E:272:ARG:HD3	1:E:292:ASP:OD2	2.15	0.46
1:C:355:VAL:HG12	1:C:357:VAL:H	1.81	0.46
1:C:679:SER:O	1:C:680:ALA:C	2.54	0.46
1:C:804:ARG:HG2	2:D:818:ALA:OXT	2.16	0.46
1:C:172:GLN:HG2	3:C:815:HOH:O	2.15	0.46
2:D:723:MET:CE	2:D:726:ILE:HD12	2.46	0.46
1:A:116:SER:H	1:A:143:VAL:CG2	2.28	0.46
1:C:327:ASP:HB3	1:C:329:PHE:CZ	2.51	0.46
2:F:813:TRP:CG	2:F:814:PRO:HD2	2.51	0.46
1:C:234:ALA:HA	1:C:244:ILE:O	2.16	0.46
1:C:241:PRO:HD3	1:C:358:PHE:CZ	2.51	0.46
1:E:675:LEU:HD21	1:E:683:LYS:HB3	1.98	0.45
1:C:680:ALA:HB1	1:C:683:LYS:HG3	1.97	0.45
2:D:779:LEU:HD23	2:D:786:GLU:CG	2.45	0.45
2:D:704:PHE:CD2	2:D:726:ILE:HG21	2.51	0.45
1:A:419:TYR:CZ	1:A:424:GLU:HB2	2.50	0.45
1:E:287:ILE:HG21	1:E:300:LEU:HD11	1.97	0.45
1:C:111:TYR:HB3	1:C:123:LEU:HD21	1.98	0.45
1:A:675:LEU:O	1:A:678:GLU:HG2	2.15	0.45
1:E:454:TYR:CE2	1:E:466:ARG:HD2	2.49	0.45
1:A:471:ALA:HB2	1:A:485:ILE:CG2	2.46	0.45
1:E:806:CYS:HB2	2:F:814:PRO:HG2	1.98	0.45
1:C:78:ARG:HH12	1:C:93:PHE:HA	1.80	0.45
1:E:665:VAL:HG23	1:E:667:GLN:HG3	1.98	0.45
2:B:726:ILE:O	2:B:730:ARG:HG3	2.16	0.45
1:E:96:HIS:ND1	1:E:122:LYS:HD2	2.31	0.45
1:A:259:THR:CG2	1:A:261:LYS:H	2.29	0.45
1:E:333:ILE:HD13	1:E:586:TYR:CD2	2.50	0.45
1:C:276:ILE:HG13	1:C:277:ALA:N	2.31	0.45
2:B:703:SER:CB	2:B:706:LYS:HD2	2.46	0.45
1:A:747:TRP:CZ2	2:B:712:LEU:HD11	2.52	0.45
1:E:366:PRO:HG2	1:E:404:SER:OG	2.16	0.45
1:E:240:LEU:HA	1:E:241:PRO:HD3	1.83	0.45
1:C:615:ILE:CD1	1:C:647:GLU:HG3	2.46	0.45
1:A:753:GLN:NE2	1:A:756:LYS:HZ1	2.13	0.45
1:C:365:SER:HA	1:C:400:TRP:CD1	2.51	0.45
1:A:377:GLY:O	1:A:394:LYS:HA	2.16	0.45
1:C:69:TRP:NE1	1:C:90:VAL:HG21	2.31	0.45
1:C:336:ASN:O	1:C:337:GLU:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:THR:OG1	1:C:75:ASP:HB2	2.17	0.45
1:C:56:THR:HG21	1:C:76:ASP:H	1.81	0.45
1:C:200:TYR:HA	1:C:213:TRP:O	2.16	0.45
1:C:672:ARG:O	1:C:674:LEU:N	2.44	0.45
1:E:476:TRP:CZ3	1:E:483:VAL:HG22	2.52	0.45
1:C:543:GLY:O	1:C:544:ASP:HB2	2.16	0.45
1:E:57:PRO:HG2	1:E:75:ASP:OD2	2.17	0.45
1:A:22:HIS:HE1	1:A:84:TYR:OH	2.00	0.45
1:C:197:ASP:O	1:C:198:LYS:HG2	2.16	0.45
1:C:420:LYS:HE2	3:C:851:HOH:O	2.16	0.45
1:E:412:GLU:OE1	1:E:412:GLU:N	2.41	0.45
1:C:22:HIS:CD2	1:C:25:GLU:H	2.35	0.45
1:A:626:VAL:HG11	1:A:635:ILE:CD1	2.46	0.45
2:B:648:ASP:HB3	2:B:651:ILE:CG1	2.46	0.45
1:C:206:ASP:OD1	1:C:230:ASN:HB3	2.17	0.45
1:E:69:TRP:HA	1:E:82:PHE:O	2.17	0.45
1:C:149:ASN:HA	1:C:192:TYR:CD1	2.52	0.45
1:E:68:ASN:HA	1:E:84:TYR:CE2	2.52	0.45
1:A:809:GLU:HG3	1:A:809:GLU:H	1.36	0.45
1:A:487:ASN:ND2	1:A:488:THR:N	2.60	0.45
1:A:556:ASN:HD22	1:A:565:ASN:HA	1.79	0.45
1:E:566:LEU:HD13	1:E:599:ILE:HD11	1.98	0.45
2:F:662:LEU:HD11	2:F:688:GLN:OE1	2.17	0.45
2:B:703:SER:HB3	2:B:706:LYS:HD2	1.98	0.45
1:C:275:CYS:O	1:C:289:SER:HA	2.17	0.45
1:E:76:ASP:O	1:E:77:PHE:CB	2.65	0.45
1:C:327:ASP:HB3	1:C:329:PHE:CE1	2.52	0.45
