



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 02:56 am BST

PDB ID : 3IBJ
Title : X-ray structure of PDE2A
Authors : Pandit, J.
Deposited on : 2009-07-16
Resolution : 3.02 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

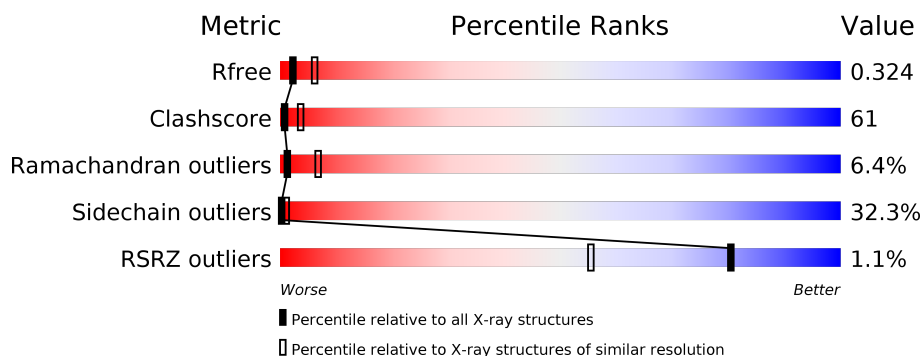
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.02 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	691	
1	B	691	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10650 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 cGMP-dependent 3',5'-cyclic phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	661	Total	C	N	O	S	0	0	0
			5291	3360	890	1000	41			
1	B	643	Total	C	N	O	S	0	0	0
			5164	3278	874	970	42			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	214	MET	-	INITIATING METHIONINE	UNP O00408
A	901	LEU	-	EXPRESSION TAG	UNP O00408
A	902	VAL	-	EXPRESSION TAG	UNP O00408
A	903	PRO	-	EXPRESSION TAG	UNP O00408
A	904	ARG	-	EXPRESSION TAG	UNP O00408
B	214	MET	-	INITIATING METHIONINE	UNP O00408
B	901	LEU	-	EXPRESSION TAG	UNP O00408
B	902	VAL	-	EXPRESSION TAG	UNP O00408
B	903	PRO	-	EXPRESSION TAG	UNP O00408
B	904	ARG	-	EXPRESSION TAG	UNP O00408

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

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

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

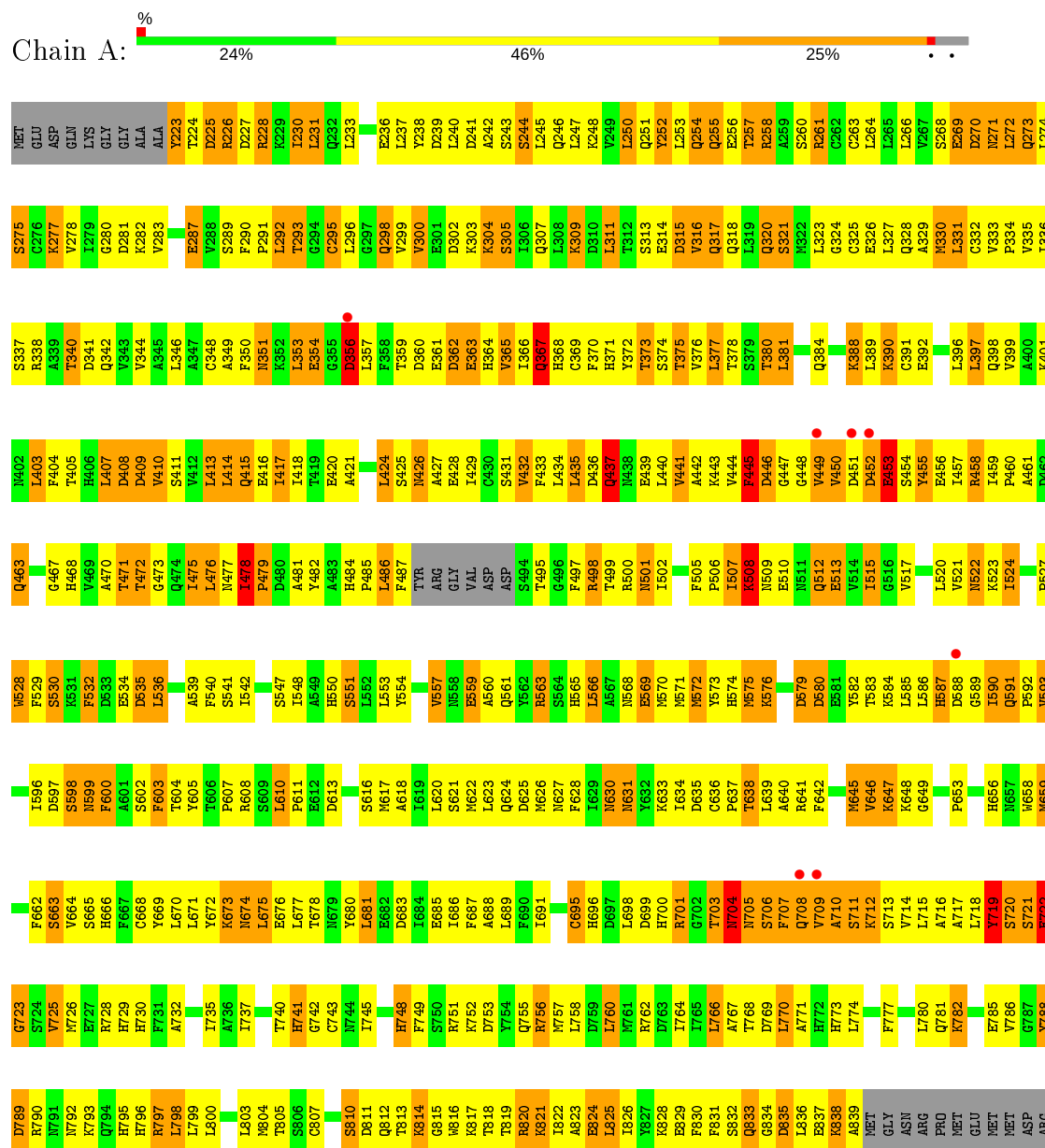
- Molecule 4 is water.

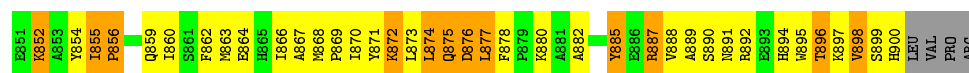
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	96	Total	O	0	0
			96	96		
4	B	95	Total	O	0	0
			95	95		

3 Residue-property plots

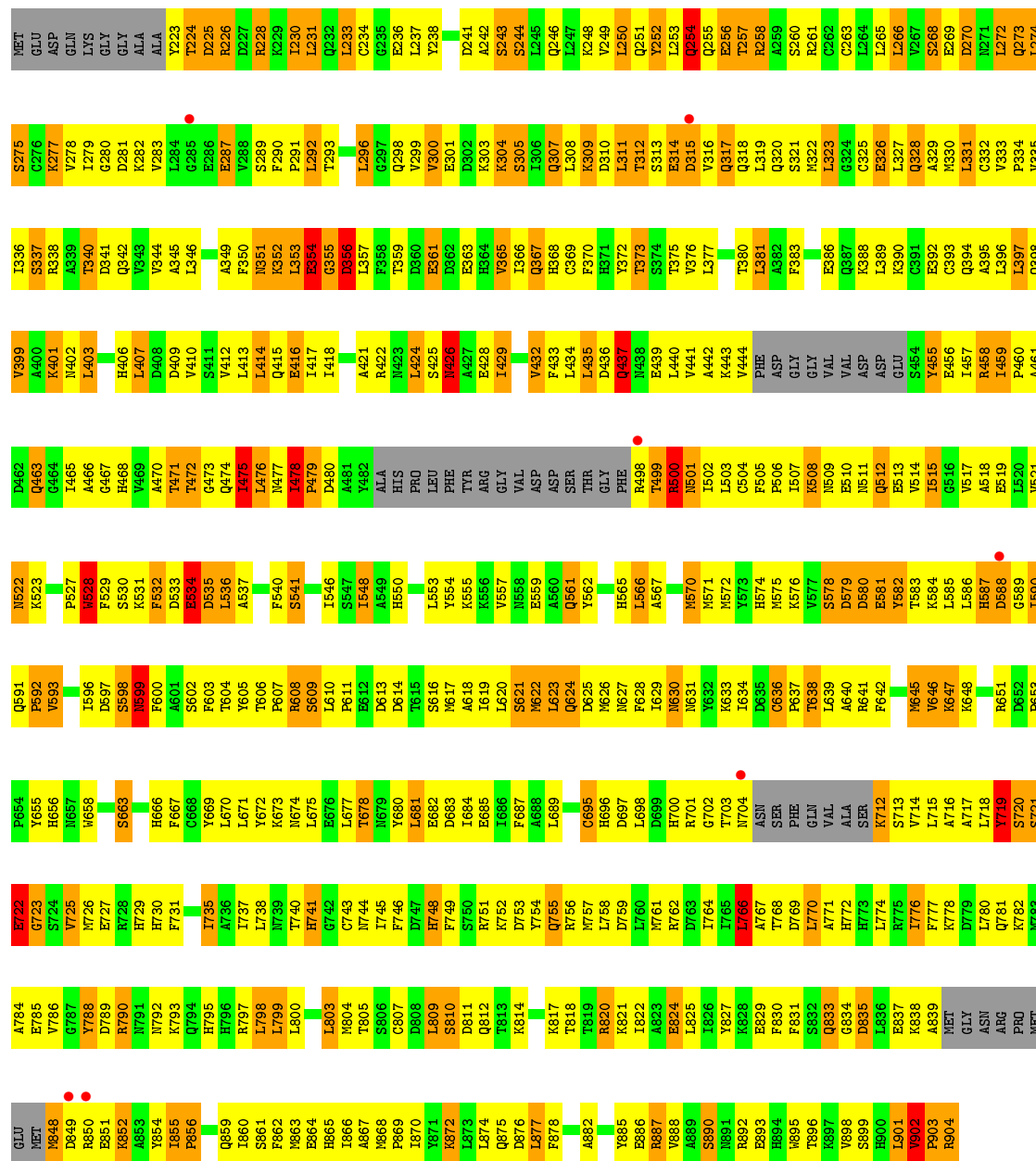
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase





• Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.23 Å 89.70 Å 264.19 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.26 – 3.02 18.17 – 3.02	Depositor EDS
% Data completeness (in resolution range)	99.5 (18.26-3.02) 99.6 (18.17-3.02)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 3.03 Å)	Xtriage
Refinement program	BUSTER-TNT 2.1.1	Depositor
R, R_{free}	0.210 , 0.311 0.217 , 0.324	Depositor DCC
R_{free} test set	1598 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	76.9	Xtriage
Anisotropy	0.567	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 82.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10650	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.66	0/5394	0.86	4/7292 (0.1%)
1	B	0.68	1/5260 (0.0%)	0.88	7/7105 (0.1%)
All	All	0.67	1/10654 (0.0%)	0.87	11/14397 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	722	GLU	CG-CD	5.25	1.59	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	855	ILE	C-N-CD	-8.18	102.61	120.60
1	A	478	ILE	C-N-CD	-7.99	103.03	120.60
1	B	902	VAL	C-N-CD	-7.13	104.91	120.60
1	B	478	ILE	C-N-CD	-6.90	105.43	120.60
1	B	723	GLY	N-CA-C	-6.66	96.44	113.10
1	B	312	THR	N-CA-C	-6.38	93.76	111.00
1	B	636	CYS	CA-CB-SG	-6.02	103.17	114.00
1	B	766	LEU	CA-CB-CG	5.90	128.88	115.30
1	A	723	GLY	N-CA-C	-5.77	98.68	113.10
1	A	264	LEU	CB-CG-CD1	-5.57	101.53	111.00
1	B	403	LEU	CA-CB-CG	5.54	128.04	115.30

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	5291	0	5225	671	0
1	B	5164	0	5128	656	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	96	0	0	10	0
4	B	95	0	0	7	0
All	All	10650	0	10353	1263	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 61.

