Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:38 AM GMT

PDB ID	:	3BJT
Title	:	Pyruvate kinase M2 is a phosphotyrosine binding protein
Authors	:	Wu, N.
Deposited on	:	2007-12-04
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 ⓘ symbol.

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

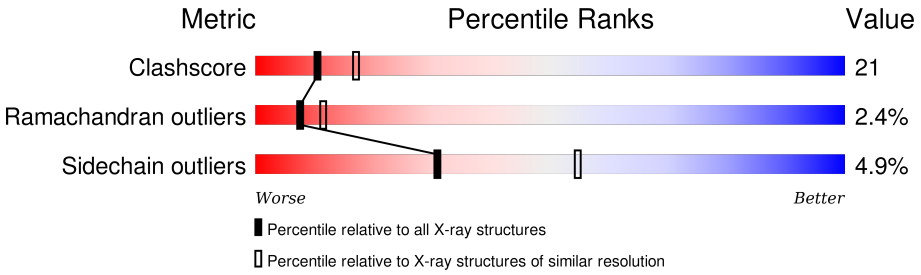
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	530	63% 28% 5% •
1	B	530	63% 32% • •
1	C	530	58% 35% • •
1	D	530	52% 41% • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15832 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.

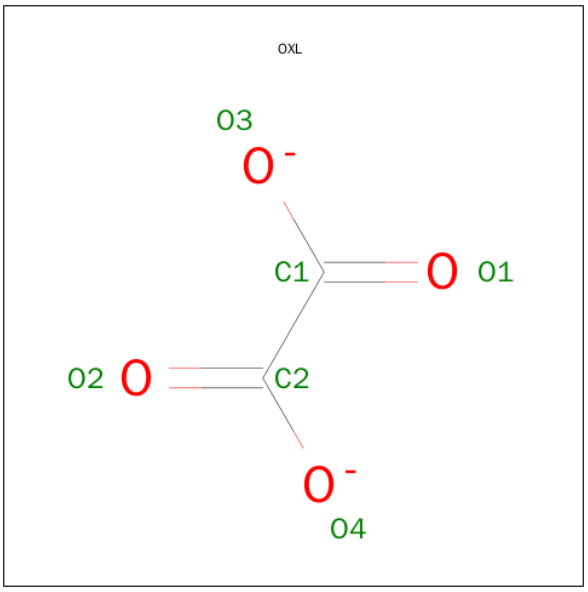
- Molecule 1 is a protein called Pyruvate kinase isozymes M1/M2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	512	Total	C	N	O	S	0	0	0
			3917	2461	693	738	25			
1	B	512	Total	C	N	O	S	0	0	0
			3917	2461	693	738	25			
1	C	512	Total	C	N	O	S	0	0	0
			3917	2461	693	738	25			
1	D	512	Total	C	N	O	S	0	0	0
			3917	2461	693	738	25			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	379	ASN	HIS	CONFLICT	UNP P14618
B	379	ASN	HIS	CONFLICT	UNP P14618
C	379	ASN	HIS	CONFLICT	UNP P14618
D	379	ASN	HIS	CONFLICT	UNP P14618

- Molecule 2 is OXALATE ION (three-letter code: OXL) (formula: C_2O_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 2 4	0	0
2	B	1	Total C O 6 2 4	0	0
2	C	1	Total C O 6 2 4	0	0
2	D	1	Total C O 6 2 4	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	41	Total O 41 41	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	38	Total O 38 38	0	0
4	C	38	Total O 38 38	0	0
4	D	19	Total O 19 19	0	0

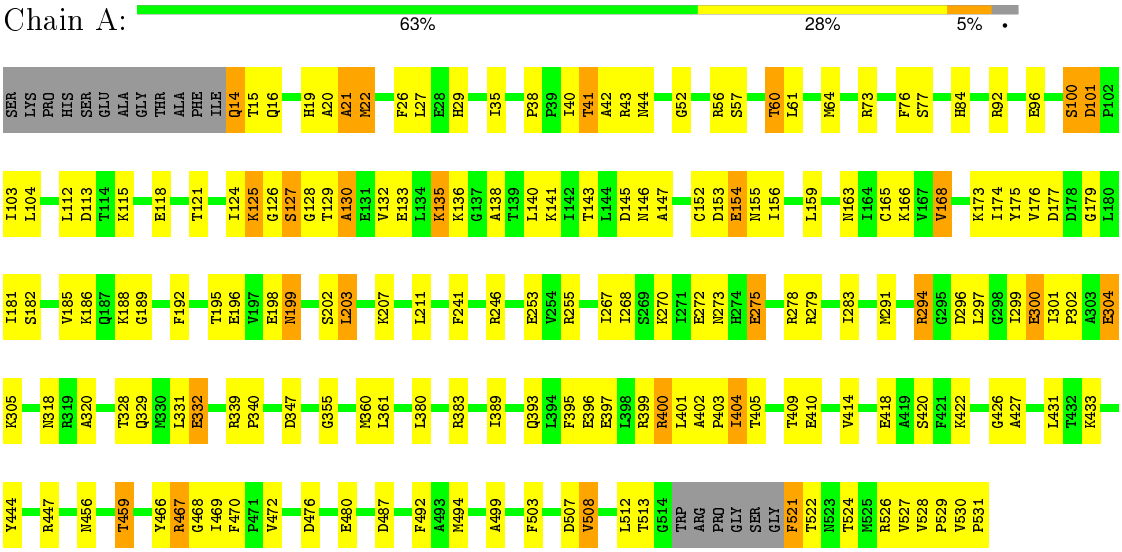
3 Residue-property plots (i)

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.

Note EDS was not executed.

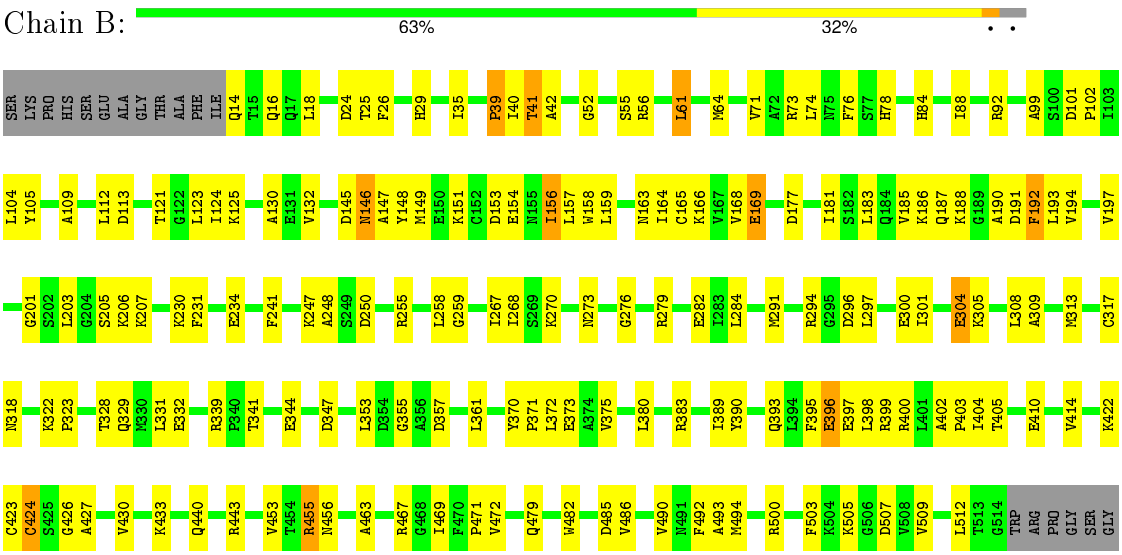
- Molecule 1: Pyruvate kinase isozymes M1/M2

Chain A:



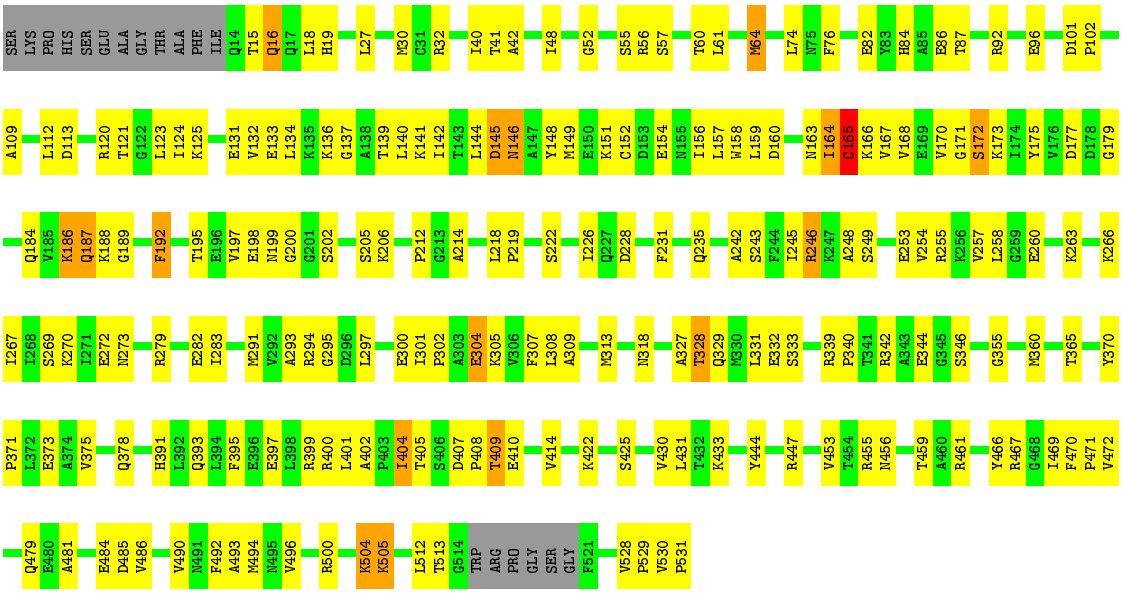
- Molecule 1: Pyruvate kinase isozymes M1/M2

