Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 07:15 PM GMT

PDB ID	:	1EQR
Title	:	CRYSTAL STRUCTURE OF FREE ASPARTYL-TRNA SYNTHETASE FROM ESCHERICHIA COLI
Authors	:	Rees, B.; Webster, G.; Delarue, M.; Boeglin, M.; Moras, D.
Deposited on	:	2000-04-06
Resolution	:	2.70 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:

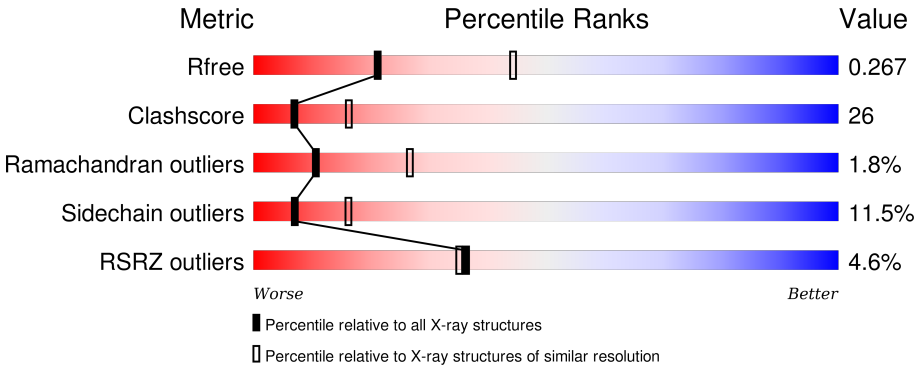
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	590	4% 55% 37% 8%
1	B	590	4% 54% 39% 6%
1	C	590	5% 52% 41% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14323 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 ASPARTYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	590	Total	C	N	O	S	0	0	0
			4631	2922	812	871	26			
1	B	590	Total	C	N	O	S	0	0	0
			4631	2922	812	871	26			
1	C	590	Total	C	N	O	S	0	0	0
			4631	2922	812	871	26			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is water.

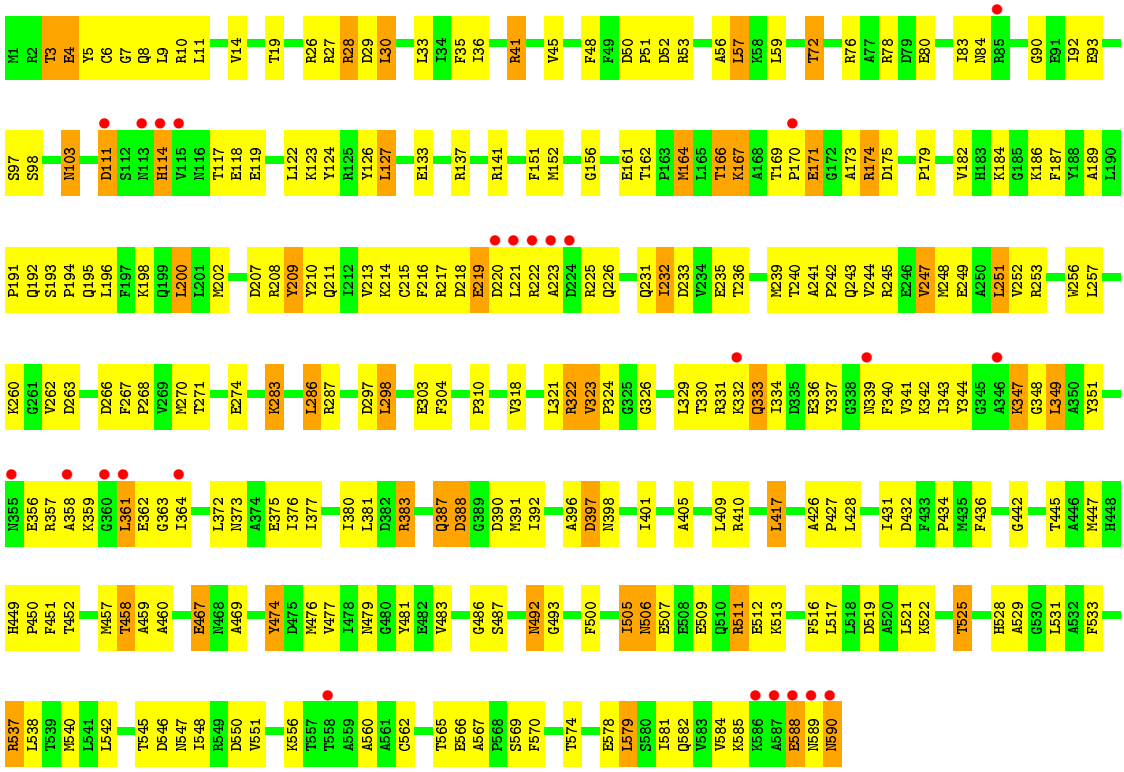
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	148	Total	O	0	0
			148	148		
3	B	131	Total	O	0	0
			131	131		
3	C	148	Total	O	0	0
			148	148		

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.

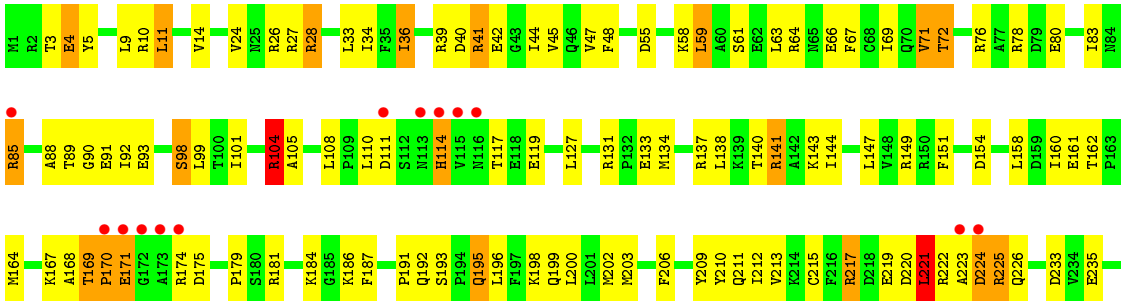
- Molecule 1: ASPARTYL-TRNA SYNTHETASE

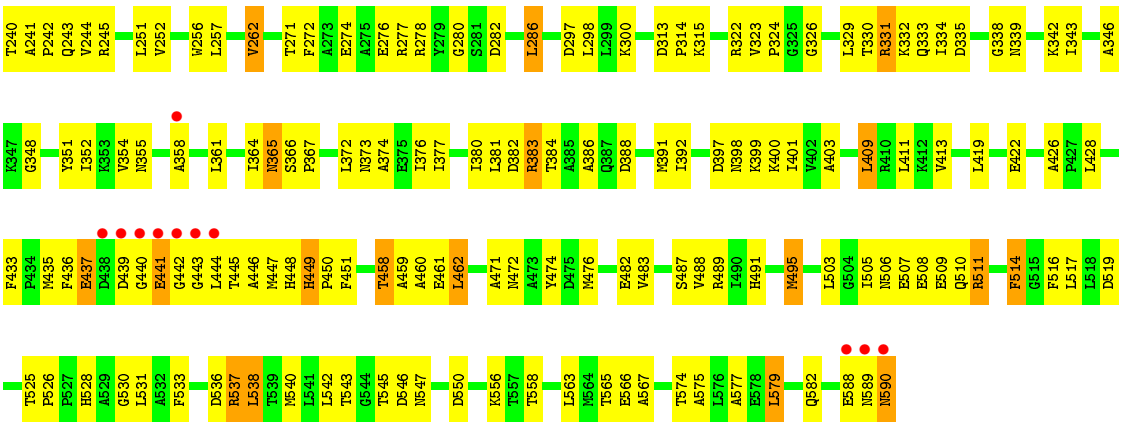
Chain A:



- Molecule 1: ASPARTYL-TRNA SYNTHETASE

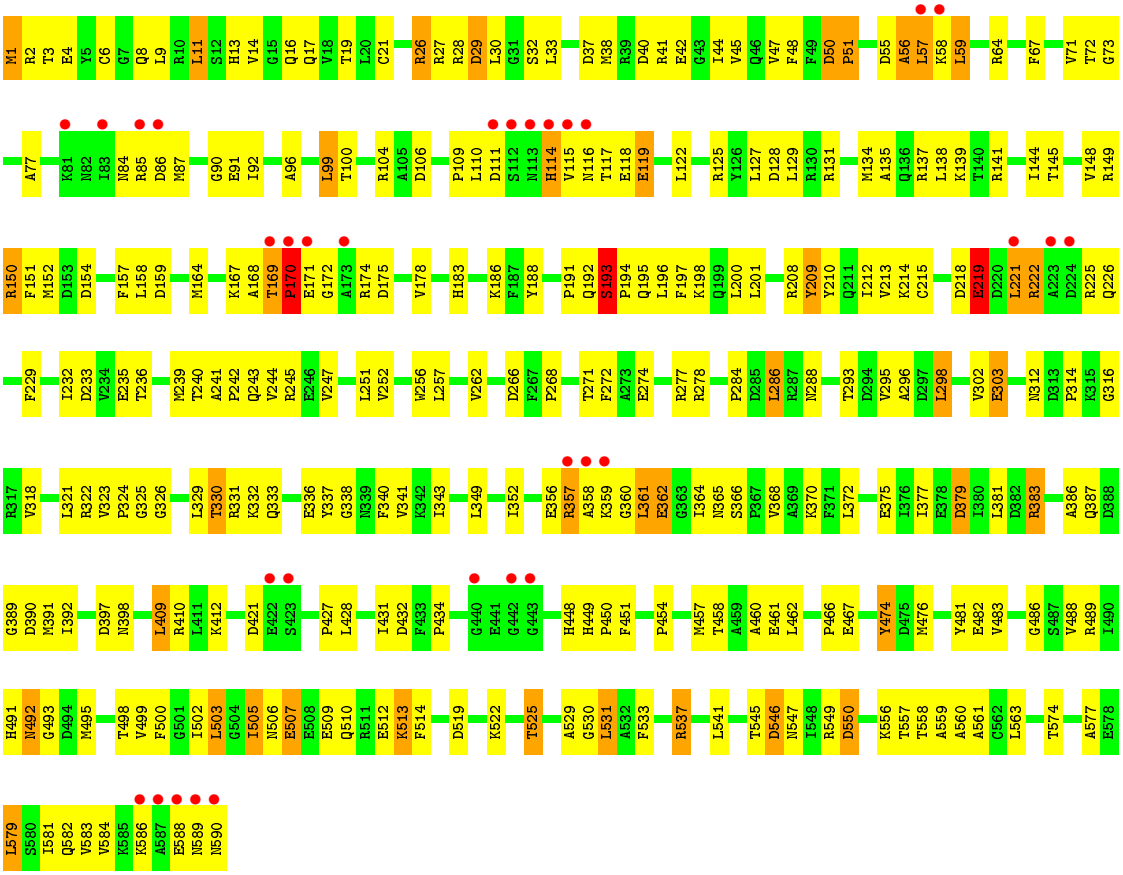
Chain B:





