



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 09:27 am BST

PDB ID : 5N8S
Title : Crystal Structure of Drosophila DHX36 helicase in complex with polyT
Authors : Chen, W.-F.; Rety, S.; Hai-Lei Guo, H.-L.; Wu, W.-Q.; Liu, N.-N.; Liu, Q.-W.;
Dai, Y.-X.; Xi, X.-G.
Deposited on : 2017-02-24
Resolution : 2.88 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
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

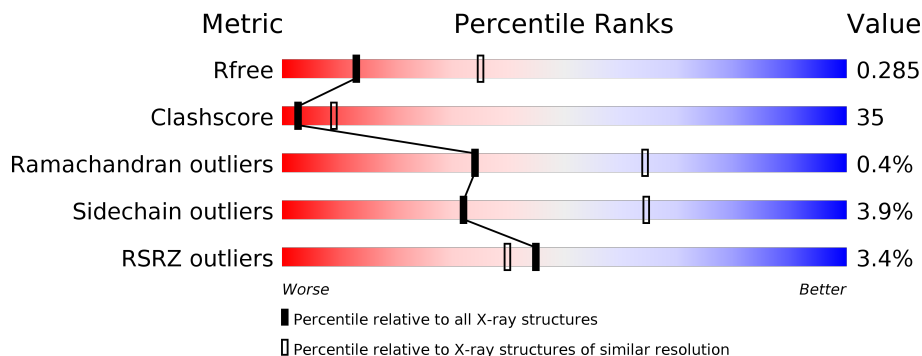
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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	944	 4% (Poor fit), 47% (0 outliers), 39% (1 outlier), 10% (2+ outliers)
1	B	944	 2% (Poor fit), 43% (0 outliers), 42% (1 outlier), 10% (2+ outliers)
2	C	16	 44% (0 outliers), 13% (1 outlier), 6% (2 outliers), 38% (Not modelled)
2	D	16	 38% (0 outliers), 25% (1 outlier), 38% (Not modelled)

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 14069 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 CG9323, isoform A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	850	6825	4310	1204	1266	45	0	0	0
1	B	851	6834	4315	1205	1269	45	0	0	0

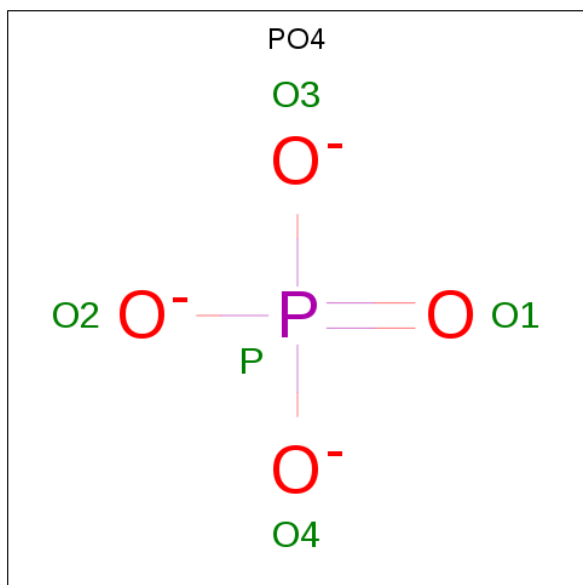
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	943	VAL	-	expression tag	UNP Q8SWT2
A	944	ASP	-	expression tag	UNP Q8SWT2
B	943	VAL	-	expression tag	UNP Q8SWT2
B	944	ASP	-	expression tag	UNP Q8SWT2

- Molecule 2 is a DNA chain called DNA (5'-D(P*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	10	200	100	20	70	10	0	0	0
2	D	10	200	100	20	70	10	0	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

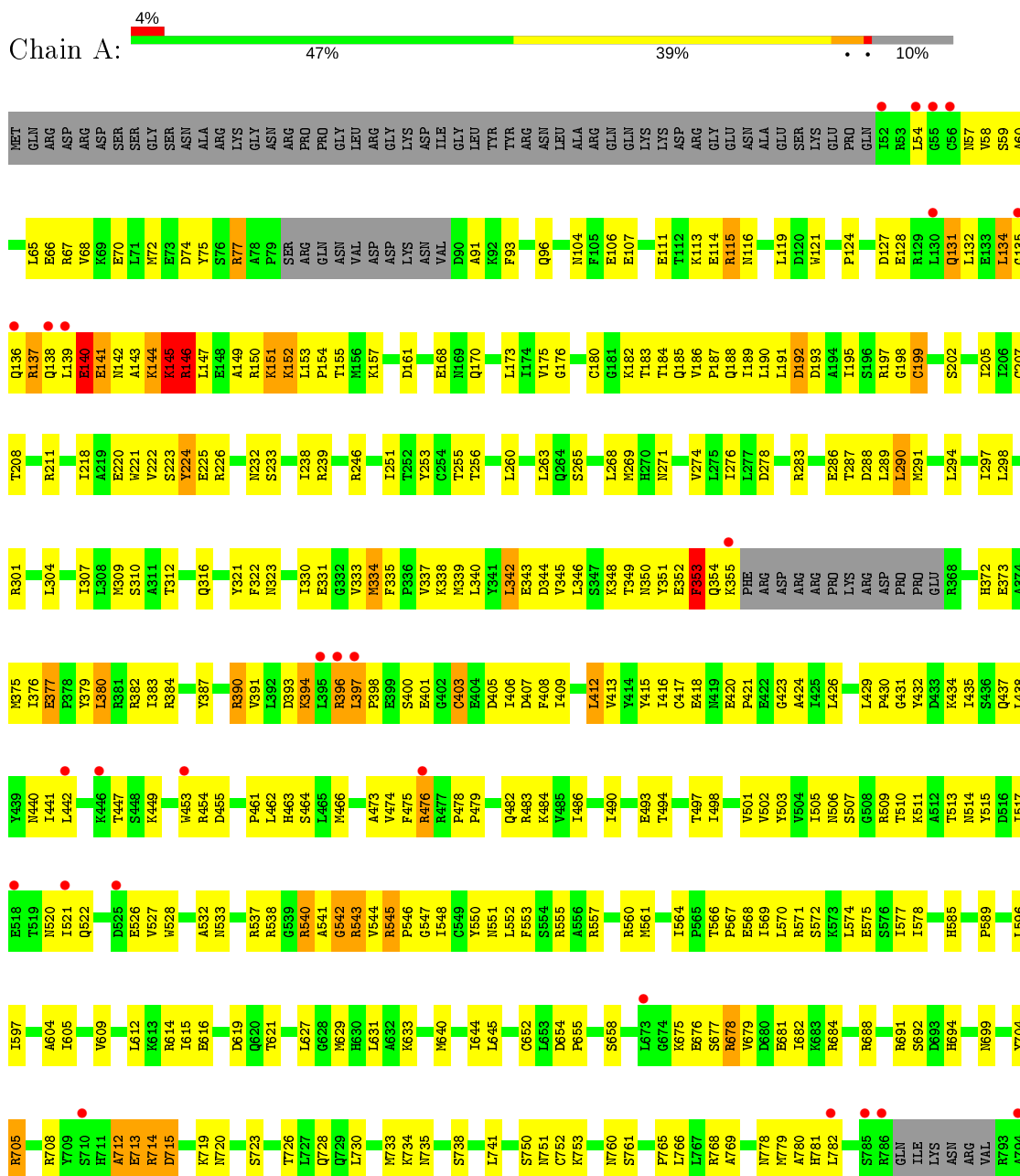


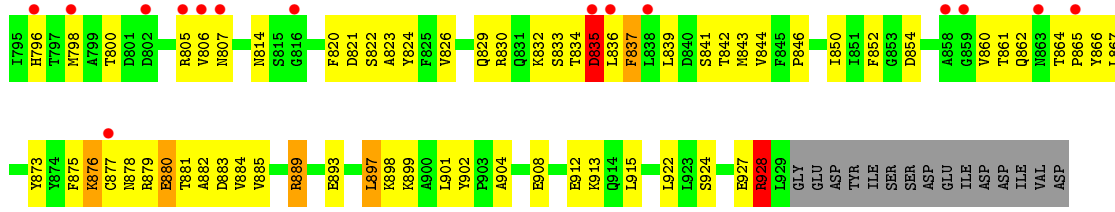
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

3 Residue-property plots [i](#)

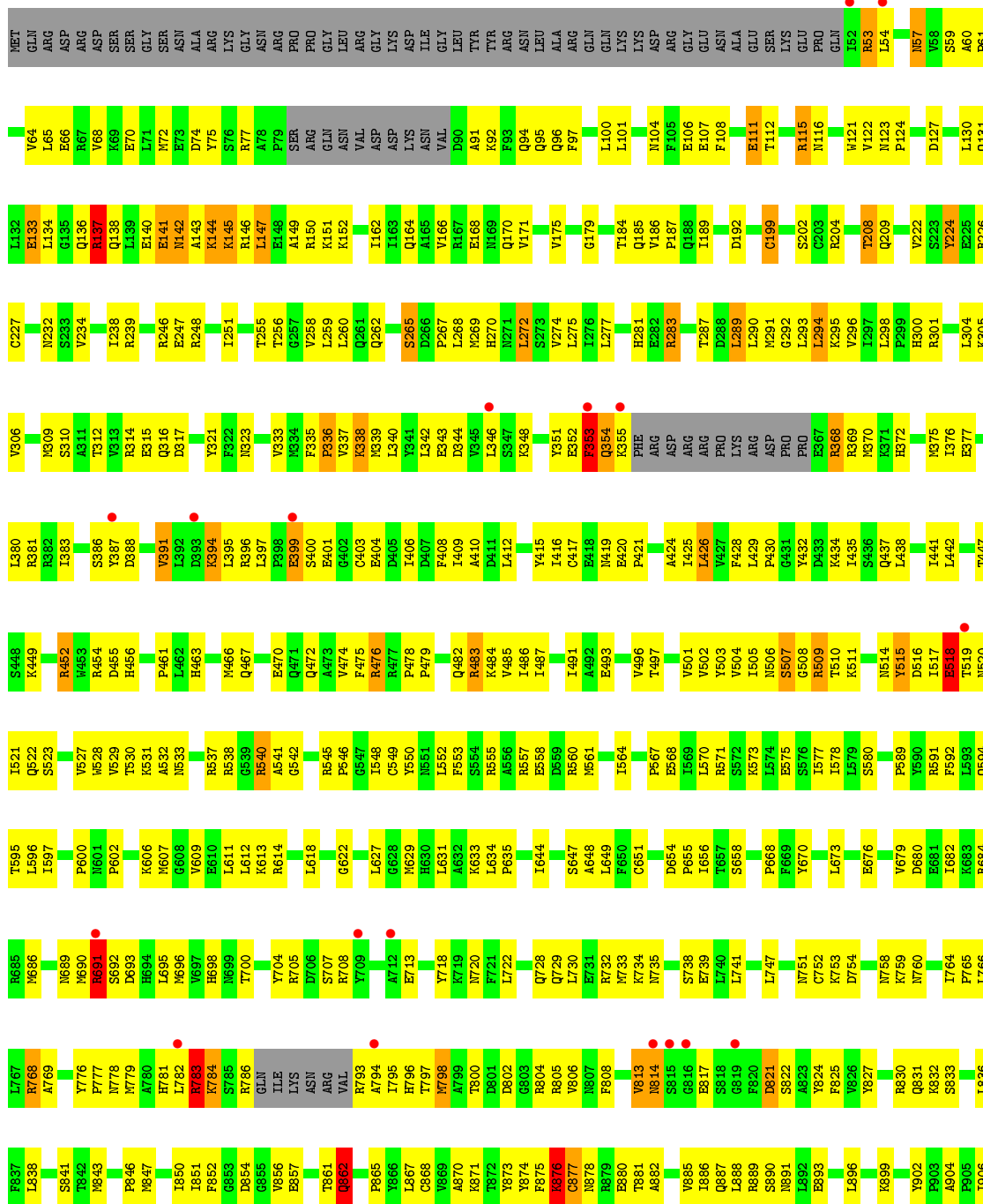
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: CG9323, isoform A





• Molecule 1: CG9323, isoform A





- Molecule 2: DNA (5'-D(P*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3')



- Molecule 2: DNA (5'-D(P*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	297.98Å 49.92Å 163.85Å 90.00° 115.01° 90.00°	Depositor
Resolution (Å)	81.10 – 2.88 83.80 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.4 (81.10-2.88) 99.4 (83.80-2.88)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.86Å)	Xtrriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.207 , 0.285 0.207 , 0.285	Depositor DCC
R_{free} test set	2480 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	70.4	Xtrriage
Anisotropy	0.079	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14069	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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: PO4

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	0.68	14/6944 (0.2%)	1.01	33/9367 (0.4%)
1	B	0.67	15/6953 (0.2%)	0.97	29/9379 (0.3%)
2	C	1.02	0/219	1.40	1/336 (0.3%)
2	D	1.04	0/219	1.42	0/336
All	All	0.69	29/14335 (0.2%)	1.01	63/19418 (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	A	0	8
1	B	0	6
All	All	0	14