Chain B:



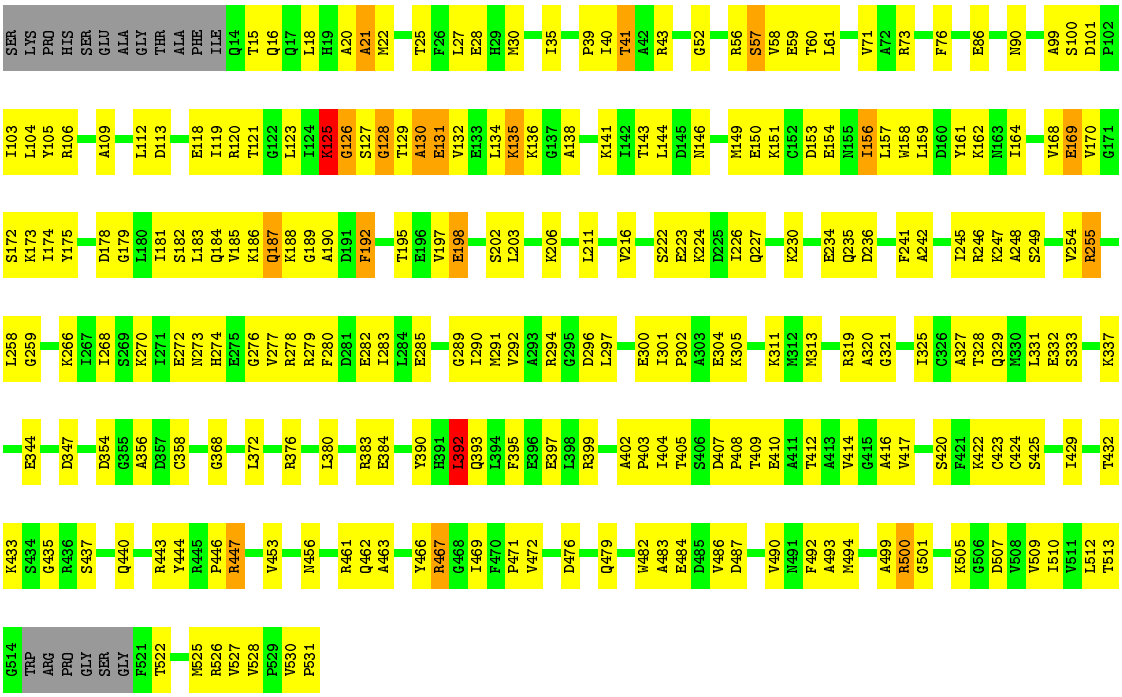
• Molecule 1: Pyruvate kinase isozymes M1/M2

Chain C:



• Molecule 1: Pyruvate kinase isozymes M1/M2

Chain D:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	74.63Å 80.71Å 107.60Å 69.82° 77.74° 67.97°	Depositor
Resolution (Å)	48.32 – 2.50	Depositor
% Data completeness (in resolution range)	89.7 (48.32-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.211 , 0.271	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15832	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OXL, 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	0.50	0/3976	0.69	0/5367
1	B	0.45	0/3976	0.66	0/5367
1	C	0.46	0/3976	0.68	0/5367
1	D	0.44	0/3976	0.65	0/5367
All	All	0.46	0/15904	0.67	0/21468

There are no bond length outliers.

There are no bond angle outliers.

