



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 03:10 PM GMT

PDB ID : 3D8K
Title : Crsytal structure of a phosphatase from a toxoplasma gondii
Authors : Damodharan, L.; Burley, S.K.; Swaminathan, S.; New York SGX Research
Center for Structural Genomics (NYSGXRC)
Deposited on : 2008-05-23
Resolution : 2.71 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

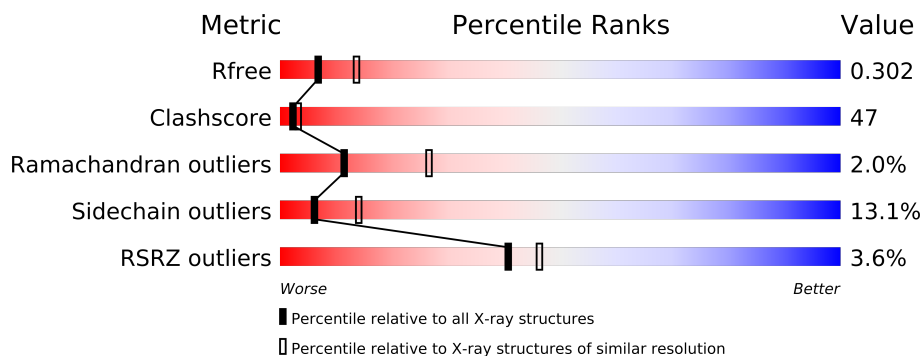
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.71 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}	66092	1770 (2.74-2.70)
Clashscore	79885	2183 (2.74-2.70)
Ramachandran outliers	78287	2147 (2.74-2.70)
Sidechain outliers	78261	2148 (2.74-2.70)
RSRZ outliers	66119	1772 (2.74-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	377	
1	B	377	
1	C	377	
1	D	377	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10892 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Protein phosphatase 2C.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	Se	0	0	0
			2664	1656	498	497	2	11			
1	B	350	Total	C	N	O	S	Se	0	0	0
			2679	1662	499	505	2	11			
1	C	351	Total	C	N	O	S	Se	0	0	0
			2696	1674	503	507	2	10			
1	D	346	Total	C	N	O	S	Se	0	0	0
			2652	1645	496	499	2	10			

There are 44 discrepancies between the modelled and reference sequences:

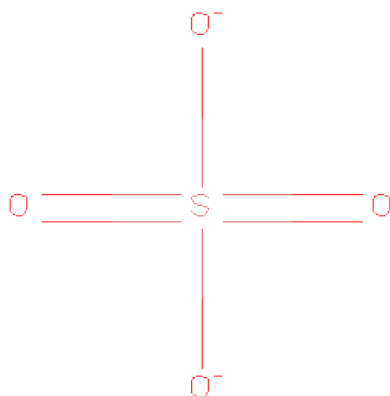
Chain	Residue	Modelled	Actual	Comment	Reference
A	76	MSE	-	expression tag	UNP A4GX63
A	77	SER	-	expression tag	UNP A4GX63
A	78	LEU	-	expression tag	UNP A4GX63
A	445	GLU	-	expression tag	UNP A4GX63
A	446	GLY	-	expression tag	UNP A4GX63
A	447	HIS	-	expression tag	UNP A4GX63
A	448	HIS	-	expression tag	UNP A4GX63
A	449	HIS	-	expression tag	UNP A4GX63
A	450	HIS	-	expression tag	UNP A4GX63
A	451	HIS	-	expression tag	UNP A4GX63
A	452	HIS	-	expression tag	UNP A4GX63
B	76	MSE	-	expression tag	UNP A4GX63
B	77	SER	-	expression tag	UNP A4GX63
B	78	LEU	-	expression tag	UNP A4GX63
B	445	GLU	-	expression tag	UNP A4GX63
B	446	GLY	-	expression tag	UNP A4GX63
B	447	HIS	-	expression tag	UNP A4GX63
B	448	HIS	-	expression tag	UNP A4GX63
B	449	HIS	-	expression tag	UNP A4GX63
B	450	HIS	-	expression tag	UNP A4GX63
B	451	HIS	-	expression tag	UNP A4GX63

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Chain	Residue	Modelled	Actual	Comment	Reference
B	452	HIS	-	expression tag	UNP A4GX63
C	76	MSE	-	expression tag	UNP A4GX63
C	77	SER	-	expression tag	UNP A4GX63
C	78	LEU	-	expression tag	UNP A4GX63
C	445	GLU	-	expression tag	UNP A4GX63
C	446	GLY	-	expression tag	UNP A4GX63
C	447	HIS	-	expression tag	UNP A4GX63
C	448	HIS	-	expression tag	UNP A4GX63
C	449	HIS	-	expression tag	UNP A4GX63
C	450	HIS	-	expression tag	UNP A4GX63
C	451	HIS	-	expression tag	UNP A4GX63
C	452	HIS	-	expression tag	UNP A4GX63
D	76	MSE	-	expression tag	UNP A4GX63
D	77	SER	-	expression tag	UNP A4GX63
D	78	LEU	-	expression tag	UNP A4GX63
D	445	GLU	-	expression tag	UNP A4GX63
D	446	GLY	-	expression tag	UNP A4GX63
D	447	HIS	-	expression tag	UNP A4GX63
D	448	HIS	-	expression tag	UNP A4GX63
D	449	HIS	-	expression tag	UNP A4GX63
D	450	HIS	-	expression tag	UNP A4GX63
D	451	HIS	-	expression tag	UNP A4GX63
D	452	HIS	-	expression tag	UNP A4GX63

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is water.

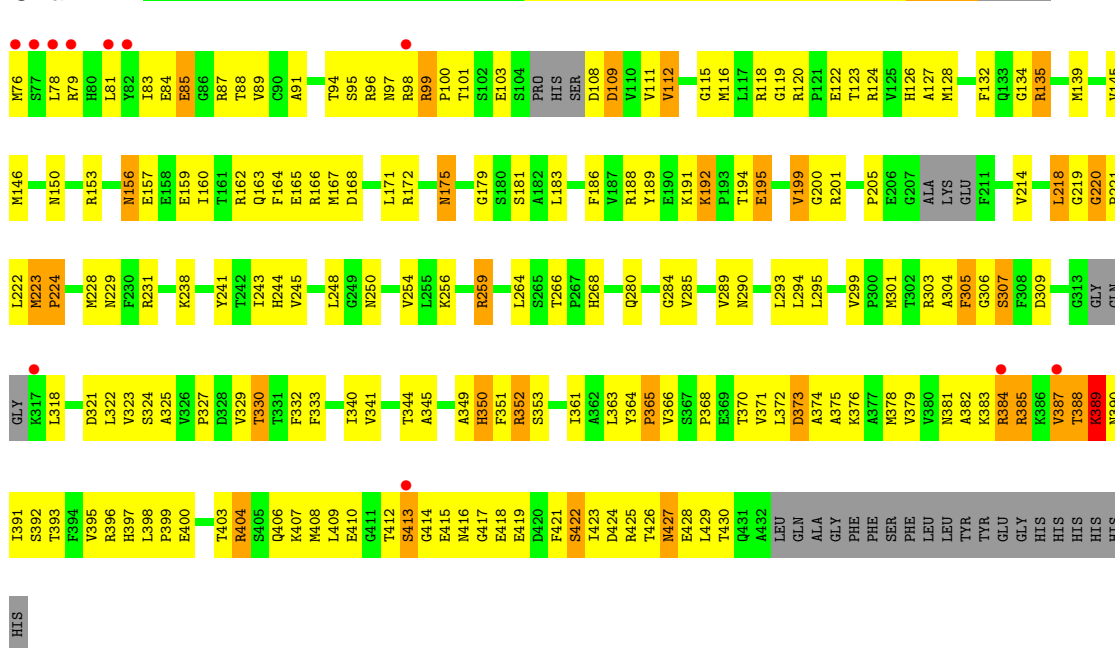
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total	O	0	0
			50	50		
3	B	42	Total	O	0	0
			42	42		
3	C	50	Total	O	0	0
			50	50		
3	D	39	Total	O	0	0
			39	39		

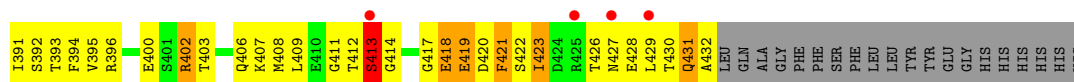
3 Residue-property plots

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: Protein phosphatase 2C

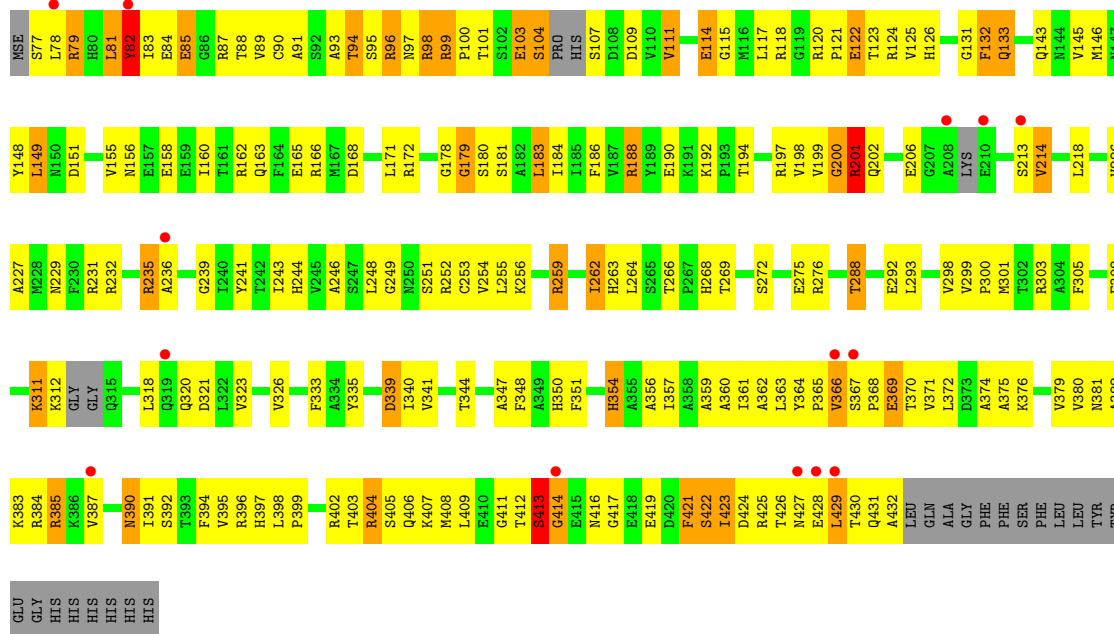
Chain A:





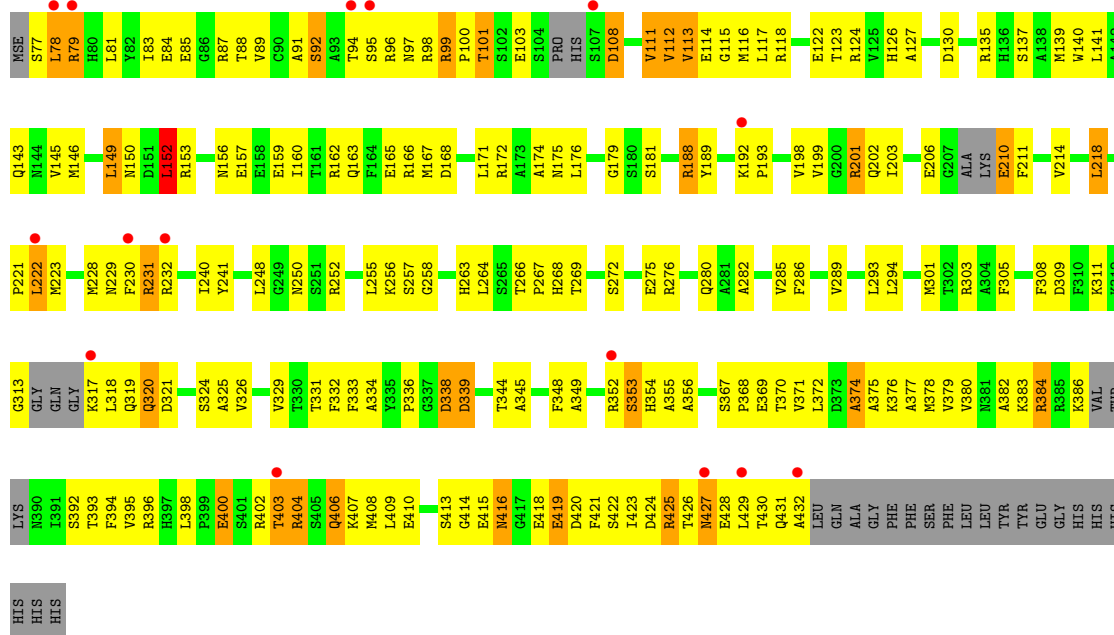
• Molecule 1: Protein phosphatase 2C

Chain C:



• Molecule 1: Protein phosphatase 2C

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.88Å 169.05Å 87.01Å 90.00° 104.47° 90.00°	Depositor
Resolution (Å)	46.71 – 2.71 46.84 – 2.59	Depositor EDS
% Data completeness (in resolution range)	94.6 (46.71-2.71) 91.8 (46.84-2.59)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.96 (at 2.58Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.251 , 0.304 0.251 , 0.302	Depositor DCC
R_{free} test set	1052 reflections (2.53%)	DCC
Wilson B-factor (Å ²)	34.8	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 26.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 48506 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	10892	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.48	0/2700	0.84	6/3628 (0.2%)
1	B	0.44	0/2714	0.74	2/3646 (0.1%)
1	C	0.45	0/2732	0.80	6/3671 (0.2%)
1	D	0.43	0/2686	0.80	5/3607 (0.1%)
All	All	0.45	0/10832	0.79	19/14552 (0.1%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	414	GLY	N-CA-C	-10.70	86.35	113.10
1	A	389	LYS	N-CA-C	-10.67	82.19	111.00
1	D	414	GLY	N-CA-C	-10.16	87.70	113.10
1	A	385	ARG	N-CA-C	-8.97	86.77	111.00
1	B	414	GLY	N-CA-C	-8.52	91.80	113.10
1	C	414	GLY	N-CA-C	-7.88	93.39	113.10
1	D	353	SER	N-CA-C	-7.46	90.86	111.00
1	C	413	SER	N-CA-C	-6.47	93.54	111.00
1	D	404	ARG	N-CA-C	-6.25	94.13	111.00
1	C	81	LEU	CA-CB-CG	6.05	129.21	115.30
1	B	413	SER	N-CA-C	-5.88	95.12	111.00
1	D	152	LEU	CA-CB-CG	5.46	127.86	115.30
1	C	385	ARG	N-CA-C	-5.44	96.31	111.00
1	A	388	THR	N-CA-C	-5.40	96.43	111.00
1	C	366	VAL	N-CA-C	-5.39	96.44	111.00
1	D	384	ARG	N-CA-C	-5.38	96.49	111.00
1	A	388	THR	OG1-CB-CG2	-5.17	98.11	110.00
1	A	387	VAL	CB-CA-C	-5.12	101.68	111.40
1	C	82	TYR	CA-CB-CG	5.04	122.98	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2664	0	2646	280	0
1	B	2679	0	2663	239	0
1	C	2696	0	2680	270	0
1	D	2652	0	2630	240	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	10	0	0	1	0
3	A	50	0	0	2	0
3	B	42	0	0	6	0
3	C	50	0	0	7	0
3	D	39	0	0	4	0
All	All	10892	0	10619	999	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 47.