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	140	GLU	CD-OE1	-11.02	1.13	1.25
1	B	691	ARG	NE-CZ	-10.27	1.19	1.33
1	A	140	GLU	CD-OE2	-9.82	1.14	1.25
1	B	691	ARG	CD-NE	-9.52	1.30	1.46
1	B	518	GLU	CD-OE1	-8.58	1.16	1.25
1	A	146	ARG	CZ-NH2	-8.34	1.22	1.33
1	B	759	LYS	CD-CE	-7.69	1.32	1.51
1	B	813	VAL	CB-CG2	-7.68	1.36	1.52
1	A	77	ARG	CZ-NH1	-7.56	1.23	1.33
1	A	146	ARG	NE-CZ	-7.10	1.23	1.33
1	B	691	ARG	CZ-NH2	-6.64	1.24	1.33
1	B	814	ASN	CB-CG	-6.28	1.36	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	77	ARG	NE-CZ	-6.26	1.25	1.33
1	A	403	CYS	CB-SG	-6.21	1.71	1.82
1	A	928	ARG	NE-CZ	-6.21	1.25	1.33
1	B	759	LYS	CE-NZ	-6.11	1.33	1.49
1	B	391	VAL	CB-CG1	-6.11	1.40	1.52
1	B	784	LYS	CD-CE	-6.02	1.36	1.51
1	B	111	GLU	CD-OE1	-5.92	1.19	1.25
1	A	928	ARG	CZ-NH1	-5.68	1.25	1.33
1	A	144	LYS	CB-CG	-5.63	1.37	1.52
1	A	928	ARG	CZ-NH2	-5.62	1.25	1.33
1	A	331	GLU	CD-OE1	-5.49	1.19	1.25
1	A	331	GLU	CD-OE2	-5.48	1.19	1.25
1	B	133	GLU	CB-CG	5.36	1.62	1.52
1	B	336	PRO	N-CD	5.28	1.55	1.47
1	B	352	GLU	CD-OE1	-5.23	1.19	1.25
1	A	145	LYS	CE-NZ	5.21	1.62	1.49
1	B	111	GLU	CD-OE2	-5.09	1.20	1.25

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	LYS	CD-CE-NZ	-16.01	74.88	111.70
1	A	146	ARG	NE-CZ-NH2	-15.51	112.55	120.30
1	A	396	ARG	NE-CZ-NH1	15.10	127.85	120.30
1	B	691	ARG	NE-CZ-NH1	-13.51	113.55	120.30
1	B	691	ARG	CD-NE-CZ	12.77	141.47	123.60
1	A	396	ARG	NE-CZ-NH2	-9.84	115.38	120.30
1	A	137	ARG	NE-CZ-NH1	-9.66	115.47	120.30
1	B	691	ARG	NH1-CZ-NH2	9.32	129.66	119.40
1	A	715	ASP	CB-CG-OD1	9.26	126.63	118.30
1	B	813	VAL	CG1-CB-CG2	-9.09	96.36	110.90
1	B	147	LEU	CA-CB-CG	8.98	135.95	115.30
1	A	715	ASP	CB-CG-OD2	-8.77	110.41	118.30
1	B	691	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	A	146	ARG	NE-CZ-NH1	8.45	124.53	120.30
1	A	476	ARG	CB-CG-CD	-7.81	91.30	111.60
1	B	928	ARG	NE-CZ-NH1	-7.62	116.49	120.30
1	A	384	ARG	NE-CZ-NH1	7.59	124.10	120.30
1	A	476	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	B	434	LYS	CD-CE-NZ	-7.54	94.36	111.70
1	B	381	ARG	NE-CZ-NH1	-7.44	116.58	120.30
1	A	134	LEU	CA-CB-CG	7.39	132.30	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	691	ARG	CA-CB-CG	-7.08	97.82	113.40
1	B	612	LEU	CA-CB-CG	7.05	131.52	115.30
1	A	396	ARG	CG-CD-NE	-7.03	97.05	111.80
1	A	540	ARG	NE-CZ-NH1	-6.96	116.82	120.30
1	A	137	ARG	NE-CZ-NH2	6.84	123.72	120.30
1	A	396	ARG	CD-NE-CZ	6.81	133.13	123.60
1	A	380	LEU	CA-CB-CG	6.70	130.72	115.30
1	A	384	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	A	342	LEU	CA-CB-CG	6.37	129.95	115.30
1	A	144	LYS	CD-CE-NZ	6.20	125.96	111.70
1	B	783	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	B	876	LYS	CD-CE-NZ	-6.05	97.77	111.70
1	B	141	GLU	CA-CB-CG	-6.02	100.15	113.40
1	A	412	LEU	CB-CG-CD2	6.00	121.20	111.00
1	A	77	ARG	CB-CG-CD	-5.96	96.12	111.60
1	B	783	ARG	CA-CB-CG	5.95	126.49	113.40
1	B	768	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	A	476	ARG	CA-CB-CG	5.80	126.17	113.40
1	B	397	LEU	CB-CG-CD1	5.76	120.80	111.00
1	A	897	LEU	CA-CB-CG	5.74	128.51	115.30
1	A	377	GLU	CA-CB-CG	5.70	125.93	113.40
2	C	8	DT	N3-C4-O4	5.67	123.30	119.90
1	A	173	LEU	CA-CB-CG	5.61	128.20	115.30
1	A	880	GLU	CA-CB-CG	-5.59	101.10	113.40
1	B	928	ARG	CB-CG-CD	-5.57	97.11	111.60
1	A	137	ARG	CG-CD-NE	5.51	123.37	111.80
1	B	606	LYS	CD-CE-NZ	5.47	124.29	111.70
1	B	476	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	A	377	GLU	N-CA-CB	5.42	120.36	110.60
1	B	515	TYR	CA-CB-CG	5.34	123.55	113.40
1	B	515	TYR	C-N-CA	5.31	134.97	121.70
1	B	426	LEU	CA-CB-CG	5.29	127.47	115.30
1	B	294	LEU	CA-CB-CG	5.26	127.39	115.30
1	B	399	GLU	CA-CB-CG	5.25	124.94	113.40
1	B	283	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	111	GLU	OE1-CD-OE2	-5.17	117.09	123.30
1	B	759	LYS	CD-CE-NZ	-5.12	99.92	111.70
1	B	813	VAL	CA-CB-CG2	-5.12	103.22	110.90
1	A	837	PHE	CB-CA-C	-5.12	100.17	110.40
1	A	396	ARG	CA-CB-CG	-5.08	102.22	113.40
1	A	290	LEU	CA-CB-CG	-5.08	103.63	115.30
1	A	397	LEU	CA-CB-CG	5.01	126.81	115.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	GLU	Peptide
1	A	141	GLU	Peptide
1	A	353	PHE	Peptide
1	A	542	GLY	Peptide
1	A	678	ARG	Peptide
1	A	712	ALA	Peptide
1	A	714	ARG	Peptide
1	A	835	ASP	Peptide
1	B	137	ARG	Peptide
1	B	142	ASN	Peptide
1	B	144	LYS	Peptide
1	B	323	ASN	Peptide
1	B	353	PHE	Peptide
1	B	862	GLN	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	A	6825	0	6925	491	1
1	B	6834	0	6930	501	0
2	C	200	0	121	4	0
2	D	200	0	121	5	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
All	All	14069	0	14097	993	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