• Molecule 1: ASPARTYL-TRNA SYNTHETASE

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	117.75Å 161.96Å 131.60Å 90.00° 110.36° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 29.46 – 2.65	Depositor EDS
% Data completeness (in resolution range)	90.2 (20.00-2.70) 90.4 (29.46-2.65)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.59 (at 2.64Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.198 , 0.269 0.197 , 0.267	Depositor DCC
R_{free} test set	2803 reflections (4.91%)	DCC
Wilson B-factor (Å^2)	34.7	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 60.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 60593 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14323	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.54	0/4717	0.77	1/6372 (0.0%)
1	B	0.55	1/4717 (0.0%)	0.78	2/6372 (0.0%)
1	C	0.49	0/4717	0.73	0/6372
All	All	0.53	1/14151 (0.0%)	0.76	3/19116 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	482	GLU	CB-CG	5.90	1.63	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	206	PHE	N-CA-C	-5.63	95.81	111.00
1	B	482	GLU	OE1-CD-OE2	-5.10	117.17	123.30
1	A	232	ILE	N-CA-C	-5.08	97.30	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	4631	0	4626	255	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4631	0	4626	252	0
1	C	4631	0	4626	251	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	148	0	0	13	0
3	B	131	0	0	12	0
3	C	148	0	0	14	0
All	All	14323	0	13878	735	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (735) 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:50:ASP:O	1:C:57:LEU:HG	1.47	1.15
1:A:51:PRO:HA	1:A:57:LEU:HD12	1.29	1.12
1:B:511:ARG:HH11	1:B:511:ARG:HG3	1.17	1.07
1:A:585:LYS:HB2	1:A:588:GLU:HB3	1.35	1.04
1:C:236:THR:HB	1:C:239:MET:HE3	1.40	1.02
1:B:240:THR:H	1:B:243:GLN:HE21	1.06	0.96
1:B:69:ILE:HG22	1:B:101:ILE:HA	1.46	0.94
1:B:226:GLN:HE22	1:B:556:LYS:H	1.10	0.93
1:C:240:THR:H	1:C:243:GLN:HE21	1.08	0.93
1:C:59:LEU:H	1:C:59:LEU:CD1	1.81	0.92
1:B:171:GLU:CG	1:B:192:GLN:HG3	2.01	0.91
1:C:225:ARG:HB3	1:C:225:ARG:HH11	1.34	0.91
1:A:347:LYS:HG3	1:A:348:GLY:H	1.33	0.91
1:A:170:PRO:HD3	1:A:513:LYS:HD2	1.53	0.91
1:A:240:THR:H	1:A:243:GLN:HE21	1.15	0.91
1:A:357:ARG:NH1	1:A:357:ARG:HB3	1.87	0.90
1:A:398:ASN:HD22	1:A:401:ILE:HG12	1.35	0.90
1:C:505:ILE:HG13	1:C:509:GLU:HG3	1.56	0.88
1:B:330:THR:HG22	1:B:332:LYS:H	1.36	0.88
1:B:161:GLU:HA	1:B:211:GLN:NE2	1.88	0.87
1:C:55:ASP:O	1:C:59:LEU:HD13	1.76	0.86
1:C:356:GLU:OE1	1:C:359:LYS:HD2	1.74	0.86
1:A:222:ARG:HB2	1:A:225:ARG:HG3	1.58	0.85
1:A:240:THR:H	1:A:243:GLN:NE2	1.73	0.84
1:C:170:PRO:HB3	3:C:1016:HOH:O	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:511:ARG:NH1	1:B:511:ARG:HG3	1.87	0.83
1:B:27:ARG:HG3	1:B:36:ILE:HG13	1.57	0.83
1:C:171:GLU:HG2	1:C:172:GLY:H	1.43	0.82
1:A:182:VAL:HG21	1:B:221:LEU:HD11	1.60	0.81
1:A:186:LYS:HE3	1:C:303:GLU:HG3	1.61	0.81
1:B:240:THR:H	1:B:243:GLN:NE2	1.78	0.80
1:A:434:PRO:HG2	1:A:447:MET:HG3	1.62	0.80
1:C:458:THR:HB	1:C:461:GLU:HG3	1.60	0.80
1:C:226:GLN:HE22	1:C:556:LYS:H	1.26	0.80
1:A:226:GLN:HE22	1:A:556:LYS:H	1.28	0.80
1:A:333:GLN:O	1:A:336:GLU:HG2	1.81	0.80
1:A:166:THR:HG23	1:A:167:LYS:N	1.97	0.79
1:C:271:THR:OG1	1:C:274:GLU:HG3	1.81	0.79
1:B:329:LEU:HA	3:B:979:HOH:O	1.80	0.79
1:A:78:ARG:HD2	1:A:92:ILE:O	1.82	0.79
1:B:36:ILE:HG22	1:B:47:VAL:CG1	2.12	0.78
1:B:331:ARG:HH22	1:C:118:GLU:HB3	1.48	0.78
1:C:59:LEU:H	1:C:59:LEU:HD13	1.48	0.78
1:C:482:GLU:OE2	3:C:1042:HOH:O	2.00	0.78
1:B:64:ARG:HB2	1:B:67:PHE:CE1	2.18	0.78
1:A:141:ARG:HD3	3:B:911:HOH:O	1.81	0.78
1:C:149:ARG:NH1	1:C:212:ILE:HD12	1.99	0.78
1:B:458:THR:HG22	1:B:460:ALA:H	1.49	0.78
1:A:357:ARG:HB3	1:A:357:ARG:HH11	1.49	0.77
1:C:359:LYS:O	1:C:362:GLU:HG3	1.84	0.77
1:B:252:VAL:HG21	1:B:476:MET:SD	2.24	0.77
1:B:240:THR:HG23	1:B:243:GLN:NE2	1.99	0.77
1:B:192:GLN:O	1:B:215:CYS:HB3	1.85	0.77
1:C:330:THR:HG22	1:C:333:GLN:H	1.46	0.77
1:A:192:GLN:O	1:A:215:CYS:HB3	1.84	0.76
1:B:342:LYS:NZ	1:B:348:GLY:HA2	2.01	0.76
1:A:506:ASN:ND2	1:A:509:GLU:H	1.84	0.76
1:A:221:LEU:HD11	1:A:560:ALA:HB2	1.67	0.76
1:B:85:ARG:HB2	1:B:85:ARG:NH1	2.01	0.76
1:C:225:ARG:NH1	1:C:225:ARG:HB3	2.01	0.76
1:C:329:LEU:HD21	1:C:337:TYR:HE2	1.50	0.76
1:A:506:ASN:ND2	1:A:509:GLU:HG3	2.00	0.76
1:C:458:THR:HG22	1:C:460:ALA:H	1.50	0.76
1:B:169:THR:N	1:B:170:PRO:HD3	2.01	0.75
1:C:194:PRO:HG2	1:C:213:VAL:HG11	1.68	0.75
1:B:169:THR:HG23	1:B:169:THR:O	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ARG:HH11	1:A:357:ARG:CB	1.99	0.75
1:A:506:ASN:C	1:A:506:ASN:HD22	1.90	0.75
1:C:169:THR:HB	1:C:170:PRO:CD	2.16	0.75
1:B:545:THR:HG22	1:B:547:ASN:H	1.50	0.75
1:C:330:THR:HG23	1:C:332:LYS:H	1.51	0.74
1:A:174:ARG:HH22	1:B:579:LEU:HD22	1.52	0.74
1:A:174:ARG:HB2	1:A:219:GLU:OE2	1.87	0.74
1:C:236:THR:CB	1:C:239:MET:HE3	2.16	0.74
1:A:166:THR:HG23	1:A:167:LYS:H	1.52	0.74
1:B:59:LEU:HB2	1:B:99:LEU:HD23	1.68	0.74
1:C:208:ARG:HE	1:C:239:MET:HE2	1.52	0.74
1:B:241:ALA:HB3	1:B:242:PRO:HD3	1.69	0.74
1:A:72:THR:HG23	1:A:98:SER:HB3	1.70	0.74
1:C:59:LEU:N	1:C:59:LEU:CD1	2.51	0.74
1:B:171:GLU:HG3	1:B:192:GLN:HG3	1.67	0.73
1:A:166:THR:CG2	1:A:167:LYS:N	2.51	0.73
1:A:26:ARG:NH1	1:A:28:ARG:HB2	2.02	0.73
1:C:509:GLU:O	1:C:513:LYS:HG3	1.89	0.73
1:B:223:ALA:O	1:B:224:ASP:HB3	1.87	0.73
1:C:170:PRO:CG	1:C:513:LYS:HD2	2.19	0.73
1:B:111:ASP:HB3	1:B:114:HIS:ND1	2.04	0.72
1:B:72:THR:HG23	1:B:98:SER:HB3	1.72	0.72
1:B:240:THR:N	1:B:243:GLN:HE21	1.84	0.72
1:B:119:GLU:HG2	3:C:1019:HOH:O	1.88	0.72
1:C:64:ARG:HB2	1:C:67:PHE:CE1	2.25	0.71
1:C:192:GLN:O	1:C:193:SER:OG	2.07	0.71
1:A:3:THR:HG22	1:A:4:GLU:OE1	1.91	0.71
1:B:346:ALA:HA	3:B:924:HOH:O	1.91	0.71
1:A:589:ASN:O	1:A:590:ASN:HB2	1.91	0.70
1:B:324:PRO:HG2	1:B:419:LEU:HD13	1.73	0.70
1:B:221:LEU:HB2	1:B:558:THR:O	1.92	0.69
1:A:247:VAL:HG22	1:A:248:MET:HE3	1.73	0.69
1:C:55:ASP:O	1:C:56:ALA:O	2.09	0.69
1:C:498:THR:O	1:C:502:ILE:HG13	1.92	0.69
1:B:545:THR:HG21	1:B:550:ASP:HB2	1.74	0.69
1:C:150:ARG:O	1:C:154:ASP:HB2	1.93	0.69
1:B:277:ARG:HH22	1:B:278:ARG:HH21	1.40	0.69
1:B:330:THR:O	1:B:334:ILE:HG13	1.92	0.69
1:B:33:LEU:HD13	1:B:48:PHE:HZ	1.58	0.69
1:A:588:GLU:HG3	1:A:589:ASN:H	1.59	0.68
1:B:36:ILE:HG22	1:B:47:VAL:HG12	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:547:ASN:O	1:C:550:ASP:HB2	1.93	0.68
1:C:333:GLN:O	1:C:336:GLU:HG2	1.93	0.68
1:C:506:ASN:HB2	3:C:958:HOH:O	1.92	0.68
1:C:296:ALA:HB2	3:C:911:HOH:O	1.91	0.68
1:B:219:GLU:HG2	1:B:220:ASP:H	1.58	0.68
1:C:505:ILE:HD12	1:C:513:LYS:HE2	1.75	0.68
1:B:240:THR:O	1:B:244:VAL:HG23	1.94	0.68
1:B:33:LEU:HB3	1:B:48:PHE:HE1	1.59	0.68
1:B:27:ARG:HG3	1:B:36:ILE:CG1	2.23	0.68
1:A:53:ARG:HD2	1:A:97:SER:HA	1.76	0.68