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	3917	0	4006	167	0
1	B	3917	0	4006	152	0
1	C	3917	0	4006	199	0
1	D	3917	0	4006	194	0
2	A	6	0	0	1	0
2	B	6	0	0	1	0
2	C	6	0	0	0	0
2	D	6	0	0	1	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	41	0	0	3	0
4	B	38	0	0	6	0
4	C	38	0	0	1	0
4	D	19	0	0	3	0
All	All	15832	0	16024	679	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 (679) 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:400:ARG:HH11	1:A:400:ARG:HB2	1.18	1.09
1:C:404:ILE:H	1:C:404:ILE:HD12	1.18	1.06
1:C:15:THR:HG22	1:C:16:GLN:HG2	1.38	1.04
1:B:380:LEU:HB3	1:D:304:GLU:HG2	1.39	1.03
1:C:57:SER:OG	1:C:60:THR:HG23	1.66	0.96
1:A:404:ILE:HD12	1:A:404:ILE:H	1.30	0.95
1:D:248:ALA:HB2	1:D:282:GLU:HG2	1.48	0.95
1:A:57:SER:OG	1:A:60:THR:HG23	1.66	0.94
1:A:405:THR:HG21	1:A:410:GLU:HG2	1.52	0.92
1:A:431:LEU:HD22	1:A:513:THR:HG22	1.51	0.91
1:A:401:LEU:HD12	1:C:27:LEU:HD23	1.53	0.90
1:C:246:ARG:HH11	1:C:246:ARG:HB2	1.36	0.90
1:C:74:LEU:HD21	1:C:87:THR:HG21	1.50	0.90
1:B:14:GLN:HB2	4:B:933:HOH:O	1.73	0.88
1:A:389:ILE:HD11	1:A:467:ARG:HH21	1.39	0.87
1:C:472:VAL:HG12	1:C:492:PHE:CE2	2.10	0.87
1:A:135:LYS:HB2	1:A:135:LYS:HZ2	1.37	0.87
1:D:15:THR:HG22	1:D:16:GLN:HG2	1.55	0.86
1:A:255:ARG:HG3	1:A:255:ARG:HH11	1.40	0.85
1:B:41:THR:HA	1:B:383:ARG:NH2	1.91	0.85
1:A:400:ARG:NH1	1:A:400:ARG:HB2	1.91	0.84
1:C:175:TYR:HB3	1:C:179:GLY:HA2	1.59	0.84
1:D:135:LYS:CD	1:D:135:LYS:H	1.89	0.84
1:A:433:LYS:O	1:A:459:THR:HG21	1.78	0.83
1:A:380:LEU:HB3	1:C:304:GLU:HG2	1.61	0.83
1:B:186:LYS:HE2	1:B:186:LYS:HA	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:ALA:HB2	1:C:282:GLU:HG2	1.61	0.82
1:A:494:MET:HG2	1:A:531:PRO:HD2	1.60	0.82
1:C:404:ILE:H	1:C:404:ILE:CD1	1.88	0.82
1:A:155:ASN:HB2	1:A:156:ILE:HD12	1.62	0.81
1:A:246:ARG:HB3	1:A:275:GLU:OE2	1.80	0.81
1:D:395:PHE:CZ	1:D:399:ARG:HD3	2.14	0.81
1:D:144:LEU:HD23	1:D:162:LYS:HA	1.62	0.80
1:D:188:LYS:HG2	1:D:189:GLY:H	1.45	0.80
1:B:404:ILE:O	1:B:404:ILE:HD12	1.81	0.79
1:C:494:MET:HG2	1:C:531:PRO:HD2	1.64	0.79
1:A:143:THR:HG22	1:A:145:ASP:H	1.47	0.79
1:C:186:LYS:HA	1:C:186:LYS:NZ	1.98	0.78
1:D:135:LYS:HD3	1:D:138:ALA:CB	2.13	0.78
1:D:135:LYS:HD2	1:D:135:LYS:H	1.49	0.77
1:C:246:ARG:HH11	1:C:246:ARG:CB	1.97	0.77
1:C:255:ARG:HG3	1:C:255:ARG:HH11	1.50	0.77
1:A:124:ILE:HD11	1:A:203:LEU:HD23	1.65	0.76
1:C:399:ARG:HH21	1:D:399:ARG:NH2	1.82	0.76
1:C:422:LYS:HE3	1:D:403:PRO:O	1.85	0.76
1:C:55:SER:O	1:C:61:LEU:HD13	1.85	0.75
1:A:395:PHE:CZ	1:A:399:ARG:HD3	2.22	0.74
1:D:135:LYS:HD2	1:D:135:LYS:N	2.01	0.74
1:C:494:MET:CG	1:C:531:PRO:HD2	2.17	0.74
1:A:399:ARG:NH2	1:B:399:ARG:HH21	1.86	0.74
1:C:121:THR:HB	1:C:157:LEU:HD11	1.70	0.73
1:C:395:PHE:CZ	1:C:399:ARG:HD3	2.22	0.73
1:C:329:GLN:HG2	1:C:332:GLU:CG	2.18	0.73
1:A:135:LYS:HB2	1:A:135:LYS:NZ	2.04	0.73
1:A:472:VAL:HG12	1:A:492:PHE:CE2	2.24	0.73
1:D:106:ARG:HE	1:D:500:ARG:NH2	1.87	0.73
1:B:453:VAL:HG21	1:B:493:ALA:HB2	1.70	0.73
1:A:472:VAL:HG12	1:A:492:PHE:HE2	1.53	0.73
1:C:504:LYS:CE	1:C:505:LYS:H	2.01	0.72
1:D:325:ILE:HG12	1:D:358:CYS:HB2	1.71	0.72
1:C:145:ASP:OD2	1:C:148:TYR:HD1	1.72	0.72
1:C:120:ARG:O	1:C:160:ASP:HB2	1.90	0.72
1:C:164:ILE:O	1:C:166:LYS:N	2.23	0.72
1:C:165:CYS:HA	1:C:168:VAL:CG1	2.19	0.71
1:A:165:CYS:HB2	1:A:166:LYS:NZ	2.05	0.71
1:B:181:ILE:HD11	1:B:201:GLY:HA3	1.72	0.71
1:D:333:SER:OG	1:D:337:LYS:HE2	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:VAL:HG13	1:C:154:GLU:HB3	1.72	0.71
1:A:135:LYS:HZ2	1:A:135:LYS:CB	2.02	0.71
1:C:246:ARG:HH11	1:C:246:ARG:CG	2.04	0.71
1:C:124:ILE:HD13	1:C:152:CYS:HB3	1.71	0.71
1:C:504:LYS:HE3	1:C:505:LYS:H	1.54	0.70
1:D:333:SER:HB3	1:D:344:GLU:OE1	1.92	0.70
1:C:431:LEU:HD22	1:C:513:THR:HG22	1.74	0.70
1:D:106:ARG:HH21	1:D:500:ARG:HH12	1.37	0.70
1:D:125:LYS:HB2	1:D:151:LYS:HA	1.74	0.69
1:A:389:ILE:HD11	1:A:467:ARG:NH2	2.07	0.69
1:C:186:LYS:HA	1:C:186:LYS:HZ2	1.57	0.69
1:D:248:ALA:HB2	1:D:282:GLU:CG	2.22	0.69
1:D:331:LEU:HA	1:D:344:GLU:HG2	1.75	0.69
1:C:279:ARG:O	1:C:283:ILE:HG13	1.93	0.69
1:D:395:PHE:O	1:D:399:ARG:HG3	1.93	0.68
1:B:494:MET:CG	1:B:531:PRO:HD2	2.23	0.68
1:D:273:ASN:ND2	1:D:276:GLY:H	1.91	0.68
1:C:164:ILE:HG23	1:C:165:CYS:H	1.58	0.68
1:B:494:MET:HG2	1:B:531:PRO:HD2	1.75	0.68
1:D:486:VAL:O	1:D:490:VAL:HG23	1.93	0.68
1:A:182:SER:HB3	1:A:198:GLU:HB2	1.75	0.68
1:C:109:ALA:HA	1:C:461:ARG:HG2	1.76	0.68
1:A:135:LYS:HZ2	1:A:135:LYS:N	1.91	0.68
1:C:466:TYR:HB2	1:C:469:ILE:HD12	1.74	0.68
1:D:505:LYS:O	1:D:530:VAL:HB	1.94	0.68
1:D:494:MET:SD	1:D:530:VAL:HG13	2.33	0.67
1:C:134:LEU:O	1:C:200:GLY:HA3	1.94	0.67
1:D:136:LYS:HG3	1:D:198:GLU:O	1.95	0.67
1:A:297:LEU:O	1:A:301:ILE:HG12	1.94	0.67
1:A:414:VAL:HG22	1:A:444:TYR:CE2	2.28	0.67
1:C:453:VAL:HG21	1:C:493:ALA:HB2	1.76	0.67
1:D:135:LYS:HD3	1:D:138:ALA:HB3	1.76	0.67
1:A:405:THR:HG21	1:A:410:GLU:CG	2.23	0.66
1:D:168:VAL:CG1	1:D:185:VAL:HG21	2.25	0.66
1:B:308:LEU:HB2	1:D:35:ILE:HG22	1.77	0.66
1:A:40:ILE:HG13	1:A:40:ILE:O	1.96	0.66
1:A:135:LYS:HZ2	1:A:135:LYS:H	1.44	0.66
1:A:156:ILE:N	1:A:156:ILE:HD12	2.11	0.66
1:A:400:ARG:HH11	1:A:400:ARG:CB	2.03	0.66
1:A:389:ILE:CD1	1:A:467:ARG:HH21	2.09	0.66
1:A:422:LYS:NZ	1:B:405:THR:HG22	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:ASN:HD21	1:C:166:LYS:HD2	1.60	0.66
1:C:124:ILE:HG12	1:C:205:SER:HB3	1.78	0.66
1:B:455:ARG:HG3	4:B:910:HOH:O	1.95	0.66
1:C:123:LEU:HA	1:C:205:SER:HB2	1.75	0.66
1:A:125:LYS:HE2	1:A:153:ASP:HB3	1.77	0.65
1:C:297:LEU:O	1:C:301:ILE:HG12	1.95	0.65
1:B:331:LEU:HD12	1:B:361:LEU:HD21	1.79	0.65
1:C:40:ILE:HG13	1:C:40:ILE:O	1.96	0.65
1:A:57:SER:OG	1:A:60:THR:CG2	2.42	0.65
1:A:135:LYS:NZ	1:A:135:LYS:H	1.95	0.65
1:C:164:ILE:HG12	1:C:165:CYS:N	2.11	0.65
1:B:258:LEU:HD12	1:B:267:ILE:HD11	1.79	0.65
1:D:479:GLN:HG3	1:D:484:GLU:OE1	1.97	0.64
1:C:248:ALA:CB	1:C:282:GLU:HG2	2.28	0.64
1:D:168:VAL:HG12	1:D:169:GLU:N	2.13	0.64
1:A:456:ASN:HB3	1:A:459:THR:HG23	1.80	0.64
1:A:14:GLN:CD	1:A:19:HIS:HB3	2.18	0.64
1:B:64:MET:HE1	1:B:371:PRO:HB2	1.80	0.64
1:D:118:GLU:OE2	1:D:120:ARG:HD2	1.98	0.64
1:C:481:ALA:HB3	1:C:484:GLU:HG3	1.79	0.64
1:D:223:GLU:O	1:D:227:GLN:HG2	1.98	0.63
1:D:410:GLU:O	1:D:414:VAL:HG23	1.99	0.63
1:D:40:ILE:HG13	1:D:40:ILE:O	1.96	0.63
1:B:64:MET:HE2	1:B:372:LEU:HD23	1.80	0.63
1:A:135:LYS:NZ	1:A:135:LYS:N	2.45	0.63
1:D:16:GLN:HG3	1:D:18:LEU:HG	1.81	0.63
1:D:71:VAL:HG22	1:D:109:ALA:HB3	1.80	0.63
1:B:528:VAL:HG13	1:B:529:PRO:HD2	1.80	0.63
1:D:134:LEU:HD22	1:D:181:ILE:HD13	1.80	0.63
1:C:168:VAL:HG23	1:C:172:SER:OG	1.98	0.62
1:D:106:ARG:HE	1:D:500:ARG:HH22	1.47	0.62
1:A:16:GLN:O	1:A:16:GLN:HG3	1.99	0.62
1:B:112:LEU:HD23	1:B:112:LEU:C	2.20	0.62
1:D:168:VAL:CG1	1:D:169:GLU:N	2.62	0.62
1:D:188:LYS:HG2	1:D:189:GLY:N	2.13	0.62
1:A:422:LYS:HG2	1:B:414:VAL:HG21	1.82	0.62
1:A:494:MET:CG	1:A:531:PRO:HD2	2.28	0.62
1:C:163:ASN:ND2	1:C:166:LYS:HD2	2.14	0.62
1:C:57:SER:O	1:C:61:LEU:HB2	2.00	0.62
1:C:140:LEU:HB3	1:C:195:THR:OG1	1.98	0.62
1:A:339:ARG:HD3	1:A:340:PRO:HD2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:TYR:HB3	1:B:373:GLU:HB2	1.81	0.62
1:C:453:VAL:CG2	1:C:493:ALA:HB2	2.30	0.61
1:B:177:ASP:OD1	1:B:207:LYS:HD2	1.99	0.61
1:C:414:VAL:HG22	1:C:444:TYR:CZ	2.34	0.61
1:B:247:LYS:HB3	1:B:279:ARG:HE	1.65	0.61
1:A:155:ASN:CB	1:A:156:ILE:HD12	2.30	0.61
1:D:144:LEU:HD21	1:D:164:ILE:HG22	1.81	0.61
1:A:112:LEU:C	1:A:112:LEU:HD23	2.21	0.61
1:D:246:ARG:HG2	1:D:273:ASN:ND2	2.15	0.61
1:A:22:MET:HG2	1:A:22:MET:O	2.01	0.61
1:B:479:GLN:HB2	1:B:485:ASP:HB2	1.83	0.61
1:C:430:VAL:HG22	1:C:512:LEU:HD12	1.81	0.61
1:D:329:GLN:HG2	1:D:332:GLU:CG	2.30	0.61