All (993) 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:141:GLU:CB	1:B:145:LYS:HZ1	1.18	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ARG:NH2	1:A:70:GLU:HB2	1.32	1.42
1:A:138:GLN:C	1:A:144:LYS:HE3	1.50	1.32
1:A:394:LYS:NZ	1:A:397:LEU:HD13	1.45	1.28
1:B:141:GLU:HB3	1:B:145:LYS:NZ	1.45	1.27
1:B:517:ILE:HD11	1:B:607:MET:CE	1.69	1.21
1:A:67:ARG:NH2	1:A:70:GLU:CB	2.02	1.20
1:B:691:ARG:HH11	1:B:814:ASN:ND2	1.41	1.18
1:A:832:LYS:HE2	1:A:835:ASP:H	1.11	1.16
1:B:691:ARG:HE	1:B:691:ARG:HA	0.99	1.15
1:B:691:ARG:NH1	1:B:814:ASN:OD1	1.78	1.15
1:A:372:HIS:CE1	1:A:376:ILE:HD11	1.81	1.14
1:A:67:ARG:HH21	1:A:70:GLU:CB	1.58	1.14
1:B:517:ILE:HD11	1:B:607:MET:HE1	1.26	1.10
1:B:141:GLU:CB	1:B:145:LYS:NZ	2.06	1.08
1:A:57:ASN:HA	1:A:876:LYS:HE2	1.29	1.07
1:A:372:HIS:NE2	1:A:376:ILE:HD11	1.70	1.06
1:B:691:ARG:HH11	1:B:814:ASN:CG	1.59	1.05
1:B:690:MET:O	1:B:768:ARG:NH2	1.88	1.04
1:A:713:GLU:HB3	1:A:714:ARG:HE	1.23	1.04
1:A:54:LEU:HD11	1:A:861:THR:HG21	1.39	1.03
1:B:522:GLN:NE2	1:B:523:SER:O	1.89	1.03
1:A:394:LYS:HZ1	1:A:397:LEU:HD13	0.86	1.02
1:A:394:LYS:HZ2	1:A:397:LEU:HB2	1.20	1.01
1:B:782:LEU:HG	1:B:798:MET:CE	1.90	1.01
1:B:141:GLU:CA	1:B:145:LYS:HZ1	1.73	1.01
1:A:394:LYS:HZ2	1:A:397:LEU:CB	1.74	0.99
1:A:138:GLN:O	1:A:144:LYS:HE3	1.63	0.98
1:B:691:ARG:HE	1:B:691:ARG:CA	1.77	0.98
1:A:490:ILE:HD12	1:A:537:ARG:HH21	1.27	0.98
1:B:691:ARG:NH1	1:B:814:ASN:CG	2.15	0.98
1:A:394:LYS:NZ	1:A:397:LEU:CD1	2.27	0.97
1:A:57:ASN:CA	1:A:876:LYS:HE2	1.93	0.97
1:B:144:LYS:H	1:B:147:LEU:H	1.12	0.96
1:A:394:LYS:HE2	1:A:394:LYS:HA	1.45	0.95
1:B:765:PRO:HG2	1:B:927:GLU:HG2	1.48	0.95
1:B:517:ILE:CD1	1:B:607:MET:HE1	1.97	0.95
1:B:60:ALA:H	1:B:881:THR:HG21	1.31	0.94
1:A:394:LYS:HZ1	1:A:397:LEU:CD1	1.80	0.93
1:A:513:THR:O	1:A:571:ARG:NH2	2.02	0.93
1:A:380:LEU:HG	1:A:396:ARG:HH21	1.33	0.93
1:A:155:THR:HA	1:A:330:ILE:HD11	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:GLU:HB3	1:B:145:LYS:HZ1	0.75	0.92
1:A:800:THR:HG23	1:A:806:VAL:HG21	1.50	0.92
1:A:58:VAL:H	1:A:876:LYS:CE	1.83	0.92
1:B:814:ASN:ND2	1:B:841:SER:OG	2.02	0.92
1:A:879:ARG:HH12	1:A:883:ASP:HB2	1.33	0.91
1:B:141:GLU:C	1:B:145:LYS:NZ	2.25	0.90
1:B:239:ARG:HB2	2:D:8:DT:H3'	1.52	0.90
1:B:782:LEU:HG	1:B:798:MET:HE3	1.53	0.90
1:A:338:LYS:HD2	1:A:339:MET:H	1.34	0.90
1:B:141:GLU:HB3	1:B:145:LYS:CE	2.00	0.90
1:B:850:ILE:O	1:B:889:ARG:NH1	2.04	0.90
1:B:141:GLU:OE2	1:B:145:LYS:NZ	2.05	0.89
1:A:372:HIS:CD2	1:A:376:ILE:HD11	2.07	0.89
1:B:144:LYS:HA	1:B:147:LEU:HB3	1.54	0.88
1:A:141:GLU:OE2	1:A:144:LYS:HD2	1.72	0.88
1:B:691:ARG:CZ	1:B:814:ASN:OD1	2.22	0.88
1:B:691:ARG:NE	1:B:691:ARG:HA	1.77	0.88
1:A:182:LYS:NZ	1:A:310:SER:O	2.08	0.87
1:B:141:GLU:C	1:B:145:LYS:HZ3	1.78	0.87
1:B:545:ARG:HH21	1:B:546:PRO:HB2	1.40	0.87
1:A:74:ASP:OD2	1:A:77:ARG:NH2	2.07	0.86
1:B:691:ARG:HH11	1:B:814:ASN:HD21	1.15	0.86
1:B:654:ASP:OD1	1:B:734:LYS:NZ	2.09	0.85
1:A:832:LYS:HE3	1:A:833:SER:H	1.40	0.85
1:A:861:THR:HG23	1:A:862:GLN:H	1.39	0.85
1:B:141:GLU:CA	1:B:145:LYS:NZ	2.34	0.85
1:A:137:ARG:HA	1:A:140:GLU:OE2	1.77	0.85
1:A:67:ARG:HH21	1:A:70:GLU:HB2	0.88	0.85
1:A:139:LEU:CA	1:A:144:LYS:HE2	2.07	0.84
1:B:136:GLN:HG3	1:B:137:ARG:H	1.42	0.84
1:A:139:LEU:C	1:A:144:LYS:HE2	1.98	0.84
1:A:333:VAL:O	1:A:543:ARG:NH1	2.09	0.84
1:A:337:VAL:HG21	1:A:541:ALA:HB3	1.60	0.84
1:B:136:GLN:HB2	1:B:137:ARG:NE	1.92	0.83
1:A:490:ILE:HD12	1:A:537:ARG:NH2	1.93	0.83
1:A:832:LYS:HE3	1:A:833:SER:N	1.94	0.83
1:A:294:LEU:O	1:A:298:LEU:HD12	1.78	0.83
1:A:879:ARG:NH1	1:A:879:ARG:O	2.11	0.83
1:A:141:GLU:OE2	1:A:141:GLU:HA	1.78	0.83
1:A:338:LYS:HD2	1:A:339:MET:N	1.94	0.83
1:B:691:ARG:NH1	1:B:814:ASN:ND2	2.25	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:ARG:NH1	1:B:317:ASP:OD1	2.11	0.83
1:B:438:LEU:CD2	1:B:487:ILE:HD13	2.10	0.82
1:A:139:LEU:HA	1:A:144:LYS:CE	2.09	0.82
1:A:146:ARG:NH1	1:A:225:GLU:HA	1.94	0.82
1:B:515:TYR:OH	1:B:520:ASN:OD1	1.97	0.82
1:B:57:ASN:HA	1:B:876:LYS:HG2	1.60	0.82
1:A:146:ARG:HA	1:A:149:ALA:HB3	1.64	0.80
1:A:138:GLN:C	1:A:144:LYS:CE	2.44	0.79
1:B:112:THR:HG21	1:B:267:PRO:HG2	1.64	0.79
1:B:782:LEU:HG	1:B:798:MET:HE2	1.65	0.79
1:B:348:LYS:HE2	1:B:415:TYR:OH	1.82	0.79
1:B:59:SER:OG	1:B:876:LYS:NZ	2.15	0.79
1:A:418:GLU:OE2	1:A:453:TRP:NE1	2.14	0.79
1:B:924:SER:O	1:B:927:GLU:HG3	1.83	0.79
1:A:139:LEU:HA	1:A:144:LYS:HE2	1.65	0.78
1:B:802:ASP:OD2	1:B:804:ARG:NH1	2.15	0.78
1:B:115:ARG:HH12	1:B:116:ASN:ND2	1.82	0.78
1:A:144:LYS:HA	1:A:147:LEU:HB3	1.66	0.77
1:A:58:VAL:H	1:A:876:LYS:HE2	1.47	0.77
1:B:224:TYR:HD2	1:B:224:TYR:O	1.66	0.77
1:A:58:VAL:N	1:A:876:LYS:HE2	2.00	0.77
1:B:387:TYR:HB3	1:B:391:VAL:HG11	1.67	0.77
1:B:784:LYS:HE2	1:B:797:THR:OG1	1.85	0.77
1:B:380:LEU:HA	1:B:383:ILE:HG12	1.66	0.77
1:A:413:VAL:HA	1:A:416:ILE:HD12	1.67	0.77
1:A:150:ARG:NH1	1:A:185:GLN:OE1	2.18	0.77
1:A:478:PRO:HG3	1:A:484:LYS:HB3	1.67	0.77
1:A:713:GLU:HB3	1:A:714:ARG:NE	2.00	0.76
1:A:193:ASP:OD2	1:A:197:ARG:NH1	2.19	0.76
1:A:350:ASN:ND2	1:A:390:ARG:HH22	1.84	0.76
1:B:343:GLU:HB3	1:B:395:LEU:HD11	1.66	0.76
1:A:334:MET:SD	1:A:335:PHE:N	2.57	0.76
1:A:407:ASP:OD2	1:A:441:ILE:HD11	1.86	0.76
1:A:515:TYR:OH	1:A:520:ASN:OD1	2.04	0.76
1:A:376:ILE:C	1:A:396:ARG:HH22	1.89	0.75
1:A:879:ARG:NH1	1:A:883:ASP:HB2	2.01	0.75
1:A:520:ASN:O	1:A:830:ARG:NH2	2.19	0.75
1:B:705:ARG:NH1	1:B:753:LYS:HD3	2.02	0.75
1:A:57:ASN:HA	1:A:876:LYS:CE	2.15	0.74
1:B:680:ASP:OD2	1:B:684:ARG:NH1	2.20	0.74
1:B:856:VAL:HG11	1:B:889:ARG:NE	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:ILE:HD11	1:B:607:MET:HE2	1.65	0.74
1:A:145:LYS:HE3	1:A:146:ARG:HE	1.51	0.74
1:A:490:ILE:CD1	1:A:537:ARG:HH21	1.98	0.74
1:A:142:ASN:OD1	1:A:143:ALA:N	2.21	0.74
1:B:136:GLN:HG3	1:B:137:ARG:N	2.03	0.74
1:B:145:LYS:H	1:B:145:LYS:HD2	1.52	0.74
1:B:136:GLN:HB2	1:B:137:ARG:HE	1.50	0.73
1:A:832:LYS:CE	1:A:835:ASP:H	1.97	0.73
1:B:644:ILE:HG22	1:B:741:LEU:HD11	1.69	0.73
1:A:372:HIS:NE2	1:A:376:ILE:CD1	2.51	0.73
1:B:531:LYS:NZ	1:B:558:GLU:O	2.18	0.73
1:B:878:ASN:OD1	1:B:881:THR:N	2.21	0.73
1:A:131:GLN:HB2	1:A:195:ILE:O	1.89	0.73
1:A:205:ILE:HG22	1:A:274:VAL:CG1	2.18	0.73
1:A:376:ILE:HB	1:A:396:ARG:NH1	2.03	0.73
1:A:463:HIS:HB3	1:A:466:MET:HE2	1.69	0.72
1:A:418:GLU:OE1	1:A:418:GLU:N	2.21	0.72
1:B:783:ARG:CB	1:B:784:LYS:HZ1	2.02	0.72
1:A:60:ALA:H	1:A:881:THR:HG21	1.54	0.72
1:A:479:PRO:HB2	1:A:482:GLN:HG3	1.72	0.72
1:B:519:THR:HG23	1:B:521:ILE:HG23	1.71	0.72
1:A:430:PRO:HA	1:A:510:THR:HA	1.72	0.72
1:A:60:ALA:HB3	1:A:65:LEU:HD21	1.72	0.71
1:A:239:ARG:HB2	2:C:8:DT:H3'	1.72	0.71
1:B:204:ARG:NH1	1:B:247:GLU:O	2.22	0.71
1:A:186:VAL:HA	1:A:189:ILE:HD12	1.72	0.71
1:A:278:ASP:HA	1:A:309:MET:HB2	1.71	0.71
1:B:66:GLU:O	1:B:70:GLU:HG3	1.90	0.71
1:A:218:ILE:O	1:A:222:VAL:HG12	1.91	0.71
1:A:437:GLN:HA	1:A:440:ASN:HD22	1.55	0.71
1:A:268:LEU:O	1:A:301:ARG:HD3	1.91	0.71
1:B:369:ARG:HH12	1:B:396:ARG:HB3	1.56	0.71
1:B:658:SER:OG	1:B:734:LYS:HE3	1.91	0.70
1:B:412:LEU:O	1:B:416:ILE:HD12	1.90	0.70
1:B:145:LYS:O	1:B:149:ALA:N	2.24	0.70
1:A:106:GLU:OE1	1:A:106:GLU:N	2.23	0.70
1:B:784:LYS:HG3	1:B:796:HIS:HA	1.73	0.70
1:A:397:LEU:O	1:A:400:SER:OG	2.09	0.70
1:B:199:CYS:O	1:B:202:SER:OG	2.08	0.70
1:B:94:GLN:OE1	1:B:95:GLN:NE2	2.22	0.70
1:B:478:PRO:HG3	1:B:484:LYS:HB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:VAL:HB	1:B:538:ARG:HG3	1.74	0.69
1:B:340:LEU:HB3	1:B:344:ASP:HB2	1.73	0.69
1:A:424:ALA:HB3	1:A:501:VAL:HA	1.72	0.69
1:B:760:ASN:HB3	1:B:766:LEU:HD23	1.74	0.69
1:B:141:GLU:CG	1:B:145:LYS:HZ1	2.04	0.69
1:B:437:GLN:O	1:B:441:ILE:HD13	1.93	0.69
1:A:57:ASN:OD1	1:A:876:LYS:NZ	2.26	0.68
1:A:878:ASN:OD1	1:A:879:ARG:N	2.26	0.68
1:B:141:GLU:CD	1:B:145:LYS:HZ2	1.96	0.68
1:A:58:VAL:N	1:A:876:LYS:CE	2.56	0.68
1:A:372:HIS:CE1	1:A:376:ILE:CD1	2.70	0.68
1:B:122:VAL:HA	1:B:248:ARG:HH22	1.58	0.68
1:A:782:LEU:HD11	1:A:796:HIS:HB3	1.74	0.68
1:A:107:GLU:O	1:A:111:GLU:HG3	1.93	0.68
1:B:692:SER:CB	1:B:695:LEU:HG	2.24	0.68
1:A:139:LEU:CA	1:A:144:LYS:CE	2.67	0.68
1:A:715:ASP:OD2	1:A:719:LYS:HE3	1.94	0.68
1:A:760:ASN:HB3	1:A:766:LEU:HD23	1.75	0.68
1:A:798:MET:H	1:A:805:ARG:HH11	1.40	0.68
1:B:122:VAL:HA	1:B:248:ARG:NH2	2.08	0.68
1:B:141:GLU:CD	1:B:145:LYS:NZ	2.47	0.68
1:B:800:THR:OG1	1:B:802:ASP:OD1	2.11	0.68
1:A:139:LEU:N	1:A:144:LYS:HE3	2.08	0.67
1:B:421:PRO:O	1:B:483:ARG:NH2	2.27	0.67
1:B:692:SER:HB3	1:B:695:LEU:HG	1.75	0.67
1:A:832:LYS:HD3	1:A:835:ASP:O	1.95	0.67
1:B:108:PHE:O	1:B:112:THR:OG1	2.09	0.67
1:B:521:ILE:HG13	1:B:521:ILE:O	1.95	0.67
1:A:832:LYS:HE2	1:A:835:ASP:N	1.96	0.67
1:B:116:ASN:HB2	1:B:270:HIS:HB2	1.76	0.67
1:A:377:GLU:HA	1:A:396:ARG:NH2	2.09	0.67
1:A:380:LEU:HG	1:A:396:ARG:NH2	2.09	0.67
1:A:394:LYS:HD3	1:A:394:LYS:O	1.94	0.67