1:A:492:ASN:HD22	1:A:493:GLY:N	1.92	0.67
1:B:330:THR:HG22	1:B:332:LYS:N	2.07	0.67
1:A:506:ASN:HD21	1:A:509:GLU:HG3	1.59	0.67
1:A:356:GLU:HG2	1:A:358:ALA:HB3	1.77	0.67
1:A:545:THR:HG22	1:A:547:ASN:H	1.59	0.67
1:B:4:GLU:HG3	3:B:928:HOH:O	1.94	0.67
1:B:286:LEU:HD22	1:B:428:LEU:HD22	1.75	0.67
1:B:226:GLN:HE22	1:B:556:LYS:N	1.90	0.66
1:B:574:THR:O	1:B:577:ALA:HB3	1.94	0.66
1:B:11:LEU:O	1:B:14:VAL:HG23	1.95	0.66
1:B:511:ARG:CG	1:B:511:ARG:HH11	2.03	0.66
1:A:198:LYS:HE3	1:A:235:GLU:OE1	1.95	0.66
1:B:588:GLU:O	1:B:590:ASN:N	2.27	0.66
1:A:321:LEU:HD23	1:A:409:LEU:HD12	1.76	0.66
1:C:492:ASN:HD22	1:C:492:ASN:C	1.98	0.66
1:C:169:THR:HB	1:C:170:PRO:HD2	1.77	0.66
1:A:240:THR:N	1:A:243:GLN:HE21	1.92	0.66
1:A:226:GLN:NE2	1:A:556:LYS:H	1.93	0.66
1:B:210:TYR:HA	1:B:233:ASP:O	1.94	0.66
1:B:458:THR:HG22	1:B:460:ALA:N	2.11	0.66
1:A:51:PRO:CA	1:A:57:LEU:HD12	2.18	0.66
1:B:459:ALA:HA	1:B:495:MET:CE	2.26	0.65
1:C:56:ALA:O	1:C:58:LYS:N	2.29	0.65
1:C:51:PRO:HA	1:C:57:LEU:CD1	2.27	0.65
1:C:171:GLU:HG2	1:C:172:GLY:N	2.10	0.65
1:C:241:ALA:HB3	1:C:242:PRO:HD3	1.79	0.65
1:A:7:GLY:O	1:A:10:ARG:NH2	2.30	0.65
1:A:481:TYR:HB3	1:A:537:ARG:HD3	1.78	0.65
1:A:56:ALA:HB3	3:A:969:HOH:O	1.96	0.65
1:A:588:GLU:HG3	1:A:589:ASN:N	2.11	0.65
1:A:248:MET:CE	1:A:248:MET:HA	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:ALA:HA	1:B:495:MET:HE2	1.79	0.64
1:A:565:THR:HG22	1:B:516:PHE:CE1	2.31	0.64
1:B:59:LEU:H	1:B:59:LEU:HD12	1.63	0.64
1:C:59:LEU:N	1:C:59:LEU:HD12	2.11	0.64
1:C:170:PRO:CD	1:C:513:LYS:HD2	2.26	0.64
1:C:361:LEU:H	1:C:361:LEU:HD23	1.61	0.64
1:B:342:LYS:HZ1	1:B:348:GLY:HA2	1.60	0.64
1:A:111:ASP:HB3	1:A:114:HIS:CD2	2.33	0.64
1:A:240:THR:O	1:A:244:VAL:HG23	1.97	0.64
1:B:326:GLY:O	1:B:329:LEU:HB2	1.98	0.64
1:C:193:SER:HA	1:C:215:CYS:SG	2.38	0.64
1:A:341:VAL:HG11	1:A:349:LEU:HD13	1.80	0.64
1:B:134:MET:HE3	3:B:989:HOH:O	1.96	0.64
1:B:352:ILE:HA	1:B:366:SER:HB2	1.80	0.63
1:C:323:VAL:CG2	1:C:326:GLY:HA3	2.28	0.63
1:A:208:ARG:HE	1:A:239:MET:HE2	1.63	0.63
1:B:274:GLU:HG2	1:B:278:ARG:NH2	2.13	0.63
1:A:356:GLU:O	1:A:363:GLY:HA3	1.99	0.63
1:C:9:LEU:HD12	1:C:45:VAL:HG21	1.80	0.63
1:A:347:LYS:HG3	1:A:348:GLY:N	2.10	0.63
1:C:499:VAL:HG12	1:C:503:LEU:HD22	1.80	0.63
1:A:585:LYS:HB2	1:A:588:GLU:CB	2.22	0.63
1:B:169:THR:O	1:B:169:THR:CG2	2.47	0.63
3:A:930:HOH:O	1:B:141:ARG:HD3	1.98	0.62
1:C:547:ASN:OD1	1:C:549:ARG:NH1	2.32	0.62
1:A:409:LEU:HD13	1:A:409:LEU:O	1.99	0.62
1:A:33:LEU:HD22	1:A:48:PHE:HE1	1.64	0.62
1:B:26:ARG:NH2	1:B:28:ARG:HG3	2.13	0.62
1:B:240:THR:OG1	1:B:243:GLN:HG3	2.00	0.62
1:C:170:PRO:HB3	1:C:174:ARG:HH12	1.64	0.62
1:C:340:PHE:CE2	1:C:412:LYS:HD2	2.35	0.62
1:C:325:GLY:HA2	1:C:389:GLY:O	1.99	0.62
1:A:3:THR:HB	1:A:19:THR:H	1.63	0.61
1:B:324:PRO:HG2	1:B:419:LEU:CD1	2.30	0.61
1:C:119:GLU:HG3	1:C:563:LEU:CD1	2.30	0.61
1:B:168:ALA:O	1:B:169:THR:HG22	2.01	0.61
1:B:174:ARG:NH1	1:B:219:GLU:HA	2.15	0.61
1:B:26:ARG:HE	1:B:28:ARG:NH1	1.98	0.61
1:B:193:SER:C	1:B:195:GLN:H	2.03	0.61
1:B:588:GLU:C	1:B:590:ASN:H	2.03	0.61
1:A:33:LEU:HD22	1:A:48:PHE:CE1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:ASP:HA	1:A:522:LYS:HE2	1.81	0.61
1:A:179:PRO:HG3	1:A:187:PHE:CE2	2.36	0.61
1:A:9:LEU:HD12	1:A:45:VAL:HG21	1.83	0.61
1:A:215:CYS:SG	1:A:231:GLN:HG3	2.39	0.61
1:C:11:LEU:HD12	1:C:91:GLU:OE1	2.00	0.61
1:C:449:HIS:HB2	1:C:450:PRO:HD2	1.83	0.61
1:B:33:LEU:HB3	1:B:48:PHE:CE1	2.36	0.61
1:C:171:GLU:CG	1:C:172:GLY:H	2.14	0.61
1:B:169:THR:N	1:B:170:PRO:CD	2.64	0.60
1:B:439:ASP:OD2	1:B:445:THR:HB	2.00	0.60
1:B:409:LEU:HD22	1:B:413:VAL:HG23	1.83	0.60
1:A:565:THR:O	1:A:566:GLU:HB2	1.99	0.60
1:B:361:LEU:HD21	1:B:374:ALA:HA	1.83	0.60
1:C:584:VAL:HG23	1:C:584:VAL:O	2.02	0.60
1:B:439:ASP:O	1:B:441:GLU:N	2.35	0.60
1:A:588:GLU:CG	1:A:589:ASN:N	2.63	0.60
1:C:6:CYS:N	1:C:40:ASP:OD2	2.35	0.60
1:C:29:ASP:O	1:C:33:LEU:O	2.19	0.60
1:B:170:PRO:HG2	1:B:171:GLU:H	1.65	0.59
1:C:329:LEU:HD21	1:C:337:TYR:CE2	2.35	0.59
1:A:359:LYS:HB3	1:A:362:GLU:HB2	1.85	0.59
1:C:111:ASP:OD2	1:C:114:HIS:HB3	2.02	0.59
1:C:492:ASN:ND2	1:C:492:ASN:C	2.55	0.59
1:A:361:LEU:O	1:A:364:ILE:HG13	2.03	0.59
1:A:361:LEU:CD2	1:A:377:ILE:HD12	2.33	0.59
1:C:244:VAL:O	1:C:247:VAL:HG12	2.03	0.59
1:A:322:ARG:O	1:A:322:ARG:HD3	2.03	0.59
1:C:586:LYS:HE2	1:C:588:GLU:OE1	2.03	0.59
1:A:194:PRO:HG2	1:A:213:VAL:HG11	1.84	0.59
1:B:339:ASN:O	1:B:342:LYS:HB2	2.02	0.59
1:C:240:THR:N	1:C:243:GLN:HE21	1.91	0.58
1:C:545:THR:HG21	1:C:550:ASP:HB2	1.85	0.58
1:B:11:LEU:HD13	1:B:92:ILE:HG23	1.85	0.58
1:C:506:ASN:OD1	1:C:509:GLU:HG2	2.03	0.58
1:A:326:GLY:O	1:A:329:LEU:HD13	2.02	0.58
1:A:387:GLN:HB2	1:A:390:ASP:OD1	2.03	0.58
1:A:249:GLU:O	1:A:253:ARG:HG3	2.03	0.58
1:C:183:HIS:HB3	1:C:186:LYS:HD2	1.85	0.58
1:A:585:LYS:HA	3:A:967:HOH:O	2.02	0.58
1:B:443:GLY:O	1:B:444:LEU:HG	2.02	0.58
1:C:109:PRO:HG2	1:C:110:LEU:H	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ILE:HB	1:A:533:PHE:HB2	1.85	0.58
1:B:161:GLU:HA	1:B:211:GLN:HE22	1.66	0.58
1:B:196:LEU:HG	1:B:517:LEU:HD22	1.85	0.58
1:B:78:ARG:HD2	1:B:92:ILE:O	2.04	0.58
1:A:398:ASN:ND2	1:A:401:ILE:HG12	2.14	0.57
1:A:174:ARG:HH22	1:B:579:LEU:CD2	2.15	0.57
1:B:83:ILE:HG23	1:B:91:GLU:HG2	1.85	0.57
1:C:505:ILE:O	1:C:505:ILE:HG12	2.03	0.57
1:A:359:LYS:O	1:A:362:GLU:HG2	2.05	0.57
1:C:26:ARG:HD2	1:C:37:ASP:OD2	2.04	0.57
1:A:449:HIS:HD2	1:A:451:PHE:H	1.51	0.57
1:C:286:LEU:HD22	1:C:428:LEU:HD22	1.86	0.57
1:A:344:TYR:HB2	1:A:405:ALA:HB2	1.87	0.57
1:C:3:THR:HG23	1:C:19:THR:HB	1.87	0.57
1:C:58:LYS:HB3	1:C:59:LEU:HD12	1.86	0.57
1:A:240:THR:OG1	1:A:243:GLN:HG3	2.05	0.57
1:C:375:GLU:O	1:C:379:ASP:OD1	2.22	0.57
1:A:123:LYS:HD3	1:A:123:LYS:O	2.04	0.57
1:A:512:GLU:O	1:A:512:GLU:HG2	2.05	0.57
1:C:557:THR:HG23	1:C:561:ALA:O	2.05	0.57
1:C:145:THR:O	1:C:149:ARG:HG3	2.05	0.57
1:A:156:GLY:O	1:B:41:ARG:NH2	2.38	0.57
1:A:540:MET:HB3	3:A:939:HOH:O	2.05	0.57
1:C:352:ILE:HA	1:C:366:SER:HB2	1.87	0.56
1:B:300:LYS:HD2	1:C:590:ASN:O	2.05	0.56
1:B:144:ILE:HD13	1:B:542:LEU:HD12	1.86	0.56
1:B:174:ARG:HG3	1:B:174:ARG:HH11	1.69	0.56
1:C:364:ILE:HD13	1:C:377:ILE:HG21	1.86	0.56
1:B:10:ARG:NH2	1:B:88:ALA:HB1	2.21	0.56
1:C:135:ALA:O	1:C:139:LYS:HG3	2.05	0.56
1:B:449:HIS:HB2	1:B:450:PRO:HD2	1.87	0.56
1:A:545:THR:HG21	1:A:550:ASP:HB2	1.87	0.56
1:B:149:ARG:NH1	1:B:212:ILE:HG13	2.20	0.56
1:A:164:MET:O	1:A:191:PRO:HD3	2.06	0.56
1:B:27:ARG:HG3	1:B:36:ILE:CD1	2.35	0.56
1:C:330:THR:CG2	1:C:332:LYS:H	2.19	0.56
1:B:83:ILE:CG2	1:B:91:GLU:HG2	2.35	0.56
1:A:458:THR:HG22	1:A:460:ALA:H	1.69	0.56
1:A:126:TYR:CE2	1:A:127:LEU:HD22	2.41	0.56
1:C:59:LEU:H	1:C:59:LEU:HD12	1.62	0.56
1:A:248:MET:HA	1:A:248:MET:HE2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ARG:HH11	1:A:26:ARG:HG2	1.70	0.56