All (1263) 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:704:ASN:ND2	1:A:705:ASN:H	1.41	1.17
1:B:312:THR:HG22	1:B:314:GLU:H	1.06	1.14
1:A:774:LEU:HD12	1:B:838:LYS:HG3	1.27	1.14
1:B:320:GLN:HG2	1:B:327:LEU:HD13	1.14	1.14
1:B:460:PRO:HG2	1:B:463:GLN:HB3	1.30	1.12
1:B:499:THR:HG22	1:B:500:ARG:H	1.11	1.12
1:A:672:TYR:HA	1:A:677:LEU:HD12	1.28	1.12
1:A:399:VAL:HG21	1:A:424:LEU:HD11	1.34	1.09
1:B:672:TYR:HA	1:B:677:LEU:HD12	1.35	1.08
1:B:789:ASP:HB3	1:B:792:ASN:HB2	1.10	1.07
1:A:303:LYS:HD3	1:A:336:ILE:HD13	1.32	1.06
1:A:440:LEU:HD12	1:A:459:ILE:HD11	1.29	1.05
1:B:223:TYR:HD2	1:B:225:ASP:HB2	1.19	1.04
1:A:458:ARG:HG2	1:A:458:ARG:HH11	1.16	1.03
1:A:566:LEU:HD11	1:B:755:GLN:HG2	1.37	1.03
1:A:704:ASN:HD22	1:A:705:ASN:N	1.55	1.02
1:A:309:LYS:HD2	1:A:309:LYS:H	1.20	1.02
1:A:789:ASP:HB3	1:A:792:ASN:HB2	1.42	1.01
1:A:695:CYS:HB3	1:A:698:LEU:HD12	1.39	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:MET:HE1	1:B:332:CYS:HB2	1.42	1.00
1:A:484:HIS:NE2	1:A:486:LEU:HD12	1.75	1.00
1:B:290:PHE:HB2	1:B:291:PRO:HD2	1.44	0.99
1:B:303:LYS:HB3	1:B:336:ILE:HD11	1.44	0.98
1:A:460:PRO:HG2	1:A:463:GLN:HB3	1.46	0.95
1:A:444:VAL:HG21	1:A:455:TYR:HD2	1.31	0.95
1:B:309:LYS:H	1:B:309:LYS:HD2	1.30	0.93
1:A:311:LEU:HD23	1:A:315:ASP:HB3	1.50	0.93
1:B:223:TYR:CD2	1:B:225:ASP:HB2	2.04	0.93
1:A:484:HIS:CD2	1:A:486:LEU:HD12	2.05	0.92
1:B:789:ASP:CB	1:B:792:ASN:HB2	1.99	0.92
1:B:270:ASP:HB2	1:B:272:LEU:CD2	2.00	0.91
1:A:270:ASP:HB2	1:A:272:LEU:CD2	2.01	0.90
1:A:799:LEU:O	1:A:803:LEU:HD12	1.71	0.90
1:B:700:HIS:HD2	1:B:702:GLY:H	1.19	0.90
1:B:270:ASP:HB2	1:B:272:LEU:HD21	1.50	0.90
1:B:623:LEU:HA	1:B:626:MET:HE2	1.51	0.90
1:A:445:PHE:HZ	1:A:450:VAL:HG22	1.37	0.89
1:A:571:MET:HA	1:A:571:MET:HE2	1.54	0.89
1:B:323:LEU:CD1	1:B:327:LEU:HD11	2.03	0.88
1:A:303:LYS:HB3	1:A:336:ILE:HD11	1.53	0.88
1:A:672:TYR:CA	1:A:677:LEU:HD12	2.03	0.88
1:A:695:CYS:HB3	1:A:698:LEU:CD1	2.03	0.87
1:A:774:LEU:HD12	1:B:838:LYS:CG	2.04	0.87
1:B:337:SER:O	1:B:341:ASP:HA	1.72	0.87
1:A:487:PHE:HZ	1:A:499:THR:HB	1.40	0.87
1:B:370:PHE:HA	1:B:373:THR:HG22	1.56	0.87
1:A:304:LYS:HA	1:A:304:LYS:HE3	1.56	0.86
1:B:312:THR:HG22	1:B:314:GLU:N	1.89	0.86
1:A:835:ASP:HA	1:A:838:LYS:CD	2.05	0.86
1:A:223:TYR:HE1	1:A:364:HIS:HE2	1.23	0.86
1:A:241:ASP:OD2	1:A:243:SER:HB2	1.76	0.85
1:B:460:PRO:HG2	1:B:463:GLN:CB	2.04	0.85
1:A:231:LEU:HD21	1:B:230:ILE:HG22	1.56	0.85
1:A:421:ALA:HB2	1:A:540:PHE:CE2	2.11	0.85
1:B:792:ASN:HB3	1:B:795:HIS:HB2	1.58	0.85
1:A:388:LYS:O	1:A:392:GLU:HG3	1.76	0.85
1:B:672:TYR:CA	1:B:677:LEU:HD12	2.07	0.84
1:B:314:GLU:HG3	1:B:315:ASP:N	1.92	0.84
1:B:499:THR:CG2	1:B:500:ARG:H	1.90	0.84
1:B:320:GLN:HG2	1:B:327:LEU:CD1	2.04	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:887:ARG:HH11	1:B:887:ARG:HG3	1.43	0.84
1:A:424:LEU:HD23	1:A:536:LEU:HD11	1.61	0.83
1:A:550:HIS:NE2	1:B:550:HIS:NE2	2.27	0.83
1:A:811:ASP:HB2	1:A:822:ILE:HD13	1.60	0.82
1:B:304:LYS:HE3	1:B:304:LYS:HA	1.60	0.82
1:B:323:LEU:HD13	1:B:327:LEU:HD11	1.58	0.82
1:A:647:LYS:HD2	1:A:658:TRP:CD1	2.14	0.82
1:B:579:ASP:O	1:B:583:THR:HG23	1.78	0.82
1:B:902:VAL:CG2	1:B:903:PRO:HD2	2.09	0.82
1:B:312:THR:HB	1:B:315:ASP:OD2	1.80	0.82
1:A:792:ASN:HB3	1:A:795:HIS:HB2	1.60	0.81
1:B:432:VAL:HG12	1:B:518:ALA:HB2	1.62	0.81
1:A:638:THR:HG22	1:A:745:ILE:HG22	1.60	0.81
1:A:330:MET:CE	1:A:332:CYS:HB2	2.10	0.81
1:A:711:SER:HB3	1:A:854:TYR:CE2	2.16	0.81
1:B:507:ILE:HG22	1:B:515:ILE:HG22	1.61	0.81
1:A:290:PHE:HB2	1:A:291:PRO:HD2	1.61	0.81
1:A:311:LEU:HD23	1:A:315:ASP:CB	2.11	0.81
1:A:666:HIS:CE1	1:A:670:LEU:HD21	2.16	0.80
1:B:656:HIS:HD2	1:B:829:GLU:OE2	1.62	0.80
1:A:399:VAL:HG21	1:A:424:LEU:CD1	2.10	0.80
1:B:638:THR:HG22	1:B:745:ILE:HG22	1.63	0.80
1:A:875:GLN:HE21	1:A:882:ALA:HA	1.45	0.80
1:B:499:THR:HG22	1:B:500:ARG:N	1.93	0.80
1:A:314:GLU:HB2	4:A:93:HOH:O	1.81	0.79
1:A:630:ASN:HD22	1:A:631:ASN:H	1.29	0.79
1:B:630:ASN:HD22	1:B:631:ASN:H	1.29	0.79
1:A:653:PRO:HB2	1:A:829:GLU:OE1	1.83	0.79
1:B:320:GLN:NE2	1:B:327:LEU:HB2	1.96	0.79
1:A:292:LEU:HD11	1:A:300:VAL:HG21	1.65	0.79
1:A:838:LYS:HD2	1:A:838:LYS:H	1.47	0.79
1:A:320:GLN:HG3	1:A:327:LEU:HD13	1.65	0.79
1:A:270:ASP:HB2	1:A:272:LEU:HD21	1.63	0.79
1:A:669:TYR:HD2	1:A:670:LEU:HD23	1.46	0.78
1:A:251:GLN:NE2	1:A:281:ASP:HA	1.98	0.78
1:B:576:LYS:O	1:B:648:LYS:HE2	1.81	0.78
1:A:837:GLU:HB2	1:A:838:LYS:HE3	1.65	0.78
1:A:789:ASP:CB	1:A:792:ASN:HB2	2.13	0.78
1:B:307:GLN:HG2	1:B:330:MET:O	1.83	0.78
1:A:238:TYR:HA	1:B:375:THR:OG1	1.84	0.78
1:A:630:ASN:ND2	1:A:631:ASN:H	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:835:ASP:HA	1:A:838:LYS:HD2	1.64	0.77
1:B:330:MET:CE	1:B:332:CYS:HB2	2.14	0.77
1:B:320:GLN:HE21	1:B:327:LEU:HB2	1.49	0.77
1:B:329:ALA:HB2	1:B:356:ASP:OD2	1.84	0.77
1:B:399:VAL:HG21	1:B:540:PHE:HE1	1.48	0.77
1:A:405:THR:HG22	1:B:546:ILE:HD12	1.65	0.77
1:A:307:GLN:HG2	1:A:330:MET:O	1.85	0.77
1:A:819:THR:HG21	1:A:891:ASN:ND2	1.99	0.77
1:B:396:LEU:HA	1:B:399:VAL:HG13	1.65	0.77
1:A:401:LYS:O	1:A:405:THR:HG23	1.84	0.77
1:A:224:THR:HG22	1:A:228:ARG:NH2	1.99	0.77
1:A:309:LYS:HD2	1:A:309:LYS:N	1.99	0.76
1:A:605:TYR:CE2	1:A:610:LEU:HD11	2.21	0.76
1:A:749:PHE:HB3	1:A:753:ASP:HB2	1.67	0.76
1:B:299:VAL:HG12	1:B:334:PRO:HG3	1.68	0.76
1:B:479:PRO:HG3	1:B:528:TRP:CZ3	2.19	0.76
1:A:711:SER:HB3	1:A:854:TYR:CD2	2.20	0.76
1:A:337:SER:OG	1:A:340:THR:HG23	1.85	0.76
1:A:340:THR:OG1	1:A:342:GLN:HG3	1.85	0.76
1:A:610:LEU:HD12	1:A:610:LEU:H	1.51	0.76
1:A:326:GLU:O	1:A:327:LEU:HD12	1.85	0.76
1:B:718:LEU:O	1:B:720:SER:N	2.17	0.76
1:A:250:LEU:HD21	1:A:263:CYS:HA	1.68	0.76
1:A:748:HIS:H	1:A:748:HIS:CD2	2.03	0.76
1:A:864:GLU:OE2	1:A:892:ARG:HD3	1.85	0.75
1:B:508:LYS:HA	1:B:513:GLU:O	1.86	0.75
1:B:789:ASP:HB3	1:B:792:ASN:CB	2.04	0.75
1:B:500:ARG:HG2	1:B:522:ASN:OD1	1.87	0.75
1:A:356:ASP:O	1:A:357:LEU:HG	1.87	0.75
1:B:605:TYR:O	1:B:814:LYS:HE3	1.86	0.75
1:B:224:THR:HG22	1:B:228:ARG:NH2	2.02	0.75
1:A:508:LYS:HA	1:A:513:GLU:O	1.86	0.75
1:B:561:GLN:HE21	1:B:561:GLN:HA	1.51	0.75
1:B:902:VAL:HG22	1:B:903:PRO:HD2	1.68	0.75
1:B:837:GLU:HB2	1:B:838:LYS:HZ3	1.51	0.75
1:A:576:LYS:HD3	1:A:576:LYS:O	1.85	0.75
1:A:410:VAL:O	1:A:414:LEU:HB2	1.87	0.75
1:B:340:THR:OG1	1:B:342:GLN:HG3	1.86	0.75
1:B:799:LEU:O	1:B:803:LEU:HD12	1.87	0.75
1:A:342:GLN:O	1:A:344:VAL:HG23	1.88	0.74
1:A:270:ASP:O	1:A:272:LEU:HD23	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:PHE:HA	1:A:373:THR:HG22	1.68	0.74
1:A:303:LYS:HD3	1:A:336:ILE:CD1	2.16	0.74
1:A:671:LEU:HD13	1:A:803:LEU:HD23	1.69	0.74
1:A:468:HIS:O	1:A:472:THR:HG23	1.88	0.74
1:A:242:ALA:O	1:A:246:GLN:HG3	1.88	0.73
1:B:381:LEU:HD12	1:B:381:LEU:O	1.87	0.73
1:A:247:LEU:HD22	1:A:251:GLN:HE22	1.53	0.73
1:A:664:VAL:HG22	1:A:807:CYS:O	1.88	0.73
1:A:484:HIS:CG	1:A:485:PRO:HD2	2.24	0.73
1:A:507:ILE:HG22	1:A:515:ILE:HG22	1.69	0.73
1:B:242:ALA:O	1:B:246:GLN:HG3	1.89	0.73
1:B:440:LEU:HG	1:B:461:ALA:HA	1.71	0.73
1:B:764:ILE:O	1:B:767:ALA:HB3	1.88	0.73
1:A:458:ARG:HG2	1:A:458:ARG:NH1	1.93	0.73
1:B:443:LYS:HD2	1:B:456:GLU:CB	2.19	0.73
1:A:700:HIS:HD2	1:A:701:ARG:H	1.36	0.72
1:A:705:ASN:O	1:A:707:PHE:N	2.22	0.72
1:A:354:GLU:HA	1:A:354:GLU:OE1	1.89	0.72
1:B:562:TYR:CZ	1:B:566:LEU:HD21	2.25	0.72
1:A:337:SER:CB	1:A:340:THR:HG23	2.19	0.72
1:A:330:MET:HE1	1:A:332:CYS:HB2	1.71	0.72
1:A:530:SER:C	1:A:532:PHE:H	1.93	0.72
1:A:410:VAL:CG1	1:A:551:SER:HB3	2.19	0.72
1:A:704:ASN:HD22	1:A:705:ASN:H	0.74	0.72
1:A:333:VAL:HB	1:A:366:ILE:HG21	1.72	0.72
1:B:671:LEU:HD13	1:B:803:LEU:HD23	1.71	0.72
1:B:468:HIS:O	1:B:472:THR:HG23	1.90	0.71
1:B:863:MET:HA	1:B:867:ALA:HB3	1.71	0.71
1:B:303:LYS:HB3	1:B:336:ILE:CD1	2.20	0.71
1:B:599:ASN:HD21	1:B:602:SER:HB3	1.54	0.71
1:A:799:LEU:O	1:A:799:LEU:HD12	1.90	0.71
1:B:714:VAL:HG12	1:B:716:ALA:H	1.56	0.71
1:A:299:VAL:HG13	1:A:304:LYS:O	1.90	0.71
1:A:835:ASP:HA	1:A:838:LYS:HD3	1.72	0.71
1:B:622:MET:HE3	1:B:666:HIS:HA	1.72	0.71
1:A:675:LEU:HD13	1:A:878:PHE:CB	2.21	0.71
1:B:875:GLN:HA	1:B:878:PHE:O	1.90	0.71
1:A:460:PRO:HG2	1:A:463:GLN:CB	2.21	0.71
1:B:299:VAL:CG1	1:B:334:PRO:HG3	2.20	0.71
1:B:642:PHE:O	1:B:646:VAL:HG12	1.90	0.71
1:A:527:PRO:HG2	1:A:528:TRP:CD1	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:740:THR:HG22	1:B:743:CYS:SG	2.31	0.71
1:B:309:LYS:N	1:B:309:LYS:HD2	2.04	0.70
1:B:681:LEU:HD13	1:B:800:LEU:HD21	1.72	0.70
1:B:572:MET:C	1:B:574:HIS:H	1.93	0.70
1:B:864:GLU:OE2	1:B:892:ARG:HD3	1.92	0.70
1:A:895:TRP:HA	1:A:898:VAL:CG2	2.21	0.70
1:B:320:GLN:HA	1:B:323:LEU:HB2	1.73	0.70
1:A:674:ASN:H	1:A:674:ASN:ND2	1.88	0.70
1:A:330:MET:HG3	1:A:350:PHE:CD1	2.27	0.70
1:A:311:LEU:CD2	1:A:315:ASP:HB3	2.21	0.70
1:A:782:LYS:O	1:A:786:VAL:HG22	1.91	0.70
1:B:605:TYR:OH	1:B:610:LEU:HD11	1.91	0.70
1:B:799:LEU:HD12	1:B:799:LEU:O	1.90	0.70
1:B:827:TYR:CD2	1:B:855:ILE:HD13	2.27	0.70
1:B:720:SER:OG	1:B:721:SER:N	2.25	0.69
1:A:329:ALA:HB2	1:A:356:ASP:OD2	1.91	0.69
1:A:410:VAL:HG12	1:A:551:SER:HB3	1.73	0.69
1:B:780:LEU:HD23	1:B:798:LEU:HB3	1.73	0.69
1:A:223:TYR:CE2	1:A:226:ARG:HG3	2.27	0.69
1:A:720:SER:CA	1:A:770:LEU:HB2	2.23	0.69
1:A:822:ILE:HA	1:A:825:LEU:HD12	1.73	0.69
1:A:669:TYR:CD2	1:A:670:LEU:HD23	2.27	0.69
1:A:311:LEU:HB3	1:A:316:VAL:HG23	1.74	0.69
1:A:444:VAL:HG21	1:A:455:TYR:CD2	2.23	0.69
1:A:484:HIS:CD2	1:A:485:PRO:HG2	2.28	0.69
1:B:261:ARG:HD3	1:B:280:GLY:HA3	1.75	0.69
1:A:231:LEU:HD12	1:B:372:TYR:CE1	2.27	0.69
1:B:479:PRO:HG3	1:B:528:TRP:HZ3	1.58	0.69
1:B:675:LEU:HD13	1:B:878:PHE:CB	2.23	0.69
1:A:666:HIS:HE1	1:A:670:LEU:HD11	1.58	0.69
1:B:433:PHE:CD2	1:B:442:ALA:HB2	2.27	0.69
1:B:829:GLU:O	1:B:831:PHE:N	2.25	0.69
1:A:720:SER:CB	1:A:770:LEU:HB2	2.23	0.68
1:B:859:GLN:NE2	1:B:859:GLN:HA	2.07	0.68
1:A:675:LEU:HD13	1:A:878:PHE:HB3	1.75	0.68
1:B:901:LEU:HD23	1:B:901:LEU:N	2.07	0.68
1:A:721:SER:HA	1:A:769:ASP:OD2	1.93	0.68
1:B:313:SER:O	1:B:316:VAL:HG12	1.92	0.68
1:A:223:TYR:OH	1:A:364:HIS:NE2	2.25	0.68
1:A:704:ASN:ND2	1:A:705:ASN:N	2.27	0.68
1:B:313:SER:C	1:B:316:VAL:HG12	2.14	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:698:LEU:O	1:A:730:HIS:HD2	1.76	0.68
1:B:315:ASP:O	1:B:319:LEU:HB2	1.93	0.68
1:A:481:ALA:O	1:A:487:PHE:HB2	1.94	0.68
1:B:461:ALA:O	1:B:467:GLY:HA2	1.94	0.68
1:B:523:LYS:NZ	1:B:533:ASP:OD2	2.26	0.68
1:B:622:MET:HE1	1:B:666:HIS:HB2	1.74	0.68
1:B:313:SER:HA	1:B:316:VAL:HG12	1.73	0.68
1:A:445:PHE:HZ	1:A:450:VAL:CG2	2.07	0.68
1:A:445:PHE:CZ	1:A:450:VAL:HG22	2.26	0.68
1:B:749:PHE:HB3	1:B:753:ASP:HB2	1.76	0.68
1:A:587:HIS:O	1:A:589:GLY:N	2.27	0.68
1:B:507:ILE:CG2	1:B:515:ILE:HG22	2.24	0.68
1:A:456:GLU:HG2	1:A:458:ARG:HE	1.58	0.67
1:A:872:LYS:HD2	1:A:885:TYR:HE1	1.59	0.67
1:B:623:LEU:HA	1:B:626:MET:CE	2.24	0.67
1:B:443:LYS:HD2	1:B:456:GLU:CG	2.24	0.67
1:A:797:ARG:HD3	4:A:59:HOH:O	1.95	0.67
1:B:354:GLU:HA	1:B:354:GLU:OE1	1.93	0.67
1:A:875:GLN:HA	1:A:878:PHE:O	1.95	0.67
1:B:667:PHE:CD2	1:B:807:CYS:HA	2.29	0.67
1:A:241:ASP:HB3	1:A:244:SER:OG	1.94	0.67
1:B:627:ASN:OD1	1:B:630:ASN:ND2	2.28	0.67
1:B:599:ASN:ND2	1:B:602:SER:HB3	2.10	0.67
1:A:428:GLU:OE2	1:A:500:ARG:NH2	2.28	0.67
1:A:837:GLU:HB2	1:A:838:LYS:CE	2.24	0.67
1:B:313:SER:CA	1:B:316:VAL:HG12	2.25	0.67