1:A:753:GLN:HE21	1:A:756:LYS:HZ1	1.65	0.45
2:D:672:LEU:HD22	2:D:674:ASP:HB2	1.99	0.45
1:E:349:THR:HG22	1:E:350:LYS:N	2.32	0.45
1:E:334:ARG:HB2	1:E:336:ASN:OD1	2.17	0.45
1:E:602:GLU:CD	1:E:602:GLU:H	2.19	0.45
1:C:665:VAL:HG23	1:C:667:GLN:HG3	1.99	0.45
1:A:623:LEU:HB3	1:A:624:PRO:HD3	1.98	0.44
1:E:333:ILE:HG21	1:E:586:TYR:CE2	2.52	0.44
1:E:330:THR:HG22	1:E:331:ALA:N	2.31	0.44
1:E:425:VAL:HG22	1:E:428:TRP:HB2	1.99	0.44
2:F:736:MET:HB3	2:F:752:ILE:HD13	1.98	0.44
1:C:585:VAL:O	1:C:596:GLY:HA2	2.17	0.44
2:D:759:LEU:N	2:D:760:PRO:CD	2.80	0.44
1:C:555:LEU:HD13	1:C:587:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:ILE:HG23	1:E:277:ALA:HB2	1.99	0.44
1:A:425:VAL:HG22	1:A:428:TRP:HB2	2.00	0.44
1:A:379:TYR:HB3	1:A:395:CYS:SG	2.57	0.44
1:A:448:LYS:HE2	1:A:470:ASN:HB2	1.99	0.44
1:E:333:ILE:O	1:E:581:ARG:NH2	2.43	0.44
2:D:736:MET:O	2:D:740:THR:HG23	2.17	0.44
1:E:692:LEU:HD13	1:E:716:LEU:HD21	1.99	0.44
1:E:486:VAL:CG1	1:E:536:ILE:HB	2.47	0.44
1:C:499:THR:HG22	1:C:529:LEU:HD23	1.99	0.44
1:C:5:ILE:CD1	1:C:300:LEU:HD22	2.47	0.44
1:C:690:ALA:O	1:C:694:ARG:HG2	2.18	0.44
1:A:197:ASP:OD1	1:A:198:LYS:HE2	2.17	0.44
1:E:68:ASN:HA	1:E:84:TYR:CZ	2.52	0.44
1:C:266:LEU:HD12	1:C:266:LEU:N	2.32	0.44
1:A:259:THR:HG22	1:A:261:LYS:H	1.81	0.44
1:C:54:THR:OG1	1:C:56:THR:HG22	2.17	0.44
1:A:513:ASN:HB2	1:A:515:ASN:ND2	2.32	0.44
1:E:418:TYR:HB2	1:E:428:TRP:CE3	2.53	0.44
1:C:589:ASP:OD2	1:C:593:HIS:HB2	2.18	0.44
1:A:531:GLU:HG3	1:A:531:GLU:O	2.18	0.44
1:E:550:THR:HG21	1:E:554:ARG:HB3	1.99	0.44
1:C:281:THR:HG23	1:C:590:ARG:NH2	2.31	0.44
1:A:515:ASN:N	1:A:515:ASN:HD22	2.07	0.44
1:E:279:HIS:CD2	1:E:281:THR:H	2.33	0.44
1:E:643:GLU:HG2	1:E:645:TYR:OH	2.18	0.44
1:A:500:LEU:CD2	1:A:528:VAL:HG22	2.47	0.44
2:F:682:ILE:HD13	2:F:697:ILE:HD12	2.00	0.44
1:C:17:LYS:HE2	1:C:17:LYS:HA	1.99	0.44
2:F:759:LEU:HD22	2:F:759:LEU:N	2.33	0.44
1:C:672:ARG:C	1:C:674:LEU:N	2.71	0.44
2:D:733:PHE:CE2	2:D:756:GLY:HA2	2.53	0.44
1:C:118:ASP:O	1:C:119:LEU:HB2	2.18	0.44
1:E:545:VAL:HG13	1:E:559:VAL:HG22	1.99	0.44
2:F:728:GLN:HG2	2:F:736:MET:CE	2.48	0.44
1:E:532:LEU:CD2	1:E:533:SER:H	2.30	0.44
1:A:281:THR:CG2	1:A:590:ARG:HH22	2.31	0.44
1:E:438:ARG:CB	1:E:438:ARG:HH11	2.29	0.44
1:E:25:GLU:HG2	1:E:27:TRP:CE2	2.53	0.43
2:D:674:ASP:HB3	2:D:677:THR:CB	2.47	0.43
1:C:365:SER:HA	1:C:400:TRP:CG	2.53	0.43
2:F:682:ILE:HD11	2:F:697:ILE:CB	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:676:THR:HB	1:C:677:ASP:H	1.48	0.43
1:C:22:HIS:HD2	1:C:25:GLU:H	1.64	0.43
1:A:603:VAL:O	1:A:607:GLN:HG3	2.18	0.43
2:B:653:PHE:CZ	2:B:677:THR:HG23	2.53	0.43
1:C:695:PHE:N	1:C:695:PHE:CD1	2.86	0.43
1:C:89:LYS:HE3	1:C:92:ASP:CB	2.44	0.43
1:C:736:THR:CG2	1:C:736:THR:O	2.64	0.43
1:A:227:HIS:HE1	1:A:251:THR:HG22	1.84	0.43
2:B:649:PRO:CB	2:B:652:ARG:HH21	2.31	0.43
1:E:315:LEU:O	1:E:330:THR:HG23	2.17	0.43