1:C:150:ARG:HH11	1:C:150:ARG:HG2	1.71	0.56
1:B:24:VAL:HG13	1:B:36:ILE:HG12	1.88	0.56
1:A:256:TRP:HD1	1:A:262:VAL:CG2	2.18	0.56
1:C:312:ASN:O	1:C:314:PRO:HD3	2.06	0.56
1:B:545:THR:HG22	1:B:546:ASP:H	1.72	0.55
1:C:167:LYS:HD2	1:C:169:THR:HG23	1.89	0.55
1:A:547:ASN:O	1:A:550:ASP:HB2	2.07	0.55
1:A:236:THR:HB	1:A:239:MET:HE3	1.89	0.55
1:A:245:ARG:NH1	3:A:914:HOH:O	2.31	0.55
1:B:476:MET:O	1:B:483:VAL:HG22	2.06	0.55
1:C:193:SER:C	1:C:195:GLN:H	2.08	0.55
1:A:323:VAL:HG22	1:A:323:VAL:O	2.06	0.55
1:B:545:THR:HG22	1:B:546:ASP:N	2.22	0.55
1:B:85:ARG:HB2	1:B:85:ARG:CZ	2.36	0.55
1:C:193:SER:O	1:C:195:GLN:HG2	2.08	0.54
1:B:277:ARG:NH2	1:B:278:ARG:HH21	2.05	0.54
1:B:439:ASP:HB3	1:B:445:THR:HG21	1.89	0.54
1:A:247:VAL:HG22	1:A:248:MET:CE	2.37	0.54
1:B:89:THR:HB	1:B:92:ILE:HD11	1.87	0.54
1:A:161:GLU:HA	1:A:211:GLN:NE2	2.22	0.54
1:A:35:PHE:O	1:A:36:ILE:HD12	2.08	0.54
1:A:167:LYS:HB2	1:B:567:ALA:HB2	1.90	0.54
1:B:462:LEU:HD12	1:B:495:MET:HE1	1.90	0.54
1:B:179:PRO:HB3	1:B:187:PHE:CE2	2.42	0.54
1:A:570:PHE:CE2	1:B:186:LYS:HE2	2.42	0.54
1:C:92:ILE:HD12	1:C:92:ILE:O	2.07	0.54
1:B:505:ILE:HG23	1:B:509:GLU:HB3	1.89	0.54
1:C:11:LEU:HD23	1:C:14:VAL:HG21	1.87	0.54
1:A:256:TRP:HD1	1:A:262:VAL:HG21	1.72	0.54
1:A:351:TYR:HA	1:A:392:ILE:O	2.08	0.54
1:B:403:ALA:HB2	3:B:986:HOH:O	2.08	0.54
1:C:491:HIS:HB2	1:C:525:THR:OG1	2.08	0.54
1:C:506:ASN:OD1	1:C:509:GLU:OE2	2.26	0.54
1:C:119:GLU:HG3	1:C:563:LEU:HD11	1.90	0.54
1:B:199:GLN:O	1:B:203:MET:HG2	2.08	0.54
1:C:333:GLN:O	1:C:336:GLU:CG	2.56	0.54
1:C:492:ASN:HD22	1:C:493:GLY:N	2.05	0.54
1:C:458:THR:HG22	1:C:460:ALA:N	2.20	0.54
1:C:498:THR:HG22	1:C:502:ILE:HD11	1.88	0.54
1:A:179:PRO:HB2	1:A:579:LEU:HG	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:ARG:HH11	1:B:225:ARG:HB3	1.73	0.53
1:C:326:GLY:O	1:C:329:LEU:HB2	2.08	0.53
1:B:9:LEU:HD12	1:B:45:VAL:HG21	1.90	0.53
1:C:387:GLN:N	1:C:390:ASP:OD2	2.41	0.53
1:A:474:TYR:CE1	1:A:487:SER:HA	2.44	0.53
1:A:505:ILE:HG13	1:A:509:GLU:HB2	1.89	0.53
1:A:474:TYR:CD1	1:A:474:TYR:N	2.76	0.53
1:A:171:GLU:HG2	3:A:1040:HOH:O	2.07	0.53
1:B:211:GLN:HG2	1:B:213:VAL:HB	1.91	0.53
1:C:131:ARG:NH1	1:C:134:MET:CG	2.71	0.53
1:C:486:GLY:HA3	1:C:531:LEU:HA	1.91	0.53
1:B:330:THR:HG21	1:B:332:LYS:HB3	1.91	0.53
1:A:216:PHE:N	1:A:216:PHE:CD1	2.77	0.53
1:C:99:LEU:HG	1:C:100:THR:N	2.24	0.53
1:B:458:THR:CG2	1:B:460:ALA:H	2.22	0.53
1:A:387:GLN:HE21	1:A:387:GLN:HA	1.74	0.53
1:A:283:LYS:HA	1:A:477:VAL:HG21	1.90	0.53
1:A:133:GLU:HG2	1:A:137:ARG:NH2	2.24	0.53
1:A:51:PRO:HA	1:A:57:LEU:CD1	2.21	0.52
1:B:462:LEU:HD12	1:B:495:MET:CE	2.39	0.52
1:C:27:ARG:O	1:C:28:ARG:HD3	2.09	0.52
1:A:537:ARG:HD2	3:A:970:HOH:O	2.08	0.52
1:A:123:LYS:HD3	1:A:123:LYS:C	2.30	0.52
1:C:545:THR:HG21	1:C:550:ASP:CB	2.38	0.52
1:A:298:LEU:HD22	1:A:383:ARG:NH2	2.25	0.52
1:C:152:MET:O	1:C:157:PHE:HB2	2.09	0.52
1:A:476:MET:O	1:A:483:VAL:HG22	2.09	0.52
1:B:27:ARG:CG	1:B:36:ILE:HG13	2.34	0.52
1:C:125:ARG:O	1:C:129:LEU:HG	2.10	0.52
1:C:451:PHE:HZ	1:C:514:PHE:CE1	2.28	0.52
1:A:50:ASP:OD2	1:A:52:ASP:HB2	2.08	0.52
1:A:506:ASN:C	1:A:506:ASN:ND2	2.62	0.52
1:B:439:ASP:HB3	1:B:445:THR:CG2	2.40	0.52
1:C:357:ARG:O	1:C:359:LYS:N	2.43	0.52
1:C:92:ILE:HD12	1:C:92:ILE:C	2.31	0.52
1:A:310:PRO:HG3	1:A:396:ALA:HB1	1.92	0.52
1:C:505:ILE:HD11	1:C:510:GLN:HA	1.92	0.51
1:C:232:ILE:HB	1:C:533:PHE:HB2	1.92	0.51
1:B:313:ASP:OD1	1:B:314:PRO:HD2	2.09	0.51
1:B:330:THR:CG2	1:B:332:LYS:HB3	2.40	0.51
1:C:109:PRO:HG2	1:C:110:LEU:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:LYS:HE3	1:B:235:GLU:OE1	2.10	0.51
1:C:213:VAL:HG22	1:C:214:LYS:O	2.10	0.51
1:A:179:PRO:HG3	1:A:187:PHE:HE2	1.72	0.51
1:A:322:ARG:NH2	1:A:387:GLN:HG2	2.25	0.51
1:B:537:ARG:NH2	1:B:540:MET:SD	2.83	0.51
1:C:474:TYR:CD1	1:C:474:TYR:N	2.78	0.51
1:A:152:MET:CE	1:A:251:LEU:HG	2.41	0.51
1:C:67:PHE:CE2	1:C:104:ARG:HG2	2.46	0.51
1:A:322:ARG:HE	1:A:324:PRO:HG3	1.76	0.51
1:A:458:THR:HG22	1:A:460:ALA:N	2.25	0.51
1:C:1:MET:HB2	1:C:21:CYS:SG	2.51	0.51
1:A:118:GLU:O	1:A:122:LEU:HG	2.11	0.51
1:A:5:TYR:O	1:A:8:GLN:HG2	2.10	0.51
1:B:85:ARG:HB2	1:B:85:ARG:HH11	1.75	0.51
1:C:387:GLN:O	1:C:390:ASP:HB2	2.10	0.51
1:A:521:LEU:HA	1:A:525:THR:HG21	1.93	0.51
1:C:386:ALA:HB2	1:C:392:ILE:HD11	1.92	0.51
1:B:588:GLU:C	1:B:590:ASN:N	2.64	0.50
1:A:244:VAL:HG21	1:A:529:ALA:HB3	1.94	0.50
1:C:505:ILE:HG12	1:C:510:GLN:HG3	1.93	0.50
1:A:506:ASN:HD22	1:A:509:GLU:H	1.54	0.50
1:C:58:LYS:HB3	1:C:59:LEU:CD1	2.41	0.50
1:B:39:ARG:HG2	1:B:40:ASP:N	2.27	0.50
1:C:77:ALA:HB1	3:C:986:HOH:O	2.11	0.50
1:A:321:LEU:HD21	1:A:410:ARG:HA	1.93	0.50
1:C:330:THR:CG2	1:C:332:LYS:HB2	2.42	0.50
1:C:33:LEU:HD22	1:C:48:PHE:CZ	2.47	0.50
1:C:284:PRO:HG2	1:C:428:LEU:HD11	1.94	0.50
1:A:436:PHE:HA	1:A:445:THR:O	2.11	0.50
1:A:270:MET:HG2	1:A:274:GLU:HB2	1.93	0.50
1:B:256:TRP:HD1	1:B:262:VAL:HG22	1.77	0.50
1:B:171:GLU:HG2	1:B:192:GLN:HG3	1.89	0.50
1:A:208:ARG:HE	1:A:239:MET:CE	2.25	0.50
1:A:528:HIS:HA	3:A:924:HOH:O	2.11	0.50
1:B:141:ARG:NH2	1:B:536:ASP:OD1	2.45	0.50
1:B:66:GLU:HG2	1:B:108:LEU:HD11	1.93	0.50
1:C:537:ARG:CG	1:C:537:ARG:HH11	2.25	0.50
1:B:196:LEU:HD21	1:B:514:PHE:HB3	1.92	0.49
1:B:164:MET:O	1:B:191:PRO:HD3	2.12	0.49
1:A:467:GLU:CD	1:A:467:GLU:H	2.14	0.49
1:C:431:ILE:HG22	1:C:474:TYR:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:GLN:HB3	3:B:996:HOH:O	2.11	0.49
1:B:342:LYS:HZ2	1:B:348:GLY:HA2	1.76	0.49
1:B:5:TYR:CZ	1:B:41:ARG:NH1	2.80	0.49
1:A:540:MET:HE1	1:A:548:ILE:HB	1.93	0.49
1:B:563:LEU:HD22	1:C:370:LYS:HE2	1.94	0.49
1:A:213:VAL:HG22	1:A:214:LYS:N	2.28	0.49
1:B:437:GLU:HG3	1:B:445:THR:HG23	1.94	0.49
1:B:437:GLU:OE1	1:B:447:MET:HG2	2.12	0.49
1:B:381:LEU:HD22	1:B:386:ALA:HB3	1.95	0.49
1:A:209:TYR:CD1	1:A:209:TYR:C	2.86	0.49
1:C:209:TYR:CG	1:C:210:TYR:N	2.81	0.49
1:C:167:LYS:HD3	1:C:168:ALA:N	2.28	0.49
1:C:357:ARG:C	1:C:359:LYS:H	2.15	0.49
1:A:339:ASN:O	1:A:342:LYS:HB3	2.13	0.49
1:A:584:VAL:HG11	1:B:582:GLN:NE2	2.27	0.49
1:B:511:ARG:NH2	1:B:519:ASP:OD1	2.46	0.49
1:A:241:ALA:N	1:A:242:PRO:CD	2.76	0.49
1:C:545:THR:HG22	1:C:547:ASN:H	1.78	0.49
1:A:356:GLU:C	1:A:358:ALA:H	2.15	0.49
1:B:433:PHE:HB3	1:B:447:MET:HE3	1.95	0.49
1:C:210:TYR:HA	1:C:233:ASP:O	2.12	0.49
1:B:221:LEU:O	1:B:558:THR:HG23	2.12	0.48
1:B:222:ARG:O	1:B:225:ARG:HB2	2.13	0.48
1:B:151:PHE:CD1	1:B:251:LEU:HD23	2.48	0.48
1:B:256:TRP:HD1	1:B:262:VAL:CG2	2.27	0.48
1:C:454:PRO:HG2	1:C:495:MET:HE1	1.95	0.48
1:C:30:LEU:HD23	1:C:30:LEU:O	2.13	0.48
1:B:354:VAL:HG12	1:B:388:ASP:HA	1.94	0.48
1:B:34:ILE:CD1	1:B:61:SER:HA	2.44	0.48
1:B:131:ARG:NH2	1:B:133:GLU:OE1	2.46	0.48
1:C:150:ARG:NH1	1:C:150:ARG:HG2	2.29	0.48
1:C:244:VAL:O	1:C:245:ARG:C	2.51	0.48
1:C:278:ARG:HG2	3:C:1033:HOH:O	2.13	0.48