All (999) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:87:ARG:HH11	1:D:84:GLU:HG2	1.05	1.16
1:D:222:LEU:O	1:D:223:MSE:HE2	1.45	1.15
1:D:371:VAL:HG23	1:D:427:ASN:HD22	0.96	1.13
1:B:98:ARG:HG2	1:B:146:MSE:HG3	1.26	1.12
1:D:221:PRO:HB2	1:D:223:MSE:HE3	1.31	1.12
1:A:248:LEU:HG	1:A:303:ARG:HG3	1.30	1.12
1:C:88:THR:HB	1:C:408:MSE:HE3	1.20	1.11
1:A:248:LEU:CG	1:A:303:ARG:HG3	1.83	1.07
1:D:420:ASP:HB2	1:D:425:ARG:NH1	1.70	1.05
1:D:108:ASP:HA	1:D:135:ARG:HB3	1.40	1.04
1:B:100:PRO:HA	1:B:111:VAL:O	1.59	1.03
1:A:248:LEU:CD1	1:A:303:ARG:CG	2.38	1.02

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:376:LYS:HA	1:B:429:LEU:HD22	1.42	1.01
1:B:389:LYS:HE2	1:B:390:ASN:H	1.25	1.01
1:A:120:ARG:HD2	1:A:123:THR:HG23	1.39	1.00
1:B:376:LYS:HG2	1:B:429:LEU:HD21	1.43	1.00
1:A:248:LEU:CD1	1:A:303:ARG:HG3	1.92	0.99
1:C:408:MSE:HE2	1:C:419:GLU:OE2	1.62	0.99
1:C:83:ILE:HG12	1:C:85:GLU:HB2	1.45	0.99
1:D:416:ASN:HB3	1:D:429:LEU:HD23	1.44	0.98
1:D:379:VAL:HG21	1:D:429:LEU:HD12	1.45	0.98
1:D:308:PHE:HA	1:D:311:LYS:HB2	1.46	0.97
1:B:108:ASP:HB2	1:B:390:ASN:HD21	1.29	0.97
1:D:124:ARG:NE	1:D:421:PHE:HZ	1.63	0.96
1:C:375:ALA:HB3	1:C:427:ASN:HD22	1.28	0.96
1:D:371:VAL:HG23	1:D:427:ASN:ND2	1.82	0.93
1:D:101:THR:HG23	1:D:111:VAL:HG13	1.49	0.93
1:B:89:VAL:HG22	1:B:406:GLN:NE2	1.83	0.93
1:B:394:PHE:HE1	1:B:426:THR:HG23	1.34	0.91
1:C:99:ARG:CZ	1:C:408:MSE:HE1	2.00	0.91
1:D:394:PHE:HE1	1:D:426:THR:HG23	1.35	0.91
1:B:99:ARG:O	1:B:113:VAL:HG22	1.72	0.90
1:D:98:ARG:HD3	1:D:146:MSE:HB2	1.53	0.90
1:C:235:ARG:HB3	1:C:235:ARG:HH11	1.36	0.90
1:C:383:LYS:HA	1:C:387:VAL:HG12	1.55	0.89
1:C:103:GLU:HG2	1:C:104:SER:H	1.36	0.88
1:A:83:ILE:CG1	1:A:85:GLU:HB2	2.03	0.88
1:C:417:GLY:H	1:C:428:GLU:HG2	1.39	0.88
1:A:98:ARG:NH1	1:A:112:VAL:HG21	1.89	0.87
1:C:292:GLU:HG3	1:C:293:LEU:HD23	1.58	0.86
1:C:293:LEU:H	1:C:293:LEU:HD23	1.40	0.86
1:D:85:GLU:OE1	1:D:407:LYS:HA	1.76	0.85
1:D:188:ARG:HG3	1:D:188:ARG:HH11	1.41	0.85
1:C:148:TYR:HB3	1:C:163:GLN:HG3	1.57	0.85
1:C:404:ARG:HH11	1:C:404:ARG:HA	1.41	0.85
1:A:120:ARG:HG2	1:A:122:GLU:H	1.41	0.85
1:A:396:ARG:NH2	1:A:424:ASP:HB3	1.92	0.85
1:C:87:ARG:NH1	1:D:84:GLU:HG2	1.90	0.85
1:A:221:PRO:HB2	1:A:223:MSE:CE	2.06	0.85
1:A:344:THR:HG23	1:A:392:SER:HB2	1.59	0.85
1:C:350:HIS:H	1:C:385:ARG:NH1	1.75	0.84
1:A:83:ILE:HG12	1:A:85:GLU:HB2	1.59	0.84
1:A:248:LEU:HG	1:A:303:ARG:CG	2.06	0.84
1:D:139:MSE:O	1:D:143:GLN:HG2	1.76	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:254:VAL:HG21	1:B:361:ILE:HD13	1.59	0.84
1:C:350:HIS:H	1:C:385:ARG:HH12	1.24	0.83
1:D:221:PRO:HB2	1:D:223:MSE:CE	2.08	0.83
1:A:156:ASN:C	1:A:156:ASN:HD22	1.81	0.83
1:B:78:LEU:HD23	1:B:79:ARG:N	1.93	0.83
1:A:248:LEU:HD11	1:A:303:ARG:CD	2.07	0.83
1:C:99:ARG:HG2	1:C:99:ARG:HH11	1.45	0.82
1:A:248:LEU:HD11	1:A:303:ARG:HD2	1.62	0.82
1:D:137:SER:O	1:D:141:LEU:HD23	1.78	0.82
1:B:172:ARG:HH12	1:B:313:GLY:HA2	1.43	0.82
1:D:221:PRO:CB	1:D:223:MSE:HE3	2.10	0.81
1:C:399:PRO:HB3	1:C:425:ARG:HE	1.46	0.81
1:B:181:SER:HB2	1:B:301:MSE:HE1	1.63	0.81
1:D:115:GLY:HA3	1:D:146:MSE:HE3	1.61	0.81
1:C:101:THR:HG22	1:C:111:VAL:HG22	1.63	0.81
1:C:375:ALA:HB3	1:C:427:ASN:ND2	1.94	0.81
1:A:78:LEU:HD21	1:A:413:SER:HB2	1.63	0.81
1:A:91:ALA:HB1	1:A:97:ASN:HB3	1.62	0.80
1:C:236:ALA:HB1	1:C:239:GLY:O	1.80	0.80
1:B:238:LYS:NZ	1:B:400:GLU:HB3	1.97	0.80
1:C:360:ALA:HA	1:C:363:LEU:HD23	1.61	0.80
1:C:96:ARG:HD3	1:C:118:ARG:CZ	2.11	0.80
1:C:87:ARG:HH11	1:D:84:GLU:CG	1.90	0.80
1:C:375:ALA:CB	1:C:427:ASN:HD22	1.93	0.80
1:C:78:LEU:HG	1:C:81:LEU:HD23	1.63	0.79
1:D:402:ARG:HG2	1:D:403:THR:HG22	1.63	0.79
1:D:139:MSE:HE2	1:D:143:GLN:OE1	1.82	0.79
1:B:83:ILE:H	1:B:83:ILE:HD12	1.46	0.79
1:B:108:ASP:HB2	1:B:390:ASN:ND2	1.96	0.78
1:D:124:ARG:HH21	1:D:421:PHE:HE2	1.30	0.78
1:A:78:LEU:HG	1:A:376:LYS:HZ2	1.48	0.78
1:C:402:ARG:NH1	1:C:422:SER:HB2	1.99	0.78
1:D:371:VAL:CG2	1:D:427:ASN:HD22	1.89	0.78
1:C:88:THR:HB	1:C:408:MSE:CE	2.10	0.78
1:C:96:ARG:HG2	1:C:118:ARG:HB3	1.64	0.78
1:B:119:GLY:O	1:B:121:PRO:HD3	1.83	0.78
1:C:403:THR:HG22	1:C:405:SER:H	1.49	0.78
1:A:392:SER:HA	1:A:430:THR:HG22	1.66	0.77
1:C:292:GLU:HG3	1:C:293:LEU:H	1.49	0.77
1:B:186:PHE:HB2	1:B:244:HIS:HB2	1.66	0.77
1:C:103:GLU:O	1:C:104:SER:HB2	1.85	0.77
1:C:85:GLU:O	1:C:88:THR:HG22	1.83	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:368:PRO:HG2	1:D:369:GLU:OE2	1.83	0.77
1:A:222:LEU:HD23	1:A:223:MSE:N	2.00	0.77
1:A:222:LEU:HD23	1:A:223:MSE:H	1.50	0.76
1:D:416:ASN:HB3	1:D:429:LEU:CD2	2.15	0.76
1:A:248:LEU:HD11	1:A:303:ARG:CG	2.15	0.76
1:C:262:ILE:HD11	3:C:480:HOH:O	1.85	0.76
1:B:98:ARG:HG2	1:B:146:MSE:CG	2.13	0.76
1:A:223:MSE:HG2	1:A:224:PRO:HD2	1.66	0.76
1:A:229:ASN:HD21	1:A:231:ARG:HB2	1.50	0.76
1:D:83:ILE:C	1:D:85:GLU:H	1.85	0.76
1:B:384:ARG:NH1	1:B:384:ARG:HB3	2.01	0.76
1:A:163:GLN:HE22	1:A:166:ARG:HE	1.30	0.76
1:A:179:GLY:H	1:A:306:GLY:HA3	1.49	0.76
1:A:84:GLU:HG2	1:A:87:ARG:HD2	1.67	0.76
1:A:264:LEU:O	1:A:330:THR:HG21	1.85	0.76
1:D:429:LEU:HD13	1:D:430:THR:N	2.01	0.75
1:C:126:HIS:CE1	1:C:426:THR:HG21	2.21	0.75
1:B:344:THR:HG23	1:B:392:SER:HB2	1.68	0.75
1:B:394:PHE:CE1	1:B:426:THR:HG23	2.21	0.75
1:A:89:VAL:HG22	1:A:406:GLN:NE2	2.02	0.75
1:B:254:VAL:CG2	1:B:341:VAL:HB	2.17	0.75
1:D:98:ARG:HG3	1:D:146:MSE:HE2	1.67	0.74
1:B:402:ARG:HA	1:B:423:ILE:HG13	1.68	0.74
1:B:101:THR:HG22	1:B:111:VAL:HB	1.70	0.74
1:A:89:VAL:HG13	1:A:406:GLN:HE22	1.52	0.74
1:A:248:LEU:HD12	1:A:303:ARG:CG	2.18	0.74
1:C:292:GLU:HG3	1:C:293:LEU:N	2.03	0.74
1:D:423:ILE:O	1:D:423:ILE:HG23	1.87	0.74
1:B:153:ARG:HG2	1:C:192:LYS:NZ	2.02	0.74
1:D:84:GLU:O	1:D:87:ARG:HB3	1.87	0.73
1:A:408:MSE:HG3	1:A:419:GLU:HG2	1.69	0.73
1:A:289:VAL:HB	1:A:294:LEU:HD22	1.71	0.73
1:D:112:VAL:O	1:D:112:VAL:HG22	1.88	0.73
1:C:417:GLY:H	1:C:428:GLU:CG	2.01	0.73
1:D:394:PHE:CE1	1:D:426:THR:HG23	2.22	0.73
1:B:78:LEU:HA	1:B:413:SER:OG	1.89	0.73
1:A:78:LEU:CD2	1:A:412:THR:O	2.37	0.73
1:A:85:GLU:O	1:A:88:THR:HG22	1.88	0.73
1:A:186:PHE:HB2	1:A:244:HIS:HB2	1.69	0.73
1:B:85:GLU:O	1:B:89:VAL:HG23	1.88	0.72
1:C:235:ARG:CB	1:C:235:ARG:HH11	2.01	0.72
1:B:372:LEU:HA	1:B:427:ASN:CG	2.10	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:83:ILE:CG1	1:C:85:GLU:HB2	2.17	0.72
1:C:198:VAL:HG13	1:C:202:GLN:O	1.88	0.72
1:A:248:LEU:CD1	1:A:303:ARG:HD2	2.19	0.72
1:B:135:ARG:HB3	1:B:135:ARG:HH11	1.54	0.72
1:B:89:VAL:HG22	1:B:406:GLN:HE21	1.53	0.72
1:D:113:VAL:HG23	1:D:426:THR:HG21	1.71	0.71
1:A:243:ILE:HD13	1:A:340:ILE:HD11	1.72	0.71
1:A:124:ARG:NE	1:A:421:PHE:HZ	1.89	0.71
1:D:79:ARG:HB3	1:D:79:ARG:CZ	2.20	0.71
1:D:199:VAL:HG11	1:D:211:PHE:CE1	2.25	0.71
1:C:78:LEU:N	1:C:413:SER:HB3	2.04	0.71
1:D:403:THR:OG1	1:D:404:ARG:N	2.19	0.71
1:B:223:MSE:HA	1:B:223:MSE:HE3	1.73	0.71
1:B:428:GLU:O	1:B:429:LEU:HD12	1.89	0.71
1:D:159:GLU:O	1:D:162:ARG:HB3	1.91	0.71
1:A:126:HIS:CE1	1:A:396:ARG:HH11	2.09	0.71
1:C:396:ARG:HB2	1:C:426:THR:HG22	1.71	0.71
1:C:252:ARG:HB2	1:C:348:PHE:CE1	2.25	0.71
1:B:317:LYS:NZ	1:B:317:LYS:HB3	2.04	0.71
1:A:126:HIS:HE1	1:A:396:ARG:HH11	1.38	0.71
1:A:115:GLY:HA3	1:A:146:MSE:HE2	1.73	0.71
1:B:336:PRO:HB3	1:B:400:GLU:HA	1.71	0.71
1:A:352:ARG:H	1:A:352:ARG:NH1	1.89	0.71
1:C:202:GLN:HE22	1:C:213:SER:HB3	1.54	0.70
1:C:78:LEU:HD21	1:C:81:LEU:HB3	1.73	0.70
1:D:289:VAL:HB	1:D:294:LEU:HD12	1.73	0.70
1:A:248:LEU:HD11	1:A:303:ARG:HG3	1.72	0.70