1:C:588:ALA:HA	1:C:593:HIS:O	2.19	0.43
1:E:134:GLN:NE2	1:E:172:GLN:O	2.51	0.43
1:A:315:LEU:O	1:A:330:THR:HA	2.19	0.43
1:C:22:HIS:CD2	1:C:24:THR:H	2.33	0.43
2:F:724:GLN:HG3	2:F:728:GLN:HE21	1.84	0.43
2:D:768:ALA:HA	2:D:795:MET:HE3	1.99	0.43
1:E:309:LEU:HD22	1:E:576:LEU:HB3	2.01	0.43
1:E:124:TRP:CZ3	1:E:132:LEU:HB2	2.54	0.43
1:E:41:ASN:ND2	1:E:41:ASN:C	2.69	0.43
1:A:308:SER:O	1:A:315:LEU:HD12	2.18	0.43
1:A:227:HIS:CE1	1:A:253:LYS:HD2	2.53	0.43
1:E:201:MET:HG3	1:E:215:TYR:CD1	2.52	0.43
1:E:553:ASN:ND2	1:E:553:ASN:N	2.67	0.43
1:E:278:THR:HG22	1:E:287:ILE:HG22	2.01	0.43
1:E:804:ARG:HA	2:F:816:LYS:HB2	2.00	0.43
1:C:202:ILE:HD12	1:C:212:ILE:CD1	2.49	0.43
2:B:740:THR:HG21	2:B:749:ARG:HB2	2.00	0.43
1:E:809:GLU:CD	1:E:809:GLU:N	2.64	0.43
1:C:67:LYS:O	1:C:68:ASN:HB2	2.18	0.43
1:C:813:GLY:O	1:C:814:SER:C	2.56	0.43
1:E:660:GLU:O	1:E:660:GLU:HG2	2.19	0.43
1:E:650:ASN:N	1:E:650:ASN:ND2	2.62	0.43
1:E:345:LEU:HD11	1:E:586:TYR:HE2	1.83	0.43
1:E:281:THR:O	1:E:281:THR:HG22	2.18	0.43
1:C:696:ASN:ND2	1:C:699:LEU:HB2	2.33	0.43
1:A:357:VAL:O	1:A:359:PRO:HD3	2.18	0.43
1:E:662:ALA:HB3	1:E:671:ALA:HB2	2.00	0.43
1:C:472:LYS:HE2	1:C:486:VAL:CG1	2.48	0.43
2:D:728:GLN:O	2:D:730:ARG:N	2.41	0.43
1:A:762:SER:O	1:A:763:GLN:HB2	2.19	0.43
1:A:672:ARG:HG3	1:A:699:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:696:MET:HA	2:F:699:GLN:OE1	2.18	0.43
1:C:237:HIS:ND1	1:C:238:PRO:HD2	2.34	0.43
1:E:679:SER:O	1:E:680:ALA:C	2.56	0.43
1:E:25:GLU:HG2	1:E:27:TRP:CZ2	2.54	0.43
1:A:626:VAL:HG11	1:A:635:ILE:HD11	2.01	0.43
1:E:739:PHE:HD2	1:E:758:LEU:HD11	1.84	0.43
2:F:729:THR:C	2:F:731:GLU:H	2.22	0.43
1:C:515:ASN:N	1:C:515:ASN:HD22	2.16	0.43
2:F:724:GLN:HE22	2:F:736:MET:CA	2.31	0.43
1:A:326:SER:O	1:A:354:SER:HB2	2.19	0.43
1:E:207:ASP:OD2	1:E:207:ASP:C	2.56	0.43
1:E:53:VAL:HG23	1:E:80:ARG:HD2	2.00	0.43
1:A:53:VAL:HG13	1:A:80:ARG:HD2	2.01	0.43
1:E:626:VAL:HG21	1:E:635:ILE:CD1	2.47	0.43
1:E:675:LEU:HA	1:E:678:GLU:HB2	2.01	0.42
2:F:728:GLN:HG2	2:F:736:MET:HE3	2.00	0.42
1:A:233:PHE:CZ	1:A:246:GLY:HA3	2.54	0.42
1:E:442:GLY:HA3	1:E:476:TRP:CD1	2.53	0.42
1:C:367:ASN:ND2	3:C:824:HOH:O	2.52	0.42
1:E:128:ASN:O	1:E:129:ASN:HB3	2.19	0.42
2:F:779:LEU:HA	2:F:779:LEU:HD12	1.89	0.42
1:C:465:ARG:HG3	1:C:526:PHE:HD1	1.84	0.42
1:E:466:ARG:HB3	1:E:466:ARG:HH11	1.84	0.42
1:C:409:LEU:N	1:C:409:LEU:CD2	2.82	0.42
1:C:804:ARG:HD2	2:D:818:ALA:OXT	2.19	0.42
1:E:591:GLU:O	1:E:592:VAL:HB	2.18	0.42
1:C:168:TRP:N	1:C:168:TRP:CD1	2.87	0.42
2:B:682:ILE:HG13	2:B:697:ILE:HG21	2.01	0.42
1:C:529:LEU:HB3	1:C:530:TYR:CD1	2.54	0.42
1:A:195:LEU:HA	1:A:196:PRO:HD3	1.83	0.42
1:E:407:TYR:CE1	1:E:419:TYR:HB2	2.53	0.42
2:D:701:GLN:HG2	2:D:701:GLN:O	2.20	0.42
1:E:76:ASP:O	1:E:77:PHE:HB2	2.19	0.42
2:D:699:GLN:HG2	2:D:707:LEU:HD11	2.02	0.42
1:A:267:ASN:ND2	1:A:267:ASN:C	2.72	0.42