1:B:472:ASN:HD22	1:B:488:VAL:HB	1.79	0.48
1:B:240:THR:HG23	1:B:243:GLN:HE21	1.77	0.48
1:C:149:ARG:CZ	1:C:212:ILE:HD12	2.44	0.48
1:C:44:ILE:HG22	1:C:87:MET:HE1	1.96	0.48
1:B:276:GLU:O	1:B:280:GLY:HA2	2.13	0.48
1:C:170:PRO:HG2	1:C:513:LYS:NZ	2.29	0.48
1:C:170:PRO:CB	1:C:174:ARG:HH12	2.27	0.48
1:A:329:LEU:HD21	1:A:337:TYR:HE2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:PHE:O	1:B:437:GLU:HB3	2.13	0.48
1:B:489:ARG:HG3	1:B:528:HIS:CD2	2.48	0.48
1:C:559:ALA:O	1:C:560:ALA:HB3	2.13	0.48
1:B:331:ARG:HH22	1:C:118:GLU:CB	2.23	0.47
1:A:336:GLU:HG3	1:A:337:TYR:N	2.29	0.47
1:A:326:GLY:C	1:A:391:MET:HB2	2.33	0.47
1:B:575:ALA:O	1:B:579:LEU:HD22	2.14	0.47
1:B:315:LYS:O	1:B:399:LYS:HG2	2.14	0.47
1:B:326:GLY:C	1:B:391:MET:HB2	2.34	0.47
1:B:11:LEU:CD1	1:B:92:ILE:HG23	2.45	0.47
1:B:386:ALA:HB2	1:B:392:ILE:HD11	1.96	0.47
1:C:251:LEU:HD13	1:C:251:LEU:C	2.34	0.47
1:C:338:GLY:O	1:C:341:VAL:HG22	2.13	0.47
1:B:174:ARG:HG3	1:B:174:ARG:NH1	2.30	0.47
1:A:30:LEU:O	1:A:33:LEU:HB2	2.14	0.47
1:C:114:HIS:CE1	1:C:116:ASN:HA	2.50	0.47
1:A:207:ASP:HB2	3:A:920:HOH:O	2.13	0.47
1:A:486:GLY:HA3	1:A:531:LEU:HA	1.95	0.47
1:A:26:ARG:HG2	1:A:27:ARG:N	2.29	0.47
1:A:492:ASN:C	1:A:492:ASN:ND2	2.68	0.47
1:C:109:PRO:CG	1:C:110:LEU:H	2.27	0.47
1:A:252:VAL:HG21	1:A:476:MET:SD	2.55	0.47
1:A:342:LYS:HD3	1:A:342:LYS:C	2.34	0.47
1:B:297:ASP:N	1:B:297:ASP:OD1	2.47	0.47
1:A:333:GLN:HA	1:A:333:GLN:OE1	2.14	0.47
1:B:41:ARG:HD2	1:B:42:GLU:OE2	2.15	0.47
1:B:458:THR:HB	1:B:461:GLU:HG3	1.97	0.47
1:C:221:LEU:O	1:C:222:ARG:CB	2.63	0.47
1:B:217:ARG:NH1	1:B:225:ARG:HD2	2.30	0.47
1:C:51:PRO:HA	1:C:57:LEU:HD12	1.96	0.46
1:C:192:GLN:C	1:C:193:SER:OG	2.53	0.46
1:C:322:ARG:NH2	1:C:387:GLN:HG3	2.29	0.46
1:B:354:VAL:HG21	1:B:381:LEU:HD22	1.97	0.46
1:A:263:ASP:HA	3:A:906:HOH:O	2.14	0.46
1:C:225:ARG:NH1	1:C:225:ARG:CB	2.75	0.46
1:B:331:ARG:NH2	1:C:118:GLU:HB3	2.24	0.46
1:C:323:VAL:HG22	1:C:391:MET:HB3	1.97	0.46
1:C:519:ASP:HA	1:C:522:LYS:HE2	1.97	0.46
1:C:8:GLN:HG3	1:C:42:GLU:HG2	1.97	0.46
1:C:218:ASP:C	1:C:219:GLU:O	2.52	0.46
1:A:192:GLN:O	1:A:215:CYS:CB	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:ILE:O	1:A:551:VAL:HG22	2.15	0.46
1:C:272:PHE:CD2	1:C:434:PRO:HD3	2.50	0.46
1:C:558:THR:O	1:C:558:THR:HG22	2.15	0.46
1:C:209:TYR:CD1	1:C:209:TYR:C	2.89	0.46
1:A:193:SER:C	1:A:195:GLN:H	2.17	0.46
1:C:277:ARG:NE	3:C:937:HOH:O	2.33	0.46
1:A:347:LYS:CG	1:A:348:GLY:H	2.10	0.46
1:B:111:ASP:HB3	1:B:114:HIS:CG	2.51	0.46
1:A:174:ARG:HD3	3:A:1021:HOH:O	2.14	0.46
1:B:222:ARG:HG2	1:B:223:ALA:N	2.31	0.46
1:B:78:ARG:HG3	1:B:93:GLU:HG2	1.98	0.46
1:C:50:ASP:OD1	1:C:96:ALA:O	2.33	0.46
1:A:184:LYS:O	1:C:303:GLU:HB3	2.15	0.46
1:B:198:LYS:O	1:B:202:MET:HG2	2.16	0.46
1:C:481:TYR:CD2	1:C:541:LEU:HD21	2.51	0.46
1:A:84:ASN:O	1:A:90:GLY:HA3	2.16	0.46
1:C:579:LEU:HB3	1:C:581:ILE:HG12	1.97	0.46
1:B:245:ARG:NH1	3:B:938:HOH:O	2.48	0.45
1:C:454:PRO:HD2	1:C:495:MET:HE3	1.98	0.45
1:C:448:HIS:HB2	3:C:1050:HOH:O	2.15	0.45
1:A:330:THR:HG22	1:A:331:ARG:H	1.80	0.45
1:C:324:PRO:HA	1:C:390:ASP:OD1	2.17	0.45
1:A:340:PHE:HA	1:A:343:ILE:HD13	1.98	0.45
1:A:442:GLY:HA3	3:A:976:HOH:O	2.15	0.45
1:B:398:ASN:ND2	1:B:400:LYS:HB3	2.31	0.45
1:A:260:LYS:HD3	1:A:542:LEU:O	2.16	0.45
1:B:474:TYR:CE2	1:B:487:SER:HA	2.51	0.45
1:B:14:VAL:HG13	1:B:76:ARG:HA	1.98	0.45
1:B:397:ASP:HB3	1:B:401:ILE:HB	1.98	0.45
1:C:170:PRO:HD2	1:C:513:LYS:HD2	1.97	0.45
1:A:6:CYS:O	1:A:45:VAL:HB	2.17	0.45
1:B:225:ARG:HH11	1:B:225:ARG:CG	2.29	0.45
1:A:492:ASN:ND2	1:A:493:GLY:N	2.63	0.45
1:B:367:PRO:HA	1:C:119:GLU:OE2	2.17	0.45
1:B:439:ASP:OD1	1:B:442:GLY:O	2.35	0.45
1:C:341:VAL:HG11	1:C:349:LEU:HD13	1.98	0.45
1:B:322:ARG:HD2	1:B:384:THR:O	2.17	0.45
1:A:103:ASN:OD1	1:B:525:THR:HG23	2.17	0.45
1:A:417:LEU:N	1:A:417:LEU:HD23	2.32	0.45
1:A:184:LYS:NZ	1:A:578:GLU:O	2.48	0.45
1:A:358:ALA:O	1:A:359:LYS:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:THR:CG2	1:A:460:ALA:H	2.30	0.45
1:C:303:GLU:CD	1:C:303:GLU:H	2.20	0.45
1:C:323:VAL:HG22	1:C:326:GLY:HA3	1.99	0.45
1:C:330:THR:HG23	1:C:332:LYS:N	2.26	0.45
1:A:111:ASP:HB3	1:A:114:HIS:HD2	1.77	0.45
1:C:178:VAL:HB	1:C:188:TYR:HB2	1.99	0.45
1:A:318:VAL:N	3:A:913:HOH:O	2.40	0.45
1:B:149:ARG:HH22	1:B:212:ILE:HB	1.82	0.45
1:A:341:VAL:HG21	1:A:348:GLY:O	2.18	0.44
1:B:69:ILE:HD13	1:B:71:VAL:CG1	2.47	0.44
1:C:33:LEU:HD22	1:C:48:PHE:CE1	2.52	0.44
1:A:196:LEU:HD23	1:A:516:PHE:CZ	2.51	0.44
1:A:103:ASN:HA	1:A:103:ASN:HD22	1.65	0.44
1:B:226:GLN:NE2	3:B:996:HOH:O	2.43	0.44
1:C:194:PRO:HG3	3:C:968:HOH:O	2.18	0.44
1:B:143:LYS:O	1:B:147:LEU:HG	2.17	0.44
1:C:321:LEU:HD23	1:C:409:LEU:HD13	1.99	0.44
1:A:376:ILE:O	1:A:380:ILE:HG13	2.17	0.44
1:C:235:GLU:HA	1:C:530:GLY:HA3	1.99	0.44
1:C:330:THR:CG2	1:C:332:LYS:N	2.81	0.44
1:A:377:ILE:O	1:A:381:LEU:HG	2.18	0.44
1:C:208:ARG:HE	1:C:239:MET:CE	2.26	0.44
1:C:71:VAL:HG12	1:C:99:LEU:HD12	2.00	0.44
1:A:481:TYR:CB	1:A:537:ARG:HD3	2.44	0.44
1:A:286:LEU:HB2	1:A:426:ALA:HB1	1.98	0.44
1:C:59:LEU:HD23	1:C:99:LEU:HD23	1.99	0.44
1:B:137:ARG:NE	1:B:545:THR:OG1	2.50	0.44
1:B:447:MET:HB3	1:B:448:HIS:CE1	2.53	0.44
1:C:13:HIS:O	1:C:16:GLN:HG3	2.18	0.44
1:C:333:GLN:HA	1:C:336:GLU:HG2	2.00	0.44
1:B:437:GLU:O	1:B:444:LEU:HA	2.18	0.44
1:C:17:GLN:HA	1:C:73:GLY:O	2.18	0.44
1:A:357:ARG:NH1	1:A:357:ARG:CB	2.61	0.44
1:A:579:LEU:O	1:A:581:ILE:HG23	2.18	0.44
1:A:387:GLN:O	1:A:390:ASP:HB2	2.18	0.44
1:B:235:GLU:OE1	1:B:530:GLY:HA3	2.17	0.44
1:C:271:THR:HA	1:C:431:ILE:O	2.17	0.44
1:C:149:ARG:NH2	1:C:212:ILE:HB	2.32	0.44
1:C:330:THR:HG23	1:C:331:ARG:N	2.33	0.44
1:A:458:THR:CG2	1:A:459:ALA:N	2.81	0.44
1:A:286:LEU:HD21	1:A:428:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:O	1:A:14:VAL:HG23	2.18	0.44
1:C:583:VAL:HB	3:C:1031:HOH:O	2.18	0.44
1:C:208:ARG:NE	1:C:239:MET:HE2	2.25	0.43
1:A:28:ARG:HD3	1:A:29:ASP:O	2.18	0.43
1:C:109:PRO:CG	1:C:110:LEU:N	2.81	0.43
1:B:297:ASP:CG	1:B:383:ARG:HH22	2.20	0.43
1:C:431:ILE:O	1:C:432:ASP:HB2	2.17	0.43
1:B:242:PRO:HG3	1:B:245:ARG:NH2	2.32	0.43
1:A:409:LEU:C	1:A:409:LEU:HD13	2.39	0.43
1:A:240:THR:CB	1:A:242:PRO:HD2	2.49	0.43
1:A:322:ARG:NH2	1:A:387:GLN:CG	2.81	0.43
1:B:330:THR:HB	1:B:333:GLN:HG3	1.99	0.43
1:B:323:VAL:HG22	1:B:323:VAL:O	2.19	0.43
1:C:137:ARG:HD3	1:C:545:THR:OG1	2.18	0.43
1:B:104:ARG:HG2	1:B:104:ARG:HH11	1.82	0.43
1:B:110:LEU:HA	1:B:110:LEU:HD12	1.90	0.43
1:A:210:TYR:HA	1:A:233:ASP:O	2.18	0.43
1:B:181:ARG:HB3	1:B:181:ARG:HE	1.47	0.43
1:C:50:ASP:OD1	1:C:50:ASP:N	2.52	0.43
1:A:26:ARG:HH12	1:A:28:ARG:HB2	1.78	0.43
1:B:225:ARG:HH11	1:B:225:ARG:CB	2.31	0.43
1:C:144:ILE:O	1:C:148:VAL:HG23	2.18	0.43
1:C:500:PHE:CD2	1:C:510:GLN:HG2	2.54	0.43
1:A:342:LYS:O	1:A:342:LYS:HD3	2.19	0.43