1:A:205:ILE:HD11	1:A:251:ILE:HG23	1.76	0.67
1:A:338:LYS:NZ	1:A:339:MET:O	2.21	0.67
1:B:124:PRO:HA	1:B:127:ASP:HB2	1.76	0.67
1:A:221:TRP:NE1	1:A:225:GLU:OE1	2.28	0.66
1:A:205:ILE:HD11	1:A:251:ILE:HD13	1.77	0.66
1:B:532:ALA:HB2	1:B:564:ILE:HG22	1.77	0.66
1:A:144:LYS:HA	1:A:147:LEU:CB	2.26	0.66
1:A:67:ARG:NH2	1:A:70:GLU:HB3	2.06	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:ARG:HD3	1:A:820:PHE:CD1	2.29	0.66
1:B:822:SER:H	1:B:843:MET:HE1	1.61	0.66
1:A:343:GLU:OE2	1:A:379:TYR:OH	2.12	0.66
1:B:144:LYS:CA	1:B:147:LEU:HB3	2.26	0.66
1:B:808:PHE:HZ	1:B:825:PHE:CE1	2.13	0.66
1:A:394:LYS:HZ2	1:A:397:LEU:CG	2.09	0.66
1:A:421:PRO:O	1:A:483:ARG:NH2	2.28	0.66
1:B:141:GLU:OE1	1:B:144:LYS:HB3	1.96	0.66
1:A:876:LYS:C	1:A:876:LYS:HD2	2.16	0.66
1:B:137:ARG:HD3	1:B:140:GLU:HB3	1.78	0.66
1:B:64:VAL:HG23	1:B:921:LEU:HD21	1.77	0.66
1:A:170:GLN:HE21	1:A:298:LEU:HD23	1.60	0.66
1:A:432:TYR:HB2	1:A:463:HIS:CE1	2.31	0.66
1:A:461:PRO:HB2	1:A:466:MET:CE	2.26	0.66
1:B:504:VAL:HG23	1:B:541:ALA:HB2	1.77	0.66
1:A:644:ILE:HG22	1:A:741:LEU:HD11	1.78	0.66
1:A:68:VAL:O	1:A:72:MET:HG3	1.96	0.66
1:B:186:VAL:HG21	1:B:309:MET:CE	2.26	0.65
1:B:430:PRO:HA	1:B:510:THR:HA	1.78	0.65
1:A:141:GLU:CD	1:A:144:LYS:HD2	2.16	0.65
1:A:186:VAL:O	1:A:190:LEU:HD12	1.96	0.65
1:A:578:ILE:HG22	1:A:589:PRO:HB3	1.77	0.65
1:A:509:ARG:NH2	1:A:526:GLU:HG2	2.11	0.65
1:A:713:GLU:HG3	1:A:714:ARG:NH2	2.11	0.65
1:B:502:VAL:HG11	1:B:545:ARG:HG2	1.78	0.65
1:B:265:SER:HB3	2:D:9:DT:H3	1.62	0.65
1:A:155:THR:HG23	1:A:180:CYS:O	1.96	0.64
1:A:146:ARG:HH11	1:A:225:GLU:HA	1.60	0.64
1:A:134:LEU:HD21	1:A:195:ILE:HG21	1.79	0.64
1:A:116:ASN:HB3	1:A:271:ASN:HD21	1.61	0.64
1:A:413:VAL:HG21	1:A:442:LEU:HD21	1.78	0.64
1:A:730:LEU:HA	1:A:733:MET:HE3	1.79	0.64
1:A:765:PRO:HG2	1:A:927:GLU:HG2	1.78	0.64
1:A:865:PRO:HB2	1:A:877:CYS:O	1.97	0.64
1:A:380:LEU:CG	1:A:396:ARG:HH21	2.10	0.64
1:B:141:GLU:CD	1:B:144:LYS:HB3	2.17	0.64
1:B:65:LEU:HD21	1:B:881:THR:HG22	1.79	0.64
1:B:342:LEU:HD21	1:B:400:SER:HB2	1.80	0.64
1:A:376:ILE:HB	1:A:396:ARG:CZ	2.28	0.64
1:B:533:ASN:O	1:B:537:ARG:HG3	1.98	0.63
1:B:146:ARG:HA	1:B:149:ALA:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:LEU:HD23	1:B:344:ASP:HB3	1.80	0.63
1:B:890:SER:O	1:B:893:GLU:HG2	1.99	0.63
1:A:675:LYS:O	1:A:679:VAL:N	2.30	0.63
1:B:260:LEU:HD21	1:B:290:LEU:HG	1.81	0.63
1:A:337:VAL:HG11	1:A:538:ARG:O	1.98	0.63
1:A:713:GLU:CB	1:A:714:ARG:HE	2.05	0.63
1:B:143:ALA:HB1	1:B:147:LEU:N	2.13	0.63
1:B:786:ARG:HG3	1:B:794:ALA:HA	1.81	0.63
1:A:137:ARG:HD2	1:A:137:ARG:N	2.12	0.63
1:A:432:TYR:HB2	1:A:463:HIS:ND1	2.13	0.63
1:A:566:THR:OG1	1:A:571:ARG:HD2	1.99	0.63
1:B:343:GLU:OE1	1:B:343:GLU:N	2.30	0.63
1:A:449:LYS:HZ1	1:A:453:TRP:HD1	1.45	0.63
1:A:483:ARG:HH21	1:A:503:TYR:HE2	1.46	0.63
1:A:67:ARG:NE	1:A:67:ARG:O	2.30	0.63
1:A:350:ASN:HD22	1:A:390:ARG:HH12	1.47	0.62
1:B:60:ALA:HB3	1:B:65:LEU:HD21	1.80	0.62
1:B:654:ASP:H	1:B:758:ASN:ND2	1.97	0.62
1:B:578:ILE:HG23	1:B:589:PRO:HG3	1.81	0.62
1:B:851:ILE:O	1:B:889:ARG:NH1	2.32	0.62
1:A:682:ILE:HD11	1:A:720:ASN:OD1	1.99	0.62
1:A:692:SER:CB	1:A:842:THR:HG22	2.29	0.62
1:A:738:SER:HB2	1:A:752:CYS:HB3	1.81	0.62
1:B:166:VAL:O	1:B:305:LYS:HE3	1.99	0.62
1:B:735:ASN:O	1:B:739:GLU:HG3	2.00	0.62
1:A:184:THR:OG1	1:A:185:GLN:HG2	1.99	0.62
1:A:713:GLU:HG3	1:A:714:ARG:HH21	1.63	0.62
1:A:333:VAL:C	1:A:543:ARG:HH12	2.03	0.61
1:B:729:GLN:O	1:B:733:MET:HG3	2.00	0.61
1:B:822:SER:H	1:B:843:MET:CE	2.13	0.61
1:A:567:PRO:HD2	1:A:570:LEU:HD12	1.82	0.61
1:B:783:ARG:HB2	1:B:784:LYS:HZ1	1.66	0.61
1:A:176:GLY:HA3	1:A:330:ILE:HG22	1.81	0.61
1:A:832:LYS:HD3	1:A:836:LEU:HA	1.80	0.61
1:A:463:HIS:HD2	1:A:464:SER:N	1.99	0.61
1:A:738:SER:OG	1:A:750:SER:O	2.17	0.61
1:A:372:HIS:CG	1:A:376:ILE:HD11	2.35	0.61
1:A:708:ARG:HH12	1:A:728:GLN:HE22	1.47	0.61
1:B:68:VAL:O	1:B:72:MET:HG3	2.01	0.61
1:A:154:PRO:O	1:A:157:LYS:HG2	2.01	0.61
1:B:274:VAL:HG22	1:B:305:LYS:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:SER:N	1:A:876:LYS:HZ1	1.99	0.61
1:B:781:HIS:C	1:B:783:ARG:HH12	2.04	0.60
1:B:60:ALA:N	1:B:881:THR:HG21	2.11	0.60
1:A:403:CYS:HB3	1:A:434:LYS:HD3	1.83	0.60
1:A:493:GLU:OE1	1:A:533:ASN:HB3	2.01	0.60
1:A:170:GLN:NE2	1:A:298:LEU:HB3	2.16	0.60
1:B:144:LYS:H	1:B:147:LEU:N	1.93	0.60
1:B:222:VAL:HG12	1:B:234:VAL:HG21	1.82	0.60
1:B:782:LEU:N	1:B:783:ARG:HH22	1.99	0.60
1:B:876:LYS:HD2	1:B:876:LYS:C	2.22	0.60
1:A:151:LYS:O	1:A:151:LYS:HG3	2.02	0.60
1:A:430:PRO:HD2	1:A:434:LYS:HD2	1.82	0.60
1:B:825:PHE:HD2	1:B:843:MET:HA	1.65	0.60
1:B:878:ASN:HD21	1:B:881:THR:CG2	2.14	0.60
1:A:321:TYR:CD1	1:A:597:ILE:HD13	2.36	0.60
1:A:352:GLU:CD	1:A:353:PHE:H	2.05	0.60
1:A:515:TYR:CD1	1:A:517:ILE:HD13	2.37	0.60
1:B:830:ARG:HD2	1:B:836:LEU:HD21	1.82	0.60
1:B:321:TYR:CD2	1:B:597:ILE:HG12	2.36	0.60
1:A:132:LEU:O	1:A:136:GLN:HG3	2.01	0.60
1:B:425:ILE:HB	1:B:485:VAL:HG22	1.82	0.60
1:B:141:GLU:OE1	1:B:141:GLU:HA	1.89	0.60
1:B:545:ARG:NE	1:B:546:PRO:O	2.34	0.60
1:A:463:HIS:HD2	1:A:464:SER:H	1.50	0.59
1:B:686:MET:CE	1:B:700:THR:HA	2.31	0.59
1:B:738:SER:OG	1:B:752:CYS:HB3	2.02	0.59
1:B:388:ASP:OD2	1:B:391:VAL:HG12	2.02	0.59
1:B:337:VAL:HG21	1:B:538:ARG:O	2.02	0.59
1:B:793:ARG:HG2	1:B:794:ALA:N	2.18	0.59
1:B:847:MET:HE2	1:B:922:LEU:HD22	1.83	0.59
1:A:654:ASP:OD2	1:A:734:LYS:NZ	2.30	0.59
1:A:899:LYS:HE2	1:A:912:GLU:OE1	2.03	0.59
1:B:691:ARG:HD3	1:B:814:ASN:ND2	2.17	0.59
1:B:141:GLU:OE2	1:B:144:LYS:HB3	2.01	0.59
1:B:438:LEU:HD23	1:B:487:ILE:HD13	1.84	0.59
1:B:417:CYS:HA	1:B:483:ARG:HH11	1.67	0.59
1:B:876:LYS:HD2	1:B:877:CYS:HA	1.84	0.59
1:A:708:ARG:HH12	1:A:728:GLN:NE2	2.00	0.59
1:B:134:LEU:HD23	1:B:138:GLN:HE21	1.68	0.59
1:B:429:LEU:HD12	1:B:435:ILE:HG22	1.84	0.59
1:B:592:PHE:O	1:B:595:THR:HG22	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:GLU:OE1	1:A:144:LYS:HB2	2.03	0.58
1:A:146:ARG:O	1:A:150:ARG:HG2	2.03	0.58
1:A:205:ILE:CD1	1:A:251:ILE:HD13	2.33	0.58
1:A:423:GLY:HA3	1:A:502:VAL:HG22	1.84	0.58
1:B:130:LEU:HA	1:B:133:GLU:HB3	1.84	0.58
1:B:192:ASP:OD1	1:B:226:ARG:NH2	2.35	0.58
1:A:175:VAL:HG12	1:A:312:THR:HG22	1.86	0.58
1:A:373:GLU:OE2	1:A:377:GLU:HG2	2.03	0.58
1:A:316:GLN:O	1:A:316:GLN:HG3	2.03	0.58
1:A:377:GLU:N	1:A:396:ARG:HH22	2.00	0.58
1:A:694:HIS:ND1	1:A:842:THR:HG23	2.18	0.58
1:B:519:THR:OG1	1:B:804:ARG:NE	2.36	0.58
1:A:676:GLU:CD	1:A:677:SER:H	2.06	0.58
1:A:832:LYS:CD	1:A:836:LEU:HA	2.33	0.58
1:A:59:SER:N	1:A:876:LYS:NZ	2.52	0.58
1:A:199:CYS:O	1:A:202:SER:OG	2.17	0.58
1:A:67:ARG:HH21	1:A:70:GLU:CA	2.13	0.58
1:A:704:TYR:O	1:A:708:ARG:HG3	2.04	0.58
1:B:295:LYS:HE3	1:B:321:TYR:CE1	2.38	0.58
1:A:104:ASN:OD1	1:A:107:GLU:HG2	2.03	0.58
1:A:751:ASN:HD21	1:A:753:LYS:HG3	1.69	0.58
1:B:354:GLN:HG3	1:B:355:LYS:H	1.68	0.58
1:B:75:TYR:CD2	1:B:915:LEU:HD12	2.38	0.58
1:A:335:PHE:CE2	1:A:545:ARG:HA	2.39	0.57
1:A:463:HIS:CD2	1:A:464:SER:N	2.72	0.57
1:A:769:ALA:HB1	1:A:852:PHE:CE2	2.39	0.57
1:B:112:THR:CG2	1:B:115:ARG:HH21	2.17	0.57
1:B:708:ARG:HG2	1:B:713:GLU:HB3	1.85	0.57
1:B:259:LEU:HD23	1:B:290:LEU:HD11	1.86	0.57
1:B:339:MET:HG3	1:B:538:ARG:HH21	1.69	0.57
1:B:609:VAL:HG12	1:B:613:LYS:HE2	1.85	0.57
1:A:283:ARG:NH1	1:A:288:ASP:OD1	2.37	0.57
1:A:515:TYR:HD1	1:A:517:ILE:HD13	1.68	0.57
1:B:136:GLN:C	1:B:137:ARG:HE	2.08	0.57
1:B:523:SER:HA	1:B:832:LYS:O	2.04	0.57
1:B:668:PRO:HB2	1:B:722:LEU:HD23	1.85	0.57
1:A:449:LYS:NZ	1:A:449:LYS:O	2.35	0.57
1:A:814:ASN:OD1	1:A:841:SER:OG	2.23	0.57
1:B:133:GLU:HA	1:B:136:GLN:NE2	2.19	0.57
1:B:426:LEU:HD11	1:B:428:PHE:CE2	2.39	0.57
1:A:145:LYS:CE	1:A:146:ARG:HE	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:ARG:CZ	1:A:526:GLU:HG2	2.35	0.57
1:B:878:ASN:HD21	1:B:881:THR:HG23	1.70	0.57
1:A:394:LYS:NZ	1:A:397:LEU:CB	2.60	0.57
1:B:484:LYS:CD	1:B:486:ILE:HD11	2.35	0.57
1:B:57:ASN:HA	1:B:876:LYS:CG	2.34	0.57
1:B:133:GLU:HG3	1:B:136:GLN:NE2	2.20	0.57
1:B:515:TYR:CB	1:B:522:GLN:OE1	2.53	0.57
1:A:91:ALA:HB2	1:A:902:TYR:HD2	1.70	0.56
1:B:463:HIS:HB3	1:B:466:MET:HG3	1.87	0.56
1:B:515:TYR:HB3	1:B:522:GLN:OE1	2.06	0.56
1:B:867:LEU:HB3	1:B:877:CYS:HB2	1.87	0.56
1:A:394:LYS:NZ	1:A:397:LEU:CG	2.67	0.56
1:B:410:ALA:HB2	1:B:441:ILE:HG21	1.87	0.56
1:A:614:ARG:NH2	1:A:854:ASP:OD1	2.36	0.56
1:B:391:VAL:HA	1:B:394:LYS:HE2	1.88	0.56
1:B:401:GLU:CD	1:B:557:ARG:HH21	2.09	0.56
1:A:861:THR:HG23	1:A:862:GLN:N	2.17	0.56
1:A:57:ASN:C	1:A:876:LYS:HE2	2.25	0.56
1:B:97:PHE:O	1:B:101:LEU:HD12	2.04	0.56
1:B:899:LYS:HE3	1:B:912:GLU:OE1	2.05	0.56
1:A:382:ARG:HB2	1:A:382:ARG:NH1	2.21	0.56
1:A:454:ARG:NH1	1:A:455:ASP:OD1	2.38	0.56
1:A:334:MET:HE1	1:A:542:GLY:HA2	1.87	0.56
1:A:568:GLU:O	1:A:572:SER:OG	2.24	0.56
1:A:121:TRP:CD2	1:B:123:ASN:HB2	2.40	0.56
1:B:377:GLU:OE2	1:B:396:ARG:NH1	2.38	0.56
1:A:629:MET:O	1:A:633:LYS:HG3	2.06	0.56