1:D:203:ILE:HD12	1:D:331:THR:HG22	1.74	0.70
1:B:181:SER:HB2	1:B:301:MSE:CE	2.21	0.70
1:C:83:ILE:O	1:C:83:ILE:HG23	1.91	0.70
1:A:78:LEU:CD2	1:A:413:SER:HB2	2.21	0.70
1:A:351:PHE:HA	1:A:352:ARG:NH1	2.07	0.70
1:D:317:LYS:O	1:D:317:LYS:HG2	1.90	0.70
1:A:97:ASN:HB2	1:A:99:ARG:NH1	2.07	0.69
1:C:194:THR:HA	1:C:231:ARG:HH11	1.55	0.69
1:D:400:GLU:CD	1:D:400:GLU:H	1.95	0.69
1:A:370:THR:HB	3:A:476:HOH:O	1.90	0.69
1:B:383:LYS:HD3	1:B:391:ILE:HD12	1.74	0.69
1:B:289:VAL:HB	1:B:294:LEU:HD13	1.74	0.69
1:D:415:GLU:O	1:D:429:LEU:HD22	1.93	0.69
1:B:99:ARG:HD3	1:B:408:MSE:SE	2.42	0.69
1:D:118:ARG:HG2	1:D:150:ASN:OD1	1.92	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:115:GLY:HA3	1:D:146:MSE:CE	2.23	0.69
1:D:84:GLU:HB3	1:D:408:MSE:HE2	1.73	0.69
1:A:248:LEU:CD1	1:A:303:ARG:CD	2.68	0.69
1:C:417:GLY:HA3	1:C:428:GLU:CD	2.14	0.69
1:A:139:MSE:O	1:A:139:MSE:HE3	1.93	0.69
1:C:372:LEU:HA	1:C:427:ASN:CG	2.13	0.69
1:B:403:THR:HG22	1:B:422:SER:CA	2.23	0.69
1:A:98:ARG:HD2	1:A:146:MSE:HG2	1.73	0.68
1:D:420:ASP:HB2	1:D:425:ARG:CZ	2.24	0.68
1:D:222:LEU:O	1:D:223:MSE:CE	2.35	0.68
1:B:139:MSE:O	1:B:143:GLN:HG3	1.93	0.68
1:A:84:GLU:CD	1:A:87:ARG:HH11	1.97	0.68
1:C:117:LEU:HD21	1:C:149:LEU:HB3	1.74	0.68
1:D:403:THR:OG1	1:D:404:ARG:O	2.12	0.68
1:C:98:ARG:HB3	1:C:146:MSE:HG3	1.76	0.68
1:C:124:ARG:NE	1:C:421:PHE:HZ	1.91	0.68
1:B:389:LYS:HE2	1:B:390:ASN:N	2.03	0.68
1:C:390:ASN:H	1:C:390:ASN:ND2	1.90	0.68
1:A:221:PRO:HB2	1:A:223:MSE:HE3	1.76	0.68
1:C:202:GLN:HE22	1:C:213:SER:CB	2.06	0.68
1:B:216:GLU:HG3	1:B:222:LEU:HB3	1.76	0.68
1:D:163:GLN:HE22	1:D:166:ARG:NH2	1.92	0.68
1:B:162:ARG:NH2	1:B:166:ARG:NH2	2.42	0.67
1:D:372:LEU:HD13	1:D:427:ASN:OD1	1.94	0.67
1:B:172:ARG:HH12	1:B:313:GLY:CA	2.06	0.67
1:C:124:ARG:HE	1:C:421:PHE:HZ	1.39	0.67
1:A:256:LYS:NZ	1:A:364:TYR:O	2.27	0.67
1:D:418:GLU:OE1	1:D:425:ARG:NH1	2.27	0.67
1:D:139:MSE:HE3	1:D:139:MSE:O	1.95	0.67
1:D:140:TRP:HE3	1:D:141:LEU:HD22	1.58	0.67
1:C:344:THR:HG23	1:C:392:SER:HB2	1.76	0.67
1:D:89:VAL:HG22	1:D:406:GLN:HG2	1.77	0.67
1:C:87:ARG:NH1	1:D:84:GLU:HA	2.08	0.67
1:A:163:GLN:NE2	1:A:166:ARG:HE	1.93	0.67
1:A:91:ALA:CB	1:A:99:ARG:HH12	2.08	0.67
1:D:407:LYS:HB3	1:D:420:ASP:HB3	1.77	0.67
1:A:396:ARG:CZ	1:A:424:ASP:HB3	2.25	0.67
1:B:90:CYS:O	1:B:94:THR:HG23	1.95	0.67
1:D:426:THR:HG22	1:D:427:ASN:N	2.10	0.66
1:A:78:LEU:HD22	1:A:412:THR:O	1.95	0.66
1:B:376:LYS:HG2	1:B:429:LEU:CD2	2.23	0.66
1:D:193:PRO:HG3	1:D:240:ILE:HG12	1.77	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:269:THR:HG22	1:B:270:ALA:N	2.10	0.66
1:C:259:ARG:HG2	1:C:259:ARG:HH11	1.60	0.66
1:B:222:LEU:O	1:B:222:LEU:HD12	1.96	0.66
1:B:146:MSE:HE3	3:B:476:HOH:O	1.95	0.66
1:A:259:ARG:N	1:A:259:ARG:HD2	2.11	0.66
1:B:161:THR:HG22	1:B:327:PRO:HG2	1.77	0.65
1:A:218:LEU:HD21	1:A:266:THR:HG22	1.78	0.65
1:D:372:LEU:HB2	1:D:427:ASN:HD21	1.62	0.65
1:C:293:LEU:H	1:C:293:LEU:CD2	2.07	0.65
1:A:172:ARG:NH1	1:D:153:ARG:HH12	1.95	0.65
1:A:164:PHE:HA	1:A:167:MSE:HE3	1.78	0.65
1:B:419:GLU:HB2	1:B:426:THR:HB	1.78	0.65
1:D:78:LEU:HD21	1:D:81:LEU:HD23	1.79	0.65
1:C:412:THR:HA	1:C:414:GLY:O	1.96	0.64
1:B:94:THR:O	1:B:95:SER:HB3	1.97	0.64
1:A:404:ARG:HA	1:A:404:ARG:NE	2.12	0.64
1:C:365:PRO:O	1:C:367:SER:N	2.30	0.64
1:C:268:HIS:CD2	1:C:303:ARG:HD2	2.32	0.64
1:C:417:GLY:N	1:C:428:GLU:CG	2.61	0.64
1:A:126:HIS:HE1	1:A:396:ARG:NH1	1.95	0.64
1:D:229:ASN:OD1	1:D:231:ARG:HG2	1.97	0.64
1:A:108:ASP:HA	1:A:135:ARG:HG3	1.79	0.64
1:B:203:ILE:HD12	1:B:331:THR:HG22	1.79	0.64
1:A:99:ARG:HG2	1:A:408:MSE:SE	2.48	0.64
1:D:96:ARG:CZ	1:D:118:ARG:HH21	2.11	0.64
1:A:101:THR:HG23	1:A:111:VAL:HB	1.79	0.64
1:C:383:LYS:HA	1:C:387:VAL:CG1	2.27	0.64
1:C:408:MSE:CE	1:C:419:GLU:OE2	2.42	0.64
1:A:368:PRO:HG3	1:A:397:HIS:CD2	2.33	0.64
1:B:145:VAL:O	1:B:149:LEU:HD13	1.96	0.64
1:B:206:GLU:HB3	1:C:206:GLU:OE2	1.98	0.64
1:B:97:ASN:O	1:B:146:MSE:HE2	1.98	0.63
1:C:91:ALA:CB	1:C:99:ARG:HH21	2.10	0.63
1:A:134:GLY:O	1:A:135:ARG:HB3	1.97	0.63
1:D:163:GLN:HE22	1:D:166:ARG:HH21	1.47	0.63
1:C:87:ARG:HH12	1:D:84:GLU:HA	1.63	0.63
1:C:99:ARG:NE	1:C:408:MSE:HE1	2.13	0.63
1:A:108:ASP:HB2	1:A:390:ASN:ND2	2.14	0.63
1:A:371:VAL:HG13	1:A:395:VAL:HG12	1.79	0.63
1:A:112:VAL:HG11	1:A:127:ALA:HB3	1.79	0.63
1:A:250:ASN:ND2	1:A:345:ALA:HB2	2.14	0.63
1:A:123:THR:HG22	1:A:188:ARG:HB2	1.81	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:110:VAL:HG21	1:B:142:ALA:HB2	1.81	0.63
1:C:186:PHE:HB2	1:C:244:HIS:HB2	1.81	0.63
1:A:248:LEU:HD12	1:A:303:ARG:HG2	1.81	0.63
1:D:91:ALA:HB1	1:D:97:ASN:HB3	1.80	0.63
1:D:95:SER:HA	1:D:116:MSE:SE	2.49	0.63
1:A:87:ARG:NH1	1:B:87:ARG:HD2	2.13	0.62
1:A:351:PHE:HA	1:A:352:ARG:HH11	1.64	0.62
1:B:403:THR:HG22	1:B:422:SER:O	1.98	0.62
1:A:375:ALA:HB2	1:A:427:ASN:HD22	1.64	0.62
1:C:132:PHE:CE2	1:C:179:GLY:HA2	2.35	0.62
1:A:124:ARG:NE	1:A:421:PHE:CZ	2.66	0.62
1:A:112:VAL:CG1	1:A:127:ALA:HB3	2.29	0.62
1:D:301:MSE:HA	1:D:301:MSE:HE3	1.81	0.62
1:A:78:LEU:HD12	1:A:376:LYS:HZ3	1.65	0.62
3:B:469:HOH:O	1:C:423:ILE:HD11	1.99	0.62
1:B:407:LYS:HB3	1:B:420:ASP:HB3	1.82	0.62
1:A:344:THR:CG2	1:A:392:SER:HB2	2.28	0.62
1:A:172:ARG:NH1	1:D:153:ARG:NH1	2.48	0.62
1:B:91:ALA:HB1	1:B:97:ASN:HB3	1.82	0.62
1:B:84:GLU:O	1:B:87:ARG:HG2	2.00	0.61
1:A:352:ARG:HH11	1:A:352:ARG:H	1.48	0.61
1:D:250:ASN:ND2	1:D:345:ALA:HB2	2.15	0.61
1:A:303:ARG:HD3	1:A:324:SER:HB3	1.82	0.61
1:C:97:ASN:C	1:C:98:ARG:HD3	2.20	0.61
1:C:81:LEU:HB2	1:C:411:GLY:HA3	1.82	0.61
1:C:344:THR:CG2	1:C:392:SER:HB2	2.31	0.61
1:A:349:ALA:O	1:A:350:HIS:HB2	2.00	0.61
1:D:83:ILE:C	1:D:85:GLU:N	2.54	0.61
1:B:83:ILE:CG2	1:B:85:GLU:OE2	2.49	0.61
1:C:417:GLY:N	1:C:428:GLU:HG2	2.11	0.61
1:C:99:ARG:HG2	1:C:99:ARG:NH1	2.14	0.61
1:D:188:ARG:HG3	1:D:188:ARG:NH1	2.13	0.61
1:A:163:GLN:HE22	1:A:166:ARG:NE	1.99	0.61
1:A:373:ASP:N	1:A:373:ASP:OD2	2.34	0.61
1:C:392:SER:OG	1:C:430:THR:HG23	2.01	0.61
1:A:259:ARG:H	1:A:259:ARG:HD2	1.66	0.61
1:B:217:ALA:C	1:B:219:GLY:H	2.02	0.61
1:A:100:PRO:HA	1:A:112:VAL:HA	1.82	0.61
1:A:352:ARG:HD2	1:A:352:ARG:N	2.15	0.61
1:A:84:GLU:CG	1:A:87:ARG:HH11	2.14	0.60
1:A:94:THR:O	1:A:95:SER:HB3	2.00	0.60
1:B:254:VAL:HG23	1:B:341:VAL:HB	1.83	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:124:ARG:NH1	1:B:421:PHE:CZ	2.69	0.60
1:D:192:LYS:HE2	1:D:193:PRO:O	2.01	0.60
1:B:114:GLU:HA	1:B:125:VAL:O	2.01	0.60
1:B:229:ASN:OD1	1:B:231:ARG:HB2	2.00	0.60
1:A:120:ARG:HH11	1:A:120:ARG:HG3	1.65	0.60
1:A:379:VAL:O	1:A:383:LYS:HG3	2.01	0.60
1:B:222:LEU:O	1:B:223:MSE:HE3	2.02	0.60
1:A:365:PRO:O	1:A:366:VAL:HG12	2.01	0.60
1:A:78:LEU:HD12	1:A:376:LYS:NZ	2.16	0.60
1:A:120:ARG:HD3	1:A:122:GLU:HB2	1.84	0.60
1:D:163:GLN:NE2	1:D:166:ARG:HH21	2.00	0.60
1:B:195:GLU:HG2	1:B:229:ASN:HA	1.84	0.60
1:D:157:GLU:HG3	1:D:329:VAL:CG1	2.32	0.60
1:D:165:GLU:OE1	1:D:165:GLU:HA	2.01	0.60
1:C:84:GLU:HG2	1:C:87:ARG:NE	2.16	0.60
1:B:99:ARG:CD	1:B:408:MSE:SE	3.00	0.60
1:C:268:HIS:CE1	1:C:303:ARG:HD2	2.37	0.60
1:D:157:GLU:HG3	1:D:329:VAL:HG11	1.83	0.60
1:A:195:GLU:HB3	1:A:229:ASN:HA	1.84	0.59
1:A:194:THR:HB	1:A:231:ARG:NH2	2.17	0.59
1:D:250:ASN:HA	1:D:267:PRO:HB3	1.83	0.59
1:A:349:ALA:O	1:A:385:ARG:NH1	2.35	0.59
1:D:175:ASN:O	1:D:176:LEU:HD23	2.01	0.59
1:A:85:GLU:HG2	1:A:407:LYS:HA	1.83	0.59
1:B:431:GLN:OE1	1:B:432:ALA:N	2.36	0.59
1:A:181:SER:HB3	1:A:301:MSE:SE	2.53	0.59
1:D:266:THR:HG23	1:D:268:HIS:HE1	1.66	0.59