1:B:591:GLN:HG3	1:B:592:PRO:N	2.09	0.67
1:A:456:GLU:OE1	1:A:458:ARG:NH2	2.28	0.67
1:A:569:GLU:HG2	1:A:570:MET:N	2.10	0.67
1:B:741:HIS:HB2	4:B:146:HOH:O	1.95	0.67
1:A:605:TYR:HE2	1:A:610:LEU:HD11	1.58	0.67
1:B:399:VAL:HG21	1:B:540:PHE:CE1	2.29	0.67
1:A:895:TRP:O	1:A:898:VAL:HG23	1.94	0.67
1:A:528:TRP:CD1	1:A:528:TRP:N	2.61	0.66
1:B:292:LEU:HD11	1:B:300:VAL:HG21	1.75	0.66
1:B:774:LEU:HD21	1:B:866:ILE:CD1	2.24	0.66
1:A:331:LEU:HD22	1:A:333:VAL:HG23	1.77	0.66
1:A:542:ILE:HG21	1:B:401:LYS:NZ	2.10	0.66
1:B:622:MET:CE	1:B:666:HIS:HA	2.25	0.66
1:B:695:CYS:HB3	1:B:698:LEU:HD12	1.77	0.66
1:A:828:LYS:HE2	4:A:122:HOH:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:LEU:HD13	1:B:397:LEU:CD1	2.25	0.66
1:A:487:PHE:CZ	1:A:499:THR:HB	2.27	0.66
1:A:231:LEU:HD12	1:B:372:TYR:CZ	2.29	0.66
1:B:530:SER:O	1:B:533:ASP:N	2.28	0.66
1:B:838:LYS:HB2	4:B:4:HOH:O	1.95	0.66
1:A:709:VAL:HB	1:A:712:LYS:H	1.59	0.66
1:A:576:LYS:H	1:A:576:LYS:CD	2.08	0.66
1:A:330:MET:HG3	1:A:350:PHE:CE1	2.31	0.66
1:A:337:SER:O	1:A:341:ASP:HA	1.96	0.66
1:A:829:GLU:O	1:A:831:PHE:N	2.29	0.66
1:B:308:LEU:O	1:B:311:LEU:HB3	1.96	0.66
1:B:320:GLN:CG	1:B:327:LEU:HD13	2.09	0.66
1:B:443:LYS:HD2	1:B:456:GLU:HG2	1.78	0.66
1:B:439:GLU:HB2	1:B:459:ILE:O	1.95	0.66
1:B:807:CYS:O	1:B:810:SER:HB3	1.95	0.66
1:B:837:GLU:HB2	1:B:838:LYS:NZ	2.10	0.66
1:B:899:SER:O	1:B:902:VAL:HG12	1.95	0.66
1:A:307:GLN:HB3	1:A:309:LYS:HD3	1.77	0.66
1:B:418:ILE:HD11	1:B:432:VAL:CG2	2.26	0.66
1:A:375:THR:HG22	1:A:376:VAL:N	2.11	0.66
1:A:535:ASP:N	1:A:535:ASP:OD1	2.28	0.66
1:A:821:LYS:O	1:A:824:GLU:HG3	1.96	0.66
1:A:444:VAL:CG2	1:A:455:TYR:HD2	2.06	0.65
1:A:479:PRO:HB3	1:A:528:TRP:CE3	2.30	0.65
1:A:572:MET:CE	1:A:737:ILE:HG12	2.26	0.65
1:A:602:SER:O	1:A:604:THR:N	2.29	0.65
1:A:897:LYS:HA	1:A:900:HIS:CD2	2.31	0.65
1:B:630:ASN:ND2	1:B:631:ASN:H	1.93	0.65
1:B:260:SER:OG	1:B:351:ASN:HB2	1.96	0.65
1:B:470:ALA:HB2	1:B:517:VAL:HG21	1.78	0.65
1:B:528:TRP:N	1:B:528:TRP:CD1	2.64	0.65
1:A:405:THR:CG2	1:B:546:ILE:HD12	2.25	0.65
1:B:578:SER:N	1:B:581:GLU:OE1	2.28	0.65
1:A:330:MET:HA	1:A:349:ALA:O	1.96	0.65
1:B:258:ARG:HD3	1:B:352:LYS:NZ	2.12	0.65
1:A:225:ASP:O	1:A:228:ARG:HB2	1.96	0.65
1:B:780:LEU:CD2	1:B:798:LEU:HB3	2.27	0.65
1:A:226:ARG:C	1:A:228:ARG:H	1.99	0.65
1:B:498:ARG:O	1:B:522:ASN:ND2	2.29	0.65
1:A:278:VAL:HG22	1:A:283:VAL:HG22	1.78	0.65
1:A:436:ASP:HB3	1:A:441:VAL:HG21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:PRO:HG2	1:B:528:TRP:CD1	2.32	0.64
1:B:580:ASP:O	1:B:584:LYS:HG3	1.96	0.64
1:B:653:PRO:HB2	1:B:829:GLU:OE1	1.96	0.64
1:A:320:GLN:HG2	1:A:325:CYS:O	1.97	0.64
1:B:270:ASP:O	1:B:272:LEU:HD23	1.96	0.64
1:B:266:LEU:HD11	1:B:277:LYS:HE2	1.78	0.64
1:A:255:GLN:O	1:A:257:THR:N	2.30	0.64
1:A:450:VAL:HG12	1:A:453:GLU:HA	1.79	0.64
1:B:786:VAL:O	1:B:786:VAL:HG23	1.97	0.64
1:B:313:SER:HA	1:B:316:VAL:CG1	2.28	0.64
1:B:328:GLN:HG2	1:B:351:ASN:OD1	1.97	0.64
1:A:436:ASP:HB3	1:A:441:VAL:CG2	2.27	0.64
1:A:645:MET:HG2	1:A:737:ILE:HG23	1.80	0.64
1:B:827:TYR:CG	1:B:855:ILE:HD13	2.32	0.64
1:A:307:GLN:HB3	1:A:309:LYS:CD	2.27	0.64
1:A:370:PHE:O	1:A:372:TYR:N	2.31	0.64
1:A:476:LEU:HD23	1:A:478:ILE:HD12	1.80	0.64
1:A:630:ASN:HD22	1:A:631:ASN:N	1.96	0.64
1:B:531:LYS:HA	1:B:534:GLU:OE1	1.98	0.64
1:A:700:HIS:CD2	1:A:701:ARG:H	2.15	0.64
1:A:680:TYR:HB3	1:A:788:TYR:CE2	2.33	0.64
1:A:856:PRO:O	1:A:860:ILE:HG12	1.98	0.64
1:A:399:VAL:HG11	1:A:540:PHE:CE1	2.33	0.64
1:A:260:SER:OG	1:A:351:ASN:HB2	1.98	0.63
1:B:460:PRO:CG	1:B:463:GLN:HB3	2.20	0.63
1:B:500:ARG:HG2	1:B:522:ASN:CG	2.18	0.63
1:B:648:LYS:HB2	1:B:648:LYS:NZ	2.12	0.63
1:A:269:GLU:O	1:A:271:ASN:ND2	2.30	0.63
1:A:813:THR:O	1:A:887:ARG:HD2	1.97	0.63
1:A:838:LYS:CD	1:A:838:LYS:H	2.10	0.63
1:A:852:LYS:O	1:A:855:ILE:HG13	1.98	0.63
1:B:768:THR:HG22	1:B:804:MET:CG	2.28	0.63
1:B:822:ILE:HA	1:B:825:LEU:CD1	2.29	0.63
1:A:863:MET:HA	1:A:867:ALA:HB3	1.80	0.63
1:A:436:ASP:CB	1:A:441:VAL:HG21	2.28	0.63
1:A:720:SER:HB2	1:A:770:LEU:HB2	1.79	0.63
1:B:303:LYS:HD3	1:B:336:ILE:HD13	1.80	0.63
1:B:630:ASN:HD22	1:B:631:ASN:N	1.96	0.63
1:B:887:ARG:NH1	1:B:887:ARG:HG3	2.08	0.63
1:B:265:LEU:HD13	1:B:274:LEU:HD12	1.80	0.63
1:A:330:MET:HE3	1:A:332:CYS:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:MET:HG3	1:B:350:PHE:CD1	2.33	0.63
1:A:768:THR:HG22	1:A:804:MET:HG3	1.80	0.63
1:B:433:PHE:CG	1:B:442:ALA:HB2	2.33	0.63
1:B:875:GLN:HG2	1:B:875:GLN:O	1.98	0.62
1:A:708:GLN:O	1:A:709:VAL:HG23	1.98	0.62
1:B:376:VAL:HG13	1:B:377:LEU:N	2.14	0.62
1:B:458:ARG:CG	1:B:458:ARG:HH11	2.13	0.62
1:B:434:LEU:HD21	1:B:548:ILE:HG21	1.80	0.62
1:B:510:GLU:OE1	1:B:510:GLU:HA	1.99	0.62
1:B:561:GLN:CA	1:B:561:GLN:HE21	2.10	0.62
1:A:456:GLU:HG2	1:A:458:ARG:NE	2.13	0.62
1:A:627:ASN:OD1	1:A:630:ASN:ND2	2.30	0.62
1:B:630:ASN:HD22	1:B:630:ASN:N	1.97	0.62
1:B:680:TYR:N	1:B:680:TYR:CD1	2.67	0.62
1:B:762:ARG:O	1:B:766:LEU:HD22	2.00	0.62
1:A:634:ILE:CG2	1:A:639:LEU:HB2	2.30	0.62
1:B:230:ILE:HG22	1:B:231:LEU:N	2.14	0.62
1:A:252:TYR:O	1:A:255:GLN:HB2	1.99	0.62
1:B:527:PRO:HB2	1:B:528:TRP:CD1	2.35	0.62
1:A:814:LYS:HB3	1:A:818:THR:HG21	1.81	0.62
1:B:328:GLN:HG3	4:B:9:HOH:O	2.00	0.62
1:B:333:VAL:HB	1:B:366:ILE:HG21	1.82	0.62
1:B:410:VAL:O	1:B:414:LEU:HB2	2.00	0.62
1:A:714:VAL:HG12	1:A:716:ALA:H	1.65	0.62
1:B:354:GLU:O	1:B:356:ASP:N	2.32	0.62
1:A:887:ARG:HG2	4:A:142:HOH:O	1.98	0.61
1:A:408:ASP:OD1	1:A:408:ASP:N	2.28	0.61
1:A:572:MET:HE1	1:A:737:ILE:HG12	1.82	0.61
1:B:596:ILE:HG21	1:B:600:PHE:CD1	2.35	0.61
1:B:475:ILE:HD13	1:B:506:PRO:HD3	1.83	0.61
1:B:762:ARG:HG2	1:B:766:LEU:CD2	2.29	0.61
1:B:837:GLU:CB	1:B:838:LYS:HZ3	2.13	0.61
1:B:417:ILE:HD13	1:B:548:ILE:HD11	1.81	0.61
1:A:223:TYR:CE2	1:A:226:ARG:HB2	2.36	0.61
1:A:610:LEU:HB3	1:A:611:PRO:HD2	1.82	0.61
1:B:875:GLN:HE21	1:B:882:ALA:CB	2.14	0.61
1:B:330:MET:HG3	1:B:350:PHE:CE1	2.36	0.61
1:B:630:ASN:ND2	1:B:630:ASN:H	1.98	0.61
1:A:484:HIS:HD2	1:A:486:LEU:H	1.47	0.61
1:A:579:ASP:O	1:A:583:THR:HG23	2.01	0.61
1:B:435:LEU:HD11	1:B:437:GLN:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:LEU:HD13	1:B:397:LEU:HD12	1.82	0.61
1:B:441:VAL:HG21	1:B:458:ARG:CZ	2.31	0.61
1:B:666:HIS:O	1:B:669:TYR:HB3	2.00	0.61
1:B:353:LEU:O	1:B:354:GLU:HB2	2.00	0.61
1:B:440:LEU:HD13	1:B:466:ALA:HB1	1.83	0.61
1:A:755:GLN:HG2	1:B:566:LEU:CD1	2.31	0.61
1:A:648:LYS:HB2	1:A:648:LYS:NZ	2.15	0.60
1:B:475:ILE:HD13	1:B:506:PRO:CD	2.31	0.60
1:B:675:LEU:HD23	1:B:675:LEU:N	2.16	0.60
1:B:530:SER:C	1:B:532:PHE:H	2.04	0.60
1:B:677:LEU:HD21	1:B:803:LEU:HD21	1.82	0.60
1:B:611:PRO:HG2	1:B:614:ASP:OD2	2.01	0.60
1:B:855:ILE:HB	1:B:856:PRO:HD3	1.83	0.60
1:A:399:VAL:CG1	1:A:540:PHE:HE1	2.14	0.60
1:A:859:GLN:O	1:A:863:MET:HG3	2.02	0.60
1:B:355:GLY:O	1:B:357:LEU:N	2.34	0.60
1:B:381:LEU:HD12	1:B:381:LEU:C	2.21	0.60
1:B:458:ARG:HG2	1:B:458:ARG:HH11	1.65	0.60
1:B:527:PRO:HG2	1:B:528:TRP:HD1	1.65	0.60
1:A:270:ASP:HB2	1:A:272:LEU:HD23	1.82	0.60
1:A:470:ALA:HB2	1:A:517:VAL:HG21	1.83	0.60
1:A:630:ASN:ND2	1:A:631:ASN:N	2.48	0.60
1:B:303:LYS:CD	1:B:336:ILE:HD13	2.31	0.60
1:B:805:THR:CG2	1:B:870:ILE:HD13	2.32	0.60
1:A:718:LEU:O	1:A:720:SER:N	2.32	0.60
1:B:399:VAL:HG11	1:B:424:LEU:HD11	1.84	0.60
1:A:251:GLN:HE22	1:A:281:ASP:HA	1.67	0.60
1:A:576:LYS:H	1:A:576:LYS:HD2	1.67	0.60
1:A:688:ALA:HA	1:A:757:MET:HE1	1.83	0.60
1:B:234:CYS:HA	1:B:237:LEU:HD12	1.83	0.60
1:B:356:ASP:OD1	4:B:9:HOH:O	2.17	0.59
1:B:443:LYS:HD2	1:B:456:GLU:HB3	1.83	0.59
1:B:678:THR:O	1:B:790:ARG:NH2	2.34	0.59
1:B:821:LYS:O	1:B:824:GLU:HG3	2.02	0.59
1:A:298:GLN:NE2	1:A:302:ASP:OD2	2.35	0.59
1:A:439:GLU:OE2	1:A:458:ARG:HB3	2.03	0.59
1:A:835:ASP:HB2	1:B:771:ALA:HB2	1.84	0.59
1:B:257:THR:O	1:B:352:LYS:HE3	2.03	0.59
1:A:237:LEU:O	1:B:375:THR:HG21	2.01	0.59
1:B:459:ILE:HG13	1:B:463:GLN:OE1	2.02	0.59
1:A:732:ALA:HB2	1:B:571:MET:HE1	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:LEU:CD1	1:B:755:GLN:HG2	2.21	0.59
1:A:431:SER:HG	1:A:433:PHE:HE1	1.51	0.59
1:A:475:ILE:HG23	1:A:505:PHE:HB3	1.83	0.59
1:A:507:ILE:CG2	1:A:515:ILE:HG22	2.32	0.59
1:A:570:MET:HE2	1:B:762:ARG:HH11	1.68	0.59
1:A:770:LEU:HD12	1:A:770:LEU:O	2.02	0.59
1:B:241:ASP:OD2	1:B:243:SER:HB2	2.02	0.59
1:A:333:VAL:CB	1:A:366:ILE:HG21	2.33	0.59
1:A:656:HIS:CD2	1:A:700:HIS:CE1	2.90	0.59
1:B:700:HIS:CD2	1:B:702:GLY:H	2.09	0.59
1:A:799:LEU:HD11	1:A:803:LEU:HD11	1.85	0.59
1:B:337:SER:OG	1:B:340:THR:HG23	2.03	0.59
1:B:432:VAL:CG1	1:B:518:ALA:HB2	2.33	0.59
1:A:418:ILE:HG12	1:A:432:VAL:HG22	1.84	0.59
1:A:576:LYS:CD	1:A:576:LYS:N	2.65	0.59
1:A:720:SER:HB2	1:A:770:LEU:CB	2.33	0.59
1:A:363:GLU:HG3	1:A:367:GLN:HE22	1.68	0.58
1:A:435:LEU:HD11	1:A:437:GLN:O	2.03	0.58
1:B:675:LEU:HD13	1:B:878:PHE:HB3	1.83	0.58
1:A:815:GLY:O	1:A:818:THR:HB	2.03	0.58
1:B:720:SER:CB	1:B:770:LEU:HB2	2.33	0.58
1:A:637:PRO:O	1:A:641:ARG:NE	2.36	0.58
1:A:575:MET:HG2	1:A:648:LYS:CD	2.33	0.58
1:A:774:LEU:HB2	1:B:838:LYS:HD2	1.84	0.58
1:A:364:HIS:HA	1:A:367:GLN:HE21	1.68	0.58
1:B:535:ASP:OD1	1:B:535:ASP:N	2.27	0.58
1:B:637:PRO:O	1:B:641:ARG:NE	2.29	0.58
1:A:872:LYS:HA	1:A:885:TYR:HD1	1.68	0.58
1:A:860:ILE:CD1	1:A:895:TRP:HB3	2.34	0.58
1:B:471:THR:HG22	1:B:472:THR:N	2.19	0.58
1:B:509:ASN:OD1	1:B:513:GLU:HG3	2.03	0.58
1:A:473:GLY:O	1:A:508:LYS:NZ	2.31	0.58
1:A:872:LYS:HD2	1:A:885:TYR:CE1	2.39	0.58
1:B:476:LEU:HD23	1:B:478:ILE:HD12	1.85	0.58
1:B:720:SER:CA	1:B:770:LEU:HB2	2.34	0.58
1:B:720:SER:HB2	1:B:770:LEU:HB2	1.85	0.58
1:A:482:TYR:CZ	1:A:487:PHE:HE2	2.22	0.58
1:B:241:ASP:HB3	1:B:244:SER:OG	2.04	0.58
1:B:721:SER:HB2	1:B:769:ASP:OD2	2.02	0.58
1:A:505:PHE:HB2	1:A:506:PRO:HD2	1.85	0.57
1:A:554:TYR:HD1	1:B:554:TYR:HD1	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:ILE:HG23	1:B:505:PHE:HB3	1.85	0.57
1:B:309:LYS:H	1:B:309:LYS:CD	2.10	0.57
1:B:398:GLN:HE22	1:B:401:LYS:HD3	1.69	0.57
1:A:875:GLN:O	1:A:875:GLN:HG2	2.03	0.57
1:B:304:LYS:HE3	1:B:304:LYS:CA	2.23	0.57
1:B:872:LYS:HE2	1:B:876:ASP:OD1	2.03	0.57
1:A:715:LEU:C	1:A:717:ALA:H	2.08	0.57
1:B:698:LEU:O	1:B:730:HIS:HD2	1.86	0.57
1:B:502:ILE:HG21	1:B:519:GLU:OE1	2.05	0.57
1:B:587:HIS:O	1:B:589:GLY:N	2.38	0.57
1:A:416:GLU:OE1	1:A:416:GLU:HA	2.03	0.57
1:B:279:ILE:HD11	1:B:322:MET:SD	2.44	0.57
1:B:459:ILE:HD12	1:B:460:PRO:CD	2.35	0.57
1:A:223:TYR:CE2	1:A:226:ARG:CG	2.88	0.57
1:A:475:ILE:HD13	1:A:506:PRO:CD	2.34	0.57
1:B:833:GLN:HG2	1:B:834:GLY:H	1.70	0.57
1:A:415:GLN:O	1:A:418:ILE:HB	2.05	0.56
1:A:885:TYR:CD2	1:A:885:TYR:C	2.78	0.56
1:B:895:TRP:HA	1:B:898:VAL:HG22	1.87	0.56
1:A:416:GLU:O	1:A:420:GLU:HB2	2.05	0.56
1:A:565:HIS:O	1:A:569:GLU:HB3	2.04	0.56
1:A:723:GLY:N	4:A:35:HOH:O	2.38	0.56
1:A:231:LEU:HD22	1:B:231:LEU:HD22	1.86	0.56
1:A:253:LEU:O	1:A:257:THR:OG1	2.23	0.56
1:A:590:ILE:HG22	1:A:624:GLN:NE2	2.20	0.56
1:A:780:LEU:CD2	1:A:798:LEU:HB3	2.34	0.56
1:A:231:LEU:HD23	1:B:231:LEU:HB2	1.87	0.56
1:B:528:TRP:N	1:B:528:TRP:HD1	2.03	0.56
1:B:607:PRO:HG2	1:B:663:SER:HB3	1.87	0.56
1:B:715:LEU:HD23	1:B:862:PHE:CD2	2.40	0.56
1:B:875:GLN:HE21	1:B:882:ALA:HB1	1.71	0.56
1:B:895:TRP:HA	1:B:898:VAL:CG2	2.35	0.56
1:A:223:TYR:HE2	1:A:226:ARG:CB	2.18	0.56
1:A:417:ILE:HD13	1:A:548:ILE:HD11	1.87	0.56