1:A:59:SER:H	1:A:876:LYS:NZ	2.03	0.56
1:B:337:VAL:O	1:B:538:ARG:NH1	2.38	0.56
1:A:372:HIS:CD2	1:A:376:ILE:CD1	2.85	0.56
1:B:649:LEU:HB3	1:B:906:ILE:HD11	1.88	0.56
1:A:170:GLN:HG3	1:A:304:LEU:O	2.05	0.56
1:B:268:LEU:HD23	1:B:300:HIS:HB2	1.87	0.56
1:B:505:ILE:HG22	1:B:550:TYR:HB2	1.87	0.56
1:A:337:VAL:HG13	1:A:538:ARG:HG3	1.88	0.55
1:A:67:ARG:CZ	1:A:70:GLU:HB2	2.24	0.55
1:A:104:ASN:C	1:A:585:HIS:HE1	2.10	0.55
1:A:527:VAL:HG12	1:A:528:TRP:O	2.05	0.55
1:A:715:ASP:OD2	1:A:719:LYS:CE	2.55	0.55
1:B:691:ARG:NH1	1:B:814:ASN:HD21	1.95	0.55
1:A:372:HIS:CD2	1:A:398:PRO:HG3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:ASN:ND2	1:A:390:ARG:HH12	2.04	0.55
1:A:434:LYS:HA	1:A:437:GLN:HG2	1.88	0.55
1:A:924:SER:O	1:A:927:GLU:HG3	2.07	0.55
1:B:553:PHE:HB2	1:B:557:ARG:HG2	1.88	0.55
1:B:908:GLU:CD	1:B:908:GLU:H	2.10	0.55
1:A:188:GLN:NE2	1:A:222:VAL:HG23	2.21	0.55
1:A:429:LEU:HD13	1:A:434:LYS:HG2	1.89	0.55
1:A:476:ARG:O	1:A:484:LYS:NZ	2.34	0.55
1:B:144:LYS:N	1:B:147:LEU:H	1.93	0.55
1:B:294:LEU:HB3	1:B:298:LEU:HG	1.88	0.55
1:A:614:ARG:HH21	1:A:854:ASP:CG	2.10	0.55
1:A:782:LEU:CD1	1:A:796:HIS:HB3	2.36	0.55
1:B:882:ALA:O	1:B:886:ILE:HG12	2.07	0.55
1:A:208:THR:CG2	1:A:256:THR:HG22	2.36	0.55
1:A:290:LEU:O	1:A:294:LEU:HD12	2.07	0.55
1:A:861:THR:HG22	1:A:864:THR:O	2.06	0.55
1:B:783:ARG:H	1:B:784:LYS:NZ	2.05	0.55
1:A:782:LEU:HD21	1:A:798:MET:SD	2.46	0.55
1:A:876:LYS:HD2	1:A:877:CYS:HA	1.88	0.55
1:B:140:GLU:HG3	1:B:142:ASN:HB2	1.88	0.55
1:A:150:ARG:HA	1:A:153:LEU:HD12	1.89	0.55
1:A:681:GLU:HG2	1:A:682:ILE:N	2.22	0.55
1:B:529:VAL:HG13	1:B:533:ASN:HB2	1.88	0.55
1:A:781:HIS:HB2	1:A:873:TYR:HE2	1.72	0.55
1:B:133:GLU:HG3	1:B:136:GLN:OE1	2.07	0.54
1:B:187:PRO:HB2	1:B:251:ILE:HD13	1.88	0.54
1:B:484:LYS:HD2	1:B:486:ILE:HD11	1.88	0.54
1:B:705:ARG:HH12	1:B:753:LYS:HD3	1.71	0.54
2:C:6:DT:H6	2:C:6:DT:H5'	1.72	0.54
1:A:405:ASP:OD2	1:A:408:PHE:N	2.40	0.54
1:A:497:THR:HA	1:A:540:ARG:NH1	2.21	0.54
1:A:899:LYS:NZ	1:A:904:ALA:O	2.35	0.54
1:B:186:VAL:HG21	1:B:309:MET:HE3	1.90	0.54
1:B:760:ASN:HB3	1:B:766:LEU:CD2	2.36	0.54
1:B:54:LEU:HA	1:B:874:TYR:O	2.07	0.54
1:A:654:ASP:O	1:A:734:LYS:NZ	2.39	0.54
1:B:428:PHE:O	1:B:507:SER:HB2	2.07	0.54
1:A:131:GLN:OE1	1:A:198:GLY:N	2.41	0.54
1:A:208:THR:HG23	1:A:256:THR:HA	1.89	0.54
1:A:205:ILE:CG1	1:A:251:ILE:HD13	2.37	0.54
1:B:454:ARG:HH11	1:B:454:ARG:HG2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:ASP:OD2	1:B:517:ILE:N	2.41	0.54
1:B:832:LYS:HB2	1:B:836:LEU:CD1	2.38	0.54
1:A:294:LEU:HA	1:A:297:ILE:HB	1.90	0.54
1:A:335:PHE:CD2	1:A:546:PRO:HD3	2.42	0.54
1:B:112:THR:HG21	1:B:267:PRO:CG	2.37	0.54
1:B:291:MET:HA	1:B:294:LEU:HD12	1.90	0.54
1:A:417:CYS:HB3	1:A:453:TRP:CH2	2.42	0.54
1:B:693:ASP:OD1	1:B:813:VAL:HG22	2.08	0.54
1:B:164:GLN:O	1:B:168:GLU:HG3	2.08	0.54
1:A:205:ILE:HG22	1:A:274:VAL:HG12	1.89	0.53
1:A:879:ARG:HH11	1:A:879:ARG:C	2.10	0.53
1:B:179:GLY:O	1:B:333:VAL:HB	2.07	0.53
1:B:515:TYR:CZ	1:B:520:ASN:HA	2.43	0.53
1:B:519:THR:OG1	1:B:804:ARG:CZ	2.55	0.53
1:B:821:ASP:N	1:B:821:ASP:OD1	2.40	0.53
1:A:372:HIS:ND1	1:A:376:ILE:HD11	2.17	0.53
1:A:506:ASN:HB3	1:A:551:ASN:OD1	2.09	0.53
1:B:142:ASN:HD21	1:B:227:CYS:HB2	1.72	0.53
1:A:268:LEU:O	1:A:301:ARG:CD	2.57	0.53
1:A:376:ILE:HB	1:A:396:ARG:NH2	2.23	0.53
1:A:682:ILE:HD13	1:A:720:ASN:HA	1.90	0.53
1:B:568:GLU:OE2	1:B:571:ARG:NH2	2.38	0.53
1:A:140:GLU:N	1:A:144:LYS:HE2	2.23	0.53
1:A:220:GLU:O	1:A:223:SER:OG	2.26	0.53
1:A:346:LEU:HA	1:A:349:THR:OG1	2.08	0.53
1:B:53:ARG:HD2	1:B:54:LEU:H	1.73	0.53
1:A:438:LEU:HA	1:A:441:ILE:HG22	1.90	0.53
1:A:232:ASN:O	1:A:246:ARG:HG2	2.08	0.53
1:A:312:THR:OG1	1:A:312:THR:O	2.22	0.53
1:A:497:THR:HA	1:A:540:ARG:HH12	1.73	0.53
1:A:898:LYS:HG3	1:A:902:TYR:HD1	1.74	0.53
1:B:281:HIS:HB3	1:B:310:SER:OG	2.08	0.53
1:A:182:LYS:HG3	1:A:183:THR:HG23	1.89	0.53
1:A:205:ILE:HG12	1:A:251:ILE:HD13	1.91	0.53
1:A:908:GLU:OE1	1:A:913:LYS:HE2	2.09	0.53
1:B:515:TYR:CE1	1:B:520:ASN:HA	2.44	0.53
1:B:57:ASN:ND2	1:B:876:LYS:HE2	2.23	0.53
1:A:377:GLU:HA	1:A:396:ARG:HH22	1.73	0.53
1:B:728:GLN:O	1:B:732:ARG:HG3	2.07	0.53
1:A:121:TRP:HZ3	1:B:248:ARG:CZ	2.21	0.53
1:A:138:GLN:O	1:A:144:LYS:CE	2.47	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ASP:HA	1:A:195:ILE:HG22	1.90	0.53
1:B:208:THR:HG23	1:B:256:THR:HG22	1.91	0.53
1:B:516:ASP:HB3	1:B:518:GLU:CD	2.28	0.53
1:B:768:ARG:HH21	1:B:843:MET:HG2	1.72	0.53
1:B:133:GLU:HG3	1:B:136:GLN:CD	2.29	0.52
1:B:321:TYR:OH	1:B:595:THR:O	2.21	0.52
1:B:654:ASP:H	1:B:758:ASN:HD21	1.56	0.52
1:B:764:ILE:O	1:B:768:ARG:HG3	2.09	0.52
1:B:861:THR:HG23	1:B:862:GLN:OE1	2.09	0.52
1:A:832:LYS:HZ3	1:A:835:ASP:C	2.13	0.52
1:A:447:THR:HG22	1:A:449:LYS:H	1.72	0.52
1:B:268:LEU:O	1:B:301:ARG:HD3	2.10	0.52
1:A:291:MET:HA	1:A:294:LEU:HD12	1.90	0.52
1:A:208:THR:HG22	1:A:256:THR:HG22	1.92	0.52
1:A:829:GLN:HB3	1:A:839:LEU:HD12	1.91	0.52
1:A:881:THR:O	1:A:885:VAL:HG13	2.09	0.52
1:B:691:ARG:CD	1:B:814:ASN:OD1	2.57	0.52
2:D:6:DT:H5'	2:D:6:DT:H6	1.74	0.52
1:B:208:THR:CG2	1:B:256:THR:HG22	2.40	0.52
1:B:594:GLN:O	1:B:594:GLN:HG2	2.09	0.52
1:A:372:HIS:O	1:A:376:ILE:HG13	2.09	0.52
1:A:515:TYR:N	1:A:522:GLN:HE21	2.07	0.52
1:B:403:CYS:HB3	1:B:507:SER:OG	2.10	0.52
1:B:137:ARG:HD3	1:B:140:GLU:CB	2.39	0.52
1:B:515:TYR:OH	1:B:520:ASN:HA	2.09	0.52
1:B:878:ASN:OD1	1:B:880:GLU:N	2.42	0.52
1:B:208:THR:HG21	1:B:277:LEU:HD12	1.90	0.52
1:B:830:ARG:HB2	1:B:838:LEU:HD23	1.92	0.52
1:B:506:ASN:OD1	1:B:508:GLY:N	2.38	0.52
1:B:907:GLU:O	1:B:913:LYS:HB2	2.10	0.52
1:B:130:LEU:O	1:B:134:LEU:N	2.44	0.51
1:B:518:GLU:HB2	1:B:519:THR:HG22	1.91	0.51
1:A:150:ARG:HD2	1:A:185:GLN:NE2	2.25	0.51
1:A:170:GLN:HE21	1:A:298:LEU:CD2	2.23	0.51
1:B:152:LYS:HD3	1:B:152:LYS:N	2.25	0.51
1:A:140:GLU:N	1:A:140:GLU:OE2	2.43	0.51
1:A:141:GLU:OE2	1:A:144:LYS:CD	2.53	0.51
1:B:417:CYS:HA	1:B:483:ARG:NH1	2.25	0.51
1:B:64:VAL:HG21	1:B:925:LEU:HD11	1.91	0.51
1:A:569:ILE:HD13	1:A:596:LEU:HD13	1.93	0.51
1:B:406:ILE:HG23	1:B:438:LEU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:LEU:HB3	1:A:344:ASP:HB2	1.91	0.51
1:A:59:SER:H	1:A:876:LYS:HZ3	1.59	0.51
1:B:784:LYS:HG3	1:B:797:THR:H	1.75	0.51
1:B:146:ARG:O	1:B:150:ARG:HG2	2.11	0.51
1:B:406:ILE:CG2	1:B:438:LEU:HB2	2.41	0.51
1:B:424:ALA:HB3	1:B:501:VAL:HA	1.93	0.51
1:A:401:GLU:HA	1:A:552:LEU:O	2.10	0.51
1:B:136:GLN:HB2	1:B:137:ARG:CZ	2.41	0.51
1:B:143:ALA:HA	1:B:146:ARG:HB2	1.93	0.51
1:B:781:HIS:CD2	1:B:783:ARG:CZ	2.94	0.51
1:A:505:ILE:HG12	1:A:550:TYR:HD1	1.74	0.50
1:B:522:GLN:O	1:B:831:GLN:HA	2.10	0.50
1:A:394:LYS:NZ	1:A:397:LEU:HB2	2.08	0.50
1:B:876:LYS:HD2	1:B:877:CYS:CA	2.40	0.50
1:B:106:GLU:N	1:B:106:GLU:OE1	2.44	0.50
1:B:686:MET:HE1	1:B:700:THR:HA	1.93	0.50
1:B:899:LYS:NZ	1:B:904:ALA:HB3	2.26	0.50
1:A:114:GLU:N	1:A:114:GLU:OE1	2.40	0.50
1:A:322:PHE:O	1:A:323:ASN:ND2	2.45	0.50
1:A:474:VAL:HG13	1:A:475:PHE:CD1	2.45	0.50
1:A:533:ASN:O	1:A:537:ARG:HG3	2.12	0.50
1:A:712:ALA:O	1:A:715:ASP:HB3	2.11	0.50
1:B:222:VAL:O	1:B:226:ARG:HG3	2.12	0.50
1:B:438:LEU:HD22	1:B:487:ILE:HD13	1.92	0.50
1:A:333:VAL:O	1:A:334:MET:HB2	2.12	0.50
1:B:529:VAL:CG1	1:B:533:ASN:HB2	2.41	0.50
1:B:865:PRO:HB2	1:B:877:CYS:O	2.11	0.50
1:A:822:SER:OG	1:A:844:VAL:O	2.22	0.50
1:A:152:LYS:HE3	1:A:153:LEU:HG	1.93	0.50
1:B:876:LYS:HD2	1:B:877:CYS:N	2.27	0.50
1:A:301:ARG:NH2	1:A:304:LEU:HB2	2.27	0.50
1:B:316:GLN:HG3	1:B:316:GLN:O	2.11	0.50
1:B:682:ILE:HD11	1:B:720:ASN:OD1	2.12	0.50
1:A:135:GLY:HA2	1:A:138:GLN:NE2	2.27	0.49
1:A:479:PRO:HG2	1:A:482:GLN:HE21	1.77	0.49
1:A:66:GLU:O	1:A:70:GLU:HG3	2.11	0.49
1:A:778:ASN:O	1:A:826:VAL:HA	2.12	0.49
1:B:691:ARG:NE	1:B:814:ASN:OD1	2.45	0.49
1:A:627:LEU:O	1:A:631:LEU:HG	2.12	0.49
1:B:491:ILE:HG12	1:B:496:VAL:HG23	1.93	0.49
1:B:145:LYS:N	1:B:145:LYS:HD2	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:ARG:NH1	1:B:528:TRP:CD1	2.81	0.49
1:B:548:ILE:HG13	1:B:550:TYR:CE2	2.46	0.49
1:B:887:GLN:O	1:B:891:ASN:ND2	2.45	0.49
1:A:187:PRO:HB2	1:A:251:ILE:HD12	1.94	0.49
1:B:429:LEU:HB3	1:B:430:PRO:HD2	1.93	0.49
1:B:730:LEU:O	1:B:734:LYS:HG3	2.12	0.49
1:A:154:PRO:HG2	1:A:180:CYS:HA	1.95	0.49
1:A:514:ASN:C	1:A:522:GLN:HG3	2.32	0.49
1:A:67:ARG:C	1:A:67:ARG:HE	2.15	0.49
1:B:170:GLN:OE1	1:B:298:LEU:HB3	2.13	0.49
1:B:312:THR:HA	1:B:315:GLU:HG3	1.95	0.49
1:B:346:LEU:HD21	1:B:408:PHE:CE2	2.47	0.49
1:B:380:LEU:HA	1:B:383:ILE:CG1	2.40	0.49
1:B:633:LYS:HA	1:B:633:LYS:HE2	1.94	0.49
1:B:391:VAL:HA	1:B:394:LYS:CE	2.43	0.49
1:B:497:THR:HG22	1:B:540:ARG:HH22	1.78	0.49
1:B:676:GLU:HA	1:B:679:VAL:HG12	1.95	0.49
1:B:781:HIS:CE1	1:B:783:ARG:NH2	2.80	0.49
1:B:782:LEU:C	1:B:783:ARG:NH2	2.66	0.49
1:B:783:ARG:CG	1:B:784:LYS:HZ1	2.24	0.49
1:A:65:LEU:HD11	1:A:881:THR:HG22	1.95	0.49