1:B:100:PRO:CA	1:B:111:VAL:O	2.44	0.59
1:B:386:LYS:HZ2	1:B:386:LYS:HB3	1.68	0.59
1:A:421:PHE:CE2	1:A:422:SER:OG	2.55	0.59
1:A:201:ARG:HD2	1:A:333:PHE:CZ	2.37	0.59
1:A:91:ALA:HB2	1:A:99:ARG:HH12	1.68	0.59
1:A:156:ASN:ND2	1:A:159:GLU:H	2.01	0.59
1:C:252:ARG:HD3	1:C:348:PHE:HD1	1.65	0.59
1:D:392:SER:OG	1:D:430:THR:HG22	2.03	0.59
1:B:158:GLU:HG3	1:C:194:THR:HG22	1.83	0.58
1:D:419:GLU:HB2	1:D:426:THR:HB	1.84	0.58
1:C:84:GLU:OE2	1:C:87:ARG:NH2	2.35	0.58
1:C:117:LEU:CD2	1:C:149:LEU:HB3	2.33	0.58
1:D:402:ARG:C	1:D:403:THR:HG22	2.23	0.58
1:B:384:ARG:HH11	1:B:384:ARG:HB3	1.68	0.58
1:C:107:SER:HA	3:C:479:HOH:O	2.03	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:84:GLU:HB3	1:D:408:MSE:CE	2.33	0.58
1:B:372:LEU:HB2	1:B:427:ASN:ND2	2.18	0.58
1:A:84:GLU:HG2	1:A:87:ARG:NH1	2.19	0.58
1:C:77:SER:C	1:C:413:SER:HB3	2.24	0.58
1:D:241:TYR:OH	1:D:423:ILE:HG12	2.03	0.58
1:A:115:GLY:CA	1:A:146:MSE:HE2	2.32	0.58
1:C:379:VAL:HG21	1:C:429:LEU:HD22	1.84	0.58
1:A:162:ARG:O	1:A:165:GLU:HG2	2.04	0.58
1:D:113:VAL:HG23	1:D:426:THR:CG2	2.34	0.58
1:A:124:ARG:CZ	1:A:421:PHE:HZ	2.17	0.58
1:C:367:SER:O	1:C:397:HIS:CD2	2.56	0.58
1:A:112:VAL:HG13	1:A:127:ALA:H	1.69	0.58
1:A:98:ARG:HH12	1:A:112:VAL:HG21	1.68	0.58
1:A:371:VAL:HG12	1:A:427:ASN:HD21	1.68	0.58
1:A:84:GLU:CG	1:A:87:ARG:NH1	2.67	0.57
1:C:350:HIS:HB2	1:C:385:ARG:HH11	1.69	0.57
1:B:241:TYR:HE1	1:B:423:ILE:HG21	1.69	0.57
1:D:248:LEU:HD12	1:D:303:ARG:HB3	1.86	0.57
1:C:197:ARG:HD2	3:C:495:HOH:O	2.04	0.57
1:D:257:SER:HB2	3:D:460:HOH:O	2.03	0.57
1:D:375:ALA:HB2	1:D:395:VAL:HG12	1.86	0.57
1:B:418:GLU:HB2	1:B:427:ASN:ND2	2.19	0.57
1:A:248:LEU:HD21	1:A:325:ALA:HA	1.85	0.57
1:A:372:LEU:HA	1:A:427:ASN:ND2	2.19	0.57
1:C:399:PRO:HB3	1:C:425:ARG:NE	2.18	0.57
1:C:348:PHE:N	1:C:348:PHE:CD2	2.72	0.57
1:D:336:PRO:HB3	1:D:400:GLU:HA	1.86	0.57
1:B:311:LYS:C	1:B:313:GLY:H	2.06	0.57
1:C:360:ALA:CA	1:C:363:LEU:HD23	2.33	0.57
1:C:312:LYS:HD3	1:C:321:ASP:OD2	2.04	0.57
1:D:367:SER:C	1:D:369:GLU:H	2.07	0.57
1:D:386:LYS:HZ2	1:D:386:LYS:HB2	1.69	0.57
1:B:372:LEU:HB2	1:B:427:ASN:HD21	1.69	0.57
1:A:134:GLY:O	1:A:135:ARG:CB	2.53	0.57
1:D:418:GLU:HG2	1:D:427:ASN:ND2	2.19	0.57
1:B:238:LYS:HZ3	1:B:400:GLU:HB3	1.69	0.57
1:C:156:ASN:O	1:C:160:ILE:HG13	2.04	0.57
1:C:131:GLY:HA2	1:C:180:SER:HA	1.86	0.56
1:C:312:LYS:HA	1:C:318:LEU:O	2.05	0.56
1:C:376:LYS:HG3	1:C:429:LEU:HD11	1.85	0.56
1:D:402:ARG:HG3	1:D:402:ARG:HH11	1.69	0.56
1:B:367:SER:OG	1:B:370:THR:HB	2.06	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:145:VAL:HG22	1:C:149:LEU:HD22	1.87	0.56
1:C:372:LEU:HA	1:C:427:ASN:ND2	2.20	0.56
1:D:199:VAL:HG11	1:D:211:PHE:HE1	1.70	0.56
1:C:124:ARG:NE	1:C:421:PHE:CZ	2.70	0.56
1:A:366:VAL:O	1:A:366:VAL:HG22	2.06	0.56
1:D:266:THR:HG23	1:D:268:HIS:CE1	2.40	0.56
1:C:82:TYR:OH	1:D:410:GLU:HB3	2.05	0.56
1:B:191:LYS:O	1:B:192:LYS:HB2	2.03	0.56
1:A:146:MSE:O	1:A:150:ASN:HB2	2.05	0.56
1:A:392:SER:CA	1:A:430:THR:HG22	2.34	0.56
1:C:416:ASN:HB3	1:C:429:LEU:HG	1.88	0.56
1:A:179:GLY:N	1:A:306:GLY:HA3	2.18	0.56
1:B:191:LYS:O	1:B:191:LYS:HG3	2.04	0.56
1:B:89:VAL:HG22	1:B:406:GLN:HE22	1.66	0.56
1:C:235:ARG:CG	1:C:235:ARG:HH11	2.17	0.56
1:A:132:PHE:CZ	1:A:179:GLY:HA2	2.40	0.56
1:A:330:THR:HG23	1:A:332:PHE:CE1	2.41	0.56
1:D:78:LEU:HD21	1:D:81:LEU:CD2	2.35	0.56
1:D:248:LEU:CD1	1:D:303:ARG:HB3	2.35	0.56
1:B:387:VAL:CG1	1:B:391:ILE:HD11	2.36	0.56
1:A:259:ARG:CD	1:A:259:ARG:N	2.67	0.56
1:B:164:PHE:CE2	1:B:327:PRO:HB3	2.41	0.56
1:C:404:ARG:NH1	1:C:404:ARG:HA	2.15	0.56
1:D:426:THR:CG2	1:D:427:ASN:N	2.68	0.56
1:B:408:MSE:HA	1:B:418:GLU:O	2.05	0.56
1:A:175:ASN:ND2	1:D:153:ARG:HH21	2.04	0.56
1:D:400:GLU:CD	1:D:400:GLU:N	2.59	0.56
1:A:156:ASN:O	1:A:160:ILE:HG12	2.06	0.55
1:A:318:LEU:N	1:A:318:LEU:HD12	2.21	0.55
1:C:431:GLN:O	1:C:432:ALA:HB2	2.06	0.55
1:C:89:VAL:HG22	1:C:406:GLN:OE1	2.06	0.55
1:A:101:THR:HG23	1:A:101:THR:O	2.07	0.55
1:C:88:THR:CB	1:C:408:MSE:HE3	2.13	0.55
1:A:172:ARG:HH12	1:D:153:ARG:NH1	2.03	0.55
1:C:268:HIS:NE2	1:C:303:ARG:HD2	2.22	0.55
1:A:163:GLN:HE22	1:A:166:ARG:HH21	1.55	0.55
1:C:390:ASN:N	1:C:390:ASN:ND2	2.54	0.55
1:A:371:VAL:HG12	1:A:427:ASN:ND2	2.21	0.55
1:C:341:VAL:HG22	1:C:395:VAL:HG22	1.89	0.55
1:C:91:ALA:HB1	1:C:97:ASN:HB3	1.88	0.55
1:B:371:VAL:HG13	1:B:395:VAL:HG22	1.89	0.55
1:D:96:ARG:CZ	1:D:118:ARG:NH2	2.69	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:269:THR:CG2	1:B:270:ALA:N	2.69	0.55
1:D:272:SER:O	1:D:276:ARG:HB2	2.07	0.55
1:D:85:GLU:O	1:D:88:THR:HG22	2.07	0.55
1:D:145:VAL:HA	1:D:167:MSE:HE3	1.89	0.55
1:C:423:ILE:O	1:C:423:ILE:CG2	2.55	0.55
1:D:379:VAL:CG2	1:D:429:LEU:HD12	2.27	0.55
1:C:293:LEU:N	1:C:293:LEU:HD23	2.12	0.55
1:C:229:ASN:HB3	1:C:232:ARG:HG2	1.88	0.55
1:A:78:LEU:CG	1:A:376:LYS:HZ2	2.17	0.54
1:A:78:LEU:HD11	1:A:416:ASN:OD1	2.07	0.54
1:B:83:ILE:HB	1:B:85:GLU:OE2	2.07	0.54
1:A:109:ASP:OD1	1:A:390:ASN:CB	2.55	0.54
1:A:389:LYS:HG3	3:A:473:HOH:O	2.07	0.54
1:B:83:ILE:HG22	1:B:85:GLU:OE2	2.08	0.54
1:C:81:LEU:HA	1:C:411:GLY:HA2	1.88	0.54
1:B:326:VAL:HG12	1:B:326:VAL:O	2.08	0.54
1:D:103:GLU:HG3	1:D:432:ALA:HA	1.88	0.54
1:A:98:ARG:HH11	1:A:146:MSE:HG2	1.72	0.54
1:C:376:LYS:HA	1:C:429:LEU:HD13	1.90	0.54
1:C:78:LEU:HD22	1:C:79:ARG:N	2.23	0.54
1:A:168:ASP:OD1	1:A:305:PHE:O	2.25	0.54
1:C:124:ARG:NH2	1:C:421:PHE:HZ	2.05	0.54
1:C:276:ARG:HD2	2:C:453:SO4:O4	2.07	0.54
1:D:89:VAL:HG22	1:D:406:GLN:CG	2.38	0.54
1:C:100:PRO:HA	1:C:111:VAL:O	2.08	0.54
1:D:149:LEU:O	1:D:152:LEU:HG	2.07	0.54
1:D:317:LYS:O	1:D:317:LYS:CG	2.54	0.54
1:C:368:PRO:HD2	1:C:370:THR:HG22	1.89	0.54
1:C:402:ARG:HG2	1:C:403:THR:H	1.72	0.54
1:D:229:ASN:OD1	1:D:231:ARG:CG	2.55	0.54
1:C:251:SER:HB2	3:C:461:HOH:O	2.07	0.54
1:C:369:GLU:HG2	1:C:369:GLU:O	2.08	0.54
1:D:218:LEU:HD23	1:D:263:HIS:CD2	2.43	0.54
1:D:111:VAL:HG11	1:D:428:GLU:CD	2.28	0.53
1:A:145:VAL:HG13	1:A:146:MSE:N	2.22	0.53
1:D:380:VAL:O	1:D:383:LYS:HB2	2.08	0.53
1:B:187:VAL:HG11	1:B:396:ARG:NH1	2.23	0.53
1:D:353:SER:C	1:D:355:ALA:N	2.60	0.53
1:D:344:THR:HG23	1:D:392:SER:HB2	1.90	0.53
1:B:418:GLU:HB2	1:B:427:ASN:HD22	1.72	0.53
1:B:403:THR:HG22	1:B:422:SER:N	2.24	0.53
1:B:354:HIS:N	1:B:354:HIS:ND1	2.56	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:135:ARG:HE	1:B:139:MSE:HE3	1.72	0.53
1:A:299:VAL:HG12	1:A:301:MSE:H	1.73	0.53
1:D:353:SER:O	1:D:354:HIS:C	2.47	0.53
1:D:116:MSE:HE2	1:D:124:ARG:CZ	2.38	0.53
1:B:254:VAL:HG22	1:B:341:VAL:HB	1.91	0.53
1:C:124:ARG:CZ	1:C:421:PHE:HZ	2.21	0.53
1:B:326:VAL:CG1	1:B:326:VAL:O	2.56	0.53
1:B:198:VAL:O	1:B:226:VAL:HG12	2.08	0.53
1:A:108:ASP:HB2	1:A:390:ASN:HD21	1.72	0.53
1:A:95:SER:O	1:A:116:MSE:HE2	2.09	0.53
1:C:326:VAL:HG23	3:C:469:HOH:O	2.08	0.53
1:C:371:VAL:O	1:C:374:ALA:HB3	2.09	0.53
1:A:115:GLY:C	1:A:146:MSE:HE2	2.28	0.53
1:B:135:ARG:HE	1:B:139:MSE:CE	2.21	0.53
1:D:377:ALA:HA	1:D:380:VAL:HG22	1.90	0.53
1:D:424:ASP:OD2	1:D:425:ARG:N	2.41	0.53
1:B:115:GLY:HA3	1:B:146:MSE:HE2	1.91	0.53
1:B:82:TYR:OH	1:B:87:ARG:NH2	2.42	0.53
1:C:103:GLU:HG2	1:C:104:SER:N	2.15	0.53
1:A:98:ARG:HH11	1:A:98:ARG:HG3	1.74	0.53
1:A:396:ARG:HG3	1:A:426:THR:HG22	1.91	0.53
1:B:159:GLU:OE1	1:C:192:LYS:HE2	2.09	0.53
1:C:414:GLY:HA3	1:C:431:GLN:OE1	2.08	0.53
1:C:371:VAL:HG12	1:C:427:ASN:HB2	1.90	0.53
1:D:103:GLU:CD	1:D:432:ALA:HA	2.29	0.53
1:D:202:GLN:HE22	1:D:214:VAL:HG23	1.74	0.53