1:A:868:MET:HG2	1:A:888:VAL:HG12	1.86	0.56
1:B:443:LYS:HA	1:B:456:GLU:HA	1.85	0.56
1:B:471:THR:HG22	1:B:472:THR:HG22	1.88	0.56
1:B:500:ARG:NE	1:B:522:ASN:HB3	2.20	0.56
1:A:421:ALA:HB2	1:A:540:PHE:HE2	1.64	0.56
1:A:573:TYR:HE1	1:A:699:ASP:OD1	1.89	0.56
1:A:590:ILE:HG21	1:A:624:GLN:OE1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:GLU:HB3	1:B:328:GLN:HE22	1.70	0.56
1:A:780:LEU:HD23	1:A:798:LEU:HB3	1.88	0.56
1:A:810:SER:HA	1:A:871:TYR:OH	2.05	0.56
1:B:312:THR:HG21	1:B:314:GLU:HB3	1.88	0.56
1:A:812:GLN:HB3	1:A:888:VAL:HG22	1.87	0.56
1:A:399:VAL:HG11	1:A:540:PHE:HE1	1.69	0.56
1:B:312:THR:CG2	1:B:314:GLU:HB3	2.36	0.56
1:B:258:ARG:HB2	1:B:352:LYS:HE2	1.87	0.56
1:B:822:ILE:HA	1:B:825:LEU:HD12	1.87	0.56
1:A:674:ASN:O	1:A:880:LYS:HD3	2.05	0.56
1:B:273:GLN:HE22	1:B:289:SER:HB2	1.71	0.56
1:A:550:HIS:CD2	1:B:550:HIS:HE2	2.21	0.56
1:A:610:LEU:H	1:A:610:LEU:CD1	2.17	0.56
1:B:471:THR:HG22	1:B:472:THR:CG2	2.36	0.56
1:A:757:MET:O	1:A:757:MET:HG3	2.06	0.55
1:B:505:PHE:HB2	1:B:506:PRO:HD2	1.88	0.55
1:A:894:HIS:O	1:A:898:VAL:HG22	2.05	0.55
1:A:479:PRO:HB3	1:A:528:TRP:CZ3	2.42	0.55
1:A:715:LEU:HD22	1:A:859:GLN:HE22	1.70	0.55
1:A:550:HIS:CD2	1:B:550:HIS:NE2	2.75	0.55
1:A:610:LEU:HD12	1:A:610:LEU:N	2.21	0.55
1:A:748:HIS:N	1:A:748:HIS:CD2	2.73	0.55
1:A:764:ILE:O	1:A:767:ALA:HB3	2.07	0.55
1:A:403:LEU:HD13	1:A:417:ILE:HG13	1.87	0.55
1:A:427:ALA:HB2	1:A:520:LEU:HD22	1.89	0.55
1:A:261:ARG:HD3	1:A:280:GLY:HA3	1.89	0.55
1:B:586:LEU:CD1	1:B:640:ALA:HB3	2.36	0.55
1:B:718:LEU:HG	1:B:719:TYR:N	2.21	0.55
1:B:827:TYR:OH	1:B:859:GLN:NE2	2.38	0.55
1:A:239:ASP:HB2	1:A:245:LEU:HD23	1.89	0.55
1:A:838:LYS:HB2	1:B:774:LEU:HD12	1.89	0.55
1:B:505:PHE:HB2	1:B:506:PRO:CD	2.37	0.55
1:A:445:PHE:CZ	1:A:450:VAL:HG13	2.42	0.55
1:A:440:LEU:O	1:A:458:ARG:HA	2.07	0.55
1:A:648:LYS:HB2	1:A:648:LYS:HZ2	1.72	0.55
1:B:837:GLU:C	1:B:838:LYS:HZ3	2.10	0.55
1:A:295:CYS:HB3	1:A:315:ASP:OD2	2.07	0.55
1:B:593:VAL:HG22	1:B:621:SER:O	2.06	0.55
1:B:666:HIS:CE1	1:B:670:LEU:HD21	2.42	0.55
1:A:709:VAL:HB	1:A:712:LYS:HB2	1.87	0.55
1:B:311:LEU:O	1:B:311:LEU:HG	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:GLU:CA	1:B:461:ALA:HB2	2.37	0.55
1:B:439:GLU:HA	1:B:461:ALA:HB2	1.88	0.55
1:B:506:PRO:O	1:B:507:ILE:HD12	2.06	0.55
1:B:530:SER:O	1:B:533:ASP:HB2	2.07	0.55
1:A:224:THR:HG22	1:A:228:ARG:CZ	2.36	0.54
1:A:476:LEU:HD23	1:A:478:ILE:CD1	2.37	0.54
1:A:607:PRO:O	1:A:610:LEU:HD13	2.07	0.54
1:A:680:TYR:HB3	1:A:788:TYR:HE2	1.72	0.54
1:A:668:CYS:SG	1:A:689:LEU:HD23	2.47	0.54
1:A:223:TYR:HE2	1:A:226:ARG:CG	2.19	0.54
1:B:500:ARG:NH2	1:B:523:LYS:O	2.39	0.54
1:B:723:GLY:C	1:B:725:VAL:H	2.11	0.54
1:A:278:VAL:CG2	1:A:283:VAL:HG22	2.36	0.54
1:A:452:ASP:O	1:A:453:GLU:O	2.25	0.54
1:A:587:HIS:C	1:A:589:GLY:H	2.10	0.54
1:B:645:MET:HE1	1:B:740:THR:HG21	1.88	0.54
1:A:275:SER:HB2	1:A:287:GLU:OE2	2.08	0.54
1:A:468:HIS:CE1	1:A:472:THR:HG21	2.42	0.54
1:A:477:ASN:HD21	1:A:529:PHE:HB2	1.72	0.54
1:A:659:MET:O	1:A:663:SER:OG	2.24	0.54
1:A:665:SER:O	1:A:668:CYS:HB3	2.07	0.54
1:B:403:LEU:HD22	1:B:417:ILE:HG13	1.87	0.54
1:B:418:ILE:CD1	1:B:444:VAL:HG21	2.37	0.54
1:B:630:ASN:N	1:B:630:ASN:ND2	2.53	0.54
1:B:721:SER:HA	1:B:769:ASP:OD2	2.07	0.54
1:B:805:THR:HG22	1:B:870:ILE:HD13	1.90	0.54
1:A:363:GLU:O	1:A:367:GLN:NE2	2.41	0.54
1:B:361:GLU:O	1:B:365:VAL:HG12	2.08	0.54
1:B:593:VAL:HG12	1:B:600:PHE:CD2	2.42	0.54
1:A:309:LYS:CD	1:A:309:LYS:H	2.04	0.54
1:A:331:LEU:HD22	1:A:333:VAL:CG2	2.38	0.54
1:A:771:ALA:HB2	1:B:835:ASP:HB2	1.89	0.54
1:B:283:VAL:HG12	1:B:283:VAL:O	2.07	0.54
1:B:687:PHE:CE1	1:B:746:PHE:HE1	2.25	0.54
1:A:376:VAL:HG21	1:B:375:THR:HG22	1.90	0.54
1:A:569:GLU:O	1:A:572:MET:HB2	2.07	0.54
1:A:231:LEU:CD2	1:B:231:LEU:HD22	2.38	0.54
1:A:542:ILE:HG21	1:B:401:LYS:HZ1	1.73	0.54
1:B:444:VAL:O	1:B:444:VAL:HG13	2.08	0.54
1:B:821:LYS:HD3	1:B:824:GLU:OE1	2.07	0.54
1:A:453:GLU:HA	1:A:453:GLU:OE1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:ARG:CG	1:A:458:ARG:NH1	2.66	0.54
1:A:575:MET:HG2	1:A:648:LYS:HD2	1.88	0.54
1:B:398:GLN:OE1	1:B:398:GLN:HA	2.06	0.54
1:B:499:THR:O	1:B:500:ARG:HD3	2.08	0.54
1:B:789:ASP:N	1:B:795:HIS:ND1	2.53	0.54
1:A:788:TYR:OH	1:A:799:LEU:HD23	2.08	0.54
1:A:815:GLY:O	1:A:818:THR:N	2.39	0.54
1:A:709:VAL:HG12	1:A:711:SER:H	1.73	0.53
1:A:720:SER:HA	1:A:770:LEU:HB2	1.89	0.53
1:B:593:VAL:HG12	1:B:600:PHE:CE2	2.44	0.53
1:B:606:THR:OG1	1:B:609:SER:HB3	2.07	0.53
1:A:666:HIS:O	1:A:669:TYR:HB3	2.07	0.53
1:B:593:VAL:CG1	1:B:600:PHE:CE2	2.91	0.53
1:A:440:LEU:HD12	1:A:459:ILE:CD1	2.20	0.53
1:A:835:ASP:CA	1:A:838:LYS:HD2	2.38	0.53
1:B:859:GLN:HE21	1:B:859:GLN:HA	1.71	0.53
1:B:877:LEU:HB2	1:B:878:PHE:CD2	2.43	0.53
1:A:642:PHE:O	1:A:646:VAL:HG12	2.08	0.53
1:A:860:ILE:HD11	1:A:895:TRP:C	2.29	0.53
1:A:599:ASN:OD1	1:A:602:SER:HB2	2.08	0.53
1:A:231:LEU:CD2	1:B:231:LEU:HB2	2.38	0.53
1:B:366:ILE:HG22	1:B:367:GLN:N	2.23	0.53
1:B:443:LYS:CD	1:B:456:GLU:HB3	2.38	0.53
1:B:457:ILE:O	1:B:457:ILE:HG22	2.07	0.53
1:B:596:ILE:HG21	1:B:600:PHE:CE1	2.43	0.53
1:A:335:VAL:HG22	1:A:370:PHE:CD2	2.44	0.53
1:A:495:THR:HG22	1:A:495:THR:O	2.09	0.53
1:A:719:TYR:O	1:A:770:LEU:HD23	2.09	0.53
1:B:331:LEU:HD22	1:B:333:VAL:HG23	1.91	0.53
1:A:550:HIS:NE2	1:B:550:HIS:CD2	2.77	0.53
1:A:420:GLU:OE2	1:A:420:GLU:HA	2.09	0.53
1:A:875:GLN:HE21	1:A:882:ALA:CA	2.20	0.53
1:A:230:ILE:HG22	1:B:231:LEU:HD21	1.91	0.53
1:B:521:VAL:HG12	1:B:522:ASN:OD1	2.08	0.53
1:A:570:MET:C	1:A:572:MET:H	2.12	0.53
1:A:675:LEU:HD13	1:A:878:PHE:CG	2.44	0.53
1:B:255:GLN:O	1:B:257:THR:N	2.41	0.53
1:B:530:SER:C	1:B:532:PHE:N	2.62	0.53
1:A:501:ASN:ND2	1:A:527:PRO:O	2.42	0.53
1:A:547:SER:O	1:A:551:SER:HB2	2.09	0.53
1:A:786:VAL:HG23	1:A:786:VAL:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:586:LEU:HD21	1:B:636:CYS:HB3	1.91	0.53
1:B:258:ARG:CG	1:B:258:ARG:HH11	2.22	0.53
1:B:768:THR:HG22	1:B:804:MET:HG3	1.91	0.52
1:A:439:GLU:HA	1:A:461:ALA:N	2.23	0.52
1:A:838:LYS:HB3	1:B:774:LEU:HB2	1.90	0.52
1:B:702:GLY:HA2	1:B:829:GLU:OE2	2.09	0.52
1:B:252:TYR:O	1:B:256:GLU:HG2	2.09	0.52
1:B:342:GLN:O	1:B:344:VAL:HG23	2.10	0.52
1:A:872:LYS:HA	1:A:885:TYR:CD1	2.44	0.52
1:B:278:VAL:HG22	1:B:283:VAL:HG22	1.91	0.52
1:A:566:LEU:HD22	1:B:755:GLN:HE21	1.75	0.52
1:B:755:GLN:OE1	1:B:759:ASP:OD2	2.28	0.52
1:A:433:PHE:CD2	1:A:442:ALA:HB2	2.44	0.52
1:B:619:ILE:O	1:B:623:LEU:HD12	2.09	0.52
1:A:270:ASP:OD2	1:A:270:ASP:N	2.39	0.52
1:A:688:ALA:HB2	1:A:760:LEU:HD12	1.92	0.52
1:B:231:LEU:HD12	1:B:231:LEU:O	2.10	0.52
1:B:435:LEU:HD13	1:B:436:ASP:N	2.24	0.52
1:B:715:LEU:C	1:B:717:ALA:H	2.13	0.52
1:A:530:SER:C	1:A:532:PHE:N	2.61	0.52
1:B:606:THR:O	1:B:609:SER:HB3	2.10	0.52
1:B:762:ARG:HG2	1:B:766:LEU:HD22	1.90	0.52
1:A:789:ASP:N	1:A:795:HIS:ND1	2.57	0.52
1:B:307:GLN:HB3	1:B:309:LYS:CD	2.40	0.52
1:B:458:ARG:O	1:B:459:ILE:HB	2.09	0.52
1:B:861:SER:O	1:B:865:HIS:HB2	2.10	0.52
1:A:721:SER:HB2	1:A:769:ASP:OD2	2.09	0.52
1:A:721:SER:O	1:A:722:GLU:OE1	2.27	0.52
1:A:721:SER:OG	1:A:722:GLU:N	2.39	0.52
1:A:770:LEU:O	1:A:774:LEU:HG	2.10	0.52
1:B:369:CYS:O	1:B:373:THR:HB	2.10	0.52
1:B:455:TYR:CD2	1:B:455:TYR:N	2.76	0.52
1:B:467:GLY:O	1:B:471:THR:HB	2.10	0.52
1:A:258:ARG:O	1:A:353:LEU:N	2.40	0.52
1:A:376:VAL:HG13	1:A:377:LEU:N	2.25	0.52
1:A:447:GLY:HA2	4:A:17:HOH:O	2.10	0.52
1:A:330:MET:CG	1:A:350:PHE:CE1	2.93	0.51
1:B:375:THR:HB	4:B:186:HOH:O	2.09	0.51
1:A:885:TYR:C	1:A:885:TYR:HD2	2.13	0.51
1:A:270:ASP:OD1	1:A:272:LEU:HG	2.10	0.51
1:A:434:LEU:O	1:A:441:VAL:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:ILE:HG21	1:A:639:LEU:HB2	1.92	0.51
1:A:698:LEU:O	1:A:730:HIS:CD2	2.62	0.51
1:B:479:PRO:HB3	1:B:528:TRP:CE3	2.45	0.51
1:A:348:CYS:HB3	1:A:350:PHE:CZ	2.45	0.51
1:A:854:TYR:CD1	1:A:854:TYR:N	2.77	0.51
1:A:439:GLU:N	1:A:461:ALA:HB2	2.25	0.51
1:A:715:LEU:CD2	1:A:859:GLN:HE22	2.23	0.51
1:B:236:GLU:O	1:B:248:LYS:NZ	2.39	0.51
1:B:307:GLN:O	1:B:310:ASP:HB2	2.10	0.51
1:A:591:GLN:HG3	1:A:592:PRO:N	2.25	0.51
1:A:597:ASP:HB3	1:A:600:PHE:HB2	1.91	0.51
1:A:833:GLN:HG2	1:A:837:GLU:OE2	2.11	0.51
1:B:273:GLN:HG2	1:B:291:PRO:HA	1.92	0.51
1:B:627:ASN:ND2	1:B:631:ASN:OD1	2.43	0.51
1:B:634:ILE:CG2	1:B:639:LEU:HB2	2.39	0.51
1:A:290:PHE:CB	1:A:291:PRO:HD2	2.29	0.51
1:B:236:GLU:O	1:B:238:TYR:CD2	2.64	0.51
1:B:799:LEU:HG	1:B:803:LEU:CD1	2.40	0.51
1:A:501:ASN:C	1:A:502:ILE:HG13	2.30	0.51
1:A:586:LEU:CD1	1:A:640:ALA:HB3	2.41	0.51
1:B:628:PHE:O	1:B:634:ILE:HD12	2.11	0.51
1:B:757:MET:HE3	1:B:761:MET:HG3	1.92	0.51
1:A:223:TYR:CZ	1:A:364:HIS:NE2	2.78	0.51
1:A:341:ASP:O	1:A:342:GLN:HG2	2.10	0.51
1:A:268:SER:HB3	1:A:273:GLN:O	2.11	0.51
1:A:820:ARG:O	1:A:824:GLU:HG2	2.11	0.51
1:B:233:LEU:O	1:B:236:GLU:N	2.36	0.51
1:B:319:LEU:O	1:B:323:LEU:HB2	2.10	0.51
1:B:465:ILE:HG22	1:B:466:ALA:N	2.25	0.51
1:A:816:TRP:CG	1:A:894:HIS:CD2	2.99	0.50
1:B:421:ALA:HB2	1:B:540:PHE:CE2	2.45	0.50
1:A:418:ILE:CG1	1:A:432:VAL:HG22	2.41	0.50
1:A:484:HIS:CD2	1:A:486:LEU:H	2.28	0.50
1:A:700:HIS:CD2	1:A:701:ARG:N	2.79	0.50
1:A:838:LYS:O	1:A:839:ALA:O	2.29	0.50
1:A:728:ARG:NE	1:B:701:ARG:NH2	2.59	0.50
1:B:782:LYS:O	1:B:786:VAL:HG22	2.11	0.50
1:A:482:TYR:CE1	1:A:487:PHE:CE2	2.99	0.50
1:A:762:ARG:O	1:A:766:LEU:HD22	2.11	0.50
1:B:307:GLN:HB3	1:B:309:LYS:HD3	1.93	0.50
1:A:317:GLN:O	1:A:321:SER:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:ALA:CB	1:A:757:MET:HE3	2.41	0.50
1:B:608:ARG:HH22	1:B:655:TYR:HE1	1.60	0.50
1:B:299:VAL:HG13	1:B:304:LYS:O	2.10	0.50
1:B:320:GLN:CA	1:B:323:LEU:HB2	2.41	0.50
1:B:477:ASN:OD1	1:B:478:ILE:N	2.44	0.50
1:B:507:ILE:O	1:B:508:LYS:O	2.30	0.50
1:B:651:ARG:HB2	1:B:700:HIS:O	2.11	0.50
1:B:667:PHE:HD2	1:B:807:CYS:HA	1.73	0.50
1:B:735:ILE:HD13	1:B:735:ILE:N	2.25	0.50
1:B:776:ILE:HG13	1:B:780:LEU:HG	1.93	0.50
1:A:239:ASP:OD1	1:A:248:LYS:HE3	2.12	0.50
1:A:523:LYS:HD3	1:A:528:TRP:O	2.12	0.50
1:B:418:ILE:CG1	1:B:432:VAL:HG22	2.41	0.50
1:B:441:VAL:HG22	1:B:458:ARG:HG3	1.94	0.50
1:A:435:LEU:HD22	1:A:440:LEU:HD23	1.94	0.50
1:A:666:HIS:CE1	1:A:670:LEU:HD11	2.43	0.50
1:A:743:CYS:O	1:A:745:ILE:HG23	2.12	0.50
1:B:252:TYR:CD2	1:B:252:TYR:C	2.85	0.50
1:B:318:GLN:OE1	1:B:318:GLN:O	2.29	0.50
1:B:320:GLN:HE21	1:B:327:LEU:N	2.10	0.50
1:B:719:TYR:OH	1:B:811:ASP:OD1	2.29	0.50
1:A:399:VAL:HG22	1:A:420:GLU:OE2	2.12	0.50
1:A:571:MET:CE	1:A:571:MET:HA	2.36	0.50
1:A:580:ASP:O	1:A:584:LYS:HG3	2.12	0.50
1:B:536:LEU:O	1:B:536:LEU:HD22	2.12	0.50
1:B:607:PRO:CG	1:B:663:SER:HB3	2.41	0.50
1:B:695:CYS:HB3	1:B:698:LEU:CD1	2.42	0.50
1:A:561:GLN:HE22	1:B:561:GLN:HA	1.77	0.50
1:B:441:VAL:HG11	1:B:443:LYS:HE3	1.93	0.50
1:B:572:MET:C	1:B:574:HIS:N	2.64	0.50
1:B:587:HIS:C	1:B:589:GLY:H	2.14	0.50
1:A:528:TRP:HD1	1:A:528:TRP:N	2.09	0.49
1:B:270:ASP:OD1	1:B:272:LEU:HG	2.12	0.49
1:A:666:HIS:CE1	1:A:670:LEU:CD2	2.93	0.49
1:B:721:SER:O	1:B:722:GLU:CD	2.51	0.49
1:A:409:ASP:C	1:A:411:SER:H	2.14	0.49
1:A:475:ILE:HD13	1:A:506:PRO:HD2	1.93	0.49
1:A:628:PHE:O	1:A:634:ILE:HD12	2.13	0.49
1:A:688:ALA:HA	1:A:757:MET:CE	2.42	0.49
1:B:265:LEU:HB3	1:B:274:LEU:HD13	1.94	0.49
1:B:305:SER:HB3	1:B:333:VAL:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:GLU:HA	1:B:416:GLU:OE1	2.12	0.49