1:B:112:THR:HG23	1:B:115:ARG:HH21	1.78	0.49
1:B:454:ARG:HG2	1:B:454:ARG:NH1	2.26	0.49
1:B:713:GLU:OE1	1:B:713:GLU:N	2.43	0.49
1:A:463:HIS:CB	1:A:466:MET:HE2	2.41	0.49
1:A:515:TYR:OH	1:A:520:ASN:HA	2.13	0.49
1:A:681:GLU:N	1:A:681:GLU:OE1	2.46	0.49
1:B:545:ARG:NH2	1:B:546:PRO:HB2	2.19	0.49
1:A:131:GLN:HA	1:A:195:ILE:HG12	1.95	0.48
1:A:548:ILE:HD11	1:A:550:TYR:OH	2.13	0.48
1:B:470:GLU:HG3	1:B:670:TYR:OH	2.12	0.48
1:B:568:GLU:OE1	1:B:571:ARG:NH1	2.28	0.48
1:B:817:GLU:N	1:B:817:GLU:OE1	2.46	0.48
1:A:155:THR:HG21	1:A:182:LYS:HA	1.94	0.48
1:A:57:ASN:OD1	1:A:876:LYS:CE	2.60	0.48
1:B:908:GLU:OE2	1:B:908:GLU:N	2.36	0.48
1:A:335:PHE:CD2	1:A:545:ARG:HA	2.48	0.48
1:B:142:ASN:HD21	1:B:227:CYS:CB	2.25	0.48
1:B:435:ILE:HD12	1:B:673:LEU:HD11	1.96	0.48
1:B:885:VAL:HA	1:B:888:LEU:HB3	1.95	0.48
1:A:342:LEU:HA	1:A:345:VAL:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ARG:HD2	1:A:185:GLN:HE22	1.77	0.48
1:A:351:TYR:HE1	1:A:353:PHE:CD1	2.32	0.48
1:B:224:TYR:C	1:B:224:TYR:HD2	2.17	0.48
1:B:343:GLU:OE2	1:B:555:ARG:NH1	2.38	0.48
1:B:857:GLU:OE2	1:B:871:LYS:NZ	2.34	0.48
1:A:574:LEU:HD11	1:A:604:ALA:HB1	1.95	0.48
1:B:184:THR:OG1	1:B:185:GLN:HG2	2.14	0.48
1:B:691:ARG:HE	1:B:691:ARG:C	2.17	0.48
2:C:4:DT:H5"	2:C:4:DT:H6	1.78	0.48
1:B:751:ASN:HB3	1:B:754:ASP:HB2	1.95	0.48
1:A:850:ILE:O	1:A:889:ARG:HD2	2.14	0.48
1:B:412:LEU:HD11	1:B:505:ILE:HG21	1.95	0.48
1:A:473:ALA:HA	1:A:476:ARG:HD2	1.96	0.48
1:A:532:ALA:HB2	1:A:564:ILE:HG22	1.96	0.48
1:B:61:PRO:HD2	1:B:925:LEU:HD21	1.96	0.48
1:A:449:LYS:NZ	1:A:453:TRP:HD1	2.11	0.47
1:B:568:GLU:CD	1:B:571:ARG:HH12	2.15	0.47
1:B:609:VAL:O	1:B:613:LYS:HG2	2.13	0.47
1:A:59:SER:OG	1:A:876:LYS:NZ	2.47	0.47
1:A:865:PRO:O	1:A:877:CYS:N	2.43	0.47
1:B:354:GLN:CG	1:B:355:LYS:N	2.77	0.47
1:B:466:MET:HE1	1:B:673:LEU:HG	1.95	0.47
1:B:133:GLU:CG	1:B:133:GLU:O	2.62	0.47
1:B:684:ARG:NH1	1:B:813:VAL:HA	2.28	0.47
1:A:354:GLN:CD	1:A:355:LYS:H	2.18	0.47
1:A:879:ARG:HH22	1:A:883:ASP:HB2	1.79	0.47
1:B:376:ILE:HD12	1:B:395:LEU:O	2.14	0.47
1:B:376:ILE:HG22	1:B:380:LEU:HG	1.96	0.47
1:B:777:PRO:O	1:B:779:MET:HG3	2.14	0.47
1:A:429:LEU:HB3	1:A:430:PRO:HD2	1.96	0.47
1:B:908:GLU:O	1:B:913:LYS:HG2	2.14	0.47
1:A:375:MET:HB2	1:A:560:ARG:NH1	2.30	0.47
1:A:93:PHE:HA	1:A:96:GLN:HG2	1.96	0.47
1:B:186:VAL:HG21	1:B:309:MET:HE1	1.97	0.47
1:A:256:THR:HG21	1:A:287:THR:HG23	1.95	0.47
1:A:337:VAL:HG13	1:A:337:VAL:O	2.14	0.47
1:A:394:LYS:NZ	1:A:397:LEU:HD22	2.29	0.47
1:A:434:LYS:HB2	1:A:434:LYS:HE3	1.61	0.47
1:A:431:GLY:O	1:A:435:ILE:HG13	2.14	0.47
1:B:185:GLN:O	1:B:189:ILE:HG13	2.14	0.47
1:B:175:VAL:HG21	1:B:315:GLU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:LEU:HD21	1:B:395:LEU:HD12	1.97	0.47
1:B:447:THR:HG22	1:B:449:LYS:H	1.80	0.47
1:A:124:PRO:O	1:A:127:ASP:HB2	2.15	0.47
1:A:376:ILE:HG22	1:A:396:ARG:NH2	2.30	0.47
1:A:412:LEU:O	1:A:416:ILE:HD12	2.15	0.47
1:A:406:ILE:CG1	1:A:438:LEU:HB2	2.44	0.47
1:A:67:ARG:HH22	1:A:70:GLU:HB3	1.77	0.47
1:A:879:ARG:O	1:A:882:ALA:HB3	2.15	0.47
1:B:131:GLN:O	1:B:131:GLN:HG2	2.13	0.47
1:B:372:HIS:CD2	1:B:396:ARG:O	2.68	0.47
1:B:880:GLU:N	1:B:880:GLU:OE1	2.41	0.47
1:A:682:ILE:CD1	1:A:720:ASN:HA	2.45	0.47
1:A:730:LEU:O	1:A:734:LYS:HG3	2.15	0.47
1:A:768:ARG:NH1	1:A:843:MET:O	2.40	0.47
1:B:224:TYR:CD2	1:B:224:TYR:O	2.57	0.47
1:B:269:MET:HB3	1:B:272:LEU:HD21	1.96	0.47
1:B:655:PRO:O	1:B:658:SER:HB2	2.15	0.47
1:A:407:ASP:CG	1:A:441:ILE:HD11	2.35	0.47
1:A:928:ARG:NE	1:A:928:ARG:HA	2.30	0.47
1:B:336:PRO:HD2	1:B:546:PRO:HA	1.97	0.47
1:B:338:LYS:HA	1:B:338:LYS:HD3	1.77	0.47
1:B:388:ASP:OD2	1:B:391:VAL:N	2.46	0.47
1:B:375:MET:HE1	1:B:557:ARG:NH2	2.30	0.47
1:B:647:SER:HB2	1:B:656:ILE:HG13	1.97	0.47
1:B:691:ARG:O	1:B:691:ARG:HG3	2.15	0.47
1:A:438:LEU:O	1:A:441:ILE:HG22	2.14	0.46
1:A:211:ARG:NH2	1:A:494:THR:HB	2.30	0.46
1:A:568:GLU:OE2	1:A:571:ARG:NH1	2.48	0.46
1:A:807:ASN:O	1:A:837:PHE:HA	2.14	0.46
1:B:256:THR:HG21	1:B:287:THR:HG23	1.97	0.46
1:B:784:LYS:HA	1:B:784:LYS:HD3	1.33	0.46
1:B:258:VAL:O	1:B:262:GLN:HG3	2.15	0.46
1:B:456:HIS:N	1:B:456:HIS:CD2	2.84	0.46
1:B:474:VAL:HG23	1:B:475:PHE:CD1	2.50	0.46
1:A:901:LEU:HA	1:A:901:LEU:HD23	1.77	0.46
1:B:776:TYR:OH	1:B:870:ALA:HB2	2.15	0.46
1:B:121:TRP:O	1:B:248:ARG:NH2	2.40	0.46
1:B:784:LYS:CG	1:B:797:THR:H	2.28	0.46
1:A:276:ILE:HG12	1:A:307:ILE:HB	1.98	0.46
1:A:394:LYS:NZ	1:A:397:LEU:H	2.13	0.46
1:A:846:PRO:HB3	1:A:875:PHE:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:893:GLU:O	1:A:897:LEU:HD12	2.15	0.46
1:B:162:ILE:O	1:B:166:VAL:HG13	2.14	0.46
1:B:419:ASN:N	1:B:419:ASN:OD1	2.45	0.46
1:B:786:ARG:CG	1:B:794:ALA:HA	2.44	0.46
1:B:846:PRO:HB3	1:B:875:PHE:CZ	2.50	0.46
1:B:769:ALA:HB1	1:B:852:PHE:CE2	2.50	0.46
1:A:473:ALA:O	1:A:476:ARG:HB2	2.14	0.46
1:A:574:LEU:O	1:A:578:ILE:HG12	2.15	0.46
1:A:605:ILE:O	1:A:609:VAL:HG23	2.15	0.46
1:B:654:ASP:HB2	1:B:752:CYS:O	2.16	0.46
1:B:784:LYS:CE	1:B:797:THR:OG1	2.60	0.46
1:A:188:GLN:HE21	1:A:222:VAL:HG23	1.81	0.46
1:A:854:ASP:HA	1:A:889:ARG:HH22	1.80	0.46
1:B:208:THR:HG23	1:B:256:THR:CG2	2.45	0.46
1:B:438:LEU:HD21	1:B:442:LEU:HD11	1.98	0.46
1:B:784:LYS:NZ	1:B:797:THR:O	2.45	0.46
1:A:176:GLY:CA	1:A:330:ILE:HG22	2.44	0.46
1:A:376:ILE:CB	1:A:396:ARG:NH2	2.79	0.46
1:B:268:LEU:CD2	1:B:300:HIS:HB2	2.46	0.46
1:B:64:VAL:HG23	1:B:921:LEU:CD2	2.45	0.46
1:B:209:GLN:O	1:B:255:THR:HA	2.16	0.46
1:B:409:ILE:HG12	1:B:552:LEU:HD11	1.98	0.46
1:B:881:THR:O	1:B:885:VAL:HG13	2.16	0.46
1:A:390:ARG:HA	1:A:393:ASP:HB2	1.97	0.46
1:A:423:GLY:HA3	1:A:502:VAL:CG2	2.44	0.46
1:A:104:ASN:C	1:A:585:HIS:CE1	2.88	0.46
1:B:141:GLU:CG	1:B:145:LYS:NZ	2.70	0.46
1:B:293:LEU:O	1:B:296:VAL:HG22	2.15	0.46
1:B:519:THR:CG2	1:B:521:ILE:HG12	2.46	0.46
1:B:515:TYR:CD1	1:B:521:ILE:O	2.69	0.46
1:B:74:ASP:HA	1:B:77:ARG:NH2	2.31	0.46
1:A:334:MET:SD	1:A:335:PHE:CD2	3.10	0.45
1:A:373:GLU:OE2	1:A:396:ARG:NH1	2.49	0.45
1:A:486:ILE:HD13	1:A:498:ILE:HD13	1.98	0.45
1:A:644:ILE:CG2	1:A:741:LEU:HD11	2.46	0.45
1:A:691:ARG:NH1	1:A:820:PHE:HA	2.31	0.45
1:B:618:LEU:HD12	1:B:618:LEU:N	2.30	0.45
1:B:686:MET:HE2	1:B:700:THR:N	2.31	0.45
1:A:860:VAL:HG22	1:A:865:PRO:HA	1.98	0.45
1:B:224:TYR:CD2	1:B:224:TYR:C	2.90	0.45
1:B:246:ARG:HD2	1:B:248:ARG:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:867:LEU:CB	1:B:877:CYS:HB2	2.45	0.45
1:A:269:MET:HB3	1:A:269:MET:HE2	1.55	0.45
1:B:141:GLU:OE2	1:B:145:LYS:CE	2.64	0.45
1:B:611:LEU:HD23	1:B:611:LEU:O	2.17	0.45
1:B:832:LYS:HB2	1:B:836:LEU:HD12	1.99	0.45
1:B:822:SER:HB3	1:B:843:MET:HE2	1.97	0.45
1:B:921:LEU:O	1:B:924:SER:OG	2.34	0.45
1:A:342:LEU:HD22	1:A:553:PHE:C	2.36	0.45
1:B:292:GLY:HA3	1:B:596:LEU:CD2	2.47	0.45
1:B:337:VAL:O	1:B:538:ARG:CZ	2.65	0.45
1:B:344:ASP:OD1	1:B:387:TYR:OH	2.27	0.45
1:B:648:ALA:HB1	1:B:747:LEU:HD21	1.98	0.45
1:A:131:GLN:HG2	1:A:132:LEU:HD12	1.99	0.45
1:B:53:ARG:NH2	1:B:54:LEU:O	2.49	0.45
1:B:878:ASN:ND2	1:B:881:THR:OG1	2.49	0.45
1:A:150:ARG:HD2	1:A:185:GLN:OE1	2.17	0.45
1:B:136:GLN:CB	1:B:137:ARG:HE	2.26	0.45
1:A:139:LEU:N	1:A:144:LYS:CE	2.74	0.45
1:A:348:LYS:HZ3	1:A:415:TYR:HE2	1.63	0.45
1:A:421:PRO:HG2	1:A:545:ARG:NH2	2.32	0.45
1:B:290:LEU:O	1:B:294:LEU:HD12	2.17	0.45
1:B:618:LEU:HD23	1:B:622:GLY:O	2.17	0.45
1:A:380:LEU:HD11	1:A:396:ARG:HE	1.82	0.45
1:A:867:LEU:HB3	1:A:877:CYS:HB2	1.98	0.45
1:B:793:ARG:CG	1:B:794:ALA:N	2.80	0.45
1:B:868:CYS:HB3	1:B:874:TYR:CD2	2.52	0.45
1:B:781:HIS:HB2	1:B:873:TYR:HE1	1.82	0.45
1:A:713:GLU:C	1:A:714:ARG:HE	2.20	0.44
1:B:527:VAL:HG23	1:B:528:TRP:O	2.16	0.44
1:B:91:ALA:HB2	1:B:902:TYR:HD1	1.82	0.44
1:A:185:GLN:O	1:A:188:GLN:N	2.50	0.44
1:A:462:LEU:HD12	1:A:462:LEU:HA	1.82	0.44
1:A:723:SER:HB3	1:A:726:THR:HB	2.00	0.44
1:A:798:MET:HE3	1:A:807:ASN:HA	1.99	0.44
1:B:519:THR:HG1	1:B:804:ARG:CZ	2.30	0.44
1:B:335:PHE:HD1	1:B:542:GLY:O	2.00	0.44
1:A:141:GLU:CA	1:A:141:GLU:OE2	2.57	0.44
1:A:409:ILE:HG12	1:A:552:LEU:HD21	1.99	0.44
1:B:412:LEU:HD12	1:B:505:ILE:HD12	1.97	0.44
1:B:693:ASP:O	1:B:696:MET:HB3	2.18	0.44
1:B:614:ARG:NH2	1:B:854:ASP:OD1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LEU:O	1:A:263:LEU:HB2	2.18	0.44
1:A:645:LEU:HA	1:A:645:LEU:HD23	1.61	0.44
1:A:691:ARG:HD3	1:A:820:PHE:CE1	2.51	0.44
1:B:112:THR:HG22	1:B:115:ARG:HH21	1.81	0.44
1:B:346:LEU:HB3	1:B:394:LYS:HE3	1.99	0.44
1:B:92:LYS:O	1:B:96:GLN:HG3	2.17	0.44
1:A:150:ARG:CA	1:A:153:LEU:HD12	2.47	0.44
1:A:337:VAL:HA	1:A:547:GLY:O	2.16	0.44
1:A:390:ARG:HD2	1:A:391:VAL:N	2.33	0.44
1:B:515:TYR:HB2	1:B:522:GLN:HA	1.99	0.44
1:A:426:LEU:HB2	1:A:501:VAL:HG11	2.00	0.44
1:B:479:PRO:HB2	1:B:482:GLN:HG3	1.99	0.44
1:B:548:ILE:HD11	1:B:550:TYR:OH	2.18	0.44
1:B:59:SER:OG	1:B:878:ASN:ND2	2.42	0.44
1:A:191:LEU:HD12	1:A:251:ILE:HG12	1.99	0.44
1:A:705:ARG:O	1:A:708:ARG:N	2.49	0.44