1:C:77:PHE:CD1	1:C:77:PHE:N	2.87	0.42
1:A:804:ARG:NH1	1:A:804:ARG:HG3	2.34	0.42
1:A:237:HIS:CG	1:A:238:PRO:HD2	2.55	0.42
1:A:237:HIS:ND1	1:A:238:PRO:HD2	2.35	0.42
1:C:697:PHE:O	1:C:701:ILE:HG13	2.19	0.42
1:C:268:VAL:HG11	1:C:296:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:685:ARG:HB2	1:C:685:ARG:HH11	1.83	0.42
1:E:310:ASP:C	1:E:310:ASP:OD2	2.58	0.42
1:E:267:ASN:C	1:E:269:GLY:H	2.23	0.42
1:C:805:VAL:HA	2:D:815:LEU:HD23	2.01	0.42
1:E:603:VAL:HG21	1:E:631:SER:HB3	2.01	0.42
1:A:234:ALA:HA	1:A:244:ILE:O	2.20	0.42
2:D:714:THR:CG2	2:D:716:ASP:HB2	2.50	0.42
1:A:120:THR:CG2	1:A:121:VAL:N	2.82	0.42
2:D:789:VAL:HG12	2:D:791:LEU:HD12	2.01	0.42
2:D:650:HIS:CE1	2:D:672:LEU:HD21	2.54	0.42
1:A:609:LEU:HB2	1:A:618:ALA:HB2	2.01	0.42
1:A:306:THR:HG22	1:A:362:LEU:CB	2.50	0.42
1:C:163:ARG:NH1	1:C:184:GLU:HG3	2.35	0.42
2:B:725:ASN:HA	2:B:728:GLN:OE1	2.18	0.42
1:C:385:LEU:HD22	1:C:386:ALA:H	1.83	0.42
1:A:412:GLU:C	1:A:414:GLY:H	2.22	0.42
1:C:106:HIS:NE2	1:C:153:PRO:HB2	2.35	0.42
2:D:720:LEU:HD21	2:D:742:TYR:HB3	2.02	0.42
1:C:56:THR:HG21	1:C:76:ASP:N	2.35	0.42
1:A:696:ASN:CG	1:A:699:LEU:HB2	2.40	0.42
1:A:475:ILE:HD13	1:A:539:GLY:O	2.20	0.42
2:D:649:PRO:HA	2:D:652:ARG:NH1	2.35	0.42
1:C:271:GLU:HB2	1:C:292:ASP:HB2	2.02	0.42
2:B:666:LEU:HG	2:B:670:LYS:HE3	2.01	0.42
1:E:233:PHE:CZ	1:E:246:GLY:HA3	2.55	0.42
1:E:532:LEU:HD23	1:E:533:SER:H	1.85	0.42
1:C:546:PHE:CE1	1:C:548:PHE:HB3	2.55	0.42
1:E:628:GLY:C	1:E:630:ASP:N	2.72	0.42
1:E:430:VAL:HG12	1:E:432:MET:HG2	2.02	0.42
1:E:102:SER:CB	1:E:145:CYS:HA	2.50	0.42
2:B:737:LEU:HA	2:B:737:LEU:HD12	1.86	0.42
1:A:120:THR:HG23	1:A:121:VAL:N	2.35	0.41
1:C:224:LEU:HD23	1:C:255:TRP:CD2	2.55	0.41
1:C:19:ILE:HG23	1:C:277:ALA:HB2	2.02	0.41
1:E:655:GLN:OE1	1:E:655:GLN:HA	2.20	0.41
1:A:330:THR:CG2	1:A:331:ALA:N	2.82	0.41
1:C:804:ARG:O	2:D:815:LEU:HA	2.21	0.41
1:E:532:LEU:HD13	1:E:536:ILE:HD11	2.01	0.41
1:E:741:LEU:HD12	1:E:741:LEU:HA	1.90	0.41
1:A:764:ARG:HD3	1:A:767:GLU:OE2	2.21	0.41
2:F:648:ASP:HA	2:F:649:PRO:HD3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:545:VAL:HG11	1:E:604:LEU:HD22	2.01	0.41
1:C:161:LEU:HA	1:C:161:LEU:HD12	1.94	0.41
1:E:283:ARG:CZ	1:E:284:LYS:HZ3	2.32	0.41
1:C:110:PRO:HA	1:C:126:TRP:CZ2	2.55	0.41
2:F:763:TYR:CZ	2:F:767:LYS:HG3	2.55	0.41
1:C:532:LEU:HD22	1:C:536:ILE:HD11	2.01	0.41
1:E:341:GLN:C	1:E:343:GLU:H	2.23	0.41
1:A:2:LYS:NZ	1:A:360:GLN:NE2	2.58	0.41
1:E:380:VAL:CG2	1:E:382:TYR:HE1	2.34	0.41
2:D:717:VAL:HG22	2:D:718:ASN:N	2.33	0.41
1:E:752:ILE:HG13	2:F:802:GLN:HG3	2.02	0.41
1:E:704:PHE:CD1	1:E:712:SER:HB3	2.55	0.41
1:E:65:ALA:C	1:E:67:LYS:N	2.73	0.41
1:E:684:TRP:HB2	1:E:707:ALA:HB2	2.03	0.41
1:A:2:LYS:HZ2	1:A:360:GLN:HE22	1.62	0.41
1:A:448:LYS:HE3	1:A:471:ALA:O	2.21	0.41
1:C:499:THR:C	1:C:500:LEU:HD23	2.40	0.41
2:D:763:TYR:CZ	2:D:767:LYS:HG3	2.56	0.41