1:A:370:PHE:HD1	1:A:373:THR:HG22	1.75	0.49
1:A:500:ARG:NH2	1:A:522:ASN:HB3	2.27	0.49
1:A:570:MET:CE	1:B:762:ARG:HH11	2.26	0.49
1:A:571:MET:CA	1:A:571:MET:HE2	2.35	0.49
1:B:376:VAL:CG1	1:B:377:LEU:N	2.75	0.49
1:B:852:LYS:CB	1:B:852:LYS:NZ	2.76	0.49
1:A:668:CYS:O	1:A:671:LEU:HB2	2.13	0.49
1:A:811:ASP:HB2	1:A:822:ILE:CD1	2.37	0.49
1:B:277:LYS:HB3	1:B:287:GLU:HG3	1.95	0.49
1:B:428:GLU:O	1:B:429:ILE:HG23	2.12	0.49
1:B:417:ILE:HD13	1:B:548:ILE:CD1	2.43	0.49
1:B:417:ILE:CD1	1:B:548:ILE:HD11	2.42	0.49
1:B:795:HIS:HA	1:B:798:LEU:HD12	1.94	0.49
1:B:872:LYS:HE2	1:B:876:ASP:CG	2.33	0.49
1:A:822:ILE:O	1:A:825:LEU:N	2.45	0.49
1:B:265:LEU:CB	1:B:274:LEU:HD13	2.41	0.49
1:B:602:SER:O	1:B:604:THR:N	2.45	0.49
1:B:882:ALA:O	1:B:886:GLU:HG2	2.13	0.49
1:A:390:LYS:HE2	1:B:386:GLU:OE1	2.12	0.49
1:A:675:LEU:N	1:A:675:LEU:HD23	2.28	0.49
1:A:715:LEU:HD22	1:A:859:GLN:NE2	2.27	0.49
1:A:572:MET:HE3	1:A:737:ILE:HG12	1.93	0.49
1:A:767:ALA:C	1:A:769:ASP:H	2.15	0.49
1:A:445:PHE:O	1:A:446:ASP:HB2	2.12	0.49
1:A:478:ILE:HG21	1:A:481:ALA:HA	1.95	0.49
1:A:709:VAL:HG12	1:A:710:ALA:N	2.28	0.49
1:A:872:LYS:HB2	1:A:885:TYR:CE1	2.48	0.49
1:B:848:MET:HA	1:B:851:GLU:HB2	1.94	0.49
1:A:337:SER:HB3	1:A:340:THR:HG23	1.92	0.49
1:A:460:PRO:HG2	1:A:463:GLN:NE2	2.28	0.49
1:B:439:GLU:HA	1:B:461:ALA:N	2.27	0.49
1:A:226:ARG:O	1:A:228:ARG:N	2.46	0.48
1:A:332:CYS:SG	1:A:346:LEU:HD13	2.53	0.48
1:A:484:HIS:CD2	1:A:485:PRO:HD2	2.47	0.48
1:A:569:GLU:HG3	1:A:574:HIS:CD2	2.48	0.48
1:A:709:VAL:HG21	1:A:712:LYS:HG3	1.95	0.48
1:B:572:MET:CE	1:B:645:MET:CE	2.91	0.48
1:B:714:VAL:HG12	1:B:716:ALA:N	2.25	0.48
1:B:788:TYR:HA	1:B:795:HIS:ND1	2.28	0.48
1:A:441:VAL:HA	1:A:457:ILE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:ILE:HG21	1:A:624:GLN:CD	2.33	0.48
1:A:873:LEU:O	1:A:877:LEU:HD12	2.12	0.48
1:B:473:GLY:HA2	1:B:514:VAL:HG21	1.93	0.48
1:B:777:PHE:CE2	1:B:781:GLN:NE2	2.81	0.48
1:B:885:TYR:CD2	1:B:885:TYR:C	2.86	0.48
1:A:223:TYR:CD2	1:A:226:ARG:HB2	2.48	0.48
1:A:440:LEU:HB2	1:A:459:ILE:HG13	1.93	0.48
1:A:810:SER:O	1:A:813:THR:OG1	2.28	0.48
1:B:402:ASN:O	1:B:406:HIS:HD2	1.95	0.48
1:B:590:ILE:O	1:B:591:GLN:HB3	2.13	0.48
1:B:799:LEU:HG	1:B:803:LEU:HD11	1.95	0.48
1:B:821:LYS:O	1:B:825:LEU:HD12	2.12	0.48
1:B:852:LYS:HG3	1:B:852:LYS:O	2.13	0.48
1:A:510:GLU:OE1	1:A:510:GLU:HA	2.14	0.48
1:A:559:GLU:O	1:A:561:GLN:N	2.47	0.48
1:B:433:PHE:CD2	1:B:442:ALA:CB	2.96	0.48
1:B:768:THR:HG22	1:B:804:MET:HG2	1.95	0.48
1:A:341:ASP:C	1:A:342:GLN:HG2	2.34	0.48
1:A:353:LEU:O	1:A:354:GLU:O	2.32	0.48
1:A:527:PRO:HB2	1:A:528:TRP:CD1	2.49	0.48
1:A:829:GLU:C	1:A:831:PHE:H	2.16	0.48
1:B:648:LYS:HE3	4:B:168:HOH:O	2.13	0.48
1:A:570:MET:CE	1:B:762:ARG:NH1	2.77	0.48
1:A:231:LEU:CD1	1:B:372:TYR:CE1	2.97	0.48
1:A:732:ALA:HB2	1:B:571:MET:CE	2.44	0.48
1:B:718:LEU:CG	1:B:719:TYR:N	2.76	0.48
1:A:247:LEU:CD2	1:A:251:GLN:HE22	2.22	0.48
1:A:305:SER:HB3	1:A:333:VAL:HA	1.94	0.48
1:A:476:LEU:CD2	1:A:478:ILE:HD11	2.44	0.48
1:B:353:LEU:HD23	1:B:353:LEU:HA	1.71	0.48
1:B:645:MET:HG2	1:B:737:ILE:HG23	1.95	0.48
1:A:246:GLN:O	1:A:250:LEU:HB2	2.13	0.48
1:A:258:ARG:HH11	1:A:258:ARG:CB	2.26	0.48
1:B:330:MET:CG	1:B:350:PHE:CD1	2.97	0.48
1:B:559:GLU:O	1:B:562:TYR:HB3	2.14	0.48
1:B:579:ASP:HA	1:B:582:TYR:CD2	2.49	0.48
1:B:667:PHE:O	1:B:670:LEU:HB2	2.14	0.48
1:B:720:SER:HB2	1:B:770:LEU:CB	2.43	0.48
1:A:428:GLU:HA	1:A:524:ILE:HD11	1.96	0.48
1:A:688:ALA:HB3	1:A:760:LEU:HD13	1.96	0.48
1:A:770:LEU:CD1	1:A:773:HIS:HB3	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:ARG:C	1:B:228:ARG:H	2.18	0.48
1:B:261:ARG:HD3	1:B:280:GLY:CA	2.44	0.48
1:B:341:ASP:O	1:B:342:GLN:HG2	2.14	0.48
1:B:501:ASN:C	1:B:502:ILE:HG13	2.35	0.48
1:B:607:PRO:HB2	1:B:663:SER:HB3	1.95	0.48
1:B:890:SER:O	1:B:893:GLU:N	2.47	0.48
1:A:258:ARG:HH11	1:A:258:ARG:HB3	1.78	0.47
1:A:591:GLN:HG3	1:A:592:PRO:CD	2.43	0.47
1:B:393:CYS:O	1:B:397:LEU:N	2.34	0.47
1:B:253:LEU:O	1:B:255:GLN:N	2.47	0.47
1:B:261:ARG:CD	1:B:280:GLY:HA3	2.43	0.47
1:A:360:ASP:HB3	4:A:110:HOH:O	2.14	0.47
1:B:433:PHE:CE2	1:B:442:ALA:HB3	2.49	0.47
1:B:479:PRO:CB	1:B:528:TRP:CE3	2.97	0.47
1:B:596:ILE:CG2	1:B:600:PHE:CD1	2.97	0.47
1:B:799:LEU:C	1:B:799:LEU:HD12	2.28	0.47
1:A:527:PRO:CG	1:A:528:TRP:CD1	2.96	0.47
1:A:593:VAL:CG1	1:A:600:PHE:CE2	2.98	0.47
1:A:590:ILE:HG22	1:A:624:GLN:HE22	1.78	0.47
1:A:668:CYS:SG	1:A:689:LEU:CD2	3.03	0.47
1:B:698:LEU:O	1:B:730:HIS:CD2	2.67	0.47
1:A:273:GLN:HG2	1:A:291:PRO:HA	1.94	0.47
1:A:563:ARG:HD3	4:A:57:HOH:O	2.14	0.47
1:B:318:GLN:HA	1:B:321:SER:OG	2.15	0.47
1:B:330:MET:CG	1:B:350:PHE:CE1	2.97	0.47
1:B:478:ILE:HG23	1:B:480:ASP:O	2.14	0.47
1:B:527:PRO:CB	1:B:528:TRP:CD1	2.97	0.47
1:A:565:HIS:HA	1:A:568:ASN:HB3	1.96	0.47
1:A:570:MET:HE3	1:B:762:ARG:NH1	2.29	0.47
1:B:352:LYS:HB3	1:B:356:ASP:HA	1.96	0.47
1:A:838:LYS:HB3	1:B:774:LEU:CB	2.45	0.47
1:B:868:MET:HG2	1:B:888:VAL:HG12	1.95	0.47
1:A:602:SER:C	1:A:604:THR:H	2.18	0.47
1:A:605:TYR:CZ	1:A:610:LEU:HD11	2.50	0.47
1:A:630:ASN:HD22	1:A:630:ASN:N	2.11	0.47
1:A:648:LYS:CB	1:A:648:LYS:NZ	2.78	0.47
1:A:814:LYS:HB3	1:A:818:THR:CG2	2.45	0.47
1:A:605:TYR:O	1:A:814:LYS:HE3	2.14	0.47
1:B:508:LYS:H	1:B:514:VAL:HA	1.79	0.47
1:B:567:ALA:O	1:B:570:MET:HB2	2.14	0.47
1:A:425:SER:OG	1:A:520:LEU:HD22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:MET:HG2	1:A:648:LYS:HG2	1.96	0.47
1:A:610:LEU:HB3	1:A:611:PRO:CD	2.44	0.47
1:A:874:LEU:HD23	1:A:874:LEU:HA	1.74	0.47
1:B:253:LEU:C	1:B:255:GLN:N	2.68	0.47
1:B:312:THR:HG22	1:B:313:SER:N	2.29	0.47
1:B:459:ILE:HD12	1:B:460:PRO:HD3	1.97	0.47
1:B:617:MET:O	1:B:620:LEU:N	2.48	0.47
1:A:440:LEU:HG	1:A:461:ALA:HA	1.97	0.47
1:B:375:THR:HG22	1:B:376:VAL:N	2.29	0.47
1:B:441:VAL:HG21	1:B:458:ARG:NH2	2.29	0.47
1:A:224:THR:CG2	1:A:228:ARG:NH2	2.74	0.47
1:A:460:PRO:CG	1:A:463:GLN:NE2	2.77	0.47
1:A:476:LEU:CD2	1:A:478:ILE:CD1	2.92	0.47
1:B:460:PRO:HG2	1:B:463:GLN:CG	2.44	0.47
1:B:636:CYS:N	1:B:637:PRO:HD2	2.30	0.47
1:B:672:TYR:N	1:B:677:LEU:HD12	2.29	0.47
1:A:230:ILE:HA	1:A:230:ILE:HD13	1.48	0.47
1:A:641:ARG:NH1	1:A:742:GLY:HA3	2.30	0.47
1:A:656:HIS:HD2	1:A:829:GLU:OE2	1.98	0.47
1:B:314:GLU:O	1:B:317:GLN:N	2.48	0.47
1:B:330:MET:HA	1:B:349:ALA:O	2.15	0.47
1:B:597:ASP:HB3	1:B:600:PHE:HB2	1.96	0.47
1:A:223:TYR:HD2	1:A:223:TYR:O	1.98	0.46
1:A:681:LEU:HB3	1:A:685:GLU:OE1	2.15	0.46
1:A:566:LEU:HD13	1:B:755:GLN:HE21	1.80	0.46
1:A:331:LEU:HD13	1:A:366:ILE:HD12	1.96	0.46
1:A:403:LEU:CD1	1:A:417:ILE:HG13	2.45	0.46
1:A:575:MET:CE	1:A:649:GLY:HA2	2.45	0.46
1:A:860:ILE:HD11	1:A:895:TRP:HB3	1.96	0.46
1:B:458:ARG:CG	1:B:458:ARG:NH1	2.73	0.46
1:B:508:LYS:N	1:B:514:VAL:HA	2.31	0.46
1:A:311:LEU:HD23	1:A:315:ASP:HB2	1.97	0.46
1:A:852:LYS:HB2	1:A:852:LYS:NZ	2.30	0.46
1:B:460:PRO:CG	1:B:463:GLN:NE2	2.78	0.46
1:B:820:ARG:O	1:B:824:GLU:HG2	2.16	0.46
1:A:593:VAL:HG12	1:A:600:PHE:CE2	2.49	0.46
1:B:270:ASP:N	1:B:270:ASP:OD2	2.48	0.46
1:B:268:SER:HB3	1:B:273:GLN:O	2.15	0.46
1:B:260:SER:HG	1:B:351:ASN:HB2	1.78	0.46
1:B:503:LEU:HD12	1:B:504:CYS:N	2.30	0.46
1:B:561:GLN:CA	1:B:561:GLN:NE2	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:TYR:CE1	1:A:364:HIS:NE2	2.65	0.46
1:A:591:GLN:HG3	1:A:592:PRO:HD2	1.97	0.46
1:A:586:LEU:HD11	1:A:636:CYS:O	2.15	0.46
1:A:816:TRP:O	1:A:820:ARG:HB2	2.14	0.46
1:B:674:ASN:H	1:B:674:ASN:ND2	2.13	0.46
1:B:748:HIS:H	1:B:748:HIS:CD2	2.33	0.46
1:B:532:PHE:C	1:B:532:PHE:CD1	2.89	0.46
1:A:732:ALA:HB1	1:B:571:MET:HE2	1.98	0.46
1:B:630:ASN:ND2	1:B:631:ASN:N	2.59	0.46
1:B:622:MET:HE1	1:B:666:HIS:CB	2.44	0.46
1:B:320:GLN:HE21	1:B:327:LEU:CB	2.23	0.46
1:A:484:HIS:CD2	1:A:485:PRO:CG	2.99	0.46
1:A:521:VAL:O	1:A:522:ASN:HB2	2.16	0.46
1:B:333:VAL:CB	1:B:366:ILE:HG21	2.46	0.46
1:B:465:ILE:CD1	1:B:502:ILE:HD13	2.46	0.46
1:B:508:LYS:HA	1:B:513:GLU:C	2.37	0.46
1:A:274:LEU:HD23	1:A:274:LEU:N	2.31	0.46
1:A:370:PHE:CD1	1:A:373:THR:HG22	2.50	0.46
1:A:388:LYS:HE3	1:A:388:LYS:HB3	1.45	0.46
1:B:671:LEU:HB3	1:B:677:LEU:HD11	1.96	0.46
1:B:818:THR:O	1:B:822:ILE:HD12	2.16	0.46
1:B:837:GLU:CB	1:B:838:LYS:NZ	2.77	0.46
1:A:223:TYR:HH	1:A:364:HIS:CE1	2.32	0.46
1:A:700:HIS:CD2	1:A:701:ARG:O	2.69	0.46
1:A:854:TYR:HE1	4:A:75:HOH:O	1.98	0.46
1:A:707:PHE:C	1:A:709:VAL:N	2.69	0.45
1:B:326:GLU:HB3	1:B:328:GLN:NE2	2.31	0.45
1:B:366:ILE:O	1:B:369:CYS:HB3	2.15	0.45
1:B:471:THR:CG2	1:B:472:THR:N	2.79	0.45
1:B:626:MET:HB2	1:B:626:MET:HE2	1.78	0.45
1:B:727:GLU:N	1:B:727:GLU:OE2	2.50	0.45
1:B:720:SER:HA	1:B:770:LEU:HB2	1.97	0.45
1:A:838:LYS:CB	1:B:774:LEU:HD12	2.46	0.45
1:A:620:LEU:HD23	1:A:639:LEU:HD21	1.98	0.45
1:A:805:THR:HG22	1:A:870:ILE:HD13	1.96	0.45
1:B:505:PHE:HE1	1:B:541:SER:HG	1.62	0.45
1:B:715:LEU:HD22	1:B:859:GLN:HE22	1.81	0.45
1:A:330:MET:CG	1:A:350:PHE:CD1	2.98	0.45
1:A:528:TRP:HD1	1:A:528:TRP:H	1.65	0.45
1:A:622:MET:SD	1:A:669:TYR:CG	3.09	0.45
1:A:777:PHE:CE2	1:A:781:GLN:NE2	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:788:TYR:CZ	1:A:799:LEU:CD2	2.99	0.45
1:A:675:LEU:CD1	1:A:878:PHE:CG	2.99	0.45
1:B:392:GLU:OE2	1:B:532:PHE:CE1	2.70	0.45
1:B:399:VAL:CG2	1:B:540:PHE:HE1	2.24	0.45
1:B:738:LEU:HD22	1:B:744:ASN:OD1	2.17	0.45
1:B:689:LEU:HA	1:B:764:ILE:HD13	1.97	0.45
1:A:366:ILE:HG22	1:A:367:GLN:N	2.30	0.45
1:A:479:PRO:CB	1:A:528:TRP:CE3	2.97	0.45
1:A:536:LEU:O	1:A:536:LEU:HD22	2.17	0.45
1:A:755:GLN:HE21	1:B:566:LEU:HD13	1.82	0.45
1:B:648:LYS:HB2	1:B:648:LYS:HZ2	1.80	0.45
1:B:852:LYS:HE3	1:B:852:LYS:HB2	1.74	0.45
1:A:484:HIS:CD2	1:A:485:PRO:CD	2.99	0.45
1:A:507:ILE:O	1:A:508:LYS:HG3	2.17	0.45
1:A:617:MET:O	1:A:620:LEU:HB2	2.16	0.45
1:A:855:ILE:N	1:A:856:PRO:CD	2.79	0.45
1:B:225:ASP:HA	1:B:228:ARG:HE	1.81	0.45
1:B:606:THR:HG1	1:B:609:SER:HB3	1.81	0.45
1:A:273:GLN:HB3	1:A:273:GLN:HE21	1.51	0.45
1:A:602:SER:HB3	4:A:184:HOH:O	2.16	0.45
1:A:862:PHE:HE1	1:A:866:ILE:HG21	1.82	0.45
1:A:610:LEU:HA	1:A:611:PRO:HD3	1.60	0.45
1:A:721:SER:CA	1:A:769:ASP:OD2	2.63	0.45
1:A:838:LYS:N	1:A:838:LYS:CD	2.78	0.45
1:A:873:LEU:HA	1:A:876:ASP:HB2	1.99	0.45
1:B:254:GLN:OE1	1:B:280:GLY:HA2	2.16	0.45
1:B:428:GLU:HB2	1:B:522:ASN:HB2	1.97	0.45
1:A:445:PHE:HB3	1:A:446:ASP:H	1.42	0.45
1:A:593:VAL:CG2	1:A:625:ASP:HB2	2.46	0.45
1:B:230:ILE:HD13	1:B:230:ILE:HA	1.64	0.45
1:B:576:LYS:H	1:B:648:LYS:HD3	1.82	0.45
1:B:755:GLN:O	1:B:758:LEU:HB2	2.16	0.45
1:A:623:LEU:HA	1:A:626:MET:HE3	1.98	0.45
1:B:290:PHE:CB	1:B:291:PRO:HD2	2.21	0.45
1:A:231:LEU:CD1	1:B:372:TYR:CZ	2.98	0.45
1:B:572:MET:CE	1:B:645:MET:HE3	2.47	0.45
1:A:277:LYS:HB3	1:A:287:GLU:CG	2.46	0.45
1:A:338:ARG:NH2	1:B:238:TYR:CD2	2.84	0.45
1:B:313:SER:O	1:B:317:GLN:HB2	2.17	0.45
1:B:389:LEU:HD23	1:B:389:LEU:HA	1.61	0.45
1:B:395:ALA:O	1:B:399:VAL:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LEU:HA	1:A:292:LEU:HD23	1.84	0.44
1:A:497:PHE:O	1:A:498:ARG:HB2	2.16	0.44
1:A:723:GLY:C	1:A:725:VAL:H	2.21	0.44
1:A:756:ARG:HB2	1:A:756:ARG:HE	1.71	0.44
1:B:258:ARG:HG2	1:B:258:ARG:NH1	2.31	0.44
1:A:240:LEU:HD11	1:B:340:THR:HG22	1.99	0.44
1:B:719:TYR:O	1:B:720:SER:HB3	2.16	0.44
1:B:735:ILE:HD12	1:B:738:LEU:HD12	1.98	0.44
1:B:754:TYR:O	1:B:758:LEU:HD13	2.18	0.44
