



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:16 pm BST

PDB ID : 6IEH
Title : Crystal structures of the hMTR4-NRDE2 complex
Authors : Chen, J.Y.; Yun, C.H.
Deposited on : 2018-09-14
Resolution : 2.89 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
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

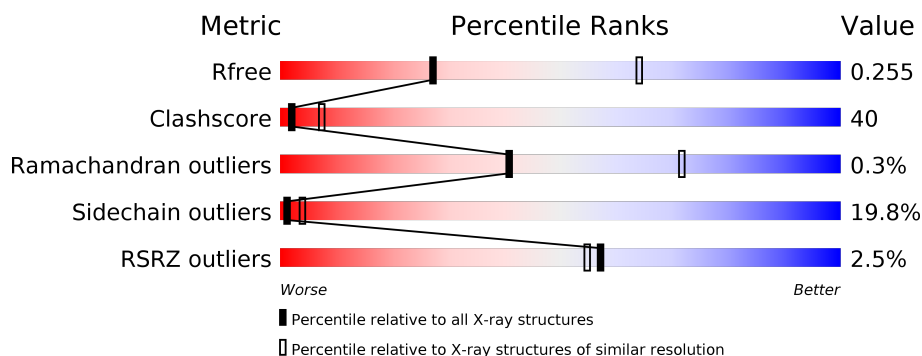
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	B	979	<div> <div>2%</div> <div> <div></div> <div>52%</div> <div>32%</div> <div>10%</div> <div>• 5%</div> </div> </div>
2	A	105	<div> <div>6%</div> <div> <div></div> <div>34%</div> <div>30%</div> <div>15%</div> <div>• 19%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ATP	B	1102	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7647 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 Exosome RNA helicase MTR4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	929	Total	C	N	O	S	0	0	0
			6907	4405	1169	1284	49			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	64	GLY	-	expression tag	UNP P42285
B	65	ALA	-	expression tag	UNP P42285
B	66	MET	-	expression tag	UNP P42285
B	67	ASP	-	expression tag	UNP P42285
B	68	PRO	-	expression tag	UNP P42285
B	69	GLU	-	expression tag	UNP P42285
B	70	PHE	-	expression tag	UNP P42285

- Molecule 2 is a protein called Protein NRDE2 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	85	Total	C	N	O	S	0	0	0
			676	432	117	124	3			

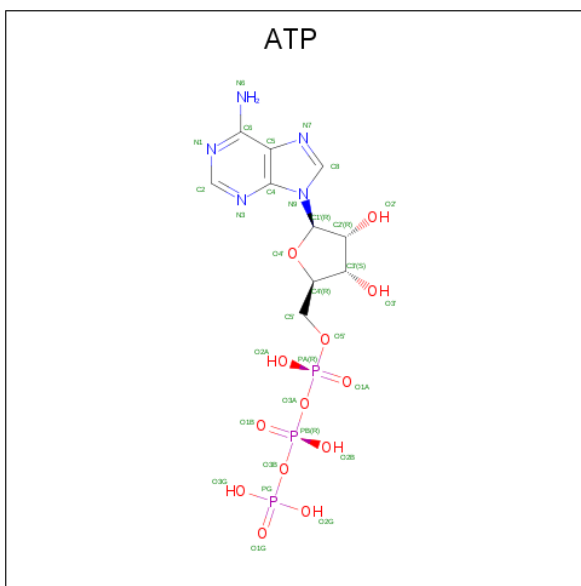
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	162	SER	-	expression tag	UNP Q9H7Z3

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:

$$\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3).$$


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

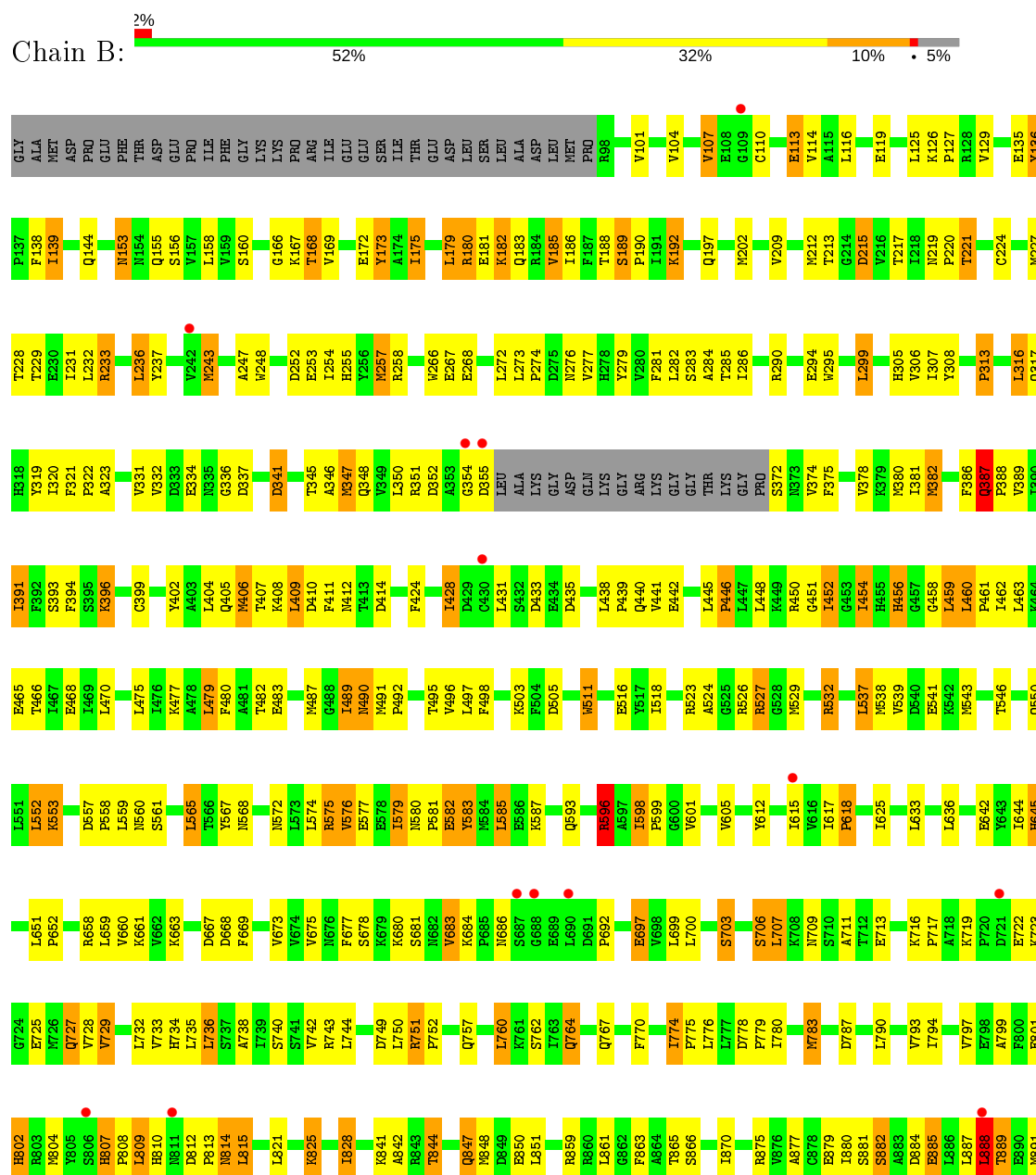
- Molecule 5 is water.

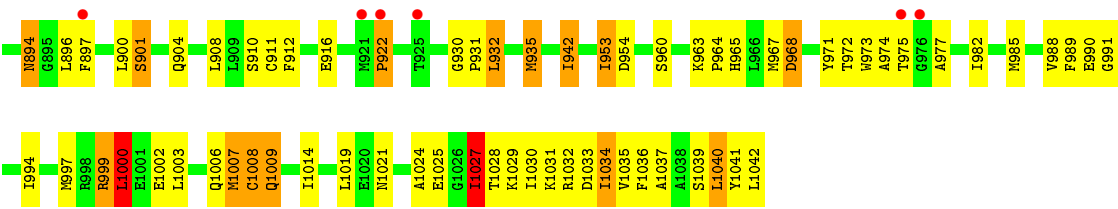
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	27	Total O 27 27	0	0
5	A	5	Total O 5 5	0	0

3 Residue-property plots

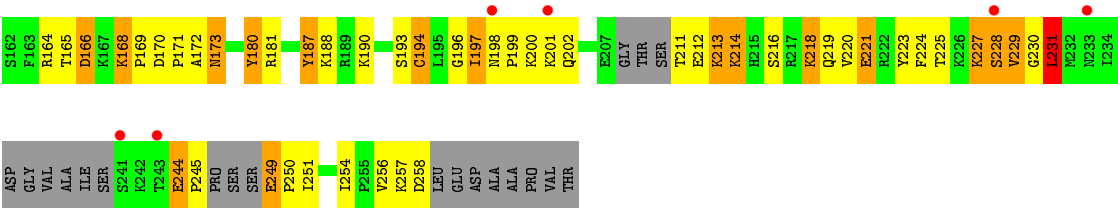
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Exosome RNA helicase MTR4





● Molecule 2: Protein NRDE2 homolog



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	148.31Å 113.73Å 80.72Å 90.00° 96.49° 90.00°	Depositor
Resolution (Å)	40.10 – 2.89 40.10 – 2.89	Depositor EDS
% Data completeness (in resolution range)	98.4 (40.10-2.89) 98.5 (40.10-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.90Å)	Xtriage
Refinement program	PHENIX (1.13 _2998: ???)	Depositor
R, R_{free}	0.235 , 0.252 0.236 , 0.255	Depositor DCC
R_{free} test set	1496 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	52.4	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7647	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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