1:C:15:THR:O	1:C:18:LEU:HG	2.00	0.61
1:B:41:THR:HA	1:B:383:ARG:HH21	1.66	0.60
1:C:142:ILE:HA	1:C:157:LEU:O	2.01	0.60
1:D:274:HIS:O	1:D:278:ARG:HG2	2.01	0.60
1:A:26:PHE:O	1:A:29:HIS:HB3	2.01	0.60
1:D:56:ARG:NH2	1:D:86:GLU:HB3	2.16	0.60
1:D:414:VAL:HG22	1:D:444:TYR:CE2	2.36	0.60
1:D:302:PRO:HG2	1:D:305:LYS:HD2	1.84	0.60
1:B:453:VAL:CG2	1:B:493:ALA:HB2	2.31	0.60
1:B:169:GLU:HA	1:B:188:LYS:HD2	1.84	0.59
1:A:405:THR:HG22	1:B:422:LYS:HE3	1.82	0.59
1:C:74:LEU:HD21	1:C:87:THR:CG2	2.27	0.59
1:B:158:TRP:O	1:B:159:LEU:HD23	2.02	0.59
1:C:144:LEU:HD22	1:C:144:LEU:N	2.18	0.59
1:D:186:LYS:O	1:D:187:GLN:HB2	2.02	0.59
1:B:248:ALA:HB2	1:B:282:GLU:HG2	1.85	0.59
1:D:182:SER:OG	1:D:198:GLU:HB2	2.03	0.59
1:D:57:SER:OG	1:D:60:THR:HG23	2.03	0.59
1:D:222:SER:O	1:D:226:ILE:HG13	2.03	0.59
1:C:414:VAL:HG22	1:C:444:TYR:CE2	2.38	0.59
1:B:297:LEU:O	1:B:301:ILE:HG12	2.03	0.59
1:B:472:VAL:HG12	1:B:492:PHE:CE2	2.38	0.59
1:D:125:LYS:CG	1:D:126:GLY:H	2.14	0.59
1:C:246:ARG:NH1	1:C:246:ARG:HB2	2.13	0.58
1:D:393:GLN:O	1:D:397:GLU:HB2	2.03	0.58
1:B:159:LEU:HD12	1:B:164:ILE:HD12	1.86	0.58
1:C:132:VAL:CG1	1:C:154:GLU:HB3	2.34	0.58
1:D:223:GLU:HA	1:D:226:ILE:HD12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:THR:HA	1:A:159:LEU:HD23	1.85	0.58
1:A:255:ARG:HG3	1:A:255:ARG:NH1	2.13	0.58
1:B:270:LYS:HD2	1:B:291:MET:SD	2.43	0.58
1:D:409:THR:HG22	1:D:522:THR:O	2.03	0.58
1:C:405:THR:HG22	1:D:422:LYS:HG3	1.85	0.58
1:D:144:LEU:HD12	1:D:144:LEU:N	2.19	0.58
1:A:165:CYS:HB2	1:A:166:LYS:HZ1	1.69	0.58
1:A:294:ARG:HB3	1:C:342:ARG:HG3	1.85	0.58
1:B:121:THR:HB	1:B:157:LEU:HD11	1.86	0.58
1:C:165:CYS:HA	1:C:168:VAL:HG12	1.85	0.57
1:A:422:LYS:HE2	1:B:403:PRO:O	2.03	0.57
1:B:55:SER:O	1:B:61:LEU:HD13	2.03	0.57
1:C:124:ILE:H	1:C:205:SER:HB3	1.69	0.57
1:C:140:LEU:HD23	1:C:141:LYS:N	2.19	0.57
1:D:433:LYS:HG3	4:D:914:HOH:O	2.04	0.57
1:B:486:VAL:O	1:B:490:VAL:HG23	2.03	0.57
1:C:258:LEU:HD12	1:C:267:ILE:HD11	1.85	0.57
1:B:148:TYR:HA	1:B:151:LYS:HB2	1.86	0.57
1:B:166:LYS:HD2	1:B:166:LYS:N	2.20	0.57
1:D:101:ASP:OD1	1:D:103:ILE:N	2.38	0.57
1:A:35:ILE:O	1:C:305:LYS:HE2	2.05	0.57
1:A:414:VAL:HG22	1:A:444:TYR:CZ	2.40	0.57
1:D:294:ARG:HD3	1:D:327:ALA:O	2.04	0.57
1:A:132:VAL:O	1:A:202:SER:HA	2.04	0.57
1:C:131:GLU:O	1:C:132:VAL:HG23	2.05	0.57
1:A:329:GLN:HG2	1:A:332:GLU:CG	2.34	0.57
1:A:124:ILE:HD11	1:A:203:LEU:CD2	2.35	0.56
1:B:396:GLU:OE2	1:B:399:ARG:CZ	2.53	0.56
1:C:131:GLU:CD	1:C:202:SER:HB2	2.26	0.56
1:D:230:LYS:O	1:D:234:GLU:HG3	2.05	0.56
1:A:175:TYR:HB3	1:A:179:GLY:HA2	1.88	0.56
1:C:255:ARG:NH1	1:C:255:ARG:HG3	2.16	0.56
1:B:329:GLN:HG2	1:B:332:GLU:CG	2.36	0.56
1:D:395:PHE:CE1	1:D:399:ARG:HD3	2.41	0.56
1:A:329:GLN:HA	1:A:332:GLU:HG2	1.88	0.56
1:C:404:ILE:N	1:C:404:ILE:HD12	2.03	0.56
1:B:410:GLU:O	1:B:414:VAL:HG23	2.06	0.56
1:D:466:TYR:HB2	1:D:469:ILE:HD12	1.88	0.56
1:A:20:ALA:O	1:A:22:MET:N	2.38	0.56
1:C:245:ILE:HG13	1:C:269:SER:HB3	1.88	0.56
1:B:323:PRO:HA	1:B:357:ASP:OD1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:THR:HG21	1:B:410:GLU:HB3	1.87	0.56
1:B:164:ILE:O	1:B:168:VAL:HG12	2.06	0.56
1:A:179:GLY:HA3	1:A:299:ILE:HD12	1.88	0.56
1:D:294:ARG:NH2	1:D:347:ASP:OD1	2.39	0.55
1:B:500:ARG:HD2	4:B:908:HOH:O	2.05	0.55
1:A:176:VAL:HB	1:A:181:ILE:HB	1.88	0.55
1:C:189:GLY:HA3	1:C:192:PHE:O	2.05	0.55
1:A:43:ARG:HB2	1:A:383:ARG:HG3	1.88	0.55
1:C:151:LYS:NZ	1:C:151:LYS:HB2	2.20	0.55
1:D:356:ALA:O	1:D:467:ARG:NH1	2.38	0.55
1:B:393:GLN:O	1:B:397:GLU:HG3	2.06	0.55
1:D:168:VAL:CG1	1:D:169:GLU:H	2.19	0.55
1:A:21:ALA:HB3	1:A:447:ARG:HH22	1.71	0.55
1:D:463:ALA:HB3	1:D:471:PRO:HG3	1.87	0.55
1:D:254:VAL:O	1:D:258:LEU:HG	2.06	0.55
1:A:380:LEU:CB	1:C:304:GLU:HG2	2.35	0.55
1:A:136:LYS:HG3	1:A:198:GLU:O	2.07	0.55
1:B:329:GLN:HA	1:B:332:GLU:HG2	1.88	0.55
1:D:372:LEU:O	1:D:376:ARG:HG3	2.06	0.55
1:A:508:VAL:HG12	1:A:527:VAL:HG12	1.89	0.55
1:C:479:GLN:OE1	1:C:479:GLN:HA	2.07	0.55
1:C:187:GLN:OE1	1:C:187:GLN:O	2.25	0.54
1:C:74:LEU:HD22	1:C:84:HIS:HD2	1.71	0.54
1:D:185:VAL:HA	1:D:195:THR:HG22	1.89	0.54
1:D:331:LEU:HD23	1:D:344:GLU:HB3	1.90	0.54
1:D:157:LEU:HD13	1:D:203:LEU:HD21	1.90	0.54
1:D:101:ASP:OD1	1:D:103:ILE:HB	2.07	0.54
1:B:71:VAL:HG22	1:B:109:ALA:HB3	1.90	0.54
1:C:243:SER:HA	1:C:270:LYS:HE2	1.89	0.54
1:D:22:MET:O	1:D:22:MET:HG2	2.06	0.54
1:C:40:ILE:O	1:C:42:ALA:N	2.40	0.54
1:C:399:ARG:HH21	1:D:399:ARG:HH21	1.53	0.54
1:A:40:ILE:O	1:A:42:ALA:N	2.40	0.54
1:C:146:ASN:O	1:C:149:MET:HG2	2.08	0.54
1:A:302:PRO:HG2	1:A:305:LYS:HD2	1.89	0.54
1:C:407:ASP:OD2	1:C:409:THR:HG23	2.07	0.54
1:D:412:THR:HG22	1:D:512:LEU:CD2	2.38	0.54
1:B:73:ARG:NH1	1:B:113:ASP:OD1	2.41	0.54
1:C:318:ASN:HD21	1:C:355:GLY:HA3	1.71	0.54
1:C:165:CYS:HA	1:C:168:VAL:HG13	1.90	0.54
1:C:391:HIS:HD2	1:C:447:ARG:CZ	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ASP:OD2	1:A:104:LEU:HD13	2.08	0.54
1:A:405:THR:O	1:B:423:CYS:HA	2.08	0.53
1:D:76:PHE:HB2	1:D:113:ASP:O	2.09	0.53
1:C:76:PHE:HB2	1:C:113:ASP:O	2.07	0.53
1:A:189:GLY:HA3	1:A:192:PHE:CE1	2.43	0.53
1:D:43:ARG:HB2	1:D:383:ARG:HG3	1.90	0.53
1:C:391:HIS:CD2	1:C:447:ARG:CZ	2.91	0.53
1:D:296:ASP:OD2	2:D:904:OXL:O2	2.26	0.53
1:C:486:VAL:O	1:C:490:VAL:HG23	2.08	0.53
1:B:395:PHE:CZ	1:B:399:ARG:HD3	2.43	0.53
1:B:294:ARG:NH2	1:B:347:ASP:OD1	2.40	0.53
1:C:393:GLN:O	1:C:397:GLU:HG3	2.08	0.53
1:D:292:VAL:HG12	1:D:294:ARG:HG3	1.89	0.53
1:A:141:LYS:NZ	4:A:929:HOH:O	2.41	0.53
1:B:191:ASP:OD2	1:B:191:ASP:N	2.41	0.53
1:C:57:SER:HG	1:C:60:THR:HG23	1.74	0.53
1:D:129:THR:O	1:D:130:ALA:C	2.47	0.53
1:B:433:LYS:HD2	4:B:910:HOH:O	2.09	0.53
1:D:319:ARG:HH11	1:D:319:ARG:HB3	1.74	0.53
1:A:92:ARG:O	1:A:96:GLU:HG2	2.09	0.53
1:C:333:SER:HB3	1:C:344:GLU:OE1	2.09	0.53
1:A:466:TYR:HB2	1:A:469:ILE:HD12	1.91	0.53
1:D:420:SER:HB2	1:D:425:SER:OG	2.09	0.53
1:C:170:VAL:HG22	1:C:188:LYS:H	1.74	0.53
1:B:304:GLU:HG2	1:D:380:LEU:HB3	1.89	0.52
1:D:505:LYS:HG3	1:D:531:PRO:C	2.29	0.52
1:D:440:GLN:O	1:D:443:ARG:HG2	2.10	0.52
1:C:156:ILE:HD12	1:C:156:ILE:N	2.23	0.52
1:B:153:ASP:OD1	1:B:156:ILE:HG13	2.10	0.52
1:A:27:LEU:HD23	1:C:401:LEU:HD12	1.90	0.52
1:C:136:LYS:HG2	1:C:137:GLY:N	2.24	0.52
1:C:339:ARG:HD3	1:C:340:PRO:HD2	1.91	0.52
1:C:16:GLN:HG3	1:C:18:LEU:HD21	1.92	0.52
1:C:139:THR:HA	1:C:195:THR:O	2.10	0.52
1:D:132:VAL:HG21	1:D:153:ASP:HA	1.90	0.52
1:C:402:ALA:HB1	1:D:422:LYS:NZ	2.23	0.52
1:C:331:LEU:HD11	1:C:378:GLN:HG3	1.92	0.52
1:D:20:ALA:C	1:D:22:MET:H	2.13	0.52
1:B:463:ALA:HB3	1:B:471:PRO:HG3	1.92	0.52
1:D:121:THR:HA	1:D:159:LEU:HD23	1.91	0.51
1:B:76:PHE:HB2	1:B:113:ASP:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:LYS:CD	1:D:138:ALA:HB3	2.40	0.51
1:D:337:LYS:N	1:D:337:LYS:HD3	2.25	0.51
1:D:121:THR:HB	1:D:157:LEU:HD11	1.91	0.51
1:B:255:ARG:HH11	1:B:255:ARG:HG3	1.75	0.51
1:A:168:VAL:O	1:A:188:LYS:HE2	2.10	0.51
1:B:187:GLN:HB2	1:B:194:VAL:HB	1.92	0.51
1:B:247:LYS:O	1:B:250:ASP:HB2	2.11	0.51
1:B:371:PRO:O	1:B:375:VAL:HG23	2.11	0.51
1:A:508:VAL:CG1	1:A:527:VAL:HG12	2.40	0.51
1:D:141:LYS:HE2	1:D:143:THR:CG2	2.40	0.51
1:A:472:VAL:CG1	1:A:492:PHE:CE2	2.92	0.51
1:B:505:LYS:O	1:B:530:VAL:O	2.28	0.51
1:A:275:GLU:CG	1:A:278:ARG:NH2	2.74	0.51
1:C:422:LYS:HZ3	1:D:410:GLU:HG3	1.76	0.51
1:D:168:VAL:HG11	1:D:185:VAL:HG21	1.93	0.51
1:B:247:LYS:HB2	1:B:282:GLU:OE2	2.10	0.51
1:B:329:GLN:HG2	1:B:332:GLU:CD	2.30	0.51
1:C:492:PHE:O	1:C:496:VAL:HG23	2.11	0.50
1:C:123:LEU:C	1:C:152:CYS:HB2	2.30	0.50
1:D:168:VAL:HG13	1:D:185:VAL:HG21	1.93	0.50
1:D:526:ARG:HG2	1:D:528:VAL:HG13	1.93	0.50
1:B:64:MET:CE	1:B:372:LEU:HD23	2.40	0.50
1:B:164:ILE:HG23	1:B:165:CYS:N	2.26	0.50