1:B:833:SER:OG	2:D:3:DT:OP1	2.26	0.44
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.66	0.44
1:A:382:ARG:CZ	1:A:382:ARG:HB2	2.48	0.44
1:A:58:VAL:H	1:A:876:LYS:HE3	1.75	0.44
1:A:735:ASN:HA	1:A:738:SER:HB3	1.98	0.44
1:A:832:LYS:NZ	1:A:837:PHE:CZ	2.86	0.44
1:B:502:VAL:CG1	1:B:545:ARG:HG2	2.47	0.44
1:B:504:VAL:O	1:B:549:CYS:HA	2.18	0.44
1:B:289:LEU:HD11	1:B:577:ILE:HG23	1.99	0.44
1:A:139:LEU:CA	1:A:144:LYS:HE3	2.43	0.43
1:A:75:TYR:CE1	1:A:915:LEU:HD22	2.53	0.43
1:A:833:SER:HB2	1:A:834:THR:HG23	1.99	0.43
1:B:570:LEU:HD23	1:B:600:PRO:HA	2.00	0.43
1:B:832:LYS:HB2	1:B:836:LEU:HD13	1.98	0.43
1:A:334:MET:HB3	1:A:335:PHE:O	2.17	0.43
1:A:403:CYS:SG	1:A:507:SER:HB2	2.58	0.43
1:A:781:HIS:HA	1:A:823:ALA:O	2.17	0.43
1:B:100:LEU:HD22	1:B:629:MET:HE2	2.00	0.43
1:B:104:ASN:ND2	1:B:107:GLU:OE1	2.52	0.43
1:B:354:GLN:HG3	1:B:355:LYS:N	2.33	0.43
1:A:396:ARG:O	1:A:398:PRO:HD3	2.18	0.43
1:A:655:PRO:O	1:A:658:SER:HB2	2.18	0.43
1:A:93:PHE:HA	1:A:96:GLN:CG	2.49	0.43
1:B:369:ARG:NH1	1:B:396:ARG:O	2.51	0.43
1:B:502:VAL:HG23	1:B:503:TYR:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:899:LYS:HZ2	1:B:904:ALA:HB3	1.83	0.43
1:B:115:ARG:HH22	1:B:116:ASN:CG	2.18	0.43
1:B:144:LYS:HD3	1:B:147:LEU:HD12	2.00	0.43
1:B:847:MET:O	1:B:851:ILE:HG13	2.17	0.43
1:A:879:ARG:HD2	1:A:879:ARG:O	2.18	0.43
1:B:247:GLU:C	1:B:248:ARG:HG2	2.39	0.43
1:B:449:LYS:O	1:B:452:ARG:HB3	2.18	0.43
1:B:682:ILE:HD13	1:B:720:ASN:HA	2.00	0.43
1:A:350:ASN:ND2	1:A:390:ARG:NH2	2.59	0.43
1:A:832:LYS:NZ	1:A:837:PHE:CE2	2.86	0.43
1:A:879:ARG:CZ	1:A:883:ASP:HB2	2.48	0.43
1:B:406:ILE:HD13	1:B:409:ILE:HD12	2.00	0.43
1:B:518:GLU:HB2	1:B:519:THR:H	1.29	0.43
1:B:283:ARG:HH12	1:B:597:ILE:HB	1.83	0.43
1:B:691:ARG:HH22	1:B:813:VAL:CG2	2.32	0.43
1:A:521:ILE:O	1:A:521:ILE:HG13	2.18	0.43
1:A:223:SER:OG	1:A:224:TYR:N	2.52	0.43
1:A:276:ILE:CG2	1:A:309:MET:HG3	2.48	0.43
1:A:447:THR:HG22	1:A:449:LYS:HB3	2.00	0.43
1:A:928:ARG:HD2	1:A:928:ARG:HH11	1.62	0.43
1:B:144:LYS:N	1:B:147:LEU:HB3	2.34	0.43
1:B:116:ASN:CB	1:B:270:HIS:HB2	2.47	0.43
1:B:339:MET:HG3	1:B:538:ARG:NH2	2.32	0.43
1:B:387:TYR:HB3	1:B:391:VAL:CG1	2.42	0.43
1:B:655:PRO:HA	1:B:698:HIS:CG	2.53	0.43
1:B:781:HIS:CG	1:B:783:ARG:NH2	2.86	0.43
1:A:146:ARG:H	1:A:146:ARG:HD2	1.82	0.43
1:B:232:ASN:O	1:B:246:ARG:HG2	2.19	0.43
1:B:515:TYR:N	1:B:522:GLN:OE1	2.52	0.43
1:B:514:ASN:C	1:B:522:GLN:OE1	2.57	0.43
1:A:406:ILE:HG13	1:A:438:LEU:HB2	2.01	0.43
1:A:416:ILE:HD11	1:A:505:ILE:HD11	2.01	0.43
1:A:139:LEU:O	1:A:139:LEU:HG	2.19	0.42
1:A:65:LEU:HD22	1:A:884:VAL:HG21	2.00	0.42
1:B:510:THR:OG1	1:B:511:LYS:N	2.52	0.42
1:B:557:ARG:O	1:B:561:MET:HG3	2.19	0.42
1:B:467:GLN:HA	1:B:670:TYR:CE1	2.54	0.42
1:A:335:PHE:HE2	1:A:544:VAL:O	2.01	0.42
1:A:515:TYR:HD2	1:A:522:GLN:HB2	1.83	0.42
1:A:832:LYS:HB2	1:A:836:LEU:HD13	2.01	0.42
1:A:879:ARG:NH2	1:A:883:ASP:HB2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:LYS:HA	1:B:348:LYS:HD2	1.88	0.42
1:A:139:LEU:HA	1:A:144:LYS:CD	2.49	0.42
1:A:289:LEU:HD11	1:A:577:ILE:HG23	2.01	0.42
1:B:111:GLU:OE1	1:B:115:ARG:N	2.53	0.42
1:B:493:GLU:OE1	1:B:533:ASN:HB3	2.19	0.42
1:A:186:VAL:CA	1:A:189:ILE:HD12	2.44	0.42
1:A:379:TYR:O	1:A:383:ILE:HG12	2.20	0.42
1:A:376:ILE:CG2	1:A:396:ARG:NH2	2.82	0.42
1:A:880:GLU:O	1:A:884:VAL:HG13	2.19	0.42
1:B:133:GLU:HG3	1:B:136:GLN:HE22	1.84	0.42
1:B:518:GLU:N	1:B:518:GLU:OE1	2.46	0.42
1:B:627:LEU:O	1:B:631:LEU:HG	2.20	0.42
1:A:511:LYS:HB2	2:C:4:DT:O4'	2.20	0.42
1:A:137:ARG:CA	1:A:140:GLU:OE2	2.59	0.42
1:A:152:LYS:HD2	1:A:152:LYS:C	2.40	0.42
1:A:260:LEU:HD21	1:A:290:LEU:HG	2.02	0.42
1:A:782:LEU:HD13	1:A:782:LEU:HA	1.71	0.42
1:B:351:TYR:HE1	1:B:353:PHE:CD1	2.37	0.42
1:B:567:PRO:HD2	1:B:570:LEU:HD12	2.00	0.42
1:B:686:MET:HE2	1:B:686:MET:HB3	1.91	0.42
1:B:283:ARG:HH21	1:B:567:PRO:HG2	1.85	0.42
1:B:505:ILE:HG22	1:B:550:TYR:CD2	2.54	0.42
1:B:53:ARG:HB3	1:B:53:ARG:HE	1.68	0.42
1:B:825:PHE:CD2	1:B:843:MET:HA	2.50	0.42
1:A:376:ILE:HB	1:A:396:ARG:HH12	1.79	0.42
1:B:339:MET:HA	1:B:549:CYS:O	2.18	0.42
1:B:573:LYS:HB3	1:B:575:GLU:OE1	2.19	0.42
1:B:65:LEU:CD2	1:B:881:THR:HG22	2.49	0.42
1:A:619:ASP:OD2	1:A:621:THR:HG23	2.19	0.42
1:A:652:CYS:HA	1:A:761:SER:OG	2.19	0.42
1:A:688:ARG:HD3	1:A:699:ASN:ND2	2.34	0.42
1:A:798:MET:H	1:A:805:ARG:NH1	2.13	0.42
1:B:419:ASN:ND2	1:B:420:GLU:HG2	2.35	0.42
1:B:600:PRO:O	1:B:602:PRO:HD3	2.20	0.42
1:A:207:CYS:HG	1:A:253:TYR:HE1	1.68	0.42
1:A:286:GLU:OE2	1:A:286:GLU:N	2.42	0.42
1:B:426:LEU:CD1	1:B:428:PHE:CE2	3.02	0.42
1:B:651:CYS:HB2	1:B:760:ASN:HD22	1.84	0.42
1:A:205:ILE:HD11	1:A:251:ILE:CD1	2.49	0.42
1:A:885:VAL:O	1:A:889:ARG:HG3	2.20	0.42
1:A:151:LYS:O	1:A:151:LYS:CG	2.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:TRP:CZ2	1:A:557:ARG:NE	2.88	0.41
1:B:655:PRO:HA	1:B:698:HIS:CD2	2.54	0.41
1:B:778:ASN:HB3	1:B:827:TYR:CE1	2.54	0.41
1:B:781:HIS:ND1	1:B:824:TYR:CE1	2.88	0.41
1:B:916:ILE:O	1:B:920:GLU:HG3	2.20	0.41
1:A:416:ILE:HG22	1:A:416:ILE:O	2.19	0.41
1:B:399:GLU:HA	1:B:404:GLU:HB3	2.01	0.41
1:B:401:GLU:OE2	1:B:557:ARG:NH2	2.48	0.41
1:B:463:HIS:HB3	1:B:466:MET:CG	2.49	0.41
1:B:783:ARG:CB	1:B:784:LYS:NZ	2.79	0.41
1:A:513:THR:OG1	1:A:571:ARG:NH2	2.53	0.41
1:A:876:LYS:HD2	1:A:877:CYS:CA	2.49	0.41
1:B:691:ARG:HD3	1:B:814:ASN:HD21	1.82	0.41
1:A:420:GLU:HA	1:A:421:PRO:HD3	1.92	0.41
1:A:545:ARG:HD2	1:A:546:PRO:N	2.35	0.41
1:A:751:ASN:ND2	1:A:753:LYS:HG3	2.33	0.41
1:B:301:ARG:HE	1:B:304:LEU:HB2	1.85	0.41
1:B:416:ILE:HG23	1:B:420:GLU:HG3	2.02	0.41
1:B:814:ASN:N	1:B:814:ASN:OD1	2.51	0.41
1:B:633:LYS:NZ	2:D:9:DT:O4	2.53	0.41
1:A:134:LEU:CD2	1:A:195:ILE:HG21	2.48	0.41
1:A:208:THR:CG2	1:A:256:THR:HA	2.50	0.41
1:A:678:ARG:HB2	1:A:681:GLU:OE2	2.20	0.41
1:A:922:LEU:HD23	1:A:922:LEU:HA	1.69	0.41
1:B:461:PRO:HB2	1:B:466:MET:SD	2.60	0.41
1:B:375:MET:HE1	1:B:557:ARG:HH22	1.85	0.41
1:B:679:VAL:HA	1:B:682:ILE:HG22	2.02	0.41
1:B:783:ARG:HB2	1:B:784:LYS:NZ	2.33	0.41
1:A:238:ILE:HG22	1:A:255:THR:HG23	2.03	0.41
1:A:290:LEU:HD23	1:A:290:LEU:HA	1.77	0.41
1:A:515:TYR:CD2	1:A:522:GLN:HB2	2.56	0.41
1:A:409:ILE:HG12	1:A:552:LEU:CD2	2.51	0.41
1:B:133:GLU:O	1:B:133:GLU:HG3	2.21	0.41
1:B:175:VAL:HG13	1:B:312:THR:HG22	2.03	0.41
1:B:53:ARG:CZ	1:B:54:LEU:O	2.69	0.41
1:B:553:PHE:CB	1:B:557:ARG:HG2	2.50	0.41
1:B:634:LEU:HA	1:B:635:PRO:HD3	1.89	0.41
1:B:786:ARG:HG2	1:B:795:ILE:HD13	2.03	0.41
1:B:915:LEU:HD23	1:B:915:LEU:O	2.20	0.41
1:A:128:GLU:O	1:A:132:LEU:HD13	2.21	0.41
1:A:387:TYR:HB3	1:A:391:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:TYR:CE1	1:A:517:ILE:HA	2.56	0.41
1:A:60:ALA:H	1:A:881:THR:CG2	2.30	0.41
1:A:779:MET:O	1:A:800:THR:HA	2.21	0.41
1:A:876:LYS:HD2	1:A:877:CYS:N	2.36	0.41
1:B:416:ILE:O	1:B:416:ILE:HG22	2.21	0.41
1:A:155:THR:HG22	1:A:330:ILE:HD13	2.02	0.41
1:A:615:ILE:C	1:A:616:GLU:HG3	2.41	0.41
1:B:472:GLN:O	1:B:476:ARG:HG3	2.21	0.41
1:B:782:LEU:HD23	1:B:782:LEU:HA	1.86	0.41
1:A:915:LEU:HD12	1:A:915:LEU:HA	1.92	0.41
1:B:696:MET:O	1:B:700:THR:HG23	2.21	0.41
1:A:140:GLU:CD	1:A:140:GLU:N	2.74	0.41
1:A:182:LYS:HG3	1:A:183:THR:CG2	2.51	0.41
1:A:339:MET:SD	1:A:538:ARG:NE	2.93	0.41
1:B:447:THR:HG22	1:B:449:LYS:N	2.36	0.41
1:B:806:VAL:HG12	1:B:836:LEU:HG	2.03	0.41
1:B:896:LEU:HD23	1:B:896:LEU:HA	1.63	0.41
1:A:233:SER:O	1:A:251:ILE:N	2.52	0.41
1:A:782:LEU:CD1	1:A:798:MET:HB2	2.51	0.41
1:B:238:ILE:HG22	1:B:255:THR:HG23	2.02	0.41
1:A:401:GLU:OE2	1:A:557:ARG:NH2	2.49	0.40
1:A:575:GLU:HB3	1:A:612:LEU:HD21	2.03	0.40
1:A:730:LEU:HD23	1:A:733:MET:HE1	2.03	0.40
1:B:171:VAL:HG12	1:B:306:VAL:HB	2.02	0.40
1:B:290:LEU:HA	1:B:290:LEU:HD23	1.86	0.40
1:B:312:THR:O	1:B:312:THR:OG1	2.33	0.40
1:B:368:ARG:HD2	1:B:369:ARG:H	1.85	0.40
1:A:692:SER:OG	1:A:842:THR:HG22	2.21	0.40
1:A:780:ALA:O	1:A:824:TYR:HA	2.21	0.40
1:B:272:LEU:CD1	1:B:275:LEU:HB2	2.52	0.40
1:B:396:ARG:H	1:B:396:ARG:HG2	1.35	0.40
1:A:183:THR:HG21	1:A:278:ASP:OD1	2.21	0.40
1:A:876:LYS:C	1:A:876:LYS:CD	2.86	0.40
1:B:136:GLN:OE1	1:B:137:ARG:HG2	2.20	0.40
1:B:247:GLU:HG3	1:B:248:ARG:HG2	2.04	0.40
1:B:704:TYR:CZ	1:B:708:ARG:HD3	2.57	0.40
1:A:861:THR:CG2	1:A:862:GLN:H	2.22	0.40
1:B:529:VAL:CG1	1:B:530:THR:N	2.84	0.40
1:B:560:ARG:HB3	1:B:560:ARG:HE	1.60	0.40
1:B:707:SER:OG	1:B:713:GLU:HA	2.21	0.40
1:B:786:ARG:HB3	1:B:795:ILE:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ASP:CG	1:A:197:ARG:NH1	2.74	0.40
1:A:226:ARG:HD2	1:A:226:ARG:HH11	1.61	0.40
1:A:377:GLU:HG2	1:A:396:ARG:NH1	2.37	0.40
1:A:461:PRO:HB2	1:A:466:MET:HE3	2.00	0.40
1:A:640:MET:HB2	1:A:640:MET:HE2	1.92	0.40
1:B:115:ARG:HH12	1:B:116:ASN:CG	2.24	0.40
1:B:454:ARG:NH1	1:B:455:ASP:OD1	2.54	0.40
1:B:401:GLU:HA	1:B:552:LEU:O	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:GLU:OE2	1:A:555:ARG:NH2[2_556]	2.17	0.03