5.1 Standard geometry

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

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	B	1.74	25/7039 (0.4%)	1.09	25/9575 (0.3%)
2	A	1.56	2/690 (0.3%)	1.18	3/922 (0.3%)
All	All	1.73	27/7729 (0.3%)	1.10	28/10497 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	187	TYR	CE1-CZ	-6.96	1.29	1.38
1	B	308	TYR	CE1-CZ	-6.95	1.29	1.38
1	B	582	GLU	CD-OE1	-6.83	1.18	1.25
1	B	567	TYR	CE1-CZ	-6.74	1.29	1.38
1	B	402	TYR	CE1-CZ	-6.44	1.30	1.38
1	B	113	GLU	CD-OE1	-6.41	1.18	1.25
1	B	172	GLU	CD-OE1	-6.33	1.18	1.25
2	A	194	CYS	CB-SG	-6.20	1.71	1.82
1	B	279	TYR	CE1-CZ	-6.05	1.30	1.38
1	B	172	GLU	CD-OE2	-5.97	1.19	1.25
1	B	295	TRP	CD2-CE2	-5.90	1.34	1.41
1	B	319	TYR	CE1-CZ	-5.88	1.30	1.38
1	B	516	GLU	CD-OE2	-5.88	1.19	1.25
1	B	173	TYR	CE1-CZ	-5.75	1.31	1.38
1	B	850	GLU	CD-OE1	-5.67	1.19	1.25
1	B	511	TRP	CE3-CZ3	-5.63	1.28	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	697	GLU	CD-OE2	-5.48	1.19	1.25
1	B	248	TRP	CG-CD1	-5.41	1.29	1.36
1	B	136	TYR	CE1-CZ	-5.41	1.31	1.38
1	B	722	GLU	CD-OE2	-5.38	1.19	1.25
1	B	319	TYR	CG-CD1	-5.36	1.32	1.39
1	B	583	TYR	CE1-CZ	-5.27	1.31	1.38
1	B	402	TYR	CG-CD1	-5.25	1.32	1.39
1	B	516	GLU	CD-OE1	-5.10	1.20	1.25
1	B	248	TRP	CD2-CE2	-5.05	1.35	1.41
1	B	295	TRP	CG-CD1	-5.04	1.29	1.36
1	B	224	CYS	CB-SG	-5.01	1.73	1.81

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	579	ILE	CG1-CB-CG2	-7.15	95.66	111.40
1	B	1037	ALA	N-CA-C	6.92	129.69	111.00
1	B	707	LEU	CB-CG-CD1	-6.85	99.36	111.00
1	B	888	LEU	CB-CG-CD2	6.76	122.50	111.00
1	B	505	ASP	CB-CA-C	-6.69	97.02	110.40
2	A	198	ASN	C-N-CD	6.57	142.19	128.40
1	B	552	LEU	CA-CB-CG	6.32	129.82	115.30
1	B	316	LEU	CA-CB-CG	6.13	129.40	115.30
1	B	954	ASP	CB-CA-C	6.11	122.61	110.40
1	B	667	ASP	CB-CA-C	6.08	122.56	110.40
1	B	1040	LEU	N-CA-C	-5.97	94.88	111.00
2	A	231	LEU	N-CA-C	5.83	126.75	111.00
1	B	387	GLN	C-N-CD	5.81	140.60	128.40
1	B	175	ILE	CB-CA-C	-5.76	100.07	111.60
1	B	529	MET	N-CA-C	5.73	126.47	111.00
2	A	229	VAL	CB-CA-C	-5.71	100.54	111.40
1	B	577	GLU	N-CA-C	5.65	126.26	111.00
1	B	596	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	306	VAL	CB-CA-C	-5.56	100.83	111.40
1	B	667	ASP	N-CA-CB	5.51	120.52	110.60
1	B	299	LEU	CB-CG-CD2	-5.46	101.72	111.00
1	B	1027	ILE	CG1-CB-CG2	-5.46	99.40	111.40
1	B	683	VAL	N-CA-CB	-5.45	99.52	111.50
1	B	1034	ILE	CB-CA-C	-5.42	100.75	111.60
1	B	107	VAL	N-CA-C	5.41	125.61	111.00
1	B	807	HIS	C-N-CD	-5.14	109.30	120.60
1	B	703	SER	CB-CA-C	-5.13	100.36	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1000	LEU	CA-CB-CG	-5.10	103.57	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	684	LYS	Peptide

5.2 Too-close contacts [i](#)

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	B	6907	0	6547	555	0
2	A	676	0	661	94	0
3	B	1	0	0	0	0
4	B	31	0	12	10	0
5	A	5	0	0	1	0
5	B	27	0	0	8	0
All	All	7647	0	7220	599	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 40.