1:A:376:VAL:O	1:A:380:THR:OG1	2.34	0.44
1:A:436:ASP:HB2	1:A:441:VAL:HG21	1.96	0.44
1:A:453:GLU:CD	1:A:453:GLU:H	2.21	0.44
1:A:505:PHE:HA	1:A:506:PRO:HD3	1.76	0.44
1:A:536:LEU:HD23	1:A:536:LEU:HA	1.76	0.44
1:B:290:PHE:CB	1:B:291:PRO:CD	2.94	0.44
1:B:433:PHE:CE2	1:B:442:ALA:CB	2.99	0.44
1:B:887:ARG:NH1	1:B:887:ARG:CG	2.78	0.44
1:A:586:LEU:HD21	1:A:636:CYS:HB3	2.00	0.44
1:A:789:ASP:HB3	1:A:792:ASN:H	1.81	0.44
1:A:709:VAL:O	1:A:710:ALA:HB2	2.16	0.44
1:A:799:LEU:CD1	1:A:803:LEU:CD1	2.95	0.44
1:A:812:GLN:CB	1:A:888:VAL:HG22	2.47	0.44
1:B:251:GLN:NE2	1:B:281:ASP:HA	2.31	0.44
1:B:851:GLU:HA	1:B:854:TYR:CE1	2.52	0.44
1:A:275:SER:CB	1:A:287:GLU:OE2	2.65	0.44
1:B:425:SER:O	1:B:426:ASN:HB2	2.17	0.44
1:B:854:TYR:CD1	1:B:854:TYR:N	2.86	0.44
1:A:251:GLN:NE2	1:A:281:ASP:CA	2.78	0.44
1:A:681:LEU:HD13	1:A:800:LEU:HD21	2.00	0.44
1:A:889:ALA:O	1:A:892:ARG:HB3	2.17	0.44
1:B:323:LEU:HD12	1:B:327:LEU:HD11	1.94	0.44
1:B:330:MET:CE	1:B:332:CYS:N	2.81	0.44
1:B:409:ASP:HB3	1:B:412:VAL:HB	1.99	0.44
1:B:459:ILE:CG1	1:B:460:PRO:HD2	2.47	0.44
1:B:459:ILE:HG13	1:B:460:PRO:HD2	2.00	0.44
1:B:508:LYS:CA	1:B:514:VAL:HA	2.48	0.44
1:A:239:ASP:HB2	1:A:245:LEU:CD2	2.48	0.44
1:A:542:ILE:HG21	1:B:401:LYS:HZ3	1.83	0.44
1:A:715:LEU:HD23	1:A:862:PHE:CD2	2.53	0.44
1:B:421:ALA:HB2	1:B:540:PHE:HE2	1.83	0.44
1:B:618:ALA:O	1:B:622:MET:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:675:LEU:HD13	1:B:878:PHE:CG	2.53	0.44
1:B:809:LEU:O	1:B:811:ASP:N	2.50	0.44
1:B:872:LYS:HD2	1:B:872:LYS:HA	1.60	0.44
1:A:413:LEU:O	1:A:416:GLU:HB2	2.17	0.44
1:A:868:MET:HB2	1:A:869:PRO:HD3	2.00	0.44
1:B:439:GLU:HA	1:B:461:ALA:H	1.83	0.44
1:B:770:LEU:HD13	1:B:770:LEU:HA	1.36	0.44
1:B:859:GLN:CA	1:B:859:GLN:HE21	2.29	0.44
1:A:299:VAL:HG12	1:A:334:PRO:HG3	1.99	0.44
1:A:805:THR:CG2	1:A:870:ILE:HD13	2.48	0.44
1:B:258:ARG:HG2	1:B:258:ARG:HH11	1.83	0.44
1:B:586:LEU:HD12	1:B:640:ALA:HB3	2.00	0.44
1:A:508:LYS:H	1:A:515:ILE:H	1.66	0.43
1:B:478:ILE:HA	1:B:479:PRO:HD2	1.61	0.43
1:B:501:ASN:OD1	1:B:522:ASN:HA	2.18	0.43
1:B:726:MET:O	1:B:729:HIS:HB3	2.18	0.43
1:B:749:PHE:N	1:B:749:PHE:CD1	2.85	0.43
1:B:848:MET:O	1:B:852:LYS:HB3	2.18	0.43
1:B:902:VAL:HA	1:B:903:PRO:HD3	1.34	0.43
1:A:719:TYR:OH	1:A:811:ASP:OD1	2.29	0.43
1:B:472:THR:O	1:B:474:GLN:HG3	2.17	0.43
1:B:682:GLU:HG3	1:B:685:GLU:OE1	2.19	0.43
1:B:855:ILE:N	1:B:856:PRO:CD	2.80	0.43
1:A:561:GLN:HE22	1:B:561:GLN:HE21	1.66	0.43
1:A:673:LYS:HB2	1:A:674:ASN:H	1.60	0.43
1:A:672:TYR:HD1	1:A:686:ILE:HG21	1.82	0.43
1:A:726:MET:O	1:A:729:HIS:HB3	2.19	0.43
1:A:689:LEU:HA	1:A:764:ILE:HD13	2.01	0.43
1:B:600:PHE:O	1:B:600:PHE:CD2	2.71	0.43
1:B:721:SER:OG	1:B:722:GLU:N	2.51	0.43
1:A:226:ARG:C	1:A:228:ARG:N	2.69	0.43
1:A:721:SER:O	1:A:722:GLU:CD	2.56	0.43
1:B:418:ILE:CG1	1:B:432:VAL:CG2	2.96	0.43
1:B:903:PRO:O	1:B:904:ARG:HG3	2.17	0.43
1:A:304:LYS:CA	1:A:304:LYS:HE3	2.31	0.43
1:A:337:SER:HB2	1:A:344:VAL:HG21	2.00	0.43
1:A:376:VAL:CG1	1:A:377:LEU:N	2.81	0.43
1:A:670:LEU:O	1:A:674:ASN:ND2	2.46	0.43
1:B:266:LEU:CD1	1:B:277:LYS:HE2	2.47	0.43
1:B:296:LEU:HD23	1:B:296:LEU:HA	1.71	0.43
1:B:356:ASP:O	1:B:357:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:VAL:CG2	1:B:375:THR:HG22	2.48	0.43
1:A:448:GLY:O	1:A:449:VAL:HG23	2.18	0.43
1:A:796:HIS:O	1:A:800:LEU:HD12	2.19	0.43
1:A:860:ILE:HD13	1:A:895:TRP:HB3	2.00	0.43
1:B:443:LYS:O	1:B:455:TYR:O	2.36	0.43
1:B:501:ASN:HB2	1:B:529:PHE:CE1	2.54	0.43
1:A:572:MET:HE3	1:A:737:ILE:N	2.34	0.43
1:A:814:LYS:N	1:A:814:LYS:CD	2.81	0.43
1:A:372:TYR:CE1	1:B:231:LEU:HD12	2.54	0.43
1:B:417:ILE:CD1	1:B:548:ILE:CD1	2.97	0.43
1:B:749:PHE:N	1:B:749:PHE:HD1	2.16	0.43
1:A:559:GLU:C	1:A:561:GLN:N	2.72	0.43
1:B:443:LYS:HA	1:B:457:ILE:H	1.84	0.43
1:B:499:THR:CG2	1:B:500:ARG:N	2.63	0.43
1:B:769:ASP:O	1:B:772:HIS:N	2.51	0.43
1:B:224:THR:HG22	1:B:228:ARG:HH21	1.80	0.43
1:B:537:ALA:O	1:B:541:SER:HB2	2.18	0.43
1:A:372:TYR:CE2	1:B:231:LEU:HD11	2.53	0.43
1:A:478:ILE:HA	1:A:479:PRO:HD2	1.48	0.43
1:A:812:GLN:O	1:A:888:VAL:HG22	2.19	0.43
1:A:855:ILE:HB	1:A:856:PRO:HD3	2.01	0.43
1:B:354:GLU:HB3	1:B:355:GLY:H	1.25	0.43
1:B:860:ILE:HD11	1:B:895:TRP:C	2.39	0.43
1:A:711:SER:CB	1:A:854:TYR:CE2	2.96	0.42
1:B:258:ARG:HD3	1:B:352:LYS:CE	2.47	0.42
1:A:656:HIS:CG	1:A:700:HIS:CE1	3.07	0.42
1:A:672:TYR:O	1:A:676:GLU:HA	2.19	0.42
1:A:788:TYR:CZ	1:A:799:LEU:HD23	2.54	0.42
1:B:250:LEU:HA	1:B:250:LEU:HD12	1.88	0.42
1:B:270:ASP:HB2	1:B:272:LEU:CG	2.46	0.42
1:A:231:LEU:HD11	1:B:372:TYR:CD2	2.54	0.42
1:B:527:PRO:CG	1:B:528:TRP:CD1	3.01	0.42
1:A:231:LEU:HD21	1:B:230:ILE:CG2	2.39	0.42
1:A:671:LEU:HD13	1:A:803:LEU:CD2	2.42	0.42
1:B:274:LEU:HD22	1:B:274:LEU:HA	1.87	0.42
1:B:627:ASN:ND2	1:B:631:ASN:CG	2.73	0.42
1:B:680:TYR:HB3	1:B:788:TYR:CE2	2.54	0.42
1:B:712:LYS:N	4:B:52:HOH:O	2.51	0.42
1:A:225:ASP:HA	1:A:228:ARG:HE	1.84	0.42
1:A:233:LEU:O	1:A:236:GLU:HB2	2.19	0.42
1:A:444:VAL:HB	1:A:454:SER:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:PHE:HA	1:A:605:TYR:CD1	2.54	0.42
1:A:834:GLY:O	1:A:838:LYS:NZ	2.49	0.42
1:B:258:ARG:HD3	1:B:352:LYS:HZ3	1.83	0.42
1:B:301:GLU:HA	1:B:301:GLU:OE1	2.19	0.42
1:B:504:CYS:SG	1:B:519:GLU:HB3	2.59	0.42
1:B:895:TRP:O	1:B:898:VAL:HG23	2.19	0.42
1:B:335:VAL:HB	1:B:345:ALA:HB3	2.01	0.42
1:B:357:LEU:HA	1:B:357:LEU:HD23	1.88	0.42
1:B:476:LEU:CD2	1:B:478:ILE:CD1	2.98	0.42
1:B:528:TRP:HB2	1:B:529:PHE:H	1.49	0.42
1:B:852:LYS:CB	1:B:852:LYS:HZ1	2.33	0.42
1:A:688:ALA:CB	1:A:760:LEU:CD1	2.98	0.42
1:B:439:GLU:N	1:B:461:ALA:HB2	2.35	0.42
1:B:476:LEU:HD23	1:B:478:ILE:CD1	2.48	0.42
1:A:540:PHE:O	1:A:542:ILE:N	2.53	0.42
1:B:821:LYS:HA	1:B:824:GLU:HG3	2.01	0.42
1:B:848:MET:O	1:B:852:LYS:N	2.52	0.42
1:A:381:LEU:O	1:A:381:LEU:HD12	2.20	0.42
1:A:735:ILE:HD13	1:A:735:ILE:HA	1.73	0.42
1:A:799:LEU:CD1	1:A:803:LEU:HD11	2.48	0.42
1:A:852:LYS:CB	1:A:852:LYS:NZ	2.83	0.42
1:B:422:ARG:HD3	1:B:429:ILE:HA	2.01	0.42
1:A:602:SER:C	1:A:604:THR:N	2.74	0.42
1:B:398:GLN:NE2	1:B:401:LYS:HD3	2.34	0.42
1:A:252:TYR:CD2	1:A:252:TYR:C	2.93	0.42
1:A:418:ILE:CG1	1:A:432:VAL:CG2	2.98	0.42
1:A:542:ILE:HD13	1:B:401:LYS:HZ1	1.85	0.42
1:A:703:THR:HB	1:A:718:LEU:HD12	2.00	0.42
1:A:726:MET:HG2	1:A:730:HIS:CE1	2.54	0.42
1:A:821:LYS:HD3	1:A:824:GLU:OE1	2.20	0.42
1:B:251:GLN:HE22	1:B:281:ASP:HA	1.84	0.42
1:A:635:ASP:OD2	1:A:638:THR:N	2.53	0.41
1:B:226:ARG:HB3	1:B:368:HIS:CE1	2.55	0.41
1:B:237:LEU:HD21	1:B:249:VAL:CG2	2.49	0.41
1:B:258:ARG:NH1	1:B:258:ARG:CG	2.83	0.41
1:B:508:LYS:H	1:B:515:ILE:H	1.68	0.41
1:B:582:TYR:O	1:B:586:LEU:HB2	2.19	0.41
1:B:697:ASP:O	1:B:700:HIS:HB2	2.20	0.41
1:A:389:LEU:HA	1:A:389:LEU:HD23	1.59	0.41
1:A:636:CYS:HB2	1:A:637:PRO:HD3	2.02	0.41
1:A:671:LEU:HD23	1:A:671:LEU:HA	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:608:ARG:NH2	1:B:655:TYR:HE1	2.17	0.41
1:A:292:LEU:O	1:A:293:THR:O	2.39	0.41
1:A:575:MET:HG2	1:A:648:LYS:CG	2.51	0.41
1:B:781:GLN:O	1:B:784:ALA:N	2.53	0.41
1:A:509:ASN:OD1	1:A:513:GLU:HG3	2.19	0.41
1:A:428:GLU:HB2	1:A:522:ASN:HB2	2.02	0.41
1:A:596:ILE:HG21	1:A:600:PHE:CD1	2.55	0.41
1:A:620:LEU:CD2	1:A:639:LEU:HD21	2.51	0.41
1:A:821:LYS:HD3	1:A:821:LYS:HA	1.80	0.41
1:B:637:PRO:C	1:B:641:ARG:HH21	2.23	0.41
1:A:571:MET:CE	1:B:731:PHE:HE2	2.33	0.41
1:A:329:ALA:O	1:A:330:MET:HB2	2.19	0.41
1:A:439:GLU:HA	1:A:461:ALA:H	1.85	0.41
1:A:467:GLY:O	1:A:471:THR:HB	2.19	0.41
1:A:481:ALA:HB1	1:A:487:PHE:CD1	2.55	0.41
1:A:819:THR:HA	1:A:822:ILE:HD12	2.02	0.41
1:B:279:ILE:CD1	1:B:322:MET:SD	3.08	0.41
1:B:629:ILE:HA	1:B:634:ILE:HD12	2.01	0.41
1:A:362:ASP:O	1:A:365:VAL:HG13	2.20	0.41
1:A:366:ILE:O	1:A:369:CYS:HB3	2.20	0.41
1:A:380:THR:O	1:A:384:GLN:HG3	2.21	0.41
1:A:399:VAL:HG13	1:A:420:GLU:HG3	2.03	0.41
1:A:427:ALA:CB	1:A:520:LEU:CD2	2.99	0.41
1:A:618:ALA:O	1:A:622:MET:N	2.53	0.41
1:A:718:LEU:C	1:A:720:SER:N	2.74	0.41
1:B:572:MET:HE3	1:B:645:MET:CE	2.51	0.41
1:B:671:LEU:HD23	1:B:671:LEU:HA	1.81	0.41
1:B:655:TYR:OH	1:B:719:TYR:OH	2.20	0.41
1:A:277:LYS:HB3	1:A:287:GLU:HG3	2.03	0.41
1:A:837:GLU:CB	1:A:838:LYS:HE3	2.41	0.41
1:B:256:GLU:H	1:B:256:GLU:HG2	1.54	0.41
1:B:586:LEU:CD1	1:B:640:ALA:CB	2.98	0.41
1:B:576:LYS:C	1:B:648:LYS:HE2	2.40	0.41
1:B:901:LEU:N	1:B:901:LEU:CD2	2.75	0.41
1:A:320:GLN:O	1:A:324:GLY:N	2.41	0.41
1:A:468:HIS:NE2	1:A:472:THR:HG21	2.34	0.41
1:A:718:LEU:CD2	1:A:826:ILE:HG23	2.51	0.41
1:B:275:SER:HB3	1:B:287:GLU:OE2	2.20	0.41
1:B:292:LEU:HD23	1:B:292:LEU:HA	1.79	0.41
1:B:812:GLN:NE2	1:B:812:GLN:HA	2.36	0.41
1:B:656:HIS:CD2	1:B:829:GLU:OE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:TYR:C	1:A:669:TYR:CD2	2.93	0.41
1:A:821:LYS:C	1:A:824:GLU:HG3	2.41	0.41
1:A:868:MET:N	1:A:869:PRO:HD2	2.35	0.41
1:B:338:ARG:HA	1:B:338:ARG:HD2	1.75	0.41
1:B:536:LEU:HD23	1:B:536:LEU:HA	1.71	0.41
1:B:677:LEU:HD21	1:B:803:LEU:CD2	2.50	0.41
1:B:740:THR:CG2	1:B:743:CYS:SG	3.05	0.41
1:B:859:GLN:HG2	1:B:895:TRP:CE2	2.56	0.41
1:A:254:GLN:OE1	1:A:280:GLY:HA2	2.21	0.41
1:A:539:ALA:O	1:A:542:ILE:HB	2.21	0.41
1:A:575:MET:HE1	1:A:649:GLY:CA	2.51	0.41
1:A:638:THR:CG2	1:A:745:ILE:HG22	2.42	0.41
1:A:688:ALA:CB	1:A:760:LEU:HD12	2.50	0.41
1:A:774:LEU:HD21	1:A:866:ILE:CD1	2.51	0.41
1:B:320:GLN:HG3	1:B:327:LEU:HD22	2.03	0.41
1:B:441:VAL:CG1	1:B:443:LYS:HD3	2.51	0.41
1:B:868:MET:HB2	1:B:869:PRO:CD	2.50	0.41
1:A:740:THR:CG2	1:A:741:HIS:N	2.84	0.41
1:B:511:ASN:N	1:B:511:ASN:ND2	2.69	0.41
1:B:578:SER:O	1:B:581:GLU:HB2	2.21	0.41
1:B:837:GLU:C	1:B:838:LYS:NZ	2.74	0.41
1:B:838:LYS:O	1:B:839:ALA:HB3	2.21	0.41
1:A:550:HIS:CD2	1:B:407:LEU:HD23	2.56	0.40
1:A:636:CYS:N	1:A:637:PRO:CD	2.83	0.40
1:A:687:PHE:O	1:A:691:ILE:HG12	2.21	0.40
1:A:707:PHE:C	1:A:709:VAL:H	2.23	0.40
1:A:709:VAL:CG2	1:A:712:LYS:HB2	2.51	0.40
1:A:720:SER:OG	1:A:721:SER:N	2.48	0.40
1:A:774:LEU:HD12	1:B:838:LYS:CB	2.51	0.40
1:B:319:LEU:HD22	1:B:322:MET:CE	2.51	0.40
1:B:572:MET:CE	1:B:645:MET:HE2	2.51	0.40
1:B:622:MET:O	1:B:626:MET:HE2	2.22	0.40
1:B:647:LYS:HD2	1:B:658:TRP:CD1	2.56	0.40
1:A:461:ALA:O	1:A:467:GLY:HA2	2.21	0.40
1:A:833:GLN:O	1:A:836:LEU:HD12	2.21	0.40
1:A:819:THR:CG2	1:A:891:ASN:ND2	2.79	0.40
1:B:620:LEU:O	1:B:624:GLN:HB3	2.21	0.40
1:A:566:LEU:CD2	1:B:755:GLN:HE21	2.33	0.40
1:A:223:TYR:CE2	1:A:226:ARG:CB	2.96	0.40
1:A:404:PHE:HA	1:A:407:LEU:HD21	2.02	0.40
1:A:647:LYS:HD2	1:A:658:TRP:CG	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:MET:CE	1:A:649:GLY:CA	2.99	0.40
1:A:788:TYR:CG	1:A:788:TYR:O	2.74	0.40
1:B:312:THR:HB	1:B:315:ASP:CG	2.38	0.40
1:B:829:GLU:C	1:B:831:PHE:H	2.24	0.40
1:A:326:GLU:C	1:A:327:LEU:HD12	2.42	0.40
1:B:629:ILE:HA	1:B:634:ILE:HB	2.04	0.40
1:A:566:LEU:CD1	1:B:755:GLN:HE21	2.34	0.40
1:B:814:LYS:HD2	1:B:814:LYS:HA	1.90	0.40
1:A:364:HIS:HA	1:A:367:GLN:NE2	2.36	0.40
1:A:770:LEU:HD13	1:A:770:LEU:HA	1.39	0.40
1:A:896:THR:O	1:A:899:SER:OG	2.33	0.40
1:B:237:LEU:HD21	1:B:249:VAL:HG22	2.04	0.40
1:B:624:GLN:CG	1:B:625:ASP:N	2.84	0.40
1:B:687:PHE:CE1	1:B:746:PHE:CE1	3.08	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	655/691 (95%)	512 (78%)	95 (14%)	48 (7%)		
1	B	633/691 (92%)	514 (81%)	84 (13%)	35 (6%)		
All	All	1288/1382 (93%)	1026 (80%)	179 (14%)	83 (6%)		