1:D:423:CYS:O	1:D:424:CYS:C	2.47	0.50
1:B:396:GLU:OE2	1:B:399:ARG:NH2	2.45	0.50
1:A:128:GLY:C	1:A:130:ALA:H	2.14	0.50
1:C:395:PHE:O	1:C:399:ARG:HG3	2.11	0.50
1:A:399:ARG:NH2	1:B:399:ARG:NH2	2.56	0.50
1:C:74:LEU:HD22	1:C:84:HIS:CD2	2.45	0.50
1:C:295:GLY:CA	1:C:328:THR:HG21	2.42	0.50
1:C:246:ARG:HH11	1:C:246:ARG:HG3	1.76	0.49
1:A:73:ARG:NH1	1:A:360:MET:CE	2.75	0.49
1:A:426:GLY:O	1:A:427:ALA:HB2	2.12	0.49
1:D:274:HIS:CD2	1:D:278:ARG:HD3	2.47	0.49
1:B:123:LEU:HA	1:B:205:SER:HB3	1.93	0.49
1:C:504:LYS:HE3	1:C:505:LYS:N	2.26	0.49
1:C:131:GLU:OE1	1:C:202:SER:HB2	2.12	0.49
1:B:389:ILE:HD11	1:B:467:ARG:HH21	1.77	0.49
1:C:272:GLU:HG2	1:C:293:ALA:HB3	1.94	0.49
1:D:73:ARG:HH12	1:D:113:ASP:CG	2.16	0.49
1:C:52:GLY:O	1:C:56:ARG:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:ARG:CD	1:C:327:ALA:O	2.61	0.49
1:D:302:PRO:CG	1:D:305:LYS:HD2	2.41	0.49
1:C:48:ILE:HB	1:C:360:MET:HG3	1.94	0.49
1:D:143:THR:C	1:D:144:LEU:HD12	2.33	0.49
1:B:168:VAL:HG13	1:B:168:VAL:O	2.12	0.49
1:C:528:VAL:HB	1:C:529:PRO:HD2	1.94	0.49
1:D:235:GLN:O	1:D:236:ASP:HB3	2.13	0.48
1:D:119:ILE:HG23	1:D:161:TYR:HB2	1.95	0.48
1:C:504:LYS:HE3	1:C:504:LYS:HA	1.95	0.48
1:A:103:ILE:HG22	1:A:104:LEU:HD12	1.94	0.48
1:A:129:THR:O	1:A:130:ALA:C	2.52	0.48
1:B:423:CYS:O	1:B:424:CYS:C	2.51	0.48
1:C:113:ASP:OD1	1:C:270:LYS:NZ	2.40	0.48
1:C:56:ARG:NH2	1:C:86:GLU:HB3	2.28	0.48
1:C:112:LEU:C	1:C:112:LEU:HD23	2.34	0.48
1:D:52:GLY:O	1:D:56:ARG:HB2	2.13	0.48
1:C:371:PRO:O	1:C:375:VAL:HG23	2.13	0.48
1:C:123:LEU:O	1:C:152:CYS:HB2	2.14	0.48
1:D:125:LYS:CG	1:D:126:GLY:N	2.76	0.48
1:B:169:GLU:OE1	1:B:169:GLU:N	2.46	0.48
1:D:329:GLN:HA	1:D:332:GLU:HG2	1.96	0.48
1:B:52:GLY:O	1:B:56:ARG:HG3	2.14	0.48
1:B:528:VAL:HG12	1:B:529:PRO:O	2.13	0.48
1:C:245:ILE:HG13	1:C:269:SER:CB	2.44	0.48
1:C:295:GLY:HA3	1:C:328:THR:HG21	1.94	0.48
1:B:398:LEU:O	1:B:402:ALA:HB2	2.13	0.48
1:A:186:LYS:HE3	1:A:196:GLU:OE1	2.14	0.48
1:A:177:ASP:OD1	1:A:207:LYS:HD2	2.13	0.48
1:A:318:ASN:HD21	1:A:355:GLY:HA3	1.78	0.48
1:B:101:ASP:OD2	1:B:104:LEU:HD23	2.13	0.48
1:D:266:LYS:HG2	1:D:462:GLN:NE2	2.28	0.47
1:C:254:VAL:HG12	1:C:267:ILE:HD13	1.96	0.47
1:C:329:GLN:HG2	1:C:332:GLU:HG3	1.94	0.47
1:C:272:GLU:O	1:C:300:GLU:HG3	2.14	0.47
1:D:453:VAL:HG21	1:D:493:ALA:HB2	1.97	0.47
1:D:255:ARG:HG3	1:D:255:ARG:HH11	1.77	0.47
1:C:27:LEU:HD12	1:C:30:MET:HE3	1.96	0.47
1:A:273:ASN:HA	1:A:300:GLU:HG2	1.96	0.47
1:C:329:GLN:HG2	1:C:332:GLU:HG2	1.92	0.47
1:C:410:GLU:O	1:C:414:VAL:HG23	2.15	0.47
1:A:456:ASN:CB	1:A:459:THR:HG23	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ASP:O	1:A:147:ALA:N	2.47	0.47
1:B:146:ASN:O	1:B:149:MET:HG2	2.14	0.47
1:A:409:THR:HG22	1:A:522:THR:O	2.14	0.47
1:A:255:ARG:HG2	1:A:267:ILE:HD12	1.96	0.47
1:A:155:ASN:HB2	1:A:156:ILE:CD1	2.41	0.47
1:C:255:ARG:HG2	1:C:267:ILE:HD12	1.96	0.47
1:D:57:SER:OG	1:D:60:THR:CG2	2.63	0.47
1:A:132:VAL:CG1	1:A:154:GLU:HB3	2.45	0.47
1:D:255:ARG:CG	1:D:255:ARG:HH11	2.27	0.47
1:B:273:ASN:ND2	1:B:276:GLY:H	2.12	0.47
1:C:218:LEU:HD11	4:C:929:HOH:O	2.15	0.47
1:A:405:THR:CG2	1:B:422:LYS:HE3	2.43	0.47
1:A:42:ALA:HB1	1:A:470:PHE:CZ	2.49	0.47
1:C:231:PHE:CZ	1:C:235:GLN:HG3	2.50	0.47
1:B:192:PHE:HD1	1:B:192:PHE:H	1.62	0.47
1:C:16:GLN:NE2	1:C:40:ILE:CG2	2.78	0.47
1:A:255:ARG:CG	1:A:255:ARG:NH1	2.72	0.47
1:B:145:ASP:O	1:B:147:ALA:N	2.48	0.47
1:C:136:LYS:HE2	1:C:198:GLU:O	2.15	0.47
1:D:417:VAL:HG22	1:D:446:PRO:HB3	1.97	0.47
1:C:400:ARG:HE	1:D:392:LEU:HD11	1.80	0.47
1:B:99:ALA:HA	1:B:105:TYR:CD1	2.49	0.47
1:D:58:VAL:HG23	1:D:90:ASN:OD1	2.15	0.47
1:D:173:LYS:HA	1:D:183:LEU:O	2.14	0.46
1:D:109:ALA:HA	1:D:461:ARG:HG2	1.97	0.46
1:B:390:TYR:CE2	1:B:393:GLN:NE2	2.82	0.46
1:C:370:TYR:HD1	1:C:373:GLU:OE2	1.98	0.46
1:B:296:ASP:OD2	2:B:902:OXL:O3	2.33	0.46
1:B:181:ILE:CD1	1:B:201:GLY:HA3	2.43	0.46
1:B:121:THR:O	1:B:206:LYS:HA	2.16	0.46
1:C:365:THR:HA	1:C:371:PRO:HB3	1.96	0.46
1:B:186:LYS:CA	1:B:186:LYS:HE2	2.39	0.46
1:B:430:VAL:HG22	1:B:512:LEU:HD12	1.98	0.46
1:A:77:SER:HB3	1:A:115:LYS:HA	1.96	0.46
1:C:246:ARG:NH1	1:C:246:ARG:HG3	2.30	0.46
1:A:129:THR:HG22	1:A:129:THR:O	2.16	0.46
1:B:241:PHE:HD1	1:B:268:ILE:HB	1.81	0.46
1:B:469:ILE:O	1:B:471:PRO:HD3	2.15	0.46
1:C:272:GLU:CG	1:C:293:ALA:HB3	2.44	0.46
1:A:246:ARG:HG3	1:A:273:ASN:HD21	1.80	0.46
1:A:73:ARG:NH1	1:A:360:MET:HE3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:PHE:HA	1:B:234:GLU:OE2	2.16	0.46
1:B:341:THR:OG1	1:B:344:GLU:HG3	2.15	0.46
1:B:183:LEU:HD23	1:B:197:VAL:HA	1.97	0.46
1:D:368:GLY:HA3	4:D:909:HOH:O	2.15	0.46
1:C:422:LYS:O	1:D:404:ILE:HG23	2.15	0.46
1:A:100:SER:O	1:A:101:ASP:HB2	2.15	0.46
1:D:416:ALA:HA	1:D:525:MET:SD	2.56	0.46
1:C:132:VAL:CG1	1:C:133:GLU:N	2.78	0.46
1:C:121:THR:O	1:C:206:LYS:HA	2.16	0.46
1:C:212:PRO:C	1:C:214:ALA:H	2.19	0.46
1:D:131:GLU:HB3	1:D:202:SER:HB3	1.97	0.46
1:B:273:ASN:HA	1:B:300:GLU:HG2	1.98	0.46
1:A:57:SER:HG	1:A:60:THR:CG2	2.27	0.45
1:B:40:ILE:C	1:B:42:ALA:H	2.19	0.45
1:D:183:LEU:HD23	1:D:197:VAL:HA	1.97	0.45
1:C:171:GLY:O	1:C:184:GLN:NE2	2.44	0.45
1:B:41:THR:CA	1:B:383:ARG:HH21	2.29	0.45
1:B:40:ILE:O	1:B:42:ALA:N	2.49	0.45
1:A:125:LYS:HE2	1:A:153:ASP:CB	2.45	0.45
1:A:270:LYS:HD2	1:A:291:MET:SD	2.56	0.45
1:A:393:GLN:O	1:A:397:GLU:HG3	2.16	0.45
1:D:135:LYS:HD3	1:D:138:ALA:HB2	1.96	0.45
1:A:422:LYS:HZ3	1:B:405:THR:HG22	1.79	0.45
1:D:56:ARG:HH21	1:D:86:GLU:HB3	1.79	0.45
1:C:132:VAL:O	1:C:202:SER:HA	2.16	0.45
1:B:279:ARG:HH11	1:B:279:ARG:HG2	1.82	0.45
1:D:390:TYR:CE1	1:D:392:LEU:HB3	2.51	0.45
1:B:24:ASP:OD2	1:B:25:THR:HG23	2.17	0.45
1:A:320:ALA:HB2	4:A:915:HOH:O	2.15	0.45
1:A:182:SER:CB	1:A:198:GLU:HB2	2.46	0.45
1:D:223:GLU:OE1	1:D:226:ILE:HD12	2.16	0.45
1:C:294:ARG:HD3	1:C:327:ALA:O	2.16	0.45
1:B:230:LYS:O	1:B:234:GLU:HG3	2.16	0.45
1:C:309:ALA:HB1	1:C:313:MET:HE2	1.98	0.45
1:B:309:ALA:HB1	1:B:313:MET:CE	2.47	0.45
1:A:16:GLN:N	1:A:38:PRO:O	2.49	0.45
1:D:99:ALA:HA	1:D:105:TYR:CD1	2.52	0.45
1:C:260:GLU:O	1:C:263:LYS:HG2	2.16	0.45
1:D:21:ALA:CB	1:D:447:ARG:HH12	2.30	0.45
1:B:181:ILE:HD11	1:B:201:GLY:CA	2.44	0.45
1:A:207:LYS:HA	1:A:207:LYS:HD3	1.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:311:LYS:NZ	1:D:354:ASP:OD1	2.49	0.45
1:B:482:TRP:O	1:B:485:ASP:N	2.48	0.45
1:B:166:LYS:HD2	1:B:166:LYS:H	1.82	0.45
1:C:479:GLN:HB2	1:C:485:ASP:HB2	1.99	0.45
1:C:407:ASP:HA	1:C:408:PRO:HD3	1.78	0.45
1:D:499:ALA:C	1:D:501:GLY:H	2.21	0.45
1:B:132:VAL:HG12	1:B:203:LEU:HB3	1.99	0.45
1:D:174:ILE:HD12	1:D:195:THR:HG21	1.98	0.45
1:D:174:ILE:HB	1:D:183:LEU:HB2	1.99	0.45
1:B:188:LYS:HA	1:B:193:LEU:HD23	1.99	0.45
1:A:73:ARG:HH11	1:A:360:MET:CE	2.30	0.45
1:B:305:LYS:HE2	1:D:384:GLU:OE1	2.17	0.45
1:B:124:ILE:HB	1:B:130:ALA:HB3	1.98	0.44
1:A:241:PHE:HD1	1:A:268:ILE:HB	1.82	0.44
1:C:125:LYS:N	1:C:152:CYS:O	2.41	0.44
1:C:146:ASN:HD22	1:C:146:ASN:N	2.14	0.44
1:C:433:LYS:O	1:C:459:THR:HG21	2.17	0.44
1:A:503:PHE:CD1	1:A:530:VAL:HG21	2.53	0.44
1:B:35:ILE:CD1	1:D:277:VAL:HG11	2.48	0.44
1:A:275:GLU:HG2	1:A:278:ARG:NH2	2.32	0.44
1:D:302:PRO:HG2	1:D:305:LYS:CD	2.47	0.44
1:A:103:ILE:HD13	1:A:499:ALA:HB1	1.98	0.44
1:D:510:ILE:CD1	1:D:527:VAL:HG22	2.48	0.44
1:D:280:PHE:CE1	1:D:313:MET:HG2	2.52	0.44
1:B:383:ARG:HB2	4:B:928:HOH:O	2.16	0.44
1:C:124:ILE:HA	1:C:152:CYS:O	2.18	0.44
1:B:158:TRP:C	1:B:159:LEU:HD23	2.38	0.44
1:B:329:GLN:CA	1:B:332:GLU:HG2	2.48	0.44
1:A:409:THR:HG22	1:A:522:THR:C	2.38	0.44
1:D:141:LYS:HE3	1:D:192:PHE:CD2	2.53	0.44
1:C:164:ILE:O	1:C:167:VAL:HG22	2.18	0.44
1:B:35:ILE:O	1:D:305:LYS:HD3	2.18	0.44
1:D:149:MET:HG3	1:D:150:GLU:HG3	1.98	0.44
1:B:16:GLN:HG3	1:B:18:LEU:HG	2.00	0.44