All (599) 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:B:686:ASN:CB	1:B:960:SER:CB	1.75	1.56
1:B:313:PRO:CB	1:B:527:ARG:NH1	1.72	1.53
1:B:686:ASN:CB	1:B:960:SER:HB3	1.07	1.49
1:B:313:PRO:CG	1:B:527:ARG:NH1	1.77	1.45
1:B:465:GLU:OE2	1:B:1040:LEU:CB	1.65	1.42
1:B:396:LYS:HG2	1:B:456:HIS:CE1	1.53	1.42
1:B:396:LYS:CG	1:B:456:HIS:ND1	1.83	1.40
1:B:615:ILE:HD11	1:B:825:LYS:CG	1.53	1.38
1:B:884:ASP:O	1:B:888:LEU:CD2	1.76	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:896:LEU:O	1:B:900:LEU:CD2	1.76	1.32
1:B:713:GLU:OE2	2:A:200:LYS:HE3	1.18	1.32
1:B:968:ASP:HB3	5:B:1221:HOH:O	1.19	1.28
1:B:168:THR:CG2	4:B:1102:ATP:O2A	1.80	1.27
1:B:468:GLU:O	1:B:491:MET:HE1	1.28	1.25
1:B:615:ILE:CD1	1:B:825:LYS:CG	2.16	1.22
1:B:897:PHE:CA	1:B:900:LEU:HD23	1.69	1.22
1:B:396:LYS:HG2	1:B:456:HIS:ND1	0.88	1.20
2:A:170:ASP:HB2	2:A:181:ARG:NH1	1.57	1.20
1:B:888:LEU:HD22	1:B:912:PHE:CE2	1.75	1.20
1:B:884:ASP:O	1:B:888:LEU:HD23	1.27	1.19
1:B:468:GLU:O	1:B:491:MET:CE	1.90	1.19
1:B:347:MET:HE2	1:B:543:MET:H	1.04	1.17
1:B:880:ILE:HD13	1:B:888:LEU:HD12	1.21	1.16
1:B:168:THR:HB	4:B:1102:ATP:O2A	1.46	1.15
1:B:375:PHE:HZ	1:B:409:LEU:HD21	1.05	1.15
1:B:880:ILE:HG21	1:B:888:LEU:HD11	1.28	1.15
1:B:615:ILE:CD1	1:B:825:LYS:HG2	1.75	1.14
1:B:168:THR:CB	4:B:1102:ATP:O2A	1.97	1.12
1:B:431:LEU:HD11	1:B:1034:ILE:CG2	1.80	1.11
1:B:375:PHE:CZ	1:B:409:LEU:HD21	1.85	1.11
2:A:244:GLU:HG2	2:A:245:PRO:HD2	1.31	1.10
2:A:249:GLU:HB3	2:A:250:PRO:HD2	1.22	1.10
1:B:233:ARG:NH2	1:B:568:ASN:OD1	1.83	1.09
1:B:897:PHE:HA	1:B:900:LEU:CD2	1.80	1.09
1:B:431:LEU:CD1	1:B:1034:ILE:HG22	1.82	1.09
1:B:896:LEU:O	1:B:900:LEU:HD21	0.92	1.09
1:B:313:PRO:HG2	1:B:527:ARG:NH1	1.62	1.07
1:B:192:LYS:HE3	1:B:213:THR:HG21	1.33	1.07
1:B:896:LEU:C	1:B:900:LEU:HD21	1.75	1.05
1:B:615:ILE:CD1	1:B:825:LYS:HG3	1.80	1.05
1:B:612:TYR:CE1	1:B:825:LYS:HD3	1.89	1.05
1:B:313:PRO:HB3	1:B:527:ARG:NH1	1.44	1.05
1:B:880:ILE:HG21	1:B:888:LEU:CD1	1.87	1.04
1:B:396:LYS:CG	1:B:456:HIS:CE1	2.31	1.04
1:B:168:THR:HG22	4:B:1102:ATP:O2A	1.51	1.04
2:A:244:GLU:HG2	2:A:245:PRO:CD	1.89	1.02
1:B:236:LEU:HB3	1:B:272:LEU:HD13	1.39	1.02
1:B:713:GLU:OE2	2:A:200:LYS:CE	2.08	1.02
1:B:968:ASP:CB	5:B:1221:HOH:O	1.85	1.02
1:B:897:PHE:HA	1:B:900:LEU:HD23	1.02	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:THR:HG21	5:B:1202:HOH:O	1.61	1.01
1:B:884:ASP:C	1:B:888:LEU:HD21	1.80	1.01
1:B:139:ILE:H	1:B:139:ILE:HD12	1.24	0.99
1:B:997:MET:HE1	1:B:1030:ILE:HG23	1.46	0.98
1:B:387:GLN:HB3	1:B:388:PRO:CD	1.94	0.97
1:B:884:ASP:O	1:B:888:LEU:HD21	1.60	0.97
1:B:406:MET:HB3	1:B:452:ILE:CD1	1.95	0.97
1:B:686:ASN:CB	1:B:960:SER:HB2	1.91	0.96
1:B:460:LEU:H	1:B:460:LEU:HD22	1.28	0.96
1:B:749:ASP:OD1	1:B:751:ARG:HG3	1.63	0.96
2:A:249:GLU:CB	2:A:250:PRO:HD2	1.94	0.94
1:B:977:ALA:O	1:B:1032:ARG:NH1	2.00	0.94
1:B:431:LEU:HD11	1:B:1034:ILE:HG22	0.95	0.93
1:B:897:PHE:C	1:B:900:LEU:HD23	1.88	0.93
1:B:347:MET:HE2	1:B:543:MET:N	1.83	0.93
1:B:258:ARG:NH1	1:B:557:ASP:O	2.02	0.93
1:B:450:ARG:NH1	1:B:450:ARG:HB2	1.84	0.93
1:B:686:ASN:CB	1:B:960:SER:CA	2.48	0.92
1:B:770:PHE:CD2	1:B:775:PRO:HD3	2.04	0.92
1:B:498:PHE:O	1:B:538:MET:HG3	1.70	0.92
1:B:598:ILE:CD1	1:B:842:ALA:HB1	2.00	0.90
1:B:897:PHE:CA	1:B:900:LEU:CD2	2.44	0.89
1:B:598:ILE:HD13	1:B:842:ALA:HB1	1.53	0.89
2:A:170:ASP:HB2	2:A:181:ARG:HH12	1.27	0.89
1:B:841:LYS:O	1:B:844:THR:HG23	1.71	0.88
1:B:888:LEU:CD2	1:B:912:PHE:CE2	2.57	0.88
1:B:490:ASN:O	1:B:490:ASN:ND2	2.07	0.87
1:B:254:ILE:HG22	1:B:283:SER:HB2	1.57	0.87
1:B:253:GLU:OE1	5:B:1201:HOH:O	1.91	0.87
1:B:751:ARG:HG3	1:B:751:ARG:HH11	1.39	0.87
2:A:231:LEU:H	2:A:231:LEU:HD23	1.39	0.86
2:A:213:LYS:HA	2:A:213:LYS:HE3	1.58	0.86
1:B:894:ASN:ND2	1:B:894:ASN:O	2.07	0.86
1:B:997:MET:CE	1:B:1030:ILE:HG23	2.07	0.85
1:B:465:GLU:OE2	1:B:1040:LEU:CA	2.25	0.85
2:A:164:ARG:HD2	5:A:302:HOH:O	1.75	0.85
1:B:700:LEU:HD12	1:B:729:VAL:CG1	2.07	0.84
1:B:442:GLU:OE1	2:A:221:GLU:OE1	1.94	0.84
1:B:254:ILE:CG2	1:B:283:SER:HB2	2.06	0.84
1:B:192:LYS:CE	1:B:213:THR:HG21	2.08	0.83
1:B:880:ILE:CG2	1:B:888:LEU:HD11	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:GLU:C	1:B:491:MET:HE1	1.97	0.83
2:A:172:ALA:HB1	2:A:180:TYR:CD2	2.13	0.83
1:B:888:LEU:HD22	1:B:912:PHE:HE2	1.44	0.83
1:B:388:PRO:HG3	1:B:526:ARG:HH12	1.44	0.82
1:B:615:ILE:HD11	1:B:825:LYS:HG2	0.84	0.82
1:B:582:GLU:HG3	1:B:848:MET:HE2	1.61	0.82
1:B:972:THR:HG21	1:B:985:MET:HE1	1.61	0.82
1:B:743:ARG:HG3	2:A:166:ASP:HB3	1.61	0.82
1:B:313:PRO:HG3	1:B:527:ARG:NH1	1.95	0.82
1:B:633:LEU:CD1	1:B:804:MET:CE	2.58	0.82
1:B:321:PHE:HE2	1:B:372:SER:HB2	1.45	0.82
1:B:388:PRO:HG3	1:B:526:ARG:NH1	1.94	0.81
1:B:727:GLN:HE22	2:A:190:LYS:HD3	1.46	0.81
1:B:336:GLY:O	1:B:553:LYS:HD3	1.79	0.81
1:B:633:LEU:CD1	1:B:804:MET:HE1	2.11	0.81
1:B:511:TRP:CZ3	1:B:543:MET:CE	2.63	0.81
1:B:458:GLY:O	1:B:991:GLY:N	2.13	0.81
1:B:404:LEU:CD2	2:A:224:PHE:CZ	2.63	0.81
1:B:735:LEU:HD11	2:A:196:GLY:HA2	1.62	0.81
1:B:703:SER:HB2	1:B:706:SER:HB2	1.61	0.81
1:B:460:LEU:H	1:B:460:LEU:CD2	1.94	0.80
1:B:815:LEU:O	1:B:815:LEU:HD22	1.81	0.80
1:B:237:TYR:OH	1:B:268:GLU:OE1	2.00	0.79
1:B:243:MET:HA	1:B:243:MET:HE2	1.65	0.79
1:B:125:LEU:HG	1:B:153:ASN:OD1	1.82	0.79
1:B:431:LEU:CD1	1:B:1034:ILE:CG2	2.52	0.79
1:B:735:LEU:HD11	2:A:196:GLY:CA	2.14	0.78
1:B:779:PRO:HA	1:B:783:MET:HG3	1.66	0.77
1:B:101:VAL:HG11	1:B:290:ARG:HD2	1.65	0.77
1:B:267:GLU:OE1	1:B:561:SER:HB2	1.84	0.77
1:B:406:MET:HB3	1:B:452:ILE:HD11	1.63	0.77
1:B:598:ILE:HD11	1:B:842:ALA:CB	2.15	0.77
1:B:884:ASP:C	1:B:888:LEU:CD2	2.45	0.76
2:A:231:LEU:HD23	2:A:231:LEU:N	2.00	0.76
1:B:897:PHE:C	1:B:900:LEU:CD2	2.54	0.76
1:B:351:ARG:O	1:B:352:ASP:HB2	1.85	0.76
1:B:404:LEU:CD2	2:A:224:PHE:HZ	1.98	0.76
1:B:582:GLU:CG	1:B:848:MET:HE2	2.14	0.75
1:B:953:ILE:HD12	1:B:953:ILE:N	2.02	0.75
1:B:633:LEU:HD11	1:B:804:MET:HE3	1.69	0.75
1:B:598:ILE:HD11	1:B:842:ALA:HA	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:751:ARG:HG3	1:B:751:ARG:NH1	2.00	0.75
1:B:880:ILE:HD13	1:B:888:LEU:CD1	2.11	0.75
1:B:711:ALA:O	2:A:190:LYS:HE3	1.86	0.75
1:B:644:ILE:HD11	1:B:779:PRO:HG3	1.67	0.74
1:B:456:HIS:HB2	1:B:482:THR:HB	1.68	0.74
1:B:598:ILE:HD11	1:B:842:ALA:CA	2.17	0.74
1:B:700:LEU:HD12	1:B:729:VAL:HG11	1.69	0.74
1:B:633:LEU:HD11	1:B:804:MET:CE	2.18	0.74
1:B:673:VAL:HG12	1:B:699:LEU:HB3	1.70	0.74
1:B:651:LEU:N	1:B:652:PRO:HD2	2.02	0.74
1:B:659:LEU:HD12	1:B:742:VAL:HB	1.68	0.74
2:A:249:GLU:HB3	2:A:250:PRO:CD	2.11	0.73
1:B:953:ILE:HD12	1:B:953:ILE:H	1.53	0.73
1:B:870:ILE:HG23	1:B:875:ARG:NH1	2.04	0.73
1:B:381:ILE:HG23	1:B:386:PHE:HB2	1.71	0.72
1:B:598:ILE:CD1	1:B:842:ALA:CB	2.68	0.72
1:B:888:LEU:HD22	1:B:912:PHE:CD2	2.21	0.72