All (83) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	GLU
1	A	293	THR
1	A	354	GLU
1	A	356	ASP

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Mol	Chain	Res	Type
1	A	371	HIS
1	A	449	VAL
1	A	453	GLU
1	A	508	LYS
1	A	512	GLN
1	A	588	ASP
1	A	598	SER
1	A	603	PHE
1	A	705	ASN
1	A	706	SER
1	A	709	VAL
1	A	710	ALA
1	A	719	TYR
1	A	720	SER
1	A	788	TYR
1	A	830	PHE
1	B	256	GLU
1	B	293	THR
1	B	355	GLY
1	B	356	ASP
1	B	475	ILE
1	B	499	THR
1	B	500	ARG
1	B	508	LYS
1	B	512	GLN
1	B	588	ASP
1	B	719	TYR
1	B	720	SER
1	B	788	TYR
1	B	830	PHE
1	A	351	ASN
1	A	367	GLN
1	A	445	PHE
1	A	534	GLU
1	A	541	SER
1	A	673	LYS
1	A	704	ASN
1	A	823	ALA
1	B	323	LEU
1	B	354	GLU
1	B	522	ASN
1	B	534	GLU

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Mol	Chain	Res	Type
1	B	598	SER
1	B	599	ASN
1	B	603	PHE
1	A	227	ASP
1	A	353	LEU
1	A	426	ASN
1	A	437	GLN
1	A	560	ALA
1	A	696	HIS
1	A	856	PRO
1	B	437	GLN
1	B	575	MET
1	B	673	LYS
1	B	696	HIS
1	B	810	SER
1	A	255	GLN
1	A	368	HIS
1	A	479	PRO
1	A	707	PHE
1	A	722	GLU
1	B	254	GLN
1	A	315	ASP
1	A	330	MET
1	A	455	TYR
1	A	522	ASN
1	B	351	ASN
1	B	479	PRO
1	B	722	GLU
1	B	856	PRO
1	A	316	VAL
1	B	426	ASN
1	B	528	TRP
1	A	475	ILE
1	B	592	PRO
1	B	903	PRO
1	A	557	VAL
1	A	591	GLN