1:B:257:SER:HA	1:B:338:ASP:OD1	2.08	0.53
1:D:85:GLU:O	1:D:89:VAL:HG23	2.08	0.52
1:C:241:TYR:CD1	1:C:398:LEU:HD22	2.44	0.52
1:C:81:LEU:CB	1:C:411:GLY:HA3	2.39	0.52
1:D:269:THR:HG22	1:D:301:MSE:HE1	1.89	0.52
1:D:174:ALA:O	1:D:176:LEU:HG	2.08	0.52
1:B:295:LEU:C	1:B:295:LEU:HD23	2.29	0.52
1:D:77:SER:O	1:D:78:LEU:CB	2.56	0.52
1:C:254:VAL:HG21	1:C:361:ILE:HG21	1.91	0.52
1:B:114:GLU:OE1	1:B:124:ARG:HD2	2.09	0.52
1:C:423:ILE:HG23	1:C:423:ILE:O	2.09	0.52
1:B:303:ARG:O	1:B:304:ALA:HB2	2.10	0.52
1:B:154:ASP:O	1:B:159:GLU:HG2	2.09	0.52
1:C:390:ASN:H	1:C:390:ASN:HD22	1.57	0.52
1:A:172:ARG:NE	1:D:162:ARG:HD2	2.25	0.52
1:C:82:TYR:OH	1:D:410:GLU:CD	2.47	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:341:VAL:HG11	1:A:361:ILE:HG21	1.91	0.52
1:A:248:LEU:HD23	1:A:304:ALA:HA	1.90	0.52
1:A:98:ARG:NH1	1:A:98:ARG:HG3	2.25	0.52
1:C:183:LEU:HD11	1:C:253:CYS:HB2	1.92	0.52
1:C:241:TYR:CE2	1:C:398:LEU:HB3	2.45	0.52
1:C:126:HIS:HE1	1:C:426:THR:HG21	1.71	0.52
1:B:110:VAL:CG2	1:B:142:ALA:HB2	2.40	0.52
1:A:238:LYS:HD2	1:A:400:GLU:OE1	2.09	0.52
1:D:99:ARG:HH11	1:D:99:ARG:HA	1.75	0.52
1:A:223:MSE:CG	1:A:224:PRO:HD2	2.36	0.52
1:C:82:TYR:C	1:C:82:TYR:CD2	2.83	0.52
1:A:248:LEU:CG	1:A:303:ARG:CG	2.64	0.52
1:C:181:SER:HB3	1:C:301:MSE:SE	2.60	0.52
1:B:372:LEU:HA	1:B:427:ASN:OD1	2.08	0.51
1:D:141:LEU:HD12	1:D:167:MSE:HE2	1.92	0.51
1:A:109:ASP:OD1	1:A:390:ASN:HB3	2.09	0.51
1:B:110:VAL:HG21	1:B:142:ALA:CB	2.40	0.51
1:D:101:THR:HG22	1:D:113:VAL:HG12	1.90	0.51
1:A:318:LEU:HD23	1:A:322:LEU:HG	1.91	0.51
1:C:181:SER:HB2	1:C:249:GLY:HA3	1.93	0.51
1:B:426:THR:HG22	1:B:427:ASN:N	2.25	0.51
1:C:390:ASN:N	1:C:390:ASN:HD22	2.07	0.51
1:A:396:ARG:CG	1:A:426:THR:HG22	2.40	0.51
1:D:272:SER:HB3	1:D:275:GLU:HB3	1.91	0.51
1:A:96:ARG:HG3	1:A:96:ARG:O	2.10	0.51
1:C:200:GLY:O	1:C:201:ARG:HB2	2.10	0.51
1:C:417:GLY:CA	1:C:428:GLU:CD	2.78	0.51
1:D:228:MSE:HE2	1:D:230:PHE:CD1	2.45	0.51
1:B:409:LEU:O	1:B:417:GLY:HA2	2.10	0.51
1:B:295:LEU:HD23	1:B:296:GLY:N	2.25	0.51
1:C:367:SER:OG	1:C:371:VAL:N	2.44	0.51
1:B:317:LYS:HB3	1:B:317:LYS:HZ3	1.73	0.51
1:D:98:ARG:HG3	1:D:146:MSE:CE	2.39	0.51
1:B:238:LYS:HZ1	1:B:400:GLU:HB3	1.72	0.51
1:A:365:PRO:O	1:A:366:VAL:CG1	2.57	0.51
1:D:130:ASP:HB3	1:D:181:SER:HB2	1.93	0.51
1:B:78:LEU:HA	1:B:413:SER:HG	1.74	0.51
1:C:148:TYR:O	1:C:151:ASP:HB2	2.10	0.51
1:A:199:VAL:HG12	1:A:199:VAL:O	2.11	0.51
1:C:99:ARG:CG	1:C:99:ARG:NH1	2.74	0.51
1:C:168:ASP:OD2	1:C:305:PHE:O	2.29	0.51
1:C:145:VAL:HG13	1:C:146:MSE:HE2	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:117:LEU:HD21	1:D:149:LEU:HB3	1.92	0.50
1:B:135:ARG:O	1:B:135:ARG:HG2	2.11	0.50
1:A:111:VAL:HG22	1:A:128:MSE:HG3	1.93	0.50
1:C:99:ARG:NH1	1:C:408:MSE:HE1	2.24	0.50
1:B:110:VAL:HG22	1:B:129:PHE:HB2	1.92	0.50
1:D:386:LYS:NZ	1:D:386:LYS:CB	2.74	0.50
1:A:378:MSE:O	1:A:382:ALA:HB2	2.11	0.50
1:A:87:ARG:HH12	1:B:87:ARG:HG3	1.76	0.50
1:B:254:VAL:HG21	1:B:361:ILE:CD1	2.37	0.50
1:C:197:ARG:HH22	1:C:206:GLU:CG	2.25	0.50
1:C:172:ARG:HB2	1:C:308:PHE:CE2	2.46	0.50
1:B:375:ALA:HB2	1:B:395:VAL:HG12	1.93	0.50
1:A:78:LEU:CD1	1:A:376:LYS:NZ	2.74	0.50
1:A:352:ARG:N	1:A:352:ARG:HH11	2.10	0.50
1:D:386:LYS:NZ	1:D:386:LYS:HB2	2.27	0.50
1:C:82:TYR:OH	1:D:410:GLU:CG	2.60	0.50
1:A:280:GLN:HA	1:A:284:GLY:O	2.11	0.50
1:A:392:SER:HA	1:A:430:THR:CG2	2.39	0.50
1:C:197:ARG:CD	3:C:495:HOH:O	2.58	0.50
1:C:424:ASP:O	1:C:425:ARG:HG3	2.11	0.50
1:C:109:ASP:OD1	1:C:344:THR:HG21	2.11	0.50
1:C:381:ASN:HD21	1:C:384:ARG:NH2	2.10	0.50
1:D:94:THR:O	1:D:95:SER:HB3	2.10	0.50
1:A:421:PHE:CG	1:A:422:SER:N	2.79	0.50
1:D:313:GLY:HA3	3:D:454:HOH:O	2.10	0.50
1:C:229:ASN:OD1	1:C:231:ARG:HG3	2.11	0.50
1:C:114:GLU:HG3	1:C:115:GLY:N	2.26	0.50
1:A:101:THR:CG2	1:A:111:VAL:HB	2.41	0.50
1:A:153:ARG:HH22	1:D:175:ASN:HB3	1.77	0.50
1:D:124:ARG:NE	1:D:421:PHE:CZ	2.52	0.49
1:D:112:VAL:HG13	1:D:127:ALA:HB3	1.94	0.49
1:D:418:GLU:CD	1:D:425:ARG:NH1	2.65	0.49
1:A:188:ARG:HH11	1:A:188:ARG:HG2	1.77	0.49
1:B:81:LEU:HA	1:B:411:GLY:HA2	1.93	0.49
1:C:90:CYS:O	1:C:93:ALA:HB3	2.12	0.49
1:D:379:VAL:O	1:D:382:ALA:HB3	2.11	0.49
1:D:99:ARG:HD2	1:D:408:MSE:HE1	1.94	0.49
1:A:396:ARG:CB	1:A:426:THR:HG22	2.42	0.49
1:D:116:MSE:HE2	1:D:124:ARG:NH2	2.27	0.49
1:D:172:ARG:HG3	1:D:308:PHE:CE2	2.48	0.49
1:A:424:ASP:C	1:A:425:ARG:HD3	2.32	0.49
1:C:96:ARG:CD	1:C:118:ARG:NH2	2.75	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:254:VAL:HB	1:A:341:VAL:HG13	1.95	0.49
1:D:201:ARG:HG3	1:D:333:PHE:O	2.12	0.49
1:B:145:VAL:HG13	1:B:146:MSE:N	2.27	0.49
1:D:382:ALA:C	1:D:384:ARG:H	2.15	0.49
1:B:98:ARG:O	1:B:99:ARG:HG3	2.13	0.49
1:A:108:ASP:HA	1:A:135:ARG:CG	2.43	0.49
1:A:366:VAL:HG13	1:A:366:VAL:O	2.13	0.49
1:D:255:LEU:HD12	1:D:339:ASP:O	2.12	0.49
1:D:376:LYS:HA	1:D:429:LEU:HG	1.94	0.49
1:C:91:ALA:CB	1:C:99:ARG:NH2	2.76	0.48
1:D:145:VAL:HG23	1:D:167:MSE:HE1	1.95	0.48
1:C:124:ARG:HH21	1:C:421:PHE:HZ	1.61	0.48
1:B:81:LEU:O	1:B:81:LEU:HG	2.13	0.48
1:D:286:PHE:HB3	1:D:293:LEU:HD11	1.96	0.48
1:A:157:GLU:HA	1:A:329:VAL:HG21	1.93	0.48
1:B:85:GLU:O	1:B:88:THR:HG22	2.13	0.48
1:A:120:ARG:CD	1:A:122:GLU:HB2	2.42	0.48
1:A:88:THR:HB	1:A:408:MSE:HE3	1.95	0.48
1:D:145:VAL:O	1:D:149:LEU:HD13	2.13	0.48
1:C:381:ASN:ND2	1:C:384:ARG:NH2	2.62	0.48
1:D:96:ARG:O	1:D:96:ARG:HG3	2.13	0.48
1:C:214:VAL:HG11	1:C:263:HIS:O	2.14	0.48
1:C:409:LEU:O	1:C:417:GLY:HA2	2.13	0.48
1:A:120:ARG:HG2	1:A:122:GLU:N	2.21	0.48
1:D:168:ASP:OD1	1:D:311:LYS:HE2	2.13	0.48
1:B:153:ARG:HG2	1:C:192:LYS:HZ3	1.78	0.48
1:A:109:ASP:CG	1:A:390:ASN:HB3	2.33	0.48
1:D:303:ARG:HA	1:D:324:SER:O	2.14	0.48
1:D:88:THR:O	1:D:92:SER:HB2	2.13	0.48
1:B:153:ARG:HG2	1:C:192:LYS:HZ1	1.73	0.48
1:A:423:ILE:O	1:A:423:ILE:HG23	2.12	0.48
1:A:120:ARG:NE	1:A:188:ARG:HE	2.11	0.48
1:D:112:VAL:HG21	1:D:146:MSE:HE1	1.94	0.48
1:B:241:TYR:HE1	1:B:423:ILE:CG2	2.25	0.48
1:A:368:PRO:O	1:A:371:VAL:HG23	2.13	0.48
1:D:372:LEU:HB2	1:D:427:ASN:ND2	2.28	0.48
1:C:359:ALA:O	1:C:362:ALA:HB3	2.13	0.48
1:B:423:ILE:CG2	1:B:423:ILE:O	2.61	0.48
1:B:107:SER:O	1:B:135:ARG:HB2	2.14	0.48
1:B:97:ASN:O	1:B:115:GLY:HA2	2.14	0.48
1:A:156:ASN:HD21	1:A:159:GLU:H	1.60	0.48
1:C:299:VAL:HA	1:C:300:PRO:HD3	1.73	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:378:MSE:HE2	1:D:393:THR:HG22	1.96	0.48
1:D:188:ARG:HH11	1:D:188:ARG:CG	2.19	0.48
1:C:376:LYS:HE2	1:C:413:SER:OG	2.14	0.48
1:C:165:GLU:OE2	1:C:166:ARG:N	2.47	0.48
1:D:85:GLU:HA	1:D:85:GLU:OE2	2.13	0.48
1:B:386:LYS:HA	1:B:386:LYS:HZ3	1.79	0.48
1:A:132:PHE:CE2	1:A:179:GLY:HA2	2.49	0.48
1:B:255:LEU:HB2	1:B:264:LEU:HD21	1.96	0.48
1:B:133:GLN:HG3	1:B:133:GLN:O	2.13	0.48
1:B:83:ILE:CB	1:B:85:GLU:OE2	2.62	0.47
1:C:91:ALA:HB3	1:C:99:ARG:HH21	1.76	0.47
1:A:156:ASN:ND2	1:A:156:ASN:C	2.55	0.47
1:D:368:PRO:HG2	1:D:369:GLU:CD	2.34	0.47
1:B:101:THR:HG21	1:B:428:GLU:HG3	1.96	0.47
1:C:350:HIS:N	1:C:385:ARG:NH1	2.54	0.47
1:C:359:ALA:O	1:C:363:LEU:CD2	2.63	0.47
1:A:393:THR:O	1:A:428:GLU:HA	2.13	0.47
1:C:259:ARG:CG	1:C:259:ARG:HH11	2.26	0.47
1:D:126:HIS:NE2	1:D:396:ARG:NH1	2.58	0.47
1:B:146:MSE:HB3	3:B:476:HOH:O	2.14	0.47
1:B:393:THR:O	1:B:428:GLU:CD	2.53	0.47
1:D:199:VAL:HG13	1:D:199:VAL:O	2.15	0.47
1:B:394:PHE:HB2	1:B:428:GLU:OE2	2.13	0.47
1:A:98:ARG:HB2	1:A:146:MSE:HG3	1.96	0.47
1:C:96:ARG:HG3	1:C:96:ARG:HH11	1.80	0.47
1:B:422:SER:OG	1:B:423:ILE:N	2.47	0.47
1:B:158:GLU:HG3	1:C:194:THR:CG2	2.43	0.47