1:B:482:THR:CG2	5:B:1202:HOH:O	2.29	0.72
1:B:511:TRP:CZ3	1:B:543:MET:HE2	2.24	0.72
1:B:236:LEU:CB	1:B:272:LEU:HD13	2.19	0.71
1:B:572:ASN:O	1:B:576:VAL:HG13	1.90	0.71
1:B:511:TRP:CZ3	1:B:543:MET:HE3	2.24	0.71
1:B:596:ARG:HH11	1:B:596:ARG:CG	2.04	0.71
1:B:406:MET:HB3	1:B:452:ILE:HD13	1.73	0.71
1:B:460:LEU:N	1:B:460:LEU:HD22	2.05	0.71
1:B:482:THR:CB	5:B:1202:HOH:O	2.35	0.71
1:B:144:GLN:NE2	1:B:169:VAL:HG13	2.05	0.71
1:B:294:GLU:OE2	1:B:596:ARG:NH2	2.24	0.70
1:B:565:LEU:HD22	1:B:847:GLN:HE21	1.56	0.70
1:B:882:SER:OG	1:B:1006:GLN:HG3	1.90	0.70
1:B:972:THR:HG21	1:B:985:MET:CE	2.20	0.70
1:B:465:GLU:OE2	1:B:1040:LEU:N	2.24	0.70
1:B:749:ASP:CG	1:B:751:ARG:NH1	2.44	0.70
1:B:974:ALA:O	1:B:1029:LYS:HB3	1.92	0.69
1:B:468:GLU:HB3	1:B:491:MET:HE3	1.72	0.69
2:A:173:ASN:N	2:A:173:ASN:OD1	2.22	0.69
1:B:334:GLU:OE2	1:B:532:ARG:HG2	1.92	0.69
1:B:881:SER:H	1:B:1006:GLN:HE21	1.39	0.69
1:B:243:MET:HG3	1:B:243:MET:O	1.90	0.69
1:B:456:HIS:CB	1:B:482:THR:HB	2.22	0.69
1:B:888:LEU:CD2	1:B:912:PHE:HE2	1.99	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:900:LEU:H	1:B:900:LEU:HD22	1.56	0.69
2:A:170:ASP:CB	2:A:181:ARG:NH1	2.48	0.69
1:B:404:LEU:HD21	2:A:224:PHE:HZ	1.58	0.69
1:B:411:PHE:HB3	1:B:477:LYS:HD2	1.74	0.69
1:B:456:HIS:HB2	5:B:1202:HOH:O	1.93	0.68
1:B:144:GLN:HE22	1:B:169:VAL:CG1	2.05	0.68
1:B:751:ARG:HH11	1:B:751:ARG:CG	2.06	0.68
1:B:387:GLN:HB3	1:B:388:PRO:HD3	1.76	0.68
1:B:465:GLU:CD	1:B:1040:LEU:N	2.47	0.68
1:B:144:GLN:NE2	1:B:166:GLY:O	2.27	0.68
1:B:770:PHE:HD2	1:B:775:PRO:HD3	1.59	0.68
1:B:1024:ALA:O	1:B:1027:ILE:HD11	1.94	0.68
1:B:511:TRP:CE3	1:B:543:MET:HE2	2.29	0.68
1:B:859:ARG:HE	1:B:866:SER:HA	1.60	0.67
1:B:347:MET:CE	1:B:543:MET:H	1.95	0.67
1:B:888:LEU:HB3	1:B:912:PHE:HE2	1.58	0.67
1:B:749:ASP:OD1	1:B:751:ARG:CG	2.42	0.67
2:A:213:LYS:HA	2:A:213:LYS:CE	2.25	0.67
1:B:334:GLU:OE2	1:B:532:ARG:CG	2.43	0.67
1:B:891:MET:HE3	1:B:935:MET:HB2	1.76	0.67
1:B:636:LEU:HD22	1:B:793:VAL:HG13	1.77	0.67
1:B:215:ASP:OD1	1:B:215:ASP:N	2.23	0.66
1:B:445:LEU:O	1:B:445:LEU:HD12	1.95	0.66
1:B:774:ILE:HD12	1:B:774:ILE:C	2.15	0.66
1:B:582:GLU:HG3	1:B:851:LEU:CD2	2.26	0.66
1:B:252:ASP:OD1	1:B:282:LEU:HD12	1.95	0.66
1:B:749:ASP:OD1	1:B:751:ARG:NH1	2.29	0.66
1:B:399:CYS:SG	1:B:480:PHE:O	2.53	0.66
1:B:797:VAL:O	1:B:801:GLU:HG3	1.96	0.66
2:A:172:ALA:HB1	2:A:180:TYR:HD2	1.60	0.66
2:A:244:GLU:CG	2:A:245:PRO:CD	2.71	0.66
1:B:188:THR:HA	1:B:227:MET:O	1.96	0.65
1:B:749:ASP:OD2	1:B:751:ARG:NH1	2.29	0.65
1:B:615:ILE:HD13	1:B:825:LYS:HG3	1.76	0.65
1:B:971:TYR:O	1:B:975:THR:HG23	1.95	0.65
1:B:973:TRP:O	1:B:1032:ARG:NH2	2.29	0.65
1:B:815:LEU:HD22	1:B:815:LEU:C	2.16	0.65
1:B:221:THR:O	1:B:221:THR:OG1	2.13	0.65
1:B:617:ILE:H	1:B:618:PRO:HD3	1.62	0.65
1:B:440:GLN:NE2	2:A:216:SER:OG	2.30	0.65
1:B:532:ARG:NH2	2:A:249:GLU:HA	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:GLN:NE2	1:B:169:VAL:CG1	2.61	0.64
1:B:968:ASP:N	1:B:968:ASP:OD1	2.29	0.64
1:B:139:ILE:H	1:B:139:ILE:CD1	2.00	0.64
1:B:382:MET:HE3	1:B:382:MET:HA	1.78	0.64
1:B:448:LEU:HD23	1:B:470:LEU:CD1	2.28	0.64
1:B:404:LEU:CD2	2:A:224:PHE:CE1	2.81	0.64
1:B:138:PHE:CD1	4:B:1102:ATP:C6	2.86	0.64
1:B:468:GLU:CA	1:B:491:MET:HE1	2.28	0.64
1:B:615:ILE:HD13	1:B:825:LYS:CG	2.22	0.64
1:B:237:TYR:O	1:B:575:ARG:NH2	2.25	0.63
1:B:932:LEU:HD22	1:B:932:LEU:O	1.97	0.63
1:B:406:MET:CB	1:B:452:ILE:CD1	2.75	0.63
1:B:450:ARG:CZ	1:B:450:ARG:HB2	2.27	0.63
1:B:686:ASN:CB	1:B:960:SER:HA	2.26	0.63
1:B:1025:GLU:OE2	1:B:1025:GLU:HA	1.97	0.63
1:B:615:ILE:C	1:B:615:ILE:HD12	2.18	0.63
1:B:633:LEU:HD12	1:B:804:MET:HE1	1.79	0.63
1:B:809:LEU:O	1:B:809:LEU:HD22	1.99	0.63
1:B:744:LEU:HD12	1:B:762:SER:HB3	1.81	0.63
1:B:450:ARG:HH11	1:B:450:ARG:HB2	1.59	0.63
1:B:233:ARG:HH11	1:B:268:GLU:CD	2.03	0.62
1:B:617:ILE:N	1:B:618:PRO:HD3	2.14	0.62
1:B:465:GLU:CD	1:B:1040:LEU:CB	2.63	0.62
1:B:732:LEU:HD23	1:B:734:HIS:HE1	1.65	0.62
1:B:274:PRO:HD2	1:B:277:VAL:HG21	1.82	0.62
1:B:387:GLN:NE2	1:B:387:GLN:HA	2.15	0.62
1:B:313:PRO:HB2	1:B:527:ARG:NH1	2.03	0.61
1:B:891:MET:CE	1:B:935:MET:HB2	2.29	0.61
2:A:170:ASP:HB2	2:A:181:ARG:HH11	1.63	0.61
1:B:888:LEU:HB3	1:B:912:PHE:CE2	2.35	0.61
1:B:460:LEU:CD1	1:B:990:GLU:HB2	2.30	0.61
1:B:1014:ILE:C	1:B:1014:ILE:HD12	2.20	0.61
1:B:375:PHE:HE2	1:B:405:GLN:O	1.84	0.61
1:B:460:LEU:HD13	1:B:990:GLU:HB2	1.81	0.61
1:B:675:VAL:HG11	2:A:187:TYR:CD2	2.36	0.61
1:B:404:LEU:HD21	2:A:224:PHE:CZ	2.32	0.61
1:B:645:HIS:CE1	1:B:734:HIS:O	2.53	0.61
1:B:532:ARG:NH2	2:A:249:GLU:N	2.48	0.61
1:B:1003:LEU:O	1:B:1003:LEU:HD12	1.99	0.61
1:B:404:LEU:HD22	2:A:224:PHE:CE1	2.35	0.61
1:B:727:GLN:HE22	2:A:190:LYS:HB2	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1009:GLN:HE21	1:B:1009:GLN:CA	2.14	0.60
1:B:930:GLY:N	1:B:931:PRO:CD	2.64	0.60
2:A:256:VAL:HG13	2:A:256:VAL:O	2.00	0.60
1:B:233:ARG:NH1	1:B:268:GLU:OE2	2.32	0.60
1:B:396:LYS:CD	1:B:456:HIS:CE1	2.84	0.60
1:B:744:LEU:N	1:B:744:LEU:HD23	2.16	0.60
1:B:372:SER:O	1:B:372:SER:OG	2.14	0.60
1:B:374:VAL:O	1:B:378:VAL:HG23	2.01	0.60
1:B:446:PRO:O	1:B:450:ARG:NH1	2.34	0.60
1:B:1009:GLN:NE2	1:B:1009:GLN:HA	2.16	0.60
1:B:912:PHE:HE1	1:B:935:MET:HE1	1.65	0.60
1:B:633:LEU:HD12	1:B:804:MET:CE	2.30	0.60
2:A:219:GLN:O	2:A:223:TYR:CE2	2.55	0.59
1:B:144:GLN:HE22	1:B:169:VAL:HG13	1.65	0.59
1:B:532:ARG:HH22	2:A:249:GLU:N	2.00	0.59
1:B:651:LEU:N	1:B:652:PRO:CD	2.66	0.59
1:B:812:ASP:CB	1:B:813:PRO:HD2	2.32	0.59
1:B:880:ILE:HG21	1:B:888:LEU:HD12	1.80	0.59
1:B:601:VAL:O	1:B:605:VAL:HG23	2.03	0.59
1:B:617:ILE:N	1:B:618:PRO:CD	2.66	0.59
1:B:465:GLU:CD	1:B:1040:LEU:CA	2.71	0.59
1:B:582:GLU:HG3	1:B:851:LEU:HD21	1.84	0.59
1:B:888:LEU:CB	1:B:912:PHE:HE2	2.15	0.59
1:B:661:LYS:HB2	1:B:738:ALA:HB3	1.85	0.58
1:B:900:LEU:N	1:B:900:LEU:HD22	2.17	0.58
2:A:219:GLN:O	2:A:223:TYR:CD2	2.56	0.58
1:B:964:PRO:HA	1:B:967:MET:HG3	1.83	0.58
1:B:450:ARG:HE	2:A:227:LYS:HZ2	1.50	0.58
1:B:347:MET:HE3	1:B:350:LEU:HD12	1.85	0.58
1:B:470:LEU:CD2	1:B:475:LEU:HD12	2.34	0.58
1:B:483:GLU:O	1:B:483:GLU:HG2	2.03	0.57
2:A:199:PRO:HB2	2:A:201:LYS:HE3	1.86	0.57
2:A:213:LYS:HG3	2:A:213:LYS:O	2.05	0.57
1:B:492:PRO:HB2	1:B:526:ARG:HG2	1.87	0.57
1:B:888:LEU:CG	1:B:912:PHE:HE2	2.18	0.57
1:B:1000:LEU:O	1:B:1000:LEU:HD23	2.05	0.57
1:B:139:ILE:HD12	1:B:139:ILE:N	2.07	0.56
1:B:396:LYS:CB	1:B:456:HIS:CE1	2.89	0.56
1:B:888:LEU:HB2	1:B:1007:MET:HE3	1.86	0.56
1:B:407:THR:O	1:B:407:THR:HG22	2.05	0.56
1:B:877:ALA:HB2	1:B:889:THR:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:GLU:C	1:B:491:MET:CE	2.64	0.56
1:B:381:ILE:HG23	1:B:386:PHE:CB	2.35	0.56
1:B:257:MET:HB3	1:B:559:LEU:HD11	1.87	0.56
1:B:410:ASP:O	2:A:230:GLY:HA2	2.06	0.56
2:A:244:GLU:HG2	2:A:245:PRO:HD3	1.82	0.56
