



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:41 pm GMT

PDB ID : 4Z6Y
Title : Structure of the TBC1D7-TSC1 complex
Authors : Gai, Z.; Wu, G.
Deposited on : 2015-04-06
Resolution : 2.81 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

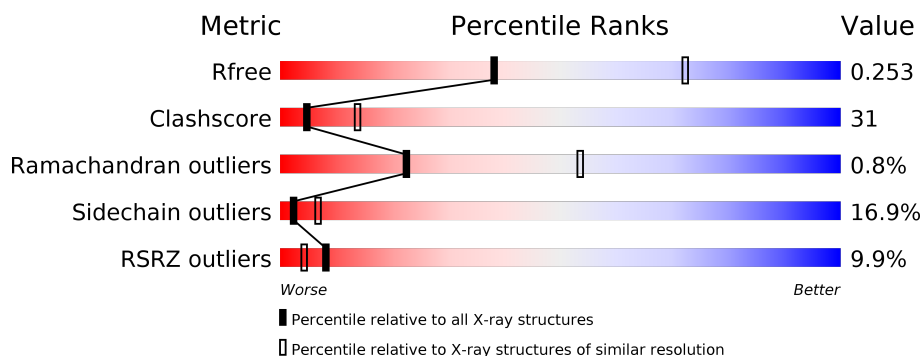
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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}	100719	2917 (2.84-2.80)
Clashscore	112137	3382 (2.84-2.80)
Ramachandran outliers	110173	3324 (2.84-2.80)
Sidechain outliers	110143	3326 (2.84-2.80)
RSRZ outliers	101464	2948 (2.84-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	273	<div> <div>3%</div> <div>67% 26% 7%</div> </div>
1	B	273	<div> <div>2%</div> <div>67% 25% 7%</div> </div>
1	E	273	<div> <div>3%</div> <div>63% 30% 6%</div> </div>
1	G	273	<div> <div>2%</div> <div>65% 27% 7%</div> </div>
2	C	56	<div> <div>50%</div> <div>32% 45% 18% 5%</div> </div>
2	D	56	<div> <div>43%</div> <div>43% 41% 11% 5%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	56	<div><div><div></div><div></div><div></div><div></div></div><div>34%45%38%14%</div><div></div></div>
2	H	56	<div><div><div></div><div></div><div></div><div></div></div><div>57%39%30%27%</div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10471 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 TBC1 domain family member 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	272	Total	C	N	O	S	0	1	0
			2200	1424	368	393	15			
1	G	272	Total	C	N	O	S	0	1	0
			2206	1427	371	393	15			
1	E	272	Total	C	N	O	S	0	1	0
			2206	1427	371	393	15			
1	A	273	Total	C	N	O	S	0	1	0
			2212	1430	372	395	15			

- Molecule 2 is a protein called Hamartin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	53	Total	C	N	O	0	0	0
			402	252	69	81			
2	H	55	Total	C	N	O	0	0	0
			415	259	71	85			
2	F	54	Total	C	N	O	0	0	0
			407	255	70	82			
2	D	53	Total	C	N	O	0	0	0
			402	252	69	81			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total	O	0	0
			4	4		
3	C	4	Total	O	0	0
			4	4		
3	G	6	Total	O	0	0
			6	6		
3	H	2	Total	O	0	0
			2	2		