1:C:248:GLU:O	1:C:272:ARG:HG2	2.20	0.41
1:E:777:LEU:HD23	1:E:777:LEU:HA	1.85	0.41
1:C:379:TYR:O	1:C:392:PHE:HA	2.21	0.41
1:C:436:ILE:HG23	1:C:447:VAL:HG23	2.01	0.41
2:D:745:SER:OG	2:D:748:GLU:HB2	2.21	0.41
1:A:470:ASN:ND2	1:A:470:ASN:N	2.66	0.41
1:E:155:THR:HA	1:E:168:TRP:O	2.20	0.41
1:A:316:VAL:HG22	1:A:330:THR:OG1	2.20	0.41
1:A:790:LYS:HE3	1:A:802:SER:O	2.21	0.41
1:C:482:LEU:CD2	1:C:544:ASP:HA	2.50	0.41
1:C:426:THR:O	1:C:427:SER:OG	2.29	0.41
2:B:730:ARG:O	2:B:731:GLU:CG	2.69	0.41
1:A:675:LEU:HD22	1:A:678:GLU:HB2	2.03	0.41
1:E:91:VAL:HG22	1:E:92:ASP:N	2.36	0.41
1:E:41:ASN:HD22	1:E:43:GLU:N	2.17	0.41
1:A:2:LYS:HZ2	1:A:360:GLN:NE2	2.17	0.41
1:A:432:MET:CB	1:A:436:ILE:HD11	2.51	0.41
1:E:123:LEU:CD1	1:E:133:GLU:HB3	2.46	0.41
2:B:728:GLN:HG2	2:B:736:MET:HE3	2.01	0.41
1:C:809:GLU:N	1:C:809:GLU:CD	2.73	0.41
2:D:648:ASP:HB3	2:D:651:ILE:CG1	2.50	0.41
1:C:8:THR:HG21	1:C:286:TYR:HE2	1.85	0.41
1:E:233:PHE:C	1:E:233:PHE:CD1	2.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:398:PHE:CD2	1:E:398:PHE:C	2.94	0.41
1:E:207:ASP:O	1:E:208:LEU:HB2	2.21	0.41
1:C:162:ASP:O	1:C:163:ARG:HB2	2.21	0.41
2:B:642:ALA:N	2:B:644:GLN:HE22	2.19	0.41
2:B:786:GLU:O	2:B:786:GLU:OE1	2.39	0.41
1:C:334:ARG:HG2	1:C:334:ARG:HH11	1.86	0.41
1:A:305:PRO:HD3	1:A:590:ARG:HA	2.03	0.41
2:B:740:THR:CG2	2:B:749:ARG:NE	2.72	0.41
1:A:120:THR:HG21	1:A:122:LYS:HE3	2.03	0.41
1:E:357:VAL:HG22	1:E:376:ASP:HB2	2.03	0.41
1:A:362:LEU:HA	1:A:372:THR:O	2.20	0.41
1:E:454:TYR:OH	1:E:466:ARG:HD2	2.21	0.40
1:A:33:TYR:HA	1:A:57:PRO:HB3	2.03	0.40
1:E:281:THR:O	1:E:590:ARG:NH2	2.53	0.40
1:E:95:ALA:HB3	1:E:100:ILE:HD11	2.03	0.40
1:E:500:LEU:HD22	1:E:528:VAL:HG22	2.04	0.40
1:A:615:ILE:HD11	1:A:644:TYR:OH	2.21	0.40
2:D:759:LEU:HD12	2:D:759:LEU:HA	1.81	0.40
1:A:281:THR:HG22	1:A:590:ARG:NH2	2.36	0.40
1:A:470:ASN:ND2	1:A:470:ASN:O	2.54	0.40
1:C:139:HIS:CE1	1:C:166:LYS:HD2	2.56	0.40
2:F:743:ASN:HD22	2:F:745:SER:N	2.20	0.40
1:C:284:LYS:HD2	1:C:286:TYR:CZ	2.56	0.40
2:B:789:VAL:HG12	2:B:790:THR:N	2.36	0.40
1:A:9:PHE:CD2	1:A:10:SER:N	2.90	0.40
1:E:657:GLN:O	1:E:658:LYS:C	2.59	0.40
1:A:546:PHE:CE2	1:A:548:PHE:HB3	2.56	0.40
1:E:512:ASN:HA	1:E:512:ASN:HD22	1.68	0.40
1:E:353:GLY:O	1:E:354:SER:HB3	2.21	0.40
1:A:676:THR:HG22	1:A:677:ASP:H	1.86	0.40
1:A:259:THR:HG23	1:A:261:LYS:CG	2.51	0.40
1:C:465:ARG:HD2	1:C:467:ILE:CD1	2.51	0.40
1:C:224:LEU:N	1:C:224:LEU:CD1	2.84	0.40
1:A:418:TYR:CB	1:A:428:TRP:CD2	3.04	0.40
1:C:575:LEU:HD21	1:C:585:VAL:CG1	2.52	0.40
1:E:185:ARG:HD2	1:E:206:ASP:CB	2.51	0.40
1:C:532:LEU:HD12	1:C:532:LEU:N	2.36	0.40
1:C:763:GLN:HA	1:C:765:PHE:CE1	2.57	0.40
1:C:556:ASN:HD22	1:C:565:ASN:HA	1.85	0.40
1:C:270:LEU:O	1:C:271:GLU:HB2	2.21	0.40
1:E:383:THR:O	1:E:387:TRP:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:692:LEU:HD11	2:F:761:LEU:CD1	2.52	0.40