1:D:156:ASN:O	1:D:160:ILE:HG13	2.14	0.47
1:D:372:LEU:CA	1:D:427:ASN:ND2	2.78	0.47
1:D:406:GLN:N	1:D:406:GLN:OE1	2.47	0.47
1:D:424:ASP:OD2	1:D:424:ASP:C	2.52	0.47
1:A:392:SER:OG	1:A:430:THR:HG22	2.15	0.47
1:B:316:GLY:O	1:B:317:LYS:HG2	2.13	0.47
1:A:219:GLY:O	1:A:220:GLY:O	2.33	0.47
1:D:353:SER:O	1:D:355:ALA:N	2.47	0.47
1:A:124:ARG:NH2	1:A:421:PHE:HZ	2.13	0.47
1:D:112:VAL:CG1	1:D:127:ALA:HB3	2.44	0.47
1:D:139:MSE:HE2	1:D:143:GLN:CD	2.35	0.47
1:D:334:ALA:HB1	1:D:338:ASP:OD1	2.15	0.47
1:A:396:ARG:HB2	1:A:426:THR:HG22	1.96	0.47
1:B:123:THR:O	1:B:124:ARG:NE	2.46	0.47
1:B:99:ARG:HG3	1:B:99:ARG:NH1	2.29	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:398:LEU:HA	1:A:399:PRO:HD3	1.71	0.47
1:A:384:ARG:HD3	1:A:384:ARG:C	2.35	0.47
1:C:95:SER:OG	1:C:118:ARG:HA	2.15	0.47
1:B:364:TYR:HA	1:B:365:PRO:HD3	1.68	0.46
1:A:396:ARG:HH21	1:A:424:ASP:HB3	1.78	0.46
1:A:417:GLY:O	1:A:427:ASN:HA	2.15	0.46
1:C:155:VAL:HG11	3:C:483:HOH:O	2.14	0.46
1:D:429:LEU:HD13	1:D:430:THR:H	1.78	0.46
1:C:396:ARG:CB	1:C:426:THR:HG22	2.42	0.46
1:B:403:THR:HG22	1:B:422:SER:HA	1.96	0.46
1:B:384:ARG:C	1:B:386:LYS:H	2.17	0.46
1:D:103:GLU:CG	1:D:432:ALA:HA	2.45	0.46
1:C:201:ARG:HA	1:C:333:PHE:CE1	2.51	0.46
1:C:226:VAL:CG2	1:C:227:ALA:N	2.79	0.46
1:B:372:LEU:HA	1:B:427:ASN:ND2	2.30	0.46
1:A:229:ASN:ND2	1:A:231:ARG:HB2	2.25	0.46
1:A:218:LEU:HD23	1:A:218:LEU:N	2.30	0.46
1:C:179:GLY:O	1:C:180:SER:HB2	2.15	0.46
1:D:201:ARG:CG	1:D:201:ARG:HH11	2.29	0.46
1:A:189:TYR:HB2	1:A:241:TYR:CE1	2.50	0.46
1:A:415:GLU:O	1:A:429:LEU:HA	2.16	0.46
1:C:97:ASN:O	1:C:98:ARG:HD3	2.16	0.46
1:D:188:ARG:CG	1:D:188:ARG:NH1	2.77	0.46
1:A:391:ILE:O	1:A:430:THR:HG22	2.14	0.46
1:D:201:ARG:HG2	1:D:201:ARG:NH1	2.29	0.46
1:B:201:ARG:HH11	1:B:201:ARG:HG2	1.81	0.46
1:A:192:LYS:HA	1:A:192:LYS:HD2	1.87	0.46
1:D:418:GLU:OE2	1:D:425:ARG:NH1	2.49	0.46
1:B:82:TYR:CD1	1:B:83:ILE:HD12	2.51	0.46
1:A:194:THR:O	1:A:195:GLU:O	2.33	0.46
1:A:89:VAL:HG22	1:A:406:GLN:HE21	1.78	0.46
1:D:96:ARG:NH1	1:D:118:ARG:NH2	2.63	0.46
1:C:120:ARG:HH11	1:C:120:ARG:HG3	1.80	0.46
1:B:78:LEU:HB2	1:B:376:LYS:NZ	2.31	0.46
1:D:163:GLN:CD	1:D:166:ARG:HH21	2.19	0.46
1:D:257:SER:HA	1:D:338:ASP:HB3	1.98	0.46
1:D:353:SER:HB2	1:D:356:ALA:H	1.80	0.46
1:D:409:LEU:N	1:D:409:LEU:HD22	2.31	0.46
1:A:84:GLU:CG	1:A:87:ARG:HD2	2.42	0.46
1:C:397:HIS:O	1:C:399:PRO:HD3	2.16	0.46
1:A:91:ALA:HB1	1:A:97:ASN:CB	2.41	0.46
1:C:256:LYS:NZ	1:C:362:ALA:HA	2.31	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:256:LYS:HZ3	1:C:362:ALA:HA	1.81	0.46
1:D:353:SER:O	1:D:356:ALA:N	2.49	0.46
1:B:253:CYS:SG	1:B:264:LEU:HD12	2.55	0.46
1:C:231:ARG:HH11	1:C:231:ARG:HG2	1.81	0.45
1:C:132:PHE:CZ	1:C:179:GLY:HA2	2.51	0.45
1:A:408:MSE:HE2	1:A:419:GLU:OE1	2.17	0.45
1:A:163:GLN:HE22	1:A:166:ARG:NH2	2.14	0.45
1:C:380:VAL:O	1:C:384:ARG:N	2.50	0.45
1:B:287:THR:C	1:B:293:LEU:HD12	2.37	0.45
1:B:372:LEU:HD13	1:B:427:ASN:HD21	1.80	0.45
1:B:84:GLU:HB3	1:B:408:MSE:CE	2.47	0.45
1:A:189:TYR:OH	1:A:191:LYS:HA	2.17	0.45
1:B:200:GLY:O	1:B:201:ARG:HB2	2.16	0.45
1:C:123:THR:OG1	1:C:188:ARG:CZ	2.64	0.45
1:D:99:ARG:NH1	1:D:99:ARG:HA	2.32	0.45
1:B:367:SER:O	1:B:371:VAL:HG23	2.16	0.45
1:D:301:MSE:CA	1:D:301:MSE:HE3	2.46	0.45
1:A:168:ASP:HB2	1:A:305:PHE:HE2	1.80	0.45
1:D:256:LYS:NZ	1:D:258:GLY:O	2.46	0.45
1:D:210:GLU:N	1:D:210:GLU:OE1	2.49	0.45
1:C:372:LEU:HD12	1:C:427:ASN:HD21	1.81	0.45
1:D:423:ILE:O	1:D:423:ILE:CG2	2.60	0.45
1:B:350:HIS:HB3	1:B:356:ALA:HB3	1.98	0.45
1:C:241:TYR:CD2	1:C:398:LEU:HB3	2.52	0.45
1:D:403:THR:HA	1:D:422:SER:O	2.16	0.45
1:A:163:GLN:NE2	1:A:166:ARG:HH21	2.15	0.45
1:A:330:THR:HG23	1:A:332:PHE:HE1	1.78	0.45
1:C:252:ARG:HB2	1:C:348:PHE:CD1	2.51	0.45
1:B:317:LYS:CG	1:B:317:LYS:O	2.65	0.45
1:A:371:VAL:C	1:A:427:ASN:HD21	2.20	0.45
1:A:81:LEU:C	1:A:81:LEU:HD12	2.37	0.45
1:C:133:GLN:OE1	1:C:133:GLN:HA	2.15	0.45
1:B:240:ILE:HD12	1:B:333:PHE:HB2	1.99	0.45
1:B:78:LEU:HB2	1:B:376:LYS:HZ3	1.82	0.45
1:B:85:GLU:HG2	1:B:407:LYS:HA	1.99	0.45
1:B:412:THR:C	1:B:413:SER:HG	2.20	0.45
1:A:78:LEU:CD1	1:A:376:LYS:HZ2	2.30	0.45
1:A:192:LYS:HE3	1:A:192:LYS:CA	2.46	0.45
1:A:303:ARG:HD3	1:A:324:SER:O	2.16	0.45
1:C:103:GLU:CG	1:C:104:SER:H	2.09	0.45
1:C:96:ARG:HD3	1:C:118:ARG:NH2	2.31	0.45
1:A:108:ASP:HA	1:A:135:ARG:HB2	1.97	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:276:ARG:HG2	1:D:280:GLN:OE1	2.16	0.45
1:D:378:MSE:CB	1:D:393:THR:HG21	2.47	0.45
1:B:263:HIS:O	1:B:264:LEU:HD23	2.16	0.45
1:A:352:ARG:HG2	1:A:353:SER:N	2.32	0.45
1:C:412:THR:HG23	1:C:412:THR:O	2.17	0.45
1:C:197:ARG:HH22	1:C:206:GLU:HG2	1.82	0.45
1:B:96:ARG:HA	1:B:116:MSE:HB3	1.98	0.45
1:D:172:ARG:HD2	3:D:454:HOH:O	2.15	0.45
1:D:308:PHE:HB3	3:D:454:HOH:O	2.17	0.45
1:D:112:VAL:O	1:D:112:VAL:CG2	2.59	0.45
1:D:117:LEU:CD2	1:D:149:LEU:HB3	2.46	0.45
1:C:96:ARG:CD	1:C:118:ARG:CZ	2.90	0.45
1:A:109:ASP:OD1	1:A:390:ASN:HB2	2.17	0.45
1:C:162:ARG:O	1:C:165:GLU:HB3	2.16	0.45
1:C:143:GLN:HE21	1:C:143:GLN:HB3	1.59	0.45
1:B:85:GLU:O	1:B:88:THR:CG2	2.65	0.44
1:A:83:ILE:O	1:A:83:ILE:HG23	2.16	0.44
1:D:326:VAL:HG12	1:D:326:VAL:O	2.17	0.44
1:B:428:GLU:C	1:B:429:LEU:HD12	2.37	0.44
1:A:124:ARG:NH2	1:A:421:PHE:CZ	2.86	0.44
1:A:83:ILE:HG13	1:A:85:GLU:HB2	1.95	0.44
1:D:282:ALA:HB1	1:D:320:GLN:NE2	2.33	0.44
1:A:87:ARG:CZ	1:B:87:ARG:HB3	2.47	0.44
1:A:421:PHE:CD2	1:A:422:SER:OG	2.67	0.44
1:B:379:VAL:O	1:B:383:LYS:HG2	2.17	0.44
1:B:82:TYR:CE1	1:B:83:ILE:HD12	2.53	0.44
1:A:303:ARG:CD	1:A:324:SER:HB3	2.46	0.44
1:C:348:PHE:HB3	1:C:357:ILE:HD13	1.99	0.44
1:B:382:ALA:O	1:B:387:VAL:HG12	2.17	0.44
1:A:164:PHE:CD2	1:A:327:PRO:HG3	2.51	0.44
1:B:376:LYS:HA	1:B:429:LEU:CD2	2.31	0.44
1:A:87:ARG:NH1	1:B:87:ARG:CG	2.80	0.44
1:C:98:ARG:HD2	1:C:146:MSE:HG3	1.99	0.44
1:C:402:ARG:HG2	1:C:403:THR:N	2.33	0.44
1:B:317:LYS:HZ2	1:B:317:LYS:HB3	1.79	0.44
1:C:90:CYS:O	1:C:94:THR:HG22	2.17	0.44
1:D:85:GLU:CA	1:D:85:GLU:OE2	2.66	0.44
1:A:87:ARG:HH12	1:B:87:ARG:CG	2.31	0.44
1:B:426:THR:CG2	1:B:427:ASN:N	2.81	0.44
1:B:384:ARG:HB3	1:B:384:ARG:CZ	2.48	0.44
1:A:109:ASP:OD2	1:A:390:ASN:HB3	2.18	0.44
1:D:377:ALA:HA	1:D:380:VAL:CG2	2.46	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:376:LYS:O	1:B:380:VAL:HG23	2.17	0.44
1:B:428:GLU:OE1	1:B:429:LEU:O	2.35	0.44
1:A:123:THR:O	1:A:124:ARG:NH1	2.50	0.44
1:D:367:SER:C	1:D:369:GLU:N	2.71	0.44
1:D:78:LEU:C	1:D:79:ARG:HE	2.21	0.44
1:C:268:HIS:CG	1:C:303:ARG:HD2	2.53	0.44
1:B:85:GLU:HA	1:B:88:THR:HG22	2.00	0.44
1:A:245:VAL:HB	1:A:330:THR:HG22	1.99	0.44
1:B:375:ALA:HB2	1:B:395:VAL:CG1	2.48	0.43
1:D:193:PRO:HG2	1:D:240:ILE:HG23	2.00	0.43
1:A:214:VAL:HG13	1:A:266:THR:HG23	1.99	0.43
1:B:187:VAL:CG1	1:B:396:ARG:NH1	2.80	0.43
1:A:145:VAL:CG1	1:A:146:MSE:N	2.81	0.43
1:C:403:THR:O	1:C:422:SER:HA	2.18	0.43
1:A:218:LEU:O	1:A:219:GLY:C	2.55	0.43
1:A:108:ASP:OD1	1:A:135:ARG:HB2	2.17	0.43
1:A:371:VAL:HG13	1:A:395:VAL:CG1	2.46	0.43
1:B:120:ARG:HB3	1:B:123:THR:HB	1.99	0.43
1:A:126:HIS:CE1	1:A:396:ARG:NH1	2.76	0.43
1:A:78:LEU:CD2	1:A:413:SER:CB	2.93	0.43
1:C:125:VAL:HG12	1:C:126:HIS:N	2.33	0.43
1:D:241:TYR:CE2	1:D:398:LEU:HB3	2.53	0.43
1:D:78:LEU:C	1:D:78:LEU:HD13	2.38	0.43
1:B:270:ALA:O	1:B:276:ARG:HD3	2.18	0.43
1:B:418:GLU:O	1:B:418:GLU:HG3	2.17	0.43
1:B:82:TYR:HE2	1:B:87:ARG:HH21	1.64	0.43
1:B:98:ARG:NH1	3:B:491:HOH:O	2.50	0.43
1:C:367:SER:HA	1:C:370:THR:HG22	1.99	0.43