1:A:456:ASN:CG	1:A:459:THR:HG23	2.38	0.44
1:D:125:LYS:NZ	1:D:125:LYS:HB3	2.33	0.44
1:D:246:ARG:HG2	1:D:273:ASN:HD21	1.83	0.44
1:C:134:LEU:HD12	1:C:134:LEU:N	2.33	0.44
1:A:132:VAL:HG12	1:A:133:GLU:N	2.32	0.44
1:A:512:LEU:HA	1:A:524:THR:O	2.17	0.44
1:B:26:PHE:O	1:B:29:HIS:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:ARG:NH1	1:C:246:ARG:CG	2.70	0.43
1:D:405:THR:HG21	1:D:410:GLU:HB3	1.99	0.43
1:D:125:LYS:HD2	1:D:126:GLY:H	1.81	0.43
1:C:302:PRO:HG2	1:C:305:LYS:HG3	2.00	0.43
1:A:304:GLU:H	1:A:304:GLU:HG3	1.28	0.43
1:C:16:GLN:HG3	1:C:18:LEU:CD2	2.48	0.43
1:A:145:ASP:C	1:A:147:ALA:H	2.21	0.43
1:A:166:LYS:N	1:A:166:LYS:HD3	2.34	0.43
1:C:132:VAL:HG12	1:C:133:GLU:N	2.33	0.43
1:C:481:ALA:HB3	1:C:484:GLU:CG	2.47	0.43
1:B:479:GLN:OE1	1:B:479:GLN:HA	2.16	0.43
1:A:409:THR:CG2	1:A:522:THR:N	2.81	0.43
1:A:174:ILE:HG12	1:A:211:LEU:CD2	2.48	0.43
1:D:242:ALA:HB1	1:D:245:ILE:HD11	2.00	0.43
1:B:318:ASN:HD21	1:B:355:GLY:HA3	1.83	0.43
1:A:404:ILE:HD12	1:A:404:ILE:N	2.13	0.43
1:C:134:LEU:HB3	1:C:197:VAL:HG21	2.01	0.43
1:A:141:LYS:HE3	1:A:192:PHE:CD2	2.52	0.43
1:C:56:ARG:HH21	1:C:86:GLU:HB3	1.83	0.43
1:A:409:THR:HG22	1:A:522:THR:N	2.33	0.43
1:D:216:VAL:HG23	1:D:216:VAL:O	2.18	0.43
1:B:284:LEU:O	1:B:322:LYS:NZ	2.43	0.43
1:D:164:ILE:HD13	1:D:211:LEU:HD11	1.99	0.43
1:C:505:LYS:O	1:C:530:VAL:O	2.37	0.43
1:B:35:ILE:HG12	4:B:920:HOH:O	2.18	0.43
1:D:268:ILE:CD1	1:D:289:GLY:HA3	2.48	0.43
1:C:279:ARG:HH11	1:C:279:ARG:HG2	1.83	0.43
1:D:99:ALA:C	1:D:101:ASP:H	2.21	0.43
1:D:499:ALA:O	1:D:501:GLY:N	2.51	0.43
1:B:40:ILE:C	1:B:383:ARG:HH21	2.22	0.43
1:A:132:VAL:HG11	1:A:154:GLU:HB3	1.99	0.43
1:C:228:ASP:O	1:C:231:PHE:HB3	2.19	0.43
1:D:432:THR:HG21	1:D:435:GLY:HA2	2.00	0.43
1:A:521:PHE:CD1	1:A:521:PHE:N	2.87	0.43
1:C:505:LYS:HG3	1:C:531:PRO:OXT	2.19	0.43
1:C:154:GLU:H	1:C:154:GLU:HG2	1.57	0.43
1:B:241:PHE:HB3	1:B:270:LYS:HD3	2.01	0.43
1:D:407:ASP:HA	1:D:408:PRO:HD3	1.88	0.43
1:A:279:ARG:O	1:A:283:ILE:HG13	2.19	0.43
1:D:472:VAL:CG1	1:D:492:PHE:CE2	3.01	0.43
1:A:124:ILE:HA	1:A:152:CYS:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:VAL:HG13	1:D:172:SER:HB2	2.01	0.43
1:A:40:ILE:O	1:A:41:THR:C	2.57	0.43
1:D:513:THR:O	1:D:522:THR:HG23	2.19	0.43
1:D:279:ARG:O	1:D:283:ILE:HG13	2.18	0.43
1:B:145:ASP:HB3	1:B:148:TYR:CD1	2.54	0.43
1:A:132:VAL:CG1	1:A:133:GLU:N	2.81	0.43
1:B:353:LEU:CD1	1:D:311:LYS:HE3	2.49	0.43
1:D:127:SER:O	1:D:128:GLY:C	2.57	0.43
1:C:253:GLU:O	1:C:257:VAL:HG23	2.19	0.43
1:B:74:LEU:HD11	1:B:88:ILE:CG1	2.48	0.43
1:C:279:ARG:NH1	1:C:279:ARG:HG2	2.34	0.43
1:C:173:LYS:HE2	1:C:198:GLU:OE1	2.19	0.43
1:A:135:LYS:HZ2	1:A:135:LYS:CA	2.32	0.42
1:C:422:LYS:NZ	1:D:410:GLU:HG3	2.34	0.42
1:D:173:LYS:HE3	1:D:184:GLN:NE2	2.34	0.42
1:A:77:SER:HB2	1:A:118:GLU:OE2	2.19	0.42
1:A:126:GLY:O	1:A:127:SER:HB2	2.19	0.42
1:C:64:MET:HE3	1:C:371:PRO:HB2	2.00	0.42
1:B:396:GLU:OE1	1:B:400:ARG:HG3	2.20	0.42
1:C:222:SER:O	1:C:226:ILE:HG13	2.19	0.42
1:D:156:ILE:HD11	4:D:913:HOH:O	2.18	0.42
1:C:266:LYS:HA	1:C:266:LYS:HD3	1.77	0.42
1:A:84:HIS:HD2	4:A:935:HOH:O	2.03	0.42
1:A:402:ALA:HA	1:A:403:PRO:HD3	1.85	0.42
1:A:329:GLN:CA	1:A:332:GLU:HG2	2.49	0.42
1:D:76:PHE:CE1	1:D:112:LEU:HG	2.55	0.42
1:A:44:ASN:HB3	1:A:468:GLY:N	2.34	0.42
1:B:74:LEU:HD11	1:B:88:ILE:HG12	2.02	0.42
1:D:247:LYS:CD	1:D:249:SER:HB2	2.48	0.42
1:A:294:ARG:NH2	1:A:347:ASP:OD1	2.52	0.42
1:A:76:PHE:HB2	1:A:113:ASP:O	2.20	0.42
1:B:78:HIS:O	1:B:84:HIS:HE1	2.02	0.42
1:C:472:VAL:HG12	1:C:492:PHE:CZ	2.54	0.42
1:B:16:GLN:HB3	1:B:39:PRO:HA	2.01	0.42
1:B:40:ILE:C	1:B:42:ALA:N	2.73	0.42
1:D:144:LEU:N	1:D:144:LEU:CD1	2.82	0.42
1:D:175:TYR:HB3	1:D:179:GLY:HA2	2.01	0.42
1:D:161:TYR:O	1:D:164:ILE:HG22	2.19	0.42
1:B:433:LYS:NZ	1:B:456:ASN:HB2	2.34	0.42
1:B:304:GLU:H	1:B:304:GLU:HG3	1.41	0.42
1:D:149:MET:HA	1:D:158:TRP:CG	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:GLY:O	1:B:427:ALA:HB2	2.20	0.42
1:C:92:ARG:O	1:C:96:GLU:HG2	2.20	0.42
1:A:331:LEU:HD12	1:A:361:LEU:HD21	2.02	0.42
1:D:27:LEU:HD12	1:D:30:MET:HE3	2.02	0.42
1:C:145:ASP:OD2	1:C:148:TYR:CD1	2.61	0.42
1:D:168:VAL:C	1:D:169:GLU:HG2	2.39	0.42
1:D:319:ARG:O	1:D:321:GLY:N	2.53	0.42
1:A:168:VAL:HG11	1:A:185:VAL:HG21	2.02	0.42
1:D:235:GLN:O	1:D:236:ASP:CB	2.68	0.42
1:B:132:VAL:HG21	1:B:154:GLU:N	2.35	0.42
1:C:109:ALA:CA	1:C:461:ARG:HG2	2.48	0.41
1:D:432:THR:HB	1:D:437:SER:HB2	2.03	0.41
1:A:528:VAL:HG13	1:A:529:PRO:HD2	2.01	0.41
1:A:329:GLN:CB	1:A:332:GLU:HG2	2.50	0.41
1:D:241:PHE:HD1	1:D:268:ILE:HB	1.84	0.41
1:C:158:TRP:CE2	1:C:159:LEU:O	2.73	0.41
1:D:456:ASN:C	1:D:456:ASN:OD1	2.58	0.41
1:B:146:ASN:C	1:B:148:TYR:H	2.22	0.41
1:D:127:SER:O	1:D:128:GLY:O	2.37	0.41
1:D:290:ILE:HG22	1:D:291:MET:N	2.35	0.41
1:B:41:THR:N	1:B:383:ARG:HH21	2.19	0.41
1:D:169:GLU:O	1:D:170:VAL:C	2.57	0.41
1:B:145:ASP:HB3	1:B:148:TYR:HD1	1.85	0.41
1:D:39:PRO:HG2	1:D:383:ARG:NH2	2.36	0.41
1:A:128:GLY:C	1:A:130:ALA:N	2.71	0.41
1:D:453:VAL:CG2	1:D:493:ALA:HB2	2.50	0.41
1:A:153:ASP:OD2	1:A:155:ASN:HB2	2.21	0.41
1:C:302:PRO:HG2	1:C:305:LYS:CG	2.51	0.41
1:C:456:ASN:CG	1:C:459:THR:HG23	2.41	0.41
1:D:297:LEU:O	1:D:301:ILE:HG12	2.20	0.41
1:C:470:PHE:HA	1:C:471:PRO:HD2	1.94	0.41
1:B:39:PRO:HB2	1:B:40:ILE:H	1.66	0.41
1:D:164:ILE:CD1	1:D:211:LEU:HD11	2.51	0.41
1:C:504:LYS:CD	1:C:505:LYS:H	2.34	0.41
1:D:402:ALA:HA	1:D:403:PRO:HD3	1.94	0.41
1:C:270:LYS:HD2	1:C:291:MET:SD	2.61	0.41
1:D:153:ASP:HB2	1:D:154:GLU:OE1	2.20	0.41
1:A:182:SER:HB3	1:A:199:ASN:H	1.86	0.41
1:D:168:VAL:HG13	1:D:169:GLU:H	1.85	0.41
1:D:25:THR:OG1	1:D:28:GLU:HB2	2.20	0.41
1:A:296:ASP:N	2:A:901:OXL:O3	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:GLY:O	1:A:56:ARG:HB2	2.20	0.41
1:A:124:ILE:HG22	1:A:125:LYS:N	2.36	0.41
1:C:490:VAL:O	1:C:494:MET:HB2	2.21	0.41
1:C:255:ARG:NH1	1:C:255:ARG:CG	2.78	0.41
1:A:21:ALA:O	1:A:22:MET:HB2	2.19	0.41
1:C:242:ALA:CB	1:C:245:ILE:HD11	2.51	0.41
1:C:101:ASP:HA	1:C:102:PRO:HD3	1.89	0.41
1:B:440:GLN:O	1:B:443:ARG:HG2	2.20	0.41
1:A:135:LYS:CE	1:A:135:LYS:N	2.84	0.41
1:B:402:ALA:HA	1:B:403:PRO:HD3	1.90	0.41
1:B:168:VAL:CG2	1:B:185:VAL:HG21	2.51	0.41
1:A:329:GLN:HG2	1:A:332:GLU:HG2	2.02	0.41
1:C:242:ALA:HB1	1:C:245:ILE:HD11	2.03	0.41
1:B:101:ASP:HA	1:B:102:PRO:HD3	1.83	0.41
1:A:275:GLU:HG2	1:A:278:ARG:HH21	1.86	0.40
1:A:526:ARG:HA	1:B:523:ASN:O	2.20	0.40
1:C:307:PHE:CZ	1:C:308:LEU:HG	2.57	0.40
1:D:412:THR:HG22	1:D:512:LEU:HD21	2.03	0.40
1:D:130:ALA:O	1:D:131:GLU:C	2.60	0.40
1:A:409:THR:CG2	1:A:522:THR:H	2.34	0.40
1:D:482:TRP:O	1:D:483:ALA:C	2.57	0.40
1:C:19:HIS:HD1	1:C:32:ARG:HD3	1.86	0.40
1:C:218:LEU:HA	1:C:219:PRO:HD3	1.94	0.40
1:D:242:ALA:O	1:D:270:LYS:HG3	2.21	0.40
1:B:317:CYS:HB3	1:B:322:LYS:O	2.22	0.40
1:C:19:HIS:ND1	1:C:32:ARG:HD3	2.36	0.40
1:A:140:LEU:HD12	1:A:155:ASN:O	2.22	0.40
1:B:404:ILE:H	1:B:404:ILE:HG13	1.63	0.40
1:C:132:VAL:HG11	1:C:154:GLU:HA	2.02	0.40
1:D:40:ILE:CG1	1:D:40:ILE:O	2.68	0.40
1:C:455:ARG:NH2	1:C:485:ASP:OD1	2.41	0.40
1:B:503:PHE:CD1	1:B:530:VAL:HG21	2.56	0.40
1:A:418:GLU:OE2	1:B:399:ARG:HD2	2.21	0.40
1:C:131:GLU:HG2	1:C:132:VAL:H	1.85	0.40
1:B:279:ARG:HG2	1:B:279:ARG:NH1	2.36	0.40
1:D:121:THR:HG22	1:D:159:LEU:HD21	2.04	0.40
1:C:96:GLU:HA	1:C:96:GLU:OE2	2.22	0.40
1:D:429:ILE:HD12	1:D:509:VAL:HG11	2.04	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	508/530 (96%)	467 (92%)	28 (6%)	13 (3%)	7 10
1	B	508/530 (96%)	469 (92%)	31 (6%)	8 (2%)	12 21
1	C	508/530 (96%)	462 (91%)	36 (7%)	10 (2%)	9 15
1	D	508/530 (96%)	453 (89%)	37 (7%)	18 (4%)	4 6
All	All	2032/2120 (96%)	1851 (91%)	132 (6%)	49 (2%)	7 11