1:A:202:ILE:HD11	1:A:210:ILE:CG2	2.51	0.40
1:C:793:LEU:HD23	1:C:802:SER:HA	2.04	0.40
1:A:240:LEU:HB2	1:A:242:ILE:HG12	2.03	0.40
1:C:176:ASN:O	1:C:177:PHE:HB3	2.20	0.40
2:D:682:ILE:HD11	2:D:697:ILE:CG2	2.52	0.40
2:F:648:ASP:OD1	2:F:651:ILE:HG13	2.22	0.40
1:C:158:SER:O	1:C:165:VAL:HA	2.21	0.40
1:C:713:LEU:HG	1:C:717:HIS:CD2	2.56	0.40
1:E:668:LEU:O	1:E:672:ARG:HB2	2.22	0.40
1:A:443:ALA:HB3	1:A:476:TRP:CZ3	2.57	0.40
1:E:764:ARG:HB3	1:E:767:GLU:OE1	2.22	0.40
1:E:421:ASN:O	1:E:422:PHE:HB2	2.21	0.40
1:A:161:LEU:HD23	1:A:161:LEU:HA	1.85	0.40
1:C:558:PHE:CZ	1:C:561:GLY:HA2	2.57	0.40
1:A:320:GLY:O	1:A:321:LYS:C	2.60	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	809/814 (99%)	755 (93%)	43 (5%)	11 (1%)	14 24
1	C	807/814 (99%)	741 (92%)	55 (7%)	11 (1%)	14 24
1	E	806/814 (99%)	749 (93%)	43 (5%)	14 (2%)	11 19
2	B	175/177 (99%)	168 (96%)	7 (4%)	0	100 100
2	D	175/177 (99%)	153 (87%)	17 (10%)	5 (3%)	6 8
2	F	173/177 (98%)	166 (96%)	7 (4%)	0	100 100
All	All	2945/2973 (99%)	2732 (93%)	172 (6%)	41 (1%)	14 24

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	339	VAL
1	A	493	ASP
1	A	494	GLU
1	C	336	ASN
1	C	679	SER
1	C	680	ALA
1	E	354	SER
1	E	592	VAL
1	E	676	THR
1	A	321	LYS
1	A	353	GLY
1	A	385	LEU
1	A	680	ALA
1	C	337	GLU
1	C	678	GLU
1	E	339	VAL
1	E	411	ASP
1	E	680	ALA
1	A	271	GLU
1	A	433	HIS
1	C	376	ASP
2	D	673	ASN
2	D	730	ARG
1	E	271	GLU
1	E	489	ASN
1	A	678	GLU
1	C	264	LYS
1	C	271	GLU
1	C	281	THR
1	C	673	ASP
2	D	773	ALA
1	E	66	ARG
1	E	184	GLU
1	C	280	PRO
2	D	785	ASP
2	D	754	ALA
1	E	342	ASP
1	A	469	VAL
1	E	153	PRO
1	E	268	VAL
1	E	23	PRO

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	698/700 (100%)	647 (93%)	51 (7%)	17	32
1	C	698/700 (100%)	643 (92%)	55 (8%)	15	28
1	E	697/700 (100%)	641 (92%)	56 (8%)	15	28
2	B	148/148 (100%)	136 (92%)	12 (8%)	15	27
2	D	148/148 (100%)	138 (93%)	10 (7%)	20	36
2	F	147/148 (99%)	136 (92%)	11 (8%)	17	31
All	All	2536/2544 (100%)	2341 (92%)	195 (8%)	16	30

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	16	VAL
1	A	41	ASN
1	A	49	ARG
1	A	77	PHE
1	A	119	LEU
1	A	120	THR
1	A	123	LEU
1	A	149	ASN
1	A	155	THR
1	A	170	LEU
1	A	251	THR
1	A	252	LEU
1	A	259	THR
1	A	267	ASN
1	A	307	LEU
1	A	336	ASN
1	A	337	GLU
1	A	342	ASP
1	A	343	GLU
1	A	367	ASN
1	A	425	VAL

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Mol	Chain	Res	Type
1	A	444	LEU
1	A	447	VAL
1	A	465	ARG
1	A	468	ASP
1	A	470	ASN
1	A	478	ASP
1	A	487	ASN
1	A	491	ASN
1	A	515	ASN
1	A	550	THR
1	A	571	LYS
1	A	576	LEU
1	A	604	LEU
1	A	615	ILE
1	A	617	GLU
1	A	639	LEU
1	A	655	GLN
1	A	665	VAL
1	A	679	SER
1	A	682	MET
1	A	699	LEU
1	A	724	GLU
1	A	738	LYS
1	A	741	LEU
1	A	771	LEU
1	A	793	LEU
1	A	800	THR
1	A	805	VAL
1	A	809	GLU
2	B	643	LEU
2	B	644	GLN
2	B	662	LEU
2	B	679	GLU
2	B	686	LEU
2	B	714	THR
2	B	740	THR
2	B	759	LEU
2	B	761	LEU