1:A:112:VAL:O	1:A:112:VAL:HG22	2.17	0.43
1:C:96:ARG:HG3	1:C:96:ARG:NH1	2.33	0.43
1:B:121:PRO:HD2	3:B:454:HOH:O	2.17	0.43
1:D:96:ARG:NE	1:D:118:ARG:HH21	2.16	0.43
1:A:341:VAL:O	1:A:341:VAL:HG13	2.19	0.43
1:A:223:MSE:CB	1:A:224:PRO:HD2	2.49	0.43
1:B:403:THR:HG22	1:B:422:SER:C	2.39	0.43
1:B:217:ALA:C	1:B:219:GLY:N	2.69	0.43
1:D:248:LEU:HD21	1:D:325:ALA:HA	2.00	0.43
1:C:82:TYR:C	1:C:82:TYR:HD2	2.19	0.43
1:B:89:VAL:HG13	1:B:406:GLN:HE22	1.83	0.43
1:C:235:ARG:CG	1:C:235:ARG:NH1	2.78	0.43
1:B:346:GLY:HA3	1:B:390:ASN:O	2.19	0.43
1:C:96:ARG:HD3	1:C:118:ARG:NE	2.32	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:172:ARG:NH2	1:D:162:ARG:HG2	2.33	0.43
1:B:269:THR:CG2	1:B:270:ALA:H	2.30	0.43
1:A:96:ARG:HB3	1:A:118:ARG:CD	2.48	0.43
1:A:84:GLU:HG2	1:A:87:ARG:HH11	1.77	0.43
1:A:408:MSE:HE2	1:A:419:GLU:HG2	2.00	0.43
1:A:98:ARG:CZ	1:A:145:VAL:HG12	2.48	0.43
1:C:396:ARG:HD2	1:C:426:THR:CG2	2.49	0.43
1:B:188:ARG:O	1:B:241:TYR:HA	2.18	0.43
1:A:101:THR:N	1:A:111:VAL:O	2.48	0.43
1:D:202:GLN:NE2	1:D:214:VAL:HG23	2.34	0.43
1:C:99:ARG:HD3	1:C:408:MSE:CE	2.48	0.43
1:C:414:GLY:CA	1:C:431:GLN:OE1	2.67	0.43
1:C:376:LYS:CG	1:C:429:LEU:HD11	2.49	0.43
1:B:152:LEU:HD22	1:B:159:GLU:HG3	2.01	0.43
1:C:311:LYS:HD2	1:C:323:VAL:O	2.19	0.43
1:B:97:ASN:O	1:B:115:GLY:CA	2.67	0.42
1:D:189:TYR:HE2	1:D:402:ARG:HH22	1.65	0.42
1:B:223:MSE:HG3	1:B:224:PRO:HD3	2.01	0.42
1:B:124:ARG:NH1	1:B:421:PHE:CE1	2.87	0.42
1:B:259:ARG:HG3	1:B:259:ARG:HH11	1.83	0.42
1:C:402:ARG:NH1	1:C:422:SER:CB	2.77	0.42
1:B:207:GLY:N	1:C:206:GLU:OE2	2.52	0.42
1:C:200:GLY:O	1:C:201:ARG:CB	2.66	0.42
1:B:350:HIS:HB3	1:B:356:ALA:CB	2.49	0.42
1:B:259:ARG:HD3	1:B:362:ALA:O	2.19	0.42
1:D:252:ARG:HB2	1:D:348:PHE:CE1	2.54	0.42
1:C:339:ASP:OD1	1:C:397:HIS:CD2	2.72	0.42
1:A:392:SER:OG	1:A:430:THR:CG2	2.67	0.42
1:B:268:HIS:CG	1:B:303:ARG:HD2	2.54	0.42
1:A:194:THR:HB	1:A:231:ARG:CZ	2.48	0.42
1:A:371:VAL:HG12	1:A:427:ASN:OD1	2.20	0.42
1:B:371:VAL:HG12	1:B:427:ASN:HB2	2.01	0.42
1:C:85:GLU:HG2	1:C:407:LYS:HA	2.02	0.42
1:C:339:ASP:OD1	1:C:397:HIS:HD2	2.02	0.42
1:A:408:MSE:HE2	1:A:419:GLU:CD	2.40	0.42
1:C:359:ALA:O	1:C:363:LEU:HD22	2.20	0.42
1:C:231:ARG:NH1	1:C:231:ARG:HG2	2.35	0.42
1:A:87:ARG:NH1	1:B:87:ARG:CD	2.81	0.42
1:C:408:MSE:O	1:C:409:LEU:HD23	2.20	0.42
1:C:408:MSE:HG3	1:C:419:GLU:OE2	2.20	0.42
1:B:308:PHE:HA	1:B:311:LYS:HB2	2.02	0.42
1:A:368:PRO:HG3	1:A:397:HIS:NE2	2.34	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:365:PRO:C	1:A:366:VAL:HG12	2.40	0.42
1:A:379:VAL:HG13	1:A:391:ILE:HG21	2.01	0.42
1:C:236:ALA:HB2	1:C:335:TYR:HD1	1.84	0.42
1:A:293:LEU:O	1:A:294:LEU:HD12	2.20	0.42
1:C:357:ILE:HG22	1:C:361:ILE:HD12	2.01	0.42
1:D:202:GLN:HB2	1:D:332:PHE:CE1	2.55	0.42
1:A:403:THR:O	1:A:403:THR:HG23	2.20	0.42
1:C:194:THR:HA	1:C:231:ARG:NH1	2.28	0.42
1:C:288:THR:HA	1:C:293:LEU:HA	2.02	0.42
1:C:347:ALA:O	1:C:385:ARG:NH2	2.53	0.42
1:A:351:PHE:CA	1:A:352:ARG:HH11	2.32	0.42
1:B:383:LYS:CD	1:B:391:ILE:HD12	2.47	0.42
1:B:321:ASP:HB3	1:B:323:VAL:O	2.20	0.42
1:B:235:ARG:HB2	1:B:335:TYR:CE1	2.55	0.42
1:D:222:LEU:C	1:D:223:MSE:HG2	2.39	0.42
1:A:248:LEU:HD23	1:A:304:ALA:CA	2.49	0.42
1:C:149:LEU:HD12	1:C:149:LEU:HA	1.76	0.42
1:D:266:THR:O	1:D:266:THR:HG23	2.20	0.42
1:C:171:LEU:HD13	1:C:171:LEU:C	2.40	0.42
1:C:382:ALA:HB3	1:C:391:ILE:HD13	2.02	0.42
1:B:394:PHE:HE1	1:B:426:THR:CG2	2.19	0.42
1:B:78:LEU:HD23	1:B:79:ARG:H	1.79	0.42
1:D:349:ALA:O	1:D:352:ARG:HG2	2.19	0.42
1:C:184:ILE:HB	1:C:246:ALA:HB3	2.01	0.42
1:C:398:LEU:HA	1:C:399:PRO:HD2	1.91	0.41
1:A:408:MSE:HG3	1:A:419:GLU:CG	2.43	0.41
1:D:156:ASN:N	1:D:156:ASN:OD1	2.53	0.41
1:D:371:VAL:O	1:D:374:ALA:HB3	2.19	0.41
1:A:83:ILE:C	1:A:85:GLU:H	2.23	0.41
1:A:410:GLU:HA	1:A:416:ASN:O	2.20	0.41
1:B:235:ARG:HB2	1:B:335:TYR:CZ	2.55	0.41
1:C:83:ILE:CG2	1:C:83:ILE:O	2.62	0.41
1:D:367:SER:OG	1:D:370:THR:HG23	2.21	0.41
1:B:382:ALA:HB1	1:B:387:VAL:HG11	2.01	0.41
1:C:248:LEU:HD12	1:C:303:ARG:HB3	2.02	0.41
1:B:198:VAL:HG13	1:B:202:GLN:O	2.20	0.41
1:A:96:ARG:HE	1:A:96:ARG:HB2	1.69	0.41
1:B:259:ARG:HD3	1:B:259:ARG:HA	1.77	0.41
1:D:114:GLU:OE2	1:D:124:ARG:HD2	2.20	0.41
1:D:141:LEU:N	1:D:141:LEU:HD22	2.35	0.41
1:B:301:MSE:SE	1:B:304:ALA:HB2	2.71	0.41
1:C:243:ILE:CD1	1:C:340:ILE:HD11	2.50	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:121:PRO:O	1:C:122:GLU:C	2.59	0.41
1:A:268:HIS:CB	1:A:303:ARG:HB3	2.50	0.41
1:A:408:MSE:C	1:A:409:LEU:HD12	2.41	0.41
1:A:98:ARG:NH2	1:A:112:VAL:HB	2.35	0.41
1:C:361:ILE:HA	1:C:364:TYR:CD1	2.55	0.41
1:C:351:PHE:HB3	1:C:356:ALA:HB3	2.03	0.41
1:D:179:GLY:HA3	1:D:305:PHE:O	2.20	0.41
1:B:372:LEU:CB	1:B:427:ASN:HD21	2.33	0.41
1:A:127:ALA:HA	1:A:183:LEU:O	2.21	0.41
1:B:387:VAL:HG13	1:B:391:ILE:HD11	2.02	0.41
1:C:272:SER:HB3	1:C:275:GLU:HB2	2.02	0.41
1:B:392:SER:HA	1:B:429:LEU:O	2.20	0.41
1:A:221:PRO:HB2	1:A:223:MSE:HE1	1.97	0.41
1:D:123:THR:O	1:D:124:ARG:NH1	2.46	0.41
1:C:101:THR:HG21	1:C:428:GLU:HB2	2.02	0.41
1:A:78:LEU:HA	1:A:78:LEU:HD23	1.72	0.41
1:A:352:ARG:HD2	1:A:352:ARG:H	1.82	0.41
1:D:382:ALA:C	1:D:384:ARG:N	2.74	0.41
1:C:101:THR:HG23	1:C:111:VAL:HG13	2.03	0.41
1:C:372:LEU:HD12	1:C:372:LEU:O	2.21	0.41
1:A:99:ARG:HD2	1:A:99:ARG:N	2.36	0.41
1:A:78:LEU:HD23	1:A:413:SER:OG	2.20	0.41
1:B:222:LEU:HG	1:B:222:LEU:H	1.61	0.41
1:A:139:MSE:O	1:A:139:MSE:CE	2.66	0.41
1:C:248:LEU:CD1	1:C:303:ARG:HB3	2.51	0.41
1:D:231:ARG:CG	1:D:231:ARG:HH11	2.33	0.41
1:B:372:LEU:CB	1:B:427:ASN:ND2	2.83	0.41
1:B:428:GLU:CG	1:B:429:LEU:N	2.84	0.41
1:C:403:THR:HG22	1:C:404:ARG:N	2.36	0.41
1:B:201:ARG:HG2	1:B:201:ARG:NH1	2.36	0.41
1:C:133:GLN:OE1	1:C:133:GLN:CA	2.69	0.41
1:C:218:LEU:O	1:C:354:HIS:HE1	2.04	0.41
1:D:264:LEU:CD1	1:D:264:LEU:N	2.84	0.41
1:D:114:GLU:CD	1:D:421:PHE:HE1	2.25	0.40
1:B:99:ARG:CG	1:B:99:ARG:HH11	2.34	0.40
1:A:97:ASN:HB2	1:A:99:ARG:HH11	1.83	0.40
1:C:190:GLU:O	1:C:190:GLU:HG2	2.21	0.40
1:B:115:GLY:HA3	1:B:146:MSE:CE	2.50	0.40
1:B:311:LYS:C	1:B:313:GLY:N	2.74	0.40
1:B:289:VAL:HB	1:B:294:LEU:CD1	2.49	0.40
1:A:404:ARG:HA	1:A:404:ARG:HE	1.83	0.40
1:A:371:VAL:O	1:A:374:ALA:HB3	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:206:GLU:CB	1:C:206:GLU:OE2	2.69	0.40
1:D:122:GLU:HA	1:D:122:GLU:OE1	2.21	0.40
1:D:123:THR:HG22	1:D:124:ARG:N	2.36	0.40
1:D:428:GLU:CD	1:D:429:LEU:N	2.75	0.40
1:B:98:ARG:NH1	3:B:492:HOH:O	2.53	0.40
1:C:376:LYS:N	1:C:429:LEU:HD13	2.37	0.40
1:B:423:ILE:HG23	1:B:423:ILE:O	2.21	0.40
1:A:351:PHE:O	1:A:352:ARG:C	2.59	0.40
1:C:199:VAL:O	1:C:200:GLY:C	2.59	0.40
1:A:295:LEU:HD13	1:A:323:VAL:HG23	2.02	0.40
1:C:365:PRO:C	1:C:367:SER:N	2.71	0.40
1:C:394:PHE:HA	1:C:427:ASN:O	2.21	0.40
1:C:363:LEU:N	1:C:363:LEU:HD22	2.36	0.40
1:B:162:ARG:NH2	1:B:166:ARG:HH22	2.19	0.40
1:B:129:PHE:CE1	1:B:141:LEU:HB3	2.55	0.40
1:B:253:CYS:O	1:B:264:LEU:N	2.54	0.40
1:D:114:GLU:OE2	1:D:424:ASP:OD1	2.38	0.40
1:C:383:LYS:HG2	1:C:387:VAL:HG11	2.04	0.40
1:C:293:LEU:N	1:C:293:LEU:CD2	2.76	0.40
1:A:195:GLU:HA	1:A:228:MSE:O	2.21	0.40
1:C:430:THR:HG22	1:C:431:GLN:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	340/377 (90%)	302 (89%)	30 (9%)	8 (2%)	9	21
1	B	342/377 (91%)	299 (87%)	36 (10%)	7 (2%)	11	26
1	C	343/377 (91%)	298 (87%)	38 (11%)	7 (2%)	11	26
1	D	336/377 (89%)	296 (88%)	35 (10%)	5 (2%)	15	36
All	All	1361/1508 (90%)	1195 (88%)	139 (10%)	27 (2%)	11	26