1:B:397:ASP:OD1	1:B:398:ASN:N	2.48	0.43
1:B:160:ILE:HG12	3:B:914:HOH:O	2.19	0.43
1:C:11:LEU:HD23	1:C:14:VAL:CG2	2.47	0.43
1:A:330:THR:O	1:A:334:ILE:HG13	2.19	0.43
1:A:457:MET:SD	1:A:469:ALA:HB2	2.58	0.43
1:B:162:THR:H	1:B:211:GLN:HE22	1.66	0.43
1:B:117:THR:C	1:B:119:GLU:N	2.72	0.43
1:B:355:ASN:O	1:B:388:ASP:HB3	2.19	0.43
1:B:282:ASP:OD1	1:B:282:ASP:C	2.57	0.43
1:C:293:THR:HG21	1:C:383:ARG:HG2	1.99	0.43
1:B:226:GLN:NE2	1:B:556:LYS:H	1.93	0.43
1:A:202:MET:HG3	1:A:235:GLU:HG3	2.01	0.43
1:A:208:ARG:NE	1:A:239:MET:HE2	2.32	0.43
1:C:229:PHE:CD1	1:C:229:PHE:N	2.87	0.43
1:B:533:PHE:HB3	1:B:538:LEU:CD2	2.49	0.42
1:A:170:PRO:HD3	1:A:513:LYS:CD	2.35	0.42
1:B:33:LEU:HD13	1:B:48:PHE:CZ	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:PHE:CE2	1:B:517:LEU:HD23	2.54	0.42
1:C:219:GLU:HG3	1:C:219:GLU:H	1.44	0.42
1:C:410:ARG:HD3	3:C:941:HOH:O	2.20	0.42
1:B:373:ASN:C	1:B:373:ASN:OD1	2.56	0.42
1:C:574:THR:O	1:C:577:ALA:HB3	2.19	0.42
1:C:336:GLU:HG3	1:C:337:TYR:H	1.84	0.42
1:A:492:ASN:C	1:A:492:ASN:HD22	2.19	0.42
1:A:359:LYS:HB2	1:A:363:GLY:CA	2.49	0.42
1:A:452:THR:HG23	1:A:487:SER:HB2	2.01	0.42
1:C:131:ARG:NH1	1:C:134:MET:HG2	2.33	0.42
1:C:221:LEU:O	1:C:222:ARG:HG3	2.18	0.42
1:B:184:LYS:HE2	3:B:917:HOH:O	2.19	0.42
1:B:365:ASN:HD22	1:B:365:ASN:HA	1.59	0.42
1:C:368:VAL:O	1:C:372:LEU:HD13	2.19	0.42
1:B:171:GLU:CD	1:B:192:GLN:HG3	2.40	0.42
1:B:436:PHE:HB3	1:B:444:LEU:HD22	2.02	0.42
1:C:159:ASP:HB2	1:C:210:TYR:CE1	2.55	0.42
1:B:343:ILE:HG23	1:C:343:ILE:HG23	2.01	0.42
1:C:240:THR:OG1	1:C:243:GLN:HG3	2.20	0.42
1:A:500:PHE:O	1:A:505:ILE:HG23	2.19	0.42
1:B:372:LEU:HB3	1:B:373:ASN:H	1.62	0.42
1:B:435:MET:HG2	1:B:471:ALA:CA	2.49	0.42
1:C:240:THR:H	1:C:243:GLN:NE2	1.93	0.42
1:A:226:GLN:HE22	1:A:556:LYS:N	2.06	0.42
1:B:323:VAL:HA	1:B:324:PRO:HD2	1.85	0.42
1:C:252:VAL:HG21	1:C:476:MET:SD	2.59	0.42
1:B:411:LEU:HA	1:B:411:LEU:HD23	1.88	0.42
1:A:200:LEU:HD12	1:A:200:LEU:HA	1.81	0.42
1:C:488:VAL:HA	1:C:529:ALA:HB2	2.01	0.42
1:A:167:LYS:CB	1:B:567:ALA:HB2	2.49	0.42
1:C:545:THR:HG22	1:C:546:ASP:N	2.33	0.42
1:B:437:GLU:CG	1:B:445:THR:HG23	2.49	0.42
1:A:271:THR:HA	1:A:431:ILE:O	2.19	0.42
1:A:303:GLU:HG3	1:A:304:PHE:N	2.35	0.42
1:B:364:ILE:HD13	1:B:377:ILE:HG21	2.02	0.42
1:C:360:GLY:C	1:C:362:GLU:N	2.72	0.42
1:B:221:LEU:CB	1:B:558:THR:O	2.64	0.42
1:C:84:ASN:CG	1:C:87:MET:HG3	2.40	0.42
1:B:506:ASN:ND2	1:B:508:GLU:H	2.17	0.42
1:C:295:VAL:O	1:C:298:LEU:HB2	2.20	0.42
1:C:316:GLY:HA2	1:C:398:ASN:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:PRO:O	1:C:467:GLU:C	2.58	0.42
1:A:240:THR:OG1	1:A:242:PRO:HD2	2.18	0.42
1:B:330:THR:HB	1:B:333:GLN:H	1.85	0.42
1:B:451:PHE:CZ	1:B:517:LEU:HD23	2.55	0.42
1:A:449:HIS:HB2	1:A:450:PRO:CD	2.50	0.42
1:C:38:MET:O	1:C:44:ILE:HA	2.20	0.42
1:C:360:GLY:C	1:C:362:GLU:H	2.21	0.42
1:A:565:THR:HG22	1:B:516:PHE:CZ	2.54	0.42
1:C:449:HIS:HE1	1:C:489:ARG:NH1	2.17	0.42
1:B:351:TYR:CD1	1:B:351:TYR:C	2.92	0.42
1:A:373:ASN:HD21	1:A:375:GLU:HB3	1.85	0.42
1:B:117:THR:C	1:B:119:GLU:H	2.21	0.41
1:A:540:MET:SD	1:A:548:ILE:HA	2.60	0.41
1:C:537:ARG:NH1	1:C:537:ARG:CG	2.82	0.41
1:B:34:ILE:HD11	1:B:61:SER:HA	2.02	0.41
1:C:288:ASN:O	1:C:410:ARG:NH2	2.53	0.41
1:C:164:MET:O	1:C:191:PRO:HD3	2.20	0.41
1:A:268:PRO:HD2	1:A:427:PRO:O	2.20	0.41
1:A:187:PHE:N	1:A:187:PHE:CD1	2.87	0.41
1:A:361:LEU:O	1:A:361:LEU:HD13	2.21	0.41
1:B:66:GLU:CG	1:B:108:LEU:HD11	2.49	0.41
1:C:221:LEU:O	1:C:222:ARG:CG	2.68	0.41
1:A:196:LEU:HD21	1:A:517:LEU:HD22	2.02	0.41
1:B:184:LYS:HD2	1:B:184:LYS:N	2.34	0.41
1:A:222:ARG:HB2	1:A:225:ARG:CG	2.41	0.41
1:B:323:VAL:CG2	1:B:323:VAL:O	2.68	0.41
1:A:322:ARG:HH11	1:A:322:ARG:HG3	1.86	0.41
1:A:297:ASP:OD1	1:A:383:ARG:NH2	2.53	0.41
1:A:195:GLN:HG3	1:A:196:LEU:H	1.85	0.41
1:C:457:MET:HG2	3:C:974:HOH:O	2.19	0.41
1:A:218:ASP:CG	1:A:218:ASP:O	2.58	0.41
1:A:59:LEU:HD23	1:A:59:LEU:HA	1.84	0.41
1:B:63:LEU:CD2	1:B:69:ILE:HG21	2.50	0.41
1:B:286:LEU:HB2	1:B:426:ALA:HB1	2.02	0.41
1:A:562:CYS:SG	1:A:565:THR:OG1	2.76	0.41
1:A:521:LEU:HA	1:A:525:THR:CG2	2.50	0.41
1:B:351:TYR:HA	1:B:392:ILE:O	2.21	0.41
1:A:80:GLU:HA	1:A:83:ILE:HD12	2.02	0.41
1:A:76:ARG:NE	1:A:93:GLU:OE2	2.51	0.41
1:A:336:GLU:HG3	1:A:337:TYR:H	1.86	0.41
1:B:331:ARG:HG3	1:B:335:ASP:OD2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:SER:C	1:B:195:GLN:N	2.72	0.41
1:A:522:LYS:O	1:B:105:ALA:HA	2.20	0.41
1:B:537:ARG:HG3	3:B:1015:HOH:O	2.21	0.41
1:C:295:VAL:HG23	1:C:318:VAL:HG12	2.02	0.41
1:B:376:ILE:O	1:B:380:ILE:HG13	2.20	0.41
1:C:208:ARG:NE	1:C:239:MET:CE	2.84	0.41
1:C:377:ILE:O	1:C:381:LEU:HG	2.21	0.41
1:A:162:THR:H	1:A:211:GLN:HE22	1.69	0.41
1:A:567:ALA:HB2	1:B:167:LYS:HA	2.02	0.41
1:A:388:ASP:N	1:A:388:ASP:OD1	2.53	0.41
1:A:357:ARG:HB3	1:A:357:ARG:CZ	2.49	0.41
1:A:217:ARG:NH1	1:A:225:ARG:NH1	2.68	0.41
1:B:437:GLU:HG3	1:B:445:THR:CG2	2.51	0.41
1:C:421:ASP:HB3	3:C:947:HOH:O	2.20	0.41
1:C:167:LYS:HD3	1:C:168:ALA:H	1.85	0.41
1:C:507:GLU:HA	1:C:510:GLN:HB2	2.02	0.41
1:A:166:THR:HG22	1:A:189:ALA:HB3	2.03	0.41
1:B:338:GLY:O	1:B:342:LYS:HD3	2.20	0.41
1:A:356:GLU:C	1:A:358:ALA:N	2.74	0.41
1:C:29:ASP:O	1:C:30:LEU:HB3	2.20	0.41
1:B:505:ILE:HG22	1:B:510:GLN:HG3	2.03	0.41
1:A:351:TYR:CD1	1:A:351:TYR:C	2.94	0.41
1:C:128:ASP:OD1	1:C:131:ARG:HD3	2.21	0.41
1:A:152:MET:HE3	1:A:251:LEU:HG	2.03	0.41
1:C:198:LYS:HE2	1:C:235:GLU:OE1	2.20	0.41
1:B:140:THR:HG21	1:B:543:THR:HG22	2.02	0.41
1:C:268:PRO:HD2	1:C:427:PRO:O	2.21	0.41
1:A:117:THR:C	1:A:119:GLU:N	2.73	0.41
1:C:151:PHE:CD1	1:C:151:PHE:C	2.94	0.41
1:A:333:GLN:O	1:A:336:GLU:CG	2.61	0.41
1:B:565:THR:O	1:B:566:GLU:HB2	2.21	0.41
1:A:507:GLU:OE2	1:A:511:ARG:HG2	2.21	0.41
1:B:334:ILE:HG22	1:B:334:ILE:O	2.21	0.40
1:C:333:GLN:C	1:C:336:GLU:HG2	2.42	0.40
1:A:545:THR:HG22	1:A:547:ASN:N	2.32	0.40
1:B:446:ALA:HB1	1:B:448:HIS:O	2.21	0.40
1:C:481:TYR:O	1:C:483:VAL:HG13	2.22	0.40
1:A:267:PHE:CD1	1:A:267:PHE:N	2.89	0.40
1:A:240:THR:HB	1:A:242:PRO:HD2	2.03	0.40
1:A:222:ARG:N	1:A:225:ARG:HB2	2.36	0.40
1:C:2:ARG:HA	1:C:19:THR:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:SER:C	1:B:186:LYS:HD2	2.42	0.40
1:B:297:ASP:OD1	1:B:383:ARG:NH2	2.55	0.40
1:C:336:GLU:HG3	1:C:337:TYR:N	2.36	0.40
1:A:236:THR:HB	1:A:239:MET:CE	2.51	0.40
1:C:588:GLU:C	1:C:590:ASN:N	2.73	0.40
1:A:123:LYS:HD2	1:A:124:TYR:CZ	2.57	0.40
1:A:151:PHE:HD1	1:A:152:MET:HE2	1.87	0.40
1:A:431:ILE:O	1:A:432:ASP:HB2	2.21	0.40
1:C:197:PHE:O	1:C:201:LEU:HG	2.22	0.40
1:A:287:ARG:HD3	1:A:479:ASN:ND2	2.36	0.40
1:A:169:THR:HB	1:A:170:PRO:HD2	2.04	0.40
1:C:118:GLU:O	1:C:122:LEU:HG	2.22	0.40
1:B:271:THR:O	1:B:272:PHE:C	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:582:GLN:NE2	1:C:582:GLN:NE2[2_654]	1.92	0.28