2	B	786	GLU
2	B	796	ASP
2	B	810	LEU
1	C	8	THR

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Mol	Chain	Res	Type
1	C	10	SER
1	C	41	ASN
1	C	55	GLU
1	C	77	PHE
1	C	89	LYS
1	C	119	LEU
1	C	123	LEU
1	C	132	LEU
1	C	155	THR
1	C	161	LEU
1	C	170	LEU
1	C	184	GLU
1	C	251	THR
1	C	256	ASN
1	C	281	THR
1	C	297	VAL
1	C	307	LEU
1	C	309	LEU
1	C	310	ASP
1	C	327	ASP
1	C	336	ASN
1	C	356	ASP
1	C	385	LEU
1	C	395	CYS
1	C	409	LEU
1	C	412	GLU
1	C	438	ARG
1	C	447	VAL
1	C	465	ARG
1	C	487	ASN
1	C	503	ASN
1	C	512	ASN
1	C	528	VAL
1	C	529	LEU
1	C	530	TYR
1	C	545	VAL
1	C	566	LEU
1	C	575	LEU
1	C	576	LEU
1	C	583	ASN
1	C	604	LEU
1	C	627	GLU

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Mol	Chain	Res	Type
1	C	649	LEU
1	C	660	GLU
1	C	672	ARG
1	C	677	ASP
1	C	694	ARG
1	C	715	LEU
1	C	726	LEU
1	C	740	ASN
1	C	758	LEU
1	C	759	LEU
1	C	793	LEU
1	C	799	ASN
2	D	672	LEU
2	D	707	LEU
2	D	710	LEU
2	D	714	THR
2	D	717	VAL
2	D	728	GLN
2	D	747	LYS
2	D	748	GLU
2	D	759	LEU
2	D	779	LEU
1	E	1	MET
1	E	3	LEU
1	E	30	THR
1	E	41	ASN
1	E	53	VAL
1	E	66	ARG
1	E	72	VAL
1	E	129	ASN
1	E	149	ASN
1	E	161	LEU
1	E	168	TRP
1	E	184	GLU
1	E	214	ASP
1	E	240	LEU
1	E	266	LEU
1	E	267	ASN
1	E	297	VAL
1	E	302	ASN
1	E	307	LEU
1	E	337	GLU

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Mol	Chain	Res	Type
1	E	352	LEU
1	E	356	ASP
1	E	357	VAL
1	E	385	LEU
1	E	390	LYS
1	E	395	CYS
1	E	425	VAL
1	E	438	ARG
1	E	441	SER
1	E	463	LEU
1	E	465	ARG
1	E	466	ARG
1	E	482	LEU
1	E	483	VAL
1	E	487	ASN
1	E	503	ASN
1	E	512	ASN
1	E	532	LEU
1	E	550	THR
1	E	576	LEU
1	E	598	GLU
1	E	611	LEU
1	E	620	GLU
1	E	623	LEU
1	E	632	LEU
1	E	650	ASN
1	E	672	ARG
1	E	673	ASP
1	E	676	THR
1	E	693	GLN
1	E	715	LEU
1	E	722	ASN
1	E	724	GLU
1	E	726	LEU
1	E	779	ASP
1	E	793	LEU
2	F	648	ASP
2	F	667	ASP
2	F	673	ASN
2	F	675	SER
2	F	696	MET
2	F	720	LEU

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Mol	Chain	Res	Type
2	F	740	THR
2	F	743	ASN
2	F	779	LEU
2	F	785	ASP
2	F	805	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	41	ASN
1	A	68	ASN
1	A	149	ASN
1	A	172	GLN
1	A	176	ASN
1	A	183	GLN
1	A	256	ASN
1	A	267	ASN
1	A	322	ASN
1	A	336	ASN
1	A	341	GLN
1	A	360	GLN
1	A	367	ASN
1	A	405	ASN
1	A	421	ASN
1	A	470	ASN
1	A	487	ASN
1	A	491	ASN
1	A	515	ASN
1	A	556	ASN
1	A	655	GLN
1	A	667	GLN
1	A	706	ASN
1	A	708	HIS
1	A	740	ASN
1	A	744	ASN
1	A	753	GLN
1	A	783	ASN
2	B	718	ASN
2	B	725	ASN
2	B	739	ASN
2	B	794	GLN

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Mol	Chain	Res	Type
1	C	22	HIS
1	C	41	ASN
1	C	52	GLN
1	C	68	ASN
1	C	139	HIS
1	C	176	ASN
1	C	183	GLN
1	C	227	HIS
1	C	256	ASN
1	C	279	HIS
1	C	336	ASN
1	C	360	GLN
1	C	396	GLN
1	C	405	ASN
1	C	421	ASN
1	C	487	ASN
1	C	503	ASN
1	C	512	ASN
1	C	513	ASN
1	C	515	ASN
1	C	556	ASN
1	C	655	GLN
1	C	693	GLN
1	C	799	ASN
2	D	644	GLN
2	D	647	GLN
2	D	688	GLN
2	D	702	HIS
2	D	724	GLN