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	842/944 (89%)	811 (96%)	27 (3%)	4 (0%)	29 59
1	B	843/944 (89%)	802 (95%)	38 (4%)	3 (0%)	34 64
All	All	1685/1888 (89%)	1613 (96%)	65 (4%)	7 (0%)	34 64

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	518	GLU
1	B	862	GLN
1	A	713	GLU
1	A	334	MET
1	A	835	ASP

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Mol	Chain	Res	Type
1	B	354	GLN
1	A	115	ARG

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	758/842 (90%)	734 (97%)	24 (3%)	39 71
1	B	759/842 (90%)	724 (95%)	35 (5%)	27 58
All	All	1517/1684 (90%)	1458 (96%)	59 (4%)	32 64

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	LYS
1	A	115	ARG
1	A	131	GLN
1	A	145	LYS
1	A	146	ARG
1	A	152	LYS
1	A	161	ASP
1	A	192	ASP
1	A	199	CYS
1	A	224	TYR
1	A	265	SER
1	A	353	PHE
1	A	390	ARG
1	A	394	LYS
1	A	543	ARG
1	A	545	ARG
1	A	561	MET
1	A	684	ARG
1	A	705	ARG
1	A	821	ASP
1	A	866	TYR

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Mol	Chain	Res	Type
1	A	876	LYS
1	A	889	ARG
1	A	928	ARG
1	B	53	ARG
1	B	57	ASN
1	B	115	ARG
1	B	137	ARG
1	B	145	LYS
1	B	151	LYS
1	B	199	CYS
1	B	208	THR
1	B	224	TYR
1	B	265	SER
1	B	272	LEU
1	B	289	LEU
1	B	338	LYS
1	B	353	PHE
1	B	368	ARG
1	B	370	MET
1	B	386	SER
1	B	394	LYS
1	B	432	TYR
1	B	452	ARG
1	B	483	ARG
1	B	507	SER
1	B	509	ARG
1	B	540	ARG
1	B	580	SER
1	B	591	ARG
1	B	689	ASN
1	B	691	ARG
1	B	718	TYR
1	B	783	ARG
1	B	798	MET
1	B	805	ARG
1	B	821	ASP
1	B	876	LYS
1	B	877	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	ASN
1	A	136	GLN
1	A	170	GLN
1	A	237	GLN
1	A	271	ASN
1	A	350	ASN
1	A	440	ASN
1	A	463	HIS
1	A	482	GLN
1	A	522	GLN
1	A	814	ASN
1	B	57	ASN
1	B	136	GLN
1	B	138	GLN
1	B	142	ASN
1	B	164	GLN
1	B	237	GLN
1	B	262	GLN
1	B	264	GLN
1	B	350	ASN
1	B	437	GLN
1	B	456	HIS
1	B	471	GLN
1	B	758	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PO4	A	1001	1	4,4,4	0.76	0	6,6,6	0.52	0
3	PO4	B	1001	-	4,4,4	0.87	0	6,6,6	0.64	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	A	850/944 (90%)	0.25	41 (4%) 30 26	43, 85, 149, 215	0
1	B	851/944 (90%)	0.09	18 (2%) 63 62	43, 78, 137, 214	0
2	C	10/16 (62%)	-0.24	0 100 100	66, 86, 131, 152	0
2	D	10/16 (62%)	-0.29	0 100 100	59, 74, 118, 140	0
All	All	1721/1920 (89%)	0.17	59 (3%) 45 40	43, 82, 142, 215	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	785	SER	5.9
1	A	136	GLN	4.9
1	A	52	ILE	4.8
1	B	355	LYS	4.3
1	B	709	TYR	3.9
1	A	395	LEU	3.9
1	A	835	ASP	3.7
1	A	446	LYS	3.5
1	B	691	ARG	3.3
1	A	518	GLU	3.2
1	B	387	TYR	3.1
1	A	805	ARG	3.1
1	A	396	ARG	3.0
1	A	858	ALA	3.0
1	A	673	LEU	3.0
1	B	712	ALA	2.9
1	A	863	ASN	2.9
1	A	397	LEU	2.9
1	A	130	LEU	2.9
1	A	838	LEU	2.8
1	A	453	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	796	HIS	2.7
1	B	54	LEU	2.7
1	A	54	LEU	2.7
1	B	794	ALA	2.7
1	B	353	PHE	2.7
1	A	836	LEU	2.6
1	A	802	ASP	2.6
1	A	806	VAL	2.6
1	A	798	MET	2.6
1	A	355	LYS	2.6
1	B	393	ASP	2.5
1	A	476	ARG	2.5
1	A	139	LEU	2.5
1	A	794	ALA	2.5
1	A	442	LEU	2.5
1	A	865	PRO	2.4
1	B	399	GLU	2.4
1	A	807	ASN	2.4
1	B	782	LEU	2.4
1	A	56	CYS	2.4
1	A	859	GLY	2.4
1	A	521	ILE	2.3
1	A	877	CYS	2.3
1	B	346	LEU	2.3
1	B	815	SER	2.2
1	A	138	GLN	2.2
1	B	52	ILE	2.2
1	A	786	ARG	2.2
1	B	816	GLY	2.2
1	A	710	SER	2.2
1	B	519	THR	2.1
1	A	525	ASP	2.1
1	A	782	LEU	2.1
1	A	135	GLY	2.1
1	A	55	GLY	2.0
1	B	814	ASN	2.0
1	B	819	GLY	2.0
1	A	816	GLY	2.0

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

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

6.3 Carbohydrates [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	PO4	A	1001	5/5	0.86	0.18	118,144,149,150	0
3	PO4	B	1001	5/5	0.94	0.22	102,111,117,121	0

6.5 Other polymers [i](#)

There are no such residues in this entry.