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	588/590 (100%)	540 (92%)	41 (7%)	7 (1%)	16 39
1	B	588/590 (100%)	529 (90%)	48 (8%)	11 (2%)	10 25
1	C	588/590 (100%)	520 (88%)	54 (9%)	14 (2%)	7 19
All	All	1764/1770 (100%)	1589 (90%)	143 (8%)	32 (2%)	11 27

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	588	GLU
1	B	58	LYS
1	B	221	LEU
1	B	440	GLY
1	B	589	ASN
1	C	56	ALA
1	C	57	LEU
1	C	169	THR
1	C	170	PRO
1	C	222	ARG
1	A	223	ALA
1	B	80	GLU
1	B	170	PRO
1	C	90	GLY
1	C	302	VAL
1	C	358	ALA
1	A	347	LYS
1	A	397	ASP
1	B	358	ALA
1	C	193	SER
1	C	219	GLU
1	C	221	LEU
1	A	41	ARG
1	A	173	ALA
1	A	349	LEU
1	B	104	ARG
1	B	422	GLU
1	C	357	ARG
1	B	437	GLU
1	C	51	PRO
1	B	90	GLY
1	C	115	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	490/490 (100%)	436 (89%)	54 (11%)	8 18
1	B	490/490 (100%)	435 (89%)	55 (11%)	7 17
1	C	490/490 (100%)	430 (88%)	60 (12%)	6 14
All	All	1470/1470 (100%)	1301 (88%)	169 (12%)	7 16