1:B:539:VAL:HG12	1:B:539:VAL:O	2.06	0.56
1:B:243:MET:CE	1:B:243:MET:HA	2.34	0.55
2:A:244:GLU:CG	2:A:245:PRO:HD2	2.20	0.55
1:B:615:ILE:O	1:B:615:ILE:HD12	2.07	0.55
1:B:1031:LYS:O	1:B:1031:LYS:HG2	2.06	0.55
1:B:908:LEU:HD22	1:B:931:PRO:HB3	1.88	0.55
1:B:190:PRO:HG3	1:B:266:TRP:CZ2	2.41	0.55
1:B:770:PHE:CE2	1:B:775:PRO:HD3	2.40	0.55
2:A:213:LYS:CA	2:A:213:LYS:CE	2.85	0.55
1:B:404:LEU:HD22	2:A:224:PHE:HE1	1.70	0.55
1:B:323:ALA:HA	1:B:372:SER:CB	2.36	0.55
1:B:408:LYS:O	2:A:228:SER:CB	2.55	0.55
1:B:387:GLN:HB3	1:B:388:PRO:HD2	1.87	0.55
1:B:341:ASP:N	1:B:341:ASP:OD1	2.27	0.54
1:B:219:ASN:N	1:B:220:PRO:HD3	2.22	0.54
1:B:409:LEU:HD23	1:B:409:LEU:N	2.22	0.54
2:A:231:LEU:CD2	2:A:231:LEU:H	2.07	0.54
1:B:243:MET:CA	1:B:243:MET:HE2	2.37	0.54
1:B:465:GLU:CD	1:B:1040:LEU:H	2.11	0.54
1:B:565:LEU:HD22	1:B:847:GLN:NE2	2.20	0.54
1:B:879:GLU:O	1:B:1006:GLN:NE2	2.40	0.54
1:B:612:TYR:CD1	1:B:825:LYS:HD3	2.39	0.54
1:B:389:VAL:HG23	1:B:495:THR:HB	1.89	0.54
1:B:380:MET:CE	2:A:254:ILE:CG2	2.86	0.53
1:B:911:CYS:SG	1:B:964:PRO:HA	2.48	0.53
1:B:560:ASN:HA	1:B:593:GLN:HE22	1.72	0.53
1:B:727:GLN:NE2	2:A:190:LYS:HB2	2.24	0.53
1:B:912:PHE:HE1	1:B:935:MET:CE	2.21	0.53
1:B:380:MET:HE1	2:A:254:ILE:HG21	1.89	0.53
1:B:190:PRO:HG3	1:B:266:TRP:CH2	2.44	0.53
1:B:113:GLU:OE1	1:B:290:ARG:HD3	2.09	0.53
1:B:532:ARG:NH2	2:A:249:GLU:CA	2.72	0.52
1:B:1039:SER:O	1:B:1041:TYR:N	2.43	0.52
1:B:703:SER:HB2	1:B:706:SER:H	1.73	0.52
1:B:751:ARG:N	1:B:752:PRO:CD	2.72	0.52
1:B:1009:GLN:CA	1:B:1009:GLN:NE2	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:799:ALA:O	1:B:802:HIS:HB3	2.09	0.52
1:B:888:LEU:HD23	1:B:888:LEU:H	1.73	0.52
1:B:252:ASP:HA	1:B:282:LEU:HB2	1.91	0.52
1:B:380:MET:HE1	2:A:254:ILE:CG2	2.40	0.52
1:B:596:ARG:HH11	1:B:596:ARG:HG2	1.73	0.52
2:A:199:PRO:CB	2:A:201:LYS:HE3	2.40	0.52
2:A:224:PHE:N	2:A:224:PHE:CD1	2.73	0.52
1:B:387:GLN:NE2	1:B:387:GLN:CA	2.73	0.52
1:B:965:HIS:CD2	1:B:965:HIS:N	2.75	0.52
2:A:249:GLU:CB	2:A:250:PRO:CD	2.63	0.52
1:B:158:LEU:HA	1:B:281:PHE:HB2	1.92	0.52
1:B:700:LEU:HD12	1:B:729:VAL:HG13	1.90	0.52
1:B:615:ILE:HD12	1:B:825:LYS:HG3	1.85	0.52
1:B:450:ARG:HD3	2:A:228:SER:OG	2.10	0.52
1:B:167:LYS:HD3	1:B:283:SER:O	2.09	0.52
1:B:217:THR:HG22	1:B:220:PRO:HG3	1.92	0.52
1:B:233:ARG:NH1	1:B:268:GLU:CD	2.63	0.52
1:B:880:ILE:CD1	1:B:888:LEU:HD12	2.15	0.52
1:B:1039:SER:O	1:B:1040:LEU:C	2.42	0.52
1:B:180:ARG:NH1	1:B:180:ARG:HG2	2.24	0.51
1:B:374:VAL:HG23	1:B:374:VAL:O	2.10	0.51
1:B:394:PHE:CD1	1:B:503:LYS:HD2	2.46	0.51
1:B:994:ILE:HG23	1:B:1035:VAL:HG13	1.92	0.51
1:B:136:TYR:OH	1:B:173:TYR:HB2	2.11	0.51
1:B:468:GLU:CA	1:B:491:MET:CE	2.88	0.51
2:A:172:ALA:CB	2:A:180:TYR:CD2	2.89	0.51
1:B:732:LEU:HD23	1:B:734:HIS:CE1	2.46	0.51
1:B:1009:GLN:HE21	1:B:1009:GLN:HA	1.72	0.51
1:B:408:LYS:HB2	1:B:409:LEU:HD23	1.93	0.51
1:B:683:VAL:O	1:B:683:VAL:HG12	2.11	0.51
1:B:236:LEU:HG	1:B:272:LEU:HB3	1.93	0.51
1:B:412:ASN:ND2	1:B:451:GLY:CA	2.73	0.51
1:B:841:LYS:HA	1:B:844:THR:CG2	2.41	0.51
2:A:187:TYR:CD1	2:A:187:TYR:C	2.84	0.51
1:B:354:GLY:O	1:B:355:ASP:O	2.29	0.51
2:A:221:GLU:O	2:A:221:GLU:HG3	2.11	0.50
1:B:227:MET:HE3	1:B:232:LEU:HD13	1.93	0.50
1:B:180:ARG:HH11	1:B:180:ARG:HG2	1.75	0.50
1:B:160:SER:OG	1:B:284:ALA:O	2.29	0.50
1:B:596:ARG:HH11	1:B:596:ARG:HG3	1.76	0.50
1:B:922:PRO:HG3	1:B:968:ASP:OD1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:THR:HG21	4:B:1102:ATP:O2A	1.99	0.50
1:B:321:PHE:CE2	1:B:372:SER:HB2	2.36	0.50
1:B:732:LEU:HD13	2:A:194:CYS:SG	2.52	0.50
1:B:841:LYS:O	1:B:844:THR:CG2	2.54	0.49
1:B:316:LEU:HD11	1:B:524:ALA:O	2.11	0.49
1:B:1021:ASN:O	1:B:1025:GLU:HG2	2.10	0.49
1:B:180:ARG:HH11	1:B:180:ARG:CG	2.24	0.49
1:B:897:PHE:O	1:B:900:LEU:HD23	2.10	0.49
1:B:406:MET:CB	1:B:452:ILE:HD13	2.38	0.49
1:B:809:LEU:HD13	1:B:815:LEU:HD23	1.94	0.49
1:B:968:ASP:HB2	5:B:1221:HOH:O	1.81	0.49
1:B:160:SER:OG	1:B:285:THR:HA	2.12	0.49
1:B:598:ILE:N	1:B:599:PRO:CD	2.75	0.49
1:B:888:LEU:HB2	1:B:1007:MET:CE	2.43	0.49
1:B:465:GLU:OE1	1:B:1040:LEU:N	2.45	0.49
1:B:706:SER:O	2:A:190:LYS:NZ	2.45	0.48
1:B:125:LEU:CG	1:B:153:ASN:OD1	2.59	0.48
1:B:446:PRO:HB2	2:A:224:PHE:CD2	2.48	0.48
1:B:456:HIS:HD2	1:B:459:LEU:HD22	1.78	0.48
1:B:804:MET:HG2	1:B:804:MET:O	2.14	0.48
1:B:997:MET:HE1	1:B:1030:ILE:CG2	2.32	0.48
1:B:790:LEU:HG	1:B:790:LEU:O	2.09	0.48
1:B:458:GLY:O	1:B:991:GLY:CA	2.62	0.48
1:B:431:LEU:CG	1:B:1034:ILE:CG2	2.91	0.48
1:B:814:ASN:ND2	1:B:814:ASN:O	2.46	0.48
1:B:233:ARG:NH1	1:B:268:GLU:OE1	2.47	0.48
1:B:126:LYS:HA	1:B:127:PRO:HD3	1.77	0.48
1:B:167:LYS:HB2	4:B:1102:ATP:O1B	2.14	0.47
1:B:243:MET:CA	1:B:243:MET:CE	2.91	0.47
1:B:445:LEU:HB3	1:B:446:PRO:HD3	1.96	0.47
1:B:410:ASP:HA	1:B:450:ARG:HG2	1.96	0.47
1:B:841:LYS:HA	1:B:844:THR:HG21	1.96	0.47
1:B:900:LEU:CD2	1:B:900:LEU:H	2.24	0.47
1:B:168:THR:CG2	4:B:1102:ATP:PA	2.95	0.47
1:B:697:GLU:OE2	2:A:187:TYR:OH	2.32	0.47
1:B:412:ASN:HD22	1:B:451:GLY:N	2.12	0.47
1:B:144:GLN:HE22	1:B:169:VAL:HG11	1.77	0.47
1:B:189:SER:O	1:B:228:THR:HA	2.13	0.47
1:B:254:ILE:HG22	1:B:282:LEU:O	2.14	0.47
1:B:257:MET:HG3	1:B:266:TRP:CB	2.45	0.47
1:B:404:LEU:CD1	2:A:220:VAL:HG22	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:PRO:HG3	1:B:346:ALA:HB1	1.97	0.47
1:B:496:VAL:HG23	1:B:524:ALA:HB2	1.95	0.47
1:B:460:LEU:HA	1:B:461:PRO:HD3	1.71	0.47
1:B:412:ASN:HD21	1:B:451:GLY:HA2	1.80	0.47
1:B:642:GLU:HA	1:B:645:HIS:NE2	2.30	0.47
1:B:1027:ILE:H	1:B:1027:ILE:HG13	1.50	0.47
1:B:267:GLU:OE1	1:B:561:SER:CB	2.60	0.47
1:B:583:TYR:CE1	1:B:587:LYS:HE3	2.50	0.47
1:B:814:ASN:C	1:B:814:ASN:HD22	2.19	0.47
1:B:1024:ALA:O	1:B:1027:ILE:CD1	2.62	0.46
1:B:197:GLN:CB	1:B:489:ILE:HG12	2.45	0.46
1:B:404:LEU:HD23	2:A:224:PHE:CZ	2.50	0.46
1:B:183:GLN:OE1	1:B:247:ALA:CB	2.62	0.46
1:B:804:MET:HG2	1:B:810:HIS:HD2	1.79	0.46
1:B:990:GLU:OE2	2:A:214:LYS:NZ	2.37	0.46
1:B:410:ASP:N	2:A:229:VAL:O	2.38	0.46
1:B:255:HIS:HB2	1:B:258:ARG:NH2	2.31	0.46
1:B:323:ALA:HA	1:B:372:SER:HB2	1.95	0.46
1:B:922:PRO:CG	1:B:968:ASP:CG	2.83	0.46
1:B:182:LYS:HA	1:B:182:LYS:HD2	1.43	0.46
1:B:320:ILE:HG13	1:B:331:VAL:HG21	1.97	0.46
1:B:559:LEU:O	1:B:559:LEU:HG	2.16	0.46
1:B:841:LYS:C	1:B:844:THR:HG23	2.33	0.46
1:B:381:ILE:HD13	1:B:389:VAL:HG21	1.98	0.46
1:B:579:ILE:HG23	1:B:579:ILE:HD12	1.53	0.46
1:B:435:ASP:OD2	1:B:1033:ASP:HB3	2.16	0.46
1:B:732:LEU:HB2	2:A:196:GLY:HA3	1.98	0.46
1:B:424:PHE:CE1	1:B:445:LEU:HD22	2.51	0.46
1:B:442:GLU:OE1	2:A:221:GLU:CD	2.53	0.46
1:B:479:LEU:HA	1:B:479:LEU:HD23	1.69	0.46
1:B:468:GLU:HA	1:B:491:MET:HE1	1.97	0.46
2:A:199:PRO:HG2	2:A:201:LYS:HD2	1.98	0.46
1:B:901:SER:HB2	1:B:904:GLN:H	1.81	0.46
1:B:911:CYS:HA	1:B:963:LYS:O	2.16	0.46
2:A:170:ASP:OD2	2:A:181:ARG:HB2	2.16	0.45