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	590/614 (96%)	393 (67%)	197 (33%)	0	1
1	B	577/614 (94%)	397 (69%)	180 (31%)	0	1
All	All	1167/1228 (95%)	790 (68%)	377 (32%)	0	1

All (377) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	223	TYR
1	A	225	ASP
1	A	226	ARG
1	A	228	ARG
1	A	230	ILE
1	A	231	LEU
1	A	244	SER
1	A	250	LEU
1	A	252	TYR
1	A	254	GLN
1	A	257	THR
1	A	258	ARG
1	A	261	ARG
1	A	266	LEU
1	A	269	GLU
1	A	270	ASP
1	A	271	ASN
1	A	272	LEU
1	A	273	GLN
1	A	275	SER
1	A	277	LYS
1	A	282	LYS
1	A	287	GLU
1	A	289	SER
1	A	292	LEU
1	A	295	CYS
1	A	296	LEU
1	A	298	GLN
1	A	300	VAL
1	A	304	LYS
1	A	305	SER

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Mol	Chain	Res	Type
1	A	309	LYS
1	A	311	LEU
1	A	313	SER
1	A	317	GLN
1	A	318	GLN
1	A	320	GLN
1	A	321	SER
1	A	323	LEU
1	A	328	GLN
1	A	331	LEU
1	A	340	THR
1	A	356	ASP
1	A	359	THR
1	A	361	GLU
1	A	362	ASP
1	A	363	GLU
1	A	365	VAL
1	A	367	GLN
1	A	373	THR
1	A	374	SER
1	A	375	THR
1	A	377	LEU
1	A	378	THR
1	A	380	THR
1	A	381	LEU
1	A	388	LYS
1	A	390	LYS
1	A	391	CYS
1	A	396	LEU
1	A	397	LEU
1	A	398	GLN
1	A	403	LEU
1	A	407	LEU
1	A	408	ASP
1	A	409	ASP
1	A	410	VAL
1	A	413	LEU
1	A	414	LEU
1	A	415	GLN
1	A	417	ILE
1	A	424	LEU
1	A	426	ASN

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Mol	Chain	Res	Type
1	A	429	ILE
1	A	432	VAL
1	A	435	LEU
1	A	437	GLN
1	A	441	VAL
1	A	443	LYS
1	A	445	PHE
1	A	446	ASP
1	A	450	VAL
1	A	451	ASP
1	A	452	ASP
1	A	453	GLU
1	A	458	ARG
1	A	463	GLN
1	A	471	THR
1	A	472	THR
1	A	476	LEU
1	A	478	ILE
1	A	486	LEU
1	A	498	ARG
1	A	501	ASN
1	A	507	ILE
1	A	508	LYS
1	A	512	GLN
1	A	513	GLU
1	A	515	ILE
1	A	524	ILE
1	A	528	TRP
1	A	530	SER
1	A	532	PHE
1	A	535	ASP
1	A	536	LEU
1	A	551	SER
1	A	553	LEU
1	A	557	VAL
1	A	559	GLU
1	A	563	ARG
1	A	566	LEU
1	A	569	GLU
1	A	572	MET
1	A	575	MET
1	A	576	LYS

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Mol	Chain	Res	Type
1	A	579	ASP
1	A	580	ASP
1	A	582	TYR
1	A	585	LEU
1	A	587	HIS
1	A	590	ILE
1	A	593	VAL
1	A	598	SER
1	A	599	ASN
1	A	600	PHE
1	A	603	PHE
1	A	608	ARG
1	A	610	LEU
1	A	613	ASP
1	A	616	SER
1	A	621	SER
1	A	630	ASN
1	A	631	ASN
1	A	633	LYS
1	A	638	THR
1	A	645	MET
1	A	646	VAL
1	A	647	LYS
1	A	659	MET
1	A	662	PHE
1	A	663	SER
1	A	674	ASN
1	A	675	LEU
1	A	678	THR
1	A	681	LEU
1	A	683	ASP
1	A	695	CYS
1	A	701	ARG
1	A	703	THR
1	A	704	ASN
1	A	706	SER
1	A	708	GLN
1	A	711	SER
1	A	712	LYS
1	A	713	SER
1	A	719	TYR
1	A	721	SER

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Mol	Chain	Res	Type
1	A	722	GLU
1	A	725	VAL
1	A	741	HIS
1	A	748	HIS
1	A	751	ARG
1	A	752	LYS
1	A	756	ARG
1	A	758	LEU
1	A	760	LEU
1	A	766	LEU
1	A	770	LEU
1	A	782	LYS
1	A	785	GLU
1	A	789	ASP
1	A	790	ARG
1	A	793	LYS
1	A	797	ARG
1	A	798	LEU
1	A	810	SER
1	A	814	LYS
1	A	817	LYS
1	A	820	ARG
1	A	821	LYS
1	A	824	GLU
1	A	825	LEU
1	A	832	SER
1	A	833	GLN
1	A	835	ASP
1	A	838	LYS
1	A	852	LYS
1	A	872	LYS
1	A	874	LEU
1	A	875	GLN
1	A	876	ASP
1	A	877	LEU
1	A	885	TYR
1	A	887	ARG
1	A	890	SER
1	A	896	THR
1	A	898	VAL
1	B	224	THR
1	B	225	ASP

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Mol	Chain	Res	Type
1	B	226	ARG
1	B	228	ARG
1	B	230	ILE
1	B	231	LEU
1	B	233	LEU
1	B	243	SER
1	B	244	SER
1	B	250	LEU
1	B	252	TYR
1	B	254	GLN
1	B	257	THR
1	B	258	ARG
1	B	263	CYS
1	B	266	LEU
1	B	268	SER
1	B	269	GLU
1	B	270	ASP
1	B	272	LEU
1	B	273	GLN
1	B	274	LEU
1	B	275	SER
1	B	277	LYS
1	B	282	LYS
1	B	287	GLU
1	B	292	LEU
1	B	296	LEU
1	B	298	GLN
1	B	300	VAL
1	B	304	LYS
1	B	305	SER
1	B	307	GLN
1	B	309	LYS
1	B	311	LEU
1	B	314	GLU
1	B	315	ASP
1	B	317	GLN
1	B	325	CYS
1	B	326	GLU
1	B	328	GLN
1	B	331	LEU
1	B	337	SER
1	B	340	THR

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Mol	Chain	Res	Type
1	B	346	LEU
1	B	352	LYS
1	B	353	LEU
1	B	354	GLU
1	B	356	ASP
1	B	359	THR
1	B	361	GLU
1	B	363	GLU
1	B	365	VAL
1	B	367	GLN
1	B	373	THR
1	B	380	THR
1	B	381	LEU
1	B	383	PHE
1	B	388	LYS
1	B	390	LYS
1	B	394	GLN
1	B	397	LEU
1	B	399	VAL
1	B	401	LYS
1	B	407	LEU
1	B	413	LEU
1	B	414	LEU
1	B	415	GLN
1	B	416	GLU
1	B	424	LEU
1	B	426	ASN
1	B	429	ILE
1	B	432	VAL
1	B	435	LEU
1	B	437	GLN
1	B	455	TYR
1	B	458	ARG
1	B	459	ILE
1	B	463	GLN
1	B	471	THR
1	B	472	THR
1	B	475	ILE
1	B	476	LEU
1	B	478	ILE
1	B	500	ARG
1	B	501	ASN

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Mol	Chain	Res	Type
1	B	512	GLN
1	B	515	ILE
1	B	528	TRP
1	B	532	PHE
1	B	534	GLU
1	B	535	ASP
1	B	536	LEU
1	B	541	SER
1	B	548	ILE
1	B	553	LEU
1	B	555	LYS
1	B	557	VAL
1	B	561	GLN
1	B	565	HIS
1	B	566	LEU
1	B	570	MET
1	B	578	SER
1	B	579	ASP
1	B	580	ASP
1	B	581	GLU
1	B	582	TYR
1	B	585	LEU
1	B	587	HIS
1	B	588	ASP
1	B	590	ILE
1	B	593	VAL
1	B	598	SER
1	B	599	ASN
1	B	608	ARG
1	B	609	SER
1	B	613	ASP
1	B	616	SER
1	B	621	SER
1	B	622	MET
1	B	623	LEU
1	B	624	GLN
1	B	630	ASN
1	B	633	LYS
1	B	638	THR
1	B	645	MET
1	B	646	VAL
1	B	647	LYS

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Mol	Chain	Res	Type
1	B	663	SER
1	B	678	THR
1	B	681	LEU
1	B	683	ASP
1	B	684	ILE
1	B	695	CYS
1	B	703	THR
1	B	704	ASN
1	B	712	LYS
1	B	713	SER
1	B	719	TYR
1	B	721	SER
1	B	722	GLU
1	B	725	VAL
1	B	735	ILE
1	B	741	HIS
1	B	748	HIS
1	B	751	ARG
1	B	752	LYS
1	B	755	GLN
1	B	756	ARG
1	B	766	LEU
1	B	770	LEU
1	B	776	ILE
1	B	778	LYS
1	B	785	GLU
1	B	790	ARG
1	B	793	LYS
1	B	797	ARG
1	B	798	LEU
1	B	799	LEU
1	B	803	LEU
1	B	809	LEU
1	B	817	LYS
1	B	820	ARG
1	B	824	GLU
1	B	833	GLN
1	B	835	ASP
1	B	848	MET
1	B	849	ASP
1	B	850	ARG
1	B	852	LYS

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Mol	Chain	Res	Type
1	B	855	ILE
1	B	872	LYS
1	B	874	LEU
1	B	877	LEU
1	B	887	ARG
1	B	890	SER
1	B	896	THR
1	B	901	LEU
1	B	902	VAL
1	B	904	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	251	GLN
1	A	271	ASN
1	A	273	GLN
1	A	298	GLN
1	A	317	GLN
1	A	367	GLN
1	A	371	HIS
1	A	398	GLN
1	A	463	GLN
1	A	484	HIS
1	A	511	ASN
1	A	574	HIS
1	A	591	GLN
1	A	624	GLN
1	A	630	ASN
1	A	656	HIS
1	A	666	HIS
1	A	674	ASN
1	A	700	HIS
1	A	704	ASN
1	A	730	HIS
1	A	748	HIS
1	A	755	GLN
1	A	781	GLN
1	A	859	GLN
1	A	875	GLN
1	A	894	HIS
1	A	900	HIS

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Mol	Chain	Res	Type
1	B	232	GLN
1	B	271	ASN
1	B	273	GLN
1	B	298	GLN
1	B	318	GLN
1	B	320	GLN
1	B	328	GLN
1	B	371	HIS
1	B	398	GLN
1	B	406	HIS
1	B	437	GLN
1	B	463	GLN
1	B	511	ASN
1	B	561	GLN
1	B	565	HIS
1	B	591	GLN
1	B	599	ASN
1	B	630	ASN
1	B	656	HIS
1	B	700	HIS
1	B	730	HIS
1	B	748	HIS
1	B	755	GLN
1	B	781	GLN
1	B	859	GLN
1	B	875	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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	661/691 (95%)	-0.36	7 (1%) 80 55	43, 79, 109, 128	0
1	B	643/691 (93%)	-0.38	7 (1%) 80 55	46, 74, 107, 125	0
All	All	1304/1382 (94%)	-0.37	14 (1%) 80 55	43, 76, 108, 128	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	588	ASP	5.1
1	A	452	ASP	4.6
1	B	588	ASP	3.4
1	A	356	ASP	3.4
1	A	708	GLN	3.0
1	A	709	VAL	2.9
1	B	849	ASP	2.7
1	B	850	ARG	2.6
1	A	451	ASP	2.4
1	B	315	ASP	2.3
1	B	498	ARG	2.3
1	A	449	VAL	2.3
1	B	285	GLY	2.3
1	B	704	ASN	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	A	905	1/1	0.86	0.89	58,58,58,58	0
3	MG	B	905	1/1	0.89	0.77	44,44,44,44	0
2	ZN	B	2	1/1	0.98	0.16	67,67,67,67	0
2	ZN	A	1	1/1	0.99	0.18	73,73,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.