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	GLU
1	A	220	GLY
1	A	413	SER
1	C	214	VAL
1	D	78	LEU
1	D	413	SER
1	A	119	GLY
1	B	200	GLY
1	B	313	GLY
1	B	349	ALA
1	B	413	SER
1	C	103	GLU
1	C	178	GLY
1	A	365	PRO
1	B	178	GLY
1	B	314	GLY
1	B	175	ASN
1	C	201	ARG
1	D	108	ASP
1	D	374	ALA
1	A	205	PRO
1	A	307	SER
1	C	200	GLY
1	D	100	PRO
1	C	179	GLY
1	C	366	VAL
1	A	200	GLY

5.3.2 Protein sidechains ⓘ

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	280/295 (95%)	243 (87%)	37 (13%)	6	14
1	B	283/295 (96%)	246 (87%)	37 (13%)	6	14
1	C	285/295 (97%)	246 (86%)	39 (14%)	5	12
1	D	280/295 (95%)	245 (88%)	35 (12%)	7	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1128/1180 (96%)	980 (87%)	148 (13%)	6 14

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	MSE
1	A	79	ARG
1	A	85	GLU
1	A	99	ARG
1	A	103	GLU
1	A	109	ASP
1	A	112	VAL
1	A	135	ARG
1	A	156	ASN
1	A	171	LEU
1	A	175	ASN
1	A	192	LYS
1	A	199	VAL
1	A	218	LEU
1	A	223	MSE
1	A	224	PRO
1	A	259	ARG
1	A	285	VAL
1	A	290	ASN
1	A	305	PHE
1	A	307	SER
1	A	309	ASP
1	A	321	ASP
1	A	330	THR
1	A	350	HIS
1	A	352	ARG
1	A	363	LEU
1	A	373	ASP
1	A	381	ASN
1	A	384	ARG
1	A	387	VAL
1	A	388	THR
1	A	389	LYS
1	A	404	ARG
1	A	418	GLU
1	A	422	SER
1	A	427	ASN

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Mol	Chain	Res	Type
1	B	76	MSE
1	B	81	LEU
1	B	83	ILE
1	B	87	ARG
1	B	102	SER
1	B	103	GLU
1	B	107	SER
1	B	108	ASP
1	B	116	MSE
1	B	117	LEU
1	B	124	ARG
1	B	135	ARG
1	B	158	GLU
1	B	183	LEU
1	B	187	VAL
1	B	201	ARG
1	B	206	GLU
1	B	210	GLU
1	B	222	LEU
1	B	223	MSE
1	B	225	VAL
1	B	228	MSE
1	B	272	SER
1	B	317	LYS
1	B	318	LEU
1	B	326	VAL
1	B	354	HIS
1	B	384	ARG
1	B	389	LYS
1	B	402	ARG
1	B	413	SER
1	B	418	GLU
1	B	419	GLU
1	B	421	PHE
1	B	423	ILE
1	B	430	THR
1	B	431	GLN
1	C	79	ARG
1	C	82	TYR
1	C	85	GLU
1	C	94	THR
1	C	96	ARG

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Mol	Chain	Res	Type
1	C	98	ARG
1	C	99	ARG
1	C	104	SER
1	C	111	VAL
1	C	114	GLU
1	C	122	GLU
1	C	132	PHE
1	C	133	GLN
1	C	149	LEU
1	C	158	GLU
1	C	183	LEU
1	C	188	ARG
1	C	201	ARG
1	C	235	ARG
1	C	255	LEU
1	C	259	ARG
1	C	262	ILE
1	C	264	LEU
1	C	266	THR
1	C	269	THR
1	C	288	THR
1	C	298	VAL
1	C	311	LYS
1	C	320	GLN
1	C	339	ASP
1	C	354	HIS
1	C	369	GLU
1	C	390	ASN
1	C	404	ARG
1	C	413	SER
1	C	421	PHE
1	C	422	SER
1	C	423	ILE
1	C	429	LEU
1	D	79	ARG
1	D	92	SER
1	D	99	ARG
1	D	101	THR
1	D	111	VAL
1	D	112	VAL
1	D	113	VAL
1	D	149	LEU

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Mol	Chain	Res	Type
1	D	152	LEU
1	D	171	LEU
1	D	188	ARG
1	D	198	VAL
1	D	201	ARG
1	D	206	GLU
1	D	210	GLU
1	D	218	LEU
1	D	222	LEU
1	D	231	ARG
1	D	232	ARG
1	D	285	VAL
1	D	309	ASP
1	D	318	LEU
1	D	319	GLN
1	D	320	GLN
1	D	321	ASP
1	D	338	ASP
1	D	339	ASP
1	D	400	GLU
1	D	403	THR
1	D	406	GLN
1	D	416	ASN
1	D	419	GLU
1	D	425	ARG
1	D	427	ASN
1	D	431	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	HIS
1	A	133	GLN
1	A	136	HIS
1	A	156	ASN
1	A	163	GLN
1	A	175	ASN
1	A	229	ASN
1	A	273	HIS
1	A	280	GLN
1	A	290	ASN
1	A	406	GLN

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Mol	Chain	Res	Type
1	B	144	ASN
1	B	156	ASN
1	B	175	ASN
1	B	280	GLN
1	B	381	ASN
1	B	390	ASN
1	B	406	GLN
1	C	143	GLN
1	C	147	ASN
1	C	163	GLN
1	C	202	GLN
1	C	280	GLN
1	C	354	HIS
1	C	381	ASN
1	C	390	ASN
1	C	397	HIS
1	C	427	ASN
1	D	147	ASN
1	D	163	GLN
1	D	263	HIS
1	D	290	ASN
1	D	320	GLN
1	D	416	ASN
1	D	427	ASN
1	D	431	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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

4 ligands are modelled in this entry.

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	SO4	A	453	-	4,4,4	0.20	0	6,6,6	0.14	0
2	SO4	B	453	-	4,4,4	0.17	0	6,6,6	0.12	0
2	SO4	C	453	-	4,4,4	0.22	0	6,6,6	0.15	0
2	SO4	C	454	-	4,4,4	0.05	0	6,6,6	0.11	0

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	SO4	A	453	-	-	0/0/0/0	0/0/0/0
2	SO4	B	453	-	-	0/0/0/0	0/0/0/0
2	SO4	C	453	-	-	0/0/0/0	0/0/0/0
2	SO4	C	454	-	-	0/0/0/0	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.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	348/377 (92%)	0.15	11 (3%)	45 51	13, 33, 56, 84	0
1	B	350/377 (92%)	0.13	10 (2%)	49 56	9, 33, 51, 90	0
1	C	351/377 (93%)	0.12	14 (3%)	36 42	10, 30, 56, 68	0
1	D	346/377 (91%)	0.19	15 (4%)	34 39	14, 33, 58, 74	0
All	All	1395/1508 (92%)	0.15	50 (3%)	41 46	9, 32, 56, 90	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	317	LYS	5.0
1	D	432	ALA	4.4
1	A	79	ARG	3.8
1	C	429	LEU	3.7
1	D	95	SER	3.6
1	C	414	GLY	3.6
1	D	352	ARG	3.6
1	C	82	TYR	3.5
1	B	314	GLY	3.5
1	A	77	SER	3.4
1	A	98	ARG	3.4
1	D	78	LEU	3.4
1	D	230	PHE	3.3
1	C	427	ASN	3.2
1	C	78	LEU	3.2
1	B	82	TYR	3.1
1	B	427	ASN	3.1
1	A	317	LYS	3.0
1	A	384	ARG	3.0
1	D	429	LEU	3.0
1	A	387	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	208	ALA	3.0
1	B	80	HIS	2.9
1	A	78	LEU	2.8
1	A	81	LEU	2.8
1	D	427	ASN	2.8
1	D	232	ARG	2.8
1	A	76	MSE	2.8
1	D	107	SER	2.7
1	C	210	GLU	2.6
1	D	403	THR	2.5
1	B	425	ARG	2.5
1	B	77	SER	2.4
1	B	429	LEU	2.4
1	C	366	VAL	2.3
1	D	79	ARG	2.3
1	B	315	GLN	2.3
1	A	82	TYR	2.3
1	C	367	SER	2.3
1	D	94	THR	2.2
1	C	236	ALA	2.2
1	B	317	LYS	2.2
1	B	413	SER	2.2
1	C	213	SER	2.2
1	D	192	LYS	2.2
1	C	428	GLU	2.1
1	D	222	LEU	2.1
1	A	413	SER	2.1
1	C	387	VAL	2.1
1	C	319	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	C	453	5/5	0.17	-0.40	82,82,82,83	0
2	SO4	C	454	5/5	0.14	-0.98	61,62,62,63	0
2	SO4	A	453	5/5	0.14	-1.23	38,39,41,42	0
2	SO4	B	453	5/5	0.17	-1.43	60,61,62,63	0

6.5 Other polymers

There are no such residues in this entry.