1:B:181:GLU:HA	1:B:181:GLU:OE2	2.14	0.45
1:B:848:MET:HE2	1:B:851:LEU:CD2	2.46	0.45
1:B:880:ILE:CG2	1:B:888:LEU:CD1	2.75	0.45
1:B:156:SER:O	1:B:305:HIS:HD2	1.99	0.45
1:B:231:ILE:HG23	1:B:231:ILE:HD12	1.64	0.45
1:B:454:ILE:HA	1:B:480:PHE:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:565:LEU:CD2	1:B:847:GLN:HE21	2.28	0.45
1:B:347:MET:CE	1:B:543:MET:N	2.65	0.45
1:B:977:ALA:O	1:B:1032:ARG:CZ	2.64	0.45
1:B:114:VAL:HB	1:B:305:HIS:HD1	1.81	0.45
1:B:489:ILE:HD12	1:B:490:ASN:H	1.81	0.45
1:B:583:TYR:HE1	1:B:587:LYS:HE3	1.82	0.45
1:B:645:HIS:HB3	1:B:736:LEU:HD12	1.98	0.45
1:B:880:ILE:HA	1:B:1006:GLN:HB3	1.98	0.45
2:A:168:LYS:HA	2:A:169:PRO:HD2	1.68	0.45
1:B:257:MET:HG3	1:B:266:TRP:HB2	1.98	0.45
1:B:450:ARG:CB	1:B:450:ARG:HH11	2.29	0.45
1:B:774:ILE:HB	1:B:775:PRO:HD2	1.99	0.45
2:A:187:TYR:CD1	2:A:187:TYR:O	2.70	0.44
1:B:456:HIS:HB2	1:B:482:THR:CB	2.43	0.44
1:B:870:ILE:CG2	1:B:875:ARG:NH1	2.77	0.44
1:B:658:ARG:NH2	2:A:166:ASP:OD2	2.50	0.44
2:A:170:ASP:HA	2:A:171:PRO:HD2	1.76	0.44
1:B:167:LYS:HE3	4:B:1102:ATP:O1B	2.17	0.44
1:B:380:MET:HE3	2:A:254:ILE:CG2	2.47	0.44
1:B:448:LEU:HD23	1:B:470:LEU:HD11	1.98	0.44
1:B:932:LEU:C	1:B:932:LEU:HD22	2.38	0.44
1:B:189:SER:HA	1:B:190:PRO:HD3	1.64	0.44
1:B:881:SER:OG	1:B:881:SER:O	2.35	0.44
1:B:1014:ILE:CD1	1:B:1014:ILE:C	2.85	0.44
1:B:922:PRO:CG	1:B:968:ASP:OD1	2.65	0.44
1:B:446:PRO:HB2	2:A:224:PHE:HD2	1.82	0.44
1:B:900:LEU:N	1:B:900:LEU:HD13	2.31	0.44
1:B:460:LEU:CD2	1:B:990:GLU:HG3	2.46	0.44
1:B:153:ASN:HA	1:B:153:ASN:HD22	1.53	0.44
1:B:814:ASN:ND2	1:B:814:ASN:C	2.71	0.44
1:B:863:PHE:HE1	1:B:889:THR:OG1	2.01	0.44
2:A:227:LYS:HD2	2:A:227:LYS:HA	1.51	0.44
1:B:119:GLU:H	1:B:119:GLU:CD	2.22	0.44
1:B:999:ARG:O	1:B:1002:GLU:HB3	2.17	0.44
1:B:307:ILE:HG22	1:B:307:ILE:O	2.18	0.44
1:B:334:GLU:OE2	1:B:532:ARG:HG3	2.17	0.44
1:B:740:SER:HA	1:B:776:LEU:HA	1.99	0.44
1:B:815:LEU:C	1:B:815:LEU:CD2	2.84	0.43
1:B:828:ILE:HG12	1:B:828:ILE:H	1.46	0.43
1:B:997:MET:CE	1:B:1030:ILE:CG2	2.87	0.43
1:B:740:SER:CB	1:B:774:ILE:HD11	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:751:ARG:HB2	1:B:752:PRO:HD3	2.00	0.43
1:B:612:TYR:HE1	1:B:825:LYS:HD3	1.69	0.43
1:B:669:PHE:N	1:B:669:PHE:CD1	2.86	0.43
1:B:431:LEU:HG	1:B:1034:ILE:HG23	2.01	0.43
1:B:582:GLU:HG2	1:B:848:MET:HE2	1.97	0.43
1:B:299:LEU:CD1	1:B:587:LYS:HD2	2.48	0.43
1:B:179:LEU:HD12	1:B:179:LEU:HA	1.66	0.43
1:B:323:ALA:HA	1:B:372:SER:HB3	2.00	0.43
1:B:404:LEU:HD11	2:A:220:VAL:HG22	2.00	0.43
1:B:428:ILE:HD11	1:B:441:VAL:HG11	2.00	0.43
1:B:863:PHE:HE1	1:B:889:THR:HG1	1.65	0.43
1:B:192:LYS:CG	1:B:213:THR:CG2	2.96	0.43
1:B:470:LEU:HD23	1:B:475:LEU:HD12	1.99	0.43
1:B:596:ARG:NH1	1:B:596:ARG:CG	2.71	0.43
2:A:218:LYS:HA	2:A:218:LYS:CE	2.48	0.43
1:B:192:LYS:CG	1:B:213:THR:HG23	2.49	0.43
1:B:274:PRO:HD2	1:B:277:VAL:CG2	2.48	0.43
1:B:404:LEU:HD11	2:A:220:VAL:CG2	2.49	0.43
1:B:744:LEU:H	1:B:744:LEU:HD23	1.82	0.43
1:B:557:ASP:HA	1:B:558:PRO:HD3	1.81	0.43
1:B:922:PRO:HG3	1:B:968:ASP:CG	2.38	0.43
2:A:224:PHE:HD1	2:A:224:PHE:N	2.17	0.42
1:B:175:ILE:O	1:B:175:ILE:HG22	2.19	0.42
1:B:537:LEU:HA	1:B:537:LEU:HD23	1.75	0.42
1:B:735:LEU:HD23	1:B:735:LEU:N	2.33	0.42
1:B:841:LYS:C	1:B:844:THR:CG2	2.87	0.42
1:B:380:MET:CE	2:A:254:ILE:HG21	2.48	0.42
1:B:336:GLY:O	1:B:553:LYS:CD	2.61	0.42
1:B:168:THR:HG22	4:B:1102:ATP:PA	2.51	0.42
1:B:683:VAL:O	1:B:683:VAL:CG1	2.67	0.42
1:B:764:GLN:HB3	1:B:764:GLN:HE21	1.60	0.42
1:B:809:LEU:C	1:B:809:LEU:HD22	2.39	0.42
1:B:770:PHE:CE2	1:B:775:PRO:HG3	2.55	0.42
1:B:942:ILE:HD12	1:B:942:ILE:HA	1.80	0.42
1:B:380:MET:HB2	1:B:380:MET:HE2	1.88	0.42
1:B:408:LYS:CD	1:B:408:LYS:N	2.81	0.42
1:B:460:LEU:HD23	1:B:463:LEU:HD12	2.00	0.42
1:B:848:MET:HG3	1:B:848:MET:O	2.18	0.42
1:B:580:ASN:HB2	1:B:581:PRO:CD	2.49	0.42
1:B:585:LEU:HD12	1:B:585:LEU:HA	1.84	0.42
1:B:727:GLN:HE21	1:B:727:GLN:HB3	1.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:809:LEU:HD23	1:B:809:LEU:HA	1.75	0.42
1:B:942:ILE:HD13	1:B:942:ILE:N	2.35	0.42
1:B:989:PHE:CD1	1:B:989:PHE:N	2.87	0.42
1:B:678:SER:OG	1:B:680:LYS:HE2	2.20	0.42
1:B:408:LYS:O	2:A:228:SER:HB2	2.18	0.42
1:B:821:LEU:HD23	1:B:821:LEU:HA	1.73	0.42
1:B:615:ILE:CD1	1:B:615:ILE:C	2.84	0.42
1:B:125:LEU:HA	1:B:125:LEU:HD12	1.67	0.42
1:B:669:PHE:HA	1:B:717:PRO:HB3	2.01	0.42
1:B:707:LEU:HD21	1:B:725:GLU:HG2	2.01	0.42
1:B:458:GLY:O	1:B:991:GLY:HA3	2.20	0.41
1:B:598:ILE:N	1:B:599:PRO:HD2	2.35	0.41
1:B:202:MET:HA	1:B:202:MET:CE	2.49	0.41
1:B:459:LEU:HD12	1:B:459:LEU:HA	1.78	0.41
1:B:550:GLN:HE21	1:B:550:GLN:HB2	1.58	0.41
1:B:897:PHE:N	1:B:900:LEU:CD2	2.83	0.41
2:A:244:GLU:CB	2:A:245:PRO:CD	2.97	0.41
1:B:273:LEU:HA	1:B:274:PRO:HD3	1.85	0.41
1:B:490:ASN:C	1:B:490:ASN:HD22	2.21	0.41
1:B:663:LYS:HA	1:B:668:ASP:HA	2.02	0.41
1:B:807:HIS:HA	1:B:808:PRO:HD3	1.22	0.41
1:B:727:GLN:NE2	2:A:190:LYS:HD3	2.24	0.41
1:B:1031:LYS:HA	1:B:1036:PHE:CE2	2.55	0.41
1:B:404:LEU:HD23	1:B:404:LEU:HA	1.75	0.41
1:B:382:MET:HG3	1:B:411:PHE:CE1	2.56	0.41
1:B:523:ARG:HD2	1:B:523:ARG:HA	1.95	0.41
1:B:1019:LEU:HA	1:B:1019:LEU:HD23	1.69	0.41
1:B:692:PRO:HG2	1:B:692:PRO:O	2.21	0.41
2:A:197:ILE:HG12	2:A:202:GLN:HB2	2.03	0.41
1:B:574:LEU:HA	1:B:574:LEU:HD23	1.79	0.41
1:B:744:LEU:CD1	1:B:762:SER:HB3	2.48	0.41
1:B:1008:CYS:SG	1:B:1024:ALA:HB2	2.61	0.41
1:B:659:LEU:HD12	1:B:742:VAL:CB	2.45	0.41
1:B:896:LEU:C	1:B:900:LEU:CD2	2.57	0.41
1:B:732:LEU:CD1	2:A:194:CYS:SG	3.09	0.41
1:B:175:ILE:HG23	1:B:185:VAL:HG11	2.03	0.41
1:B:332:VAL:HA	1:B:337:ASP:O	2.20	0.41
1:B:431:LEU:HG	1:B:1034:ILE:CG2	2.50	0.41
1:B:470:LEU:HD22	1:B:475:LEU:HD12	2.01	0.41
1:B:764:GLN:HA	1:B:767:GLN:HB2	2.03	0.41
1:B:433:ASP:OD1	1:B:433:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:ASN:C	1:B:490:ASN:ND2	2.72	0.41
1:B:885:GLU:HA	1:B:888:LEU:HG	2.02	0.41
1:B:997:MET:HE1	1:B:1030:ILE:HG12	2.02	0.41
1:B:456:HIS:HB3	1:B:482:THR:HB	2.01	0.40
1:B:391:ILE:HG23	1:B:497:LEU:HD23	2.02	0.40
1:B:953:ILE:CD1	1:B:953:ILE:O	2.69	0.40
2:A:227:LYS:HD2	2:A:228:SER:H	1.86	0.40
1:B:129:VAL:O	1:B:129:VAL:CG2	2.68	0.40
1:B:645:HIS:HB3	1:B:736:LEU:CD1	2.52	0.40
1:B:847:GLN:HB3	1:B:847:GLN:HE21	1.65	0.40
1:B:848:MET:HE2	1:B:851:LEU:HD23	2.03	0.40
1:B:438:LEU:HA	1:B:439:PRO:HD3	1.79	0.40
1:B:644:ILE:CG2	1:B:644:ILE:O	2.69	0.40
1:B:760:LEU:HD23	1:B:760:LEU:HA	1.64	0.40
1:B:450:ARG:HE	2:A:227:LYS:NZ	2.16	0.40
1:B:459:LEU:HD13	1:B:459:LEU:N	2.35	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	B	925/979 (94%)	905 (98%)	18 (2%)	2 (0%)	47	78
2	A	77/105 (73%)	72 (94%)	4 (5%)	1 (1%)	12	37
All	All	1002/1084 (92%)	977 (98%)	22 (2%)	3 (0%)	41	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	387	GLN
2	A	244	GLU