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	MET
1	A	127	SER
1	A	507	ASP
1	B	507	ASP
1	C	41	THR
1	C	164	ILE
1	C	165	CYS
1	C	425	SER
1	A	21	ALA
1	A	41	THR
1	A	146	ASN
1	B	259	GLY
1	C	172	SER
1	D	126	GLY
1	D	128	GLY
1	D	130	ALA
1	D	187	GLN
1	D	190	ALA
1	A	100	SER
1	B	39	PRO
1	B	41	THR
1	B	146	ASN

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Mol	Chain	Res	Type
1	B	424	CYS
1	C	16	GLN
1	C	146	ASN
1	C	177	ASP
1	D	21	ALA
1	D	41	THR
1	D	131	GLU
1	D	198	GLU
1	D	320	ALA
1	D	392	LEU
1	D	500	ARG
1	D	507	ASP
1	A	125	LYS
1	A	138	ALA
1	B	190	ALA
1	C	505	LYS
1	D	125	LYS
1	D	146	ASN
1	D	328	THR
1	A	101	ASP
1	A	130	ALA
1	A	332	GLU
1	C	328	THR
1	D	100	SER
1	D	259	GLY
1	A	328	THR
1	B	328	THR

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	422/435 (97%)	392 (93%)	30 (7%)	18 34
1	B	422/435 (97%)	410 (97%)	12 (3%)	51 78
1	C	422/435 (97%)	404 (96%)	18 (4%)	35 61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	422/435 (97%)	399 (94%)	23 (6%)	27 48
All	All	1688/1740 (97%)	1605 (95%)	83 (5%)	31 55