2	D	725	ASN
2	D	728	GLN
2	D	739	ASN
2	D	744	ASN
1	E	22	HIS
1	E	41	ASN
1	E	68	ASN
1	E	128	ASN
1	E	129	ASN
1	E	149	ASN
1	E	176	ASN
1	E	183	GLN
1	E	256	ASN

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Mol	Chain	Res	Type
1	E	267	ASN
1	E	279	HIS
1	E	285	ASN
1	E	360	GLN
1	E	405	ASN
1	E	415	GLN
1	E	421	ASN
1	E	487	ASN
1	E	489	ASN
1	E	503	ASN
1	E	512	ASN
1	E	513	ASN
1	E	553	ASN
1	E	565	ASN
1	E	650	ASN
1	E	706	ASN
1	E	708	HIS
1	E	717	HIS
1	E	722	ASN
1	E	753	GLN
2	F	644	GLN
2	F	673	ASN
2	F	724	GLN
2	F	728	GLN
2	F	739	ASN
2	F	743	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	811/814 (99%)	0.05	23 (2%) 56 61	17, 39, 62, 84	0
1	C	811/814 (99%)	0.14	29 (3%) 46 51	20, 43, 66, 89	0
1	E	810/814 (99%)	0.13	20 (2%) 61 65	19, 42, 67, 89	0
2	B	177/177 (100%)	0.18	6 (3%) 49 54	29, 44, 68, 74	0
2	D	177/177 (100%)	0.65	12 (6%) 20 23	32, 55, 77, 83	0
2	F	175/177 (98%)	0.40	10 (5%) 27 31	30, 53, 73, 80	0
All	All	2961/2973 (99%)	0.16	100 (3%) 49 54	17, 43, 68, 89	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	818	ALA	9.3
1	C	814	SER	7.5
2	B	818	ALA	7.1
1	C	679	SER	6.3
1	A	676	THR	5.8
1	C	491	ASN	5.6
1	E	490	SER	5.6
1	A	353	GLY	5.3
2	D	785	ASP	4.7
1	C	813	GLY	4.6
1	A	338	GLU	4.6
2	B	642	ALA	4.5
1	C	490	SER	4.3
1	A	491	ASN	4.3
2	D	731	GLU	4.2
1	A	339	VAL	4.1
1	E	427	SER	4.0
1	A	493	ASP	4.0
1	E	433	HIS	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	385	LEU	3.9
1	C	676	THR	3.8
2	B	787	GLN	3.8
1	E	739	PHE	3.6
1	C	338	GLU	3.6
2	F	642	ALA	3.6
1	E	340	GLU	3.6
1	E	676	THR	3.5
2	F	816	LYS	3.5
1	E	677	ASP	3.4
1	A	490	SER	3.4
1	E	339	VAL	3.4
2	D	718	ASN	3.4
1	C	433	HIS	3.4
1	C	427	SER	3.3
1	C	339	VAL	3.3
1	A	678	GLU	3.2
1	C	322	ASN	3.2
2	D	817	GLU	3.2
1	E	797	GLY	3.1
1	A	433	HIS	3.1
2	D	787	GLN	3.1
2	F	785	ASP	3.0
1	E	2	LYS	2.9
2	F	787	GLN	2.9
1	E	4	ASP	2.9
2	D	722	LYS	2.8
1	A	386	ALA	2.8
1	E	794	ILE	2.8
2	D	642	ALA	2.7
1	C	348	GLN	2.7
1	C	627	GLU	2.6
2	F	718	ASN	2.6
1	E	627	GLU	2.6
1	A	660	GLU	2.5
1	C	88	GLU	2.5
1	E	426	THR	2.5
1	C	809	GLU	2.5
1	E	629	LYS	2.5
2	D	721	SER	2.5
1	A	494	GLU	2.5
1	A	336	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	629	LYS	2.5
1	E	680	ALA	2.5
2	F	679	GLU	2.4
1	A	492	GLY	2.4
1	C	450	ASP	2.4
1	E	185	ARG	2.3
1	C	343	GLU	2.3
1	E	338	GLU	2.3
1	E	1	MET	2.3
1	A	627	GLU	2.3
2	F	731	GLU	2.2
1	A	366	PRO	2.2
1	A	348	GLN	2.2
1	A	679	SER	2.2
1	C	412	GLU	2.2
2	F	672	LEU	2.2
2	F	717	VAL	2.1
1	C	495	ALA	2.1
2	B	817	GLU	2.1
1	A	587	LEU	2.1
1	E	342	ASP	2.1
1	C	302	ASN	2.1
1	A	322	ASN	2.1
1	C	376	ASP	2.1
1	C	494	GLU	2.1
2	F	702	HIS	2.1
1	C	597	TYR	2.1
1	C	431	PRO	2.1
1	A	343	GLU	2.1
1	C	2	LYS	2.1
2	D	667	ASP	2.1
1	C	808	ALA	2.1
1	C	628	GLY	2.1
1	A	2	LYS	2.1
2	D	700	THR	2.1
2	B	731	GLU	2.0
2	B	783	GLU	2.0
1	C	340	GLU	2.0
2	D	761	LEU	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.