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Mol	Chain	Res	Type
1	B	922	PRO

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	B	689/860 (80%)	560 (81%)	129 (19%)	1	5
2	A	72/94 (77%)	50 (69%)	22 (31%)	0	1
All	All	761/954 (80%)	610 (80%)	151 (20%)	1	4

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	104	VAL
1	B	107	VAL
1	B	110	CYS
1	B	116	LEU
1	B	135	GLU
1	B	139	ILE
1	B	153	ASN
1	B	155	GLN
1	B	168	THR
1	B	179	LEU
1	B	180	ARG
1	B	182	LYS
1	B	185	VAL
1	B	186	ILE
1	B	189	SER
1	B	192	LYS
1	B	209	VAL
1	B	212	MET
1	B	215	ASP
1	B	221	THR
1	B	229	THR
1	B	233	ARG

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Mol	Chain	Res	Type
1	B	236	LEU
1	B	243	MET
1	B	257	MET
1	B	276	ASN
1	B	286	ILE
1	B	313	PRO
1	B	317	GLN
1	B	341	ASP
1	B	345	THR
1	B	347	MET
1	B	348	GLN
1	B	382	MET
1	B	387	GLN
1	B	391	ILE
1	B	393	SER
1	B	396	LYS
1	B	406	MET
1	B	409	LEU
1	B	414	ASP
1	B	428	ILE
1	B	446	PRO
1	B	452	ILE
1	B	454	ILE
1	B	456	HIS
1	B	459	LEU
1	B	460	LEU
1	B	462	ILE
1	B	466	THR
1	B	479	LEU
1	B	487	MET
1	B	489	ILE
1	B	490	ASN
1	B	518	ILE
1	B	527	ARG
1	B	532	ARG
1	B	537	LEU
1	B	541	GLU
1	B	546	THR
1	B	552	LEU
1	B	553	LYS
1	B	565	LEU
1	B	575	ARG

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Mol	Chain	Res	Type
1	B	576	VAL
1	B	585	LEU
1	B	596	ARG
1	B	598	ILE
1	B	618	PRO
1	B	625	ILE
1	B	645	HIS
1	B	660	VAL
1	B	677	PHE
1	B	681	SER
1	B	706	SER
1	B	709	ASN
1	B	716	LYS
1	B	719	LYS
1	B	723	LYS
1	B	727	GLN
1	B	728	VAL
1	B	729	VAL
1	B	733	VAL
1	B	736	LEU
1	B	750	LEU
1	B	751	ARG
1	B	757	GLN
1	B	760	LEU
1	B	764	GLN
1	B	774	ILE
1	B	778	ASP
1	B	780	ILE
1	B	783	MET
1	B	787	ASP
1	B	794	ILE
1	B	802	HIS
1	B	809	LEU
1	B	814	ASN
1	B	815	LEU
1	B	825	LYS
1	B	828	ILE
1	B	844	THR
1	B	847	GLN
1	B	861	LEU
1	B	865	THR
1	B	882	SER

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Mol	Chain	Res	Type
1	B	885	GLU
1	B	887	LEU
1	B	888	LEU
1	B	889	THR
1	B	894	ASN
1	B	901	SER
1	B	910	SER
1	B	916	GLU
1	B	932	LEU
1	B	935	MET
1	B	942	ILE
1	B	953	ILE
1	B	968	ASP
1	B	982	ILE
1	B	988	VAL
1	B	999	ARG
1	B	1000	LEU
1	B	1007	MET
1	B	1008	CYS
1	B	1009	GLN
1	B	1027	ILE
1	B	1028	THR
1	B	1042	LEU
2	A	165	THR
2	A	166	ASP
2	A	168	LYS
2	A	173	ASN
2	A	180	TYR
2	A	188	LYS
2	A	193	SER
2	A	197	ILE
2	A	211	THR
2	A	212	GLU
2	A	213	LYS
2	A	214	LYS
2	A	218	LYS
2	A	221	GLU
2	A	225	THR
2	A	227	LYS
2	A	228	SER
2	A	231	LEU
2	A	249	GLU

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Mol	Chain	Res	Type
2	A	251	ILE
2	A	257	LYS
2	A	258	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	112	HIS
1	B	144	GLN
1	B	255	HIS
1	B	317	GLN
1	B	344	ASN
1	B	387	GLN
1	B	405	GLN
1	B	412	ASN
1	B	440	GLN
1	B	550	GLN
1	B	593	GLN
1	B	727	GLN
1	B	734	HIS
1	B	764	GLN
1	B	810	HIS
1	B	814	ASN
1	B	827	GLN
1	B	847	GLN
1	B	894	ASN
1	B	965	HIS
1	B	1006	GLN
1	B	1009	GLN
2	A	202	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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	B	1102	-	26,33,33	2.00	10 (38%)	31,52,52	1.43	6 (19%)

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
4	ATP	B	1102	-	-	1/18/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1102	ATP	C4-N3	-4.07	1.30	1.35
4	B	1102	ATP	C2'-C1'	-3.64	1.48	1.53
4	B	1102	ATP	O4'-C4'	-3.20	1.37	1.45
4	B	1102	ATP	C5-N7	-2.72	1.29	1.39
4	B	1102	ATP	PB-O2B	-2.62	1.43	1.55
4	B	1102	ATP	PG-O3G	-2.56	1.45	1.54
4	B	1102	ATP	PA-O1A	-2.47	1.42	1.50
4	B	1102	ATP	PA-O2A	-2.28	1.44	1.55
4	B	1102	ATP	PG-O2G	-2.25	1.46	1.54
4	B	1102	ATP	PB-O1B	-2.23	1.43	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1102	ATP	N3-C2-N1	-3.22	123.65	128.68
4	B	1102	ATP	O4'-C1'-C2'	-2.90	102.68	106.93
4	B	1102	ATP	C4-C5-N7	-2.81	106.47	109.40
4	B	1102	ATP	C5-C6-N6	2.80	124.61	120.35
4	B	1102	ATP	PB-O3B-PG	2.16	140.23	132.83
4	B	1102	ATP	O3G-PG-O1G	2.04	118.66	110.68

There are no chirality outliers.