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	4	GLU
1	A	28	ARG
1	A	30	LEU
1	A	41	ARG
1	A	57	LEU
1	A	72	THR
1	A	103	ASN
1	A	111	ASP
1	A	114	HIS
1	A	127	LEU
1	A	164	MET
1	A	166	THR
1	A	167	LYS
1	A	171	GLU
1	A	174	ARG
1	A	175	ASP
1	A	200	LEU
1	A	209	TYR
1	A	219	GLU
1	A	220	ASP
1	A	247	VAL
1	A	251	LEU
1	A	257	LEU
1	A	266	ASP
1	A	283	LYS
1	A	286	LEU
1	A	298	LEU
1	A	322	ARG
1	A	323	VAL
1	A	332	LYS
1	A	333	GLN
1	A	361	LEU
1	A	372	LEU

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Mol	Chain	Res	Type
1	A	383	ARG
1	A	387	GLN
1	A	388	ASP
1	A	397	ASP
1	A	417	LEU
1	A	458	THR
1	A	467	GLU
1	A	474	TYR
1	A	492	ASN
1	A	505	ILE
1	A	506	ASN
1	A	511	ARG
1	A	525	THR
1	A	537	ARG
1	A	538	LEU
1	A	546	ASP
1	A	574	THR
1	A	579	LEU
1	A	582	GLN
1	A	590	ASN
1	B	3	THR
1	B	4	GLU
1	B	11	LEU
1	B	28	ARG
1	B	36	ILE
1	B	41	ARG
1	B	44	ILE
1	B	55	ASP
1	B	59	LEU
1	B	71	VAL
1	B	72	THR
1	B	85	ARG
1	B	98	SER
1	B	104	ARG
1	B	114	HIS
1	B	127	LEU
1	B	138	LEU
1	B	141	ARG
1	B	154	ASP
1	B	158	LEU
1	B	169	THR
1	B	171	GLU

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Mol	Chain	Res	Type
1	B	175	ASP
1	B	195	GLN
1	B	200	LEU
1	B	209	TYR
1	B	217	ARG
1	B	221	LEU
1	B	224	ASP
1	B	225	ARG
1	B	257	LEU
1	B	262	VAL
1	B	286	LEU
1	B	298	LEU
1	B	331	ARG
1	B	365	ASN
1	B	382	ASP
1	B	383	ARG
1	B	409	LEU
1	B	441	GLU
1	B	449	HIS
1	B	458	THR
1	B	462	LEU
1	B	491	HIS
1	B	495	MET
1	B	503	LEU
1	B	507	GLU
1	B	511	ARG
1	B	514	PHE
1	B	526	PRO
1	B	531	LEU
1	B	537	ARG
1	B	538	LEU
1	B	579	LEU
1	B	590	ASN
1	C	1	MET
1	C	4	GLU
1	C	11	LEU
1	C	26	ARG
1	C	29	ASP
1	C	32	SER
1	C	41	ARG
1	C	47	VAL
1	C	50	ASP

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Mol	Chain	Res	Type
1	C	59	LEU
1	C	72	THR
1	C	85	ARG
1	C	86	ASP
1	C	99	LEU
1	C	106	ASP
1	C	114	HIS
1	C	117	THR
1	C	119	GLU
1	C	127	LEU
1	C	138	LEU
1	C	141	ARG
1	C	150	ARG
1	C	158	LEU
1	C	170	PRO
1	C	175	ASP
1	C	193	SER
1	C	196	LEU
1	C	200	LEU
1	C	209	TYR
1	C	219	GLU
1	C	256	TRP
1	C	257	LEU
1	C	262	VAL
1	C	266	ASP
1	C	286	LEU
1	C	298	LEU
1	C	303	GLU
1	C	330	THR
1	C	361	LEU
1	C	362	GLU
1	C	365	ASN
1	C	379	ASP
1	C	383	ARG
1	C	397	ASP
1	C	409	LEU
1	C	462	LEU
1	C	474	TYR
1	C	492	ASN
1	C	503	LEU
1	C	505	ILE
1	C	507	GLU

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Mol	Chain	Res	Type
1	C	512	GLU
1	C	513	LYS
1	C	525	THR
1	C	531	LEU
1	C	537	ARG
1	C	546	ASP
1	C	550	ASP
1	C	579	LEU
1	C	589	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	65	ASN
1	A	103	ASN
1	A	211	GLN
1	A	226	GLN
1	A	231	GLN
1	A	243	GLN
1	A	339	ASN
1	A	387	GLN
1	A	398	ASN
1	A	449	HIS
1	A	492	ASN
1	A	497	GLN
1	A	506	ASN
1	A	582	GLN
1	A	590	ASN
1	B	16	GLN
1	B	65	ASN
1	B	70	GLN
1	B	192	GLN
1	B	199	GLN
1	B	211	GLN
1	B	226	GLN
1	B	243	GLN
1	B	365	ASN
1	B	398	ASN
1	B	472	ASN
1	B	506	ASN
1	B	582	GLN

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Mol	Chain	Res	Type
1	B	590	ASN
1	C	16	GLN
1	C	65	ASN
1	C	195	GLN
1	C	226	GLN
1	C	243	GLN
1	C	365	ASN
1	C	449	HIS
1	C	492	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	590/590 (100%)	-0.17	25 (4%)	40	39	9, 31, 75, 101	0
1	B	590/590 (100%)	-0.18	24 (4%)	41	41	10, 33, 73, 101	0
1	C	590/590 (100%)	-0.07	32 (5%)	29	28	15, 37, 82, 101	0
All	All	1770/1770 (100%)	-0.14	81 (4%)	36	35	9, 34, 78, 101	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	588	GLU	8.3
1	C	590	ASN	7.9
1	A	590	ASN	7.8
1	A	589	ASN	7.8
1	B	170	PRO	5.5
1	C	587	ALA	5.4
1	B	115	VAL	5.3
1	B	590	ASN	5.2
1	C	358	ALA	5.2
1	B	443	GLY	5.2
1	C	589	ASN	4.9
1	C	115	VAL	4.8
1	A	587	ALA	4.7
1	A	224	ASP	4.7
1	B	441	GLU	4.6
1	B	113	ASN	4.3
1	B	439	ASP	4.1
1	C	114	HIS	4.0
1	A	115	VAL	3.9
1	A	223	ALA	3.9
1	A	361	LEU	3.7
1	B	440	GLY	3.7
1	B	223	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	224	ASP	3.7
1	B	588	GLU	3.7
1	C	112	SER	3.6
1	C	113	ASN	3.6
1	C	443	GLY	3.6
1	B	589	ASN	3.5
1	B	111	ASP	3.5
1	B	438	ASP	3.5
1	C	173	ALA	3.4
1	B	174	ARG	3.3
1	B	114	HIS	3.3
1	A	586	LYS	3.3
1	A	358	ALA	3.2
1	A	114	HIS	3.2
1	B	171	GLU	3.2
1	B	173	ALA	3.2
1	A	170	PRO	3.2
1	C	116	ASN	3.2
1	C	586	LYS	3.1
1	B	172	GLY	3.1
1	A	221	LEU	3.0
1	C	223	ALA	3.0
1	C	440	GLY	2.9
1	C	81	LYS	2.8
1	C	170	PRO	2.8
1	C	111	ASP	2.8
1	C	423	SER	2.8
1	A	222	ARG	2.8
1	B	85	ARG	2.8
1	C	359	LYS	2.8
1	A	346	ALA	2.7
1	C	57	LEU	2.7
1	C	85	ARG	2.7
1	C	221	LEU	2.7
1	A	558	THR	2.7
1	C	58	LYS	2.6
1	B	116	ASN	2.6
1	A	113	ASN	2.5
1	B	224	ASP	2.5
1	A	364	ILE	2.3
1	B	444	LEU	2.3
1	A	355	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	357	ARG	2.3
1	A	111	ASP	2.3
1	C	169	THR	2.3
1	A	339	ASN	2.2
1	C	442	GLY	2.2
1	B	358	ALA	2.2
1	A	588	GLU	2.2
1	C	83	ILE	2.1
1	A	360	GLY	2.1
1	A	220	ASP	2.1
1	C	422	GLU	2.1
1	B	442	GLY	2.1
1	A	332	LYS	2.1
1	A	85	ARG	2.0
1	C	171	GLU	2.0
1	C	86	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MG	C	903	1/1	0.97	0.27	-	2,2,2,2	0
2	MG	B	902	1/1	0.98	0.26	-	2,2,2,2	0
2	MG	A	901	1/1	0.98	0.30	-	2,2,2,2	0

6.5 Other polymers (i)

There are no such residues in this entry.