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	15	THR
1	A	60	THR
1	A	61	LEU
1	A	64	MET
1	A	135	LYS
1	A	154	GLU
1	A	163	ASN
1	A	168	VAL
1	A	173	LYS
1	A	195	THR
1	A	199	ASN
1	A	203	LEU
1	A	253	GLU
1	A	272	GLU
1	A	275	GLU
1	A	294	ARG
1	A	300	GLU
1	A	304	GLU
1	A	396	GLU
1	A	400	ARG
1	A	404	ILE
1	A	420	SER
1	A	459	THR
1	A	467	ARG
1	A	476	ASP
1	A	480	GLU
1	A	487	ASP
1	A	508	VAL
1	A	521	PHE
1	B	61	LEU
1	B	92	ARG
1	B	125	LYS
1	B	156	ILE
1	B	163	ASN
1	B	169	GLU

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Mol	Chain	Res	Type
1	B	192	PHE
1	B	304	GLU
1	B	339	ARG
1	B	396	GLU
1	B	455	ARG
1	B	509	VAL
1	C	64	MET
1	C	82	GLU
1	C	145	ASP
1	C	165	CYS
1	C	186	LYS
1	C	187	GLN
1	C	192	PHE
1	C	199	ASN
1	C	246	ARG
1	C	249	SER
1	C	273	ASN
1	C	304	GLU
1	C	346	SER
1	C	404	ILE
1	C	409	THR
1	C	467	ARG
1	C	500	ARG
1	C	504	LYS
1	D	41	THR
1	D	57	SER
1	D	59	GLU
1	D	61	LEU
1	D	104	LEU
1	D	123	LEU
1	D	125	LYS
1	D	135	LYS
1	D	156	ILE
1	D	169	GLU
1	D	178	ASP
1	D	192	PHE
1	D	206	LYS
1	D	224	LYS
1	D	255	ARG
1	D	272	GLU
1	D	285	GLU
1	D	300	GLU

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Mol	Chain	Res	Type
1	D	392	LEU
1	D	447	ARG
1	D	467	ARG
1	D	476	ASP
1	D	487	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	HIS
1	A	163	ASN
1	A	274	HIS
1	A	393	GLN
1	B	14	GLN
1	B	84	HIS
1	B	163	ASN
1	B	264	ASN
1	B	273	ASN
1	B	439	HIS
1	B	495	ASN
1	C	16	GLN
1	C	78	HIS
1	C	84	HIS
1	C	146	ASN
1	C	264	ASN
1	C	273	ASN
1	C	318	ASN
1	C	391	HIS
1	C	393	GLN
1	C	491	ASN
1	D	14	GLN
1	D	163	ASN
1	D	199	ASN
1	D	273	ASN
1	D	318	ASN
1	D	393	GLN
1	D	439	HIS
1	D	440	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	OXL	A	901	-	0,5,5	0.00	-	0,6,6	0.00	-
2	OXL	B	902	-	0,5,5	0.00	-	0,6,6	0.00	-
2	OXL	C	903	-	0,5,5	0.00	-	0,6,6	0.00	-
2	OXL	D	904	-	0,5,5	0.00	-	0,6,6	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OXL	A	901	-	-	0/0/4/4	0/0/0/0
2	OXL	B	902	-	-	0/0/4/4	0/0/0/0
2	OXL	C	903	-	-	0/0/4/4	0/0/0/0
2	OXL	D	904	-	-	0/0/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	OXL	1	0
2	B	902	OXL	1	0
2	D	904	OXL	1	0

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.