All (1) torsion outliers are listed below:

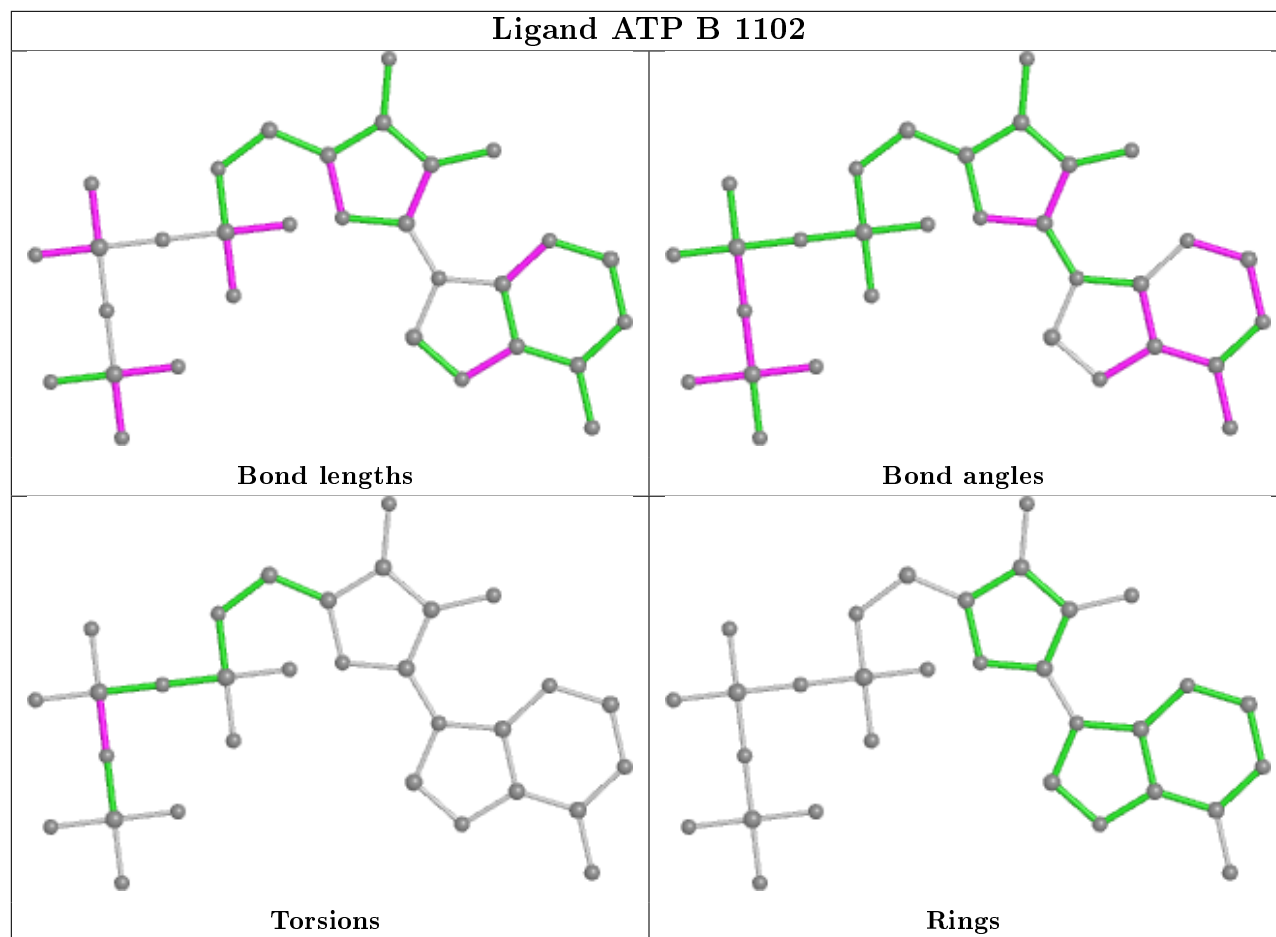
Mol	Chain	Res	Type	Atoms
4	B	1102	ATP	PG-O3B-PB-O1B

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1102	ATP	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	B	929/979 (94%)	-0.11	19 (2%) 65 63	25, 48, 71, 99	0
2	A	85/105 (80%)	0.27	6 (7%) 16 12	35, 55, 84, 102	0
All	All	1014/1084 (93%)	-0.08	25 (2%) 57 55	25, 48, 74, 102	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	355	ASP	5.2
2	A	198	ASN	4.8
2	A	243	THR	4.0
1	B	688	GLY	4.0
1	B	687	SER	3.7
1	B	976	GLY	3.7
1	B	897	PHE	3.2
1	B	354	GLY	3.1
1	B	430	CYS	2.9
1	B	721	ASP	2.8
2	A	201	LYS	2.7
2	A	241	SER	2.6
1	B	811	ASN	2.6
2	A	233	ASN	2.6
1	B	806	SER	2.6
2	A	228	SER	2.5
1	B	921	MET	2.4
1	B	690	LEU	2.4
1	B	922	PRO	2.3
1	B	925	THR	2.3
1	B	975	THR	2.2
1	B	888	LEU	2.2
1	B	109	GLY	2.1
1	B	615	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	242	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

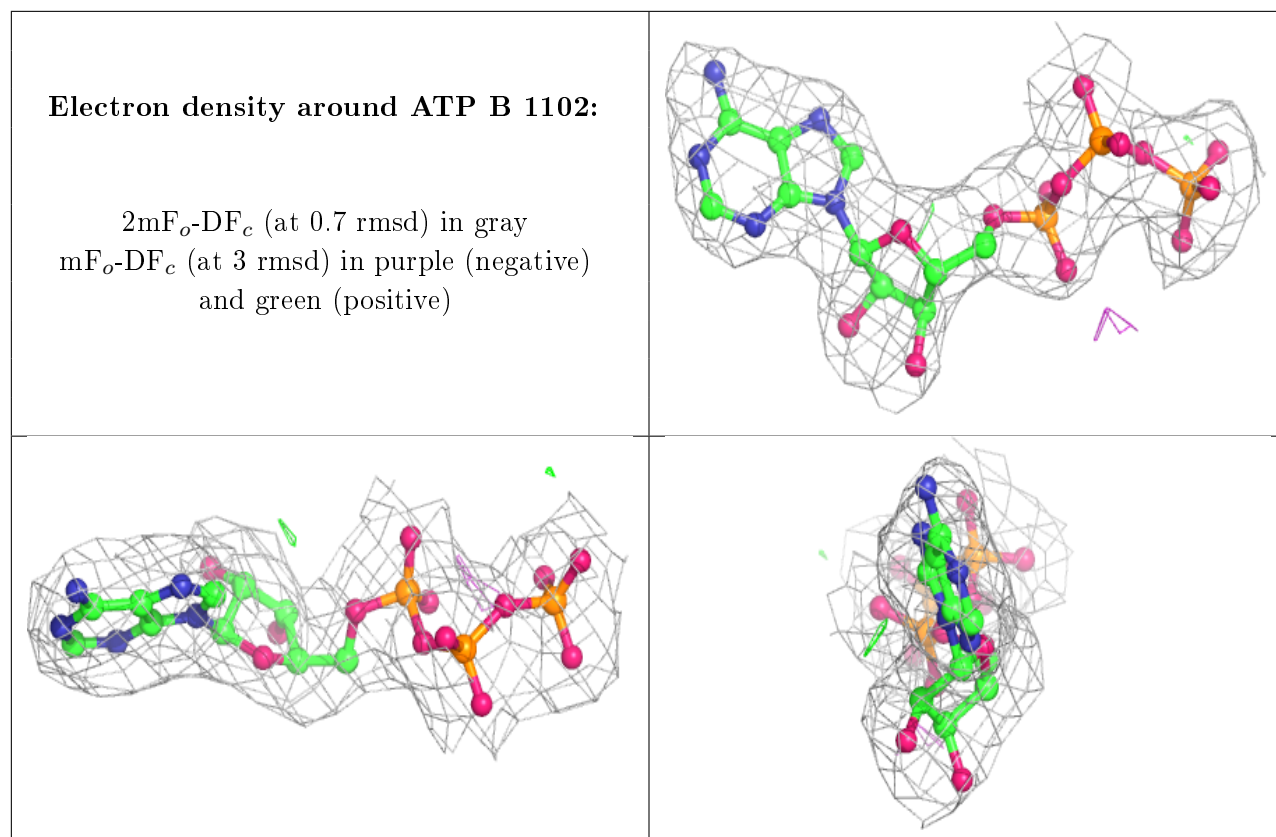
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	CL	B	1101	1/1	0.91	0.11	52,52,52,52	0
4	ATP	B	1102	31/31	0.95	0.14	33,43,53,62	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.