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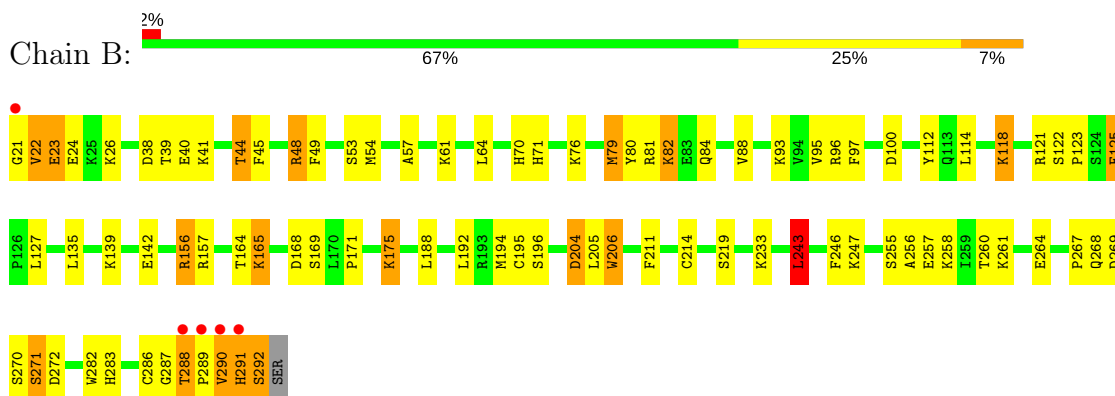
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total 1	O 1	0	0
3	F	1	Total 1	O 1	0	0
3	A	1	Total 1	O 1	0	0
3	D	2	Total 2	O 2	0	0

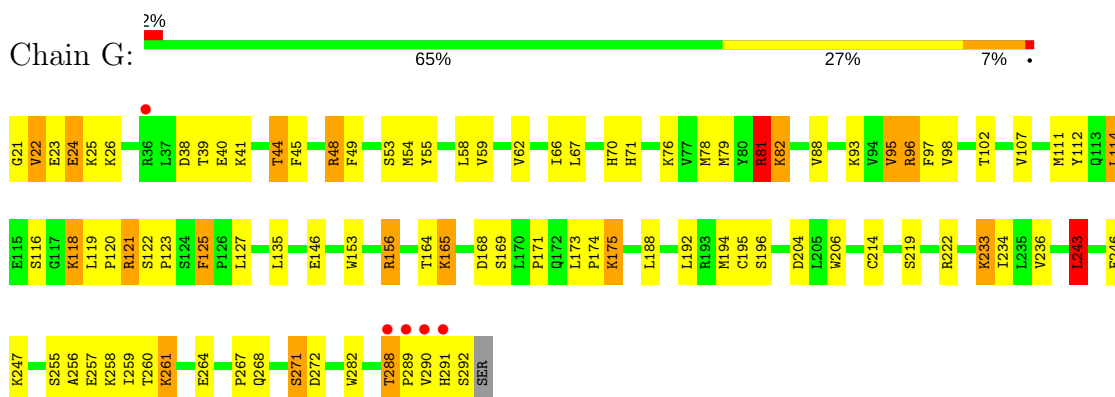
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

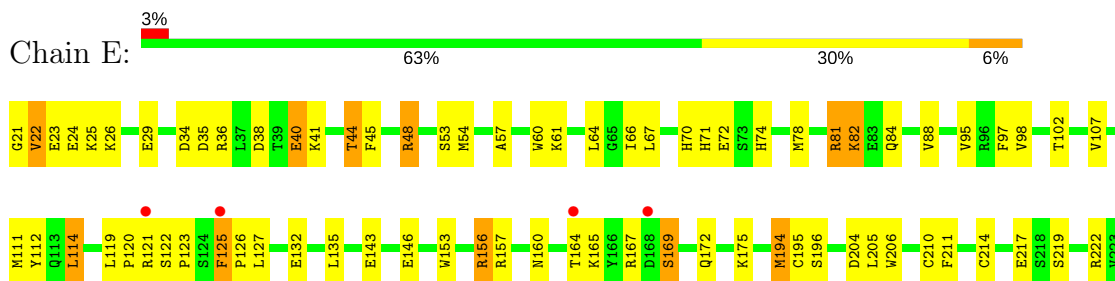
- Molecule 1: TBC1 domain family member 7



- Molecule 1: TBC1 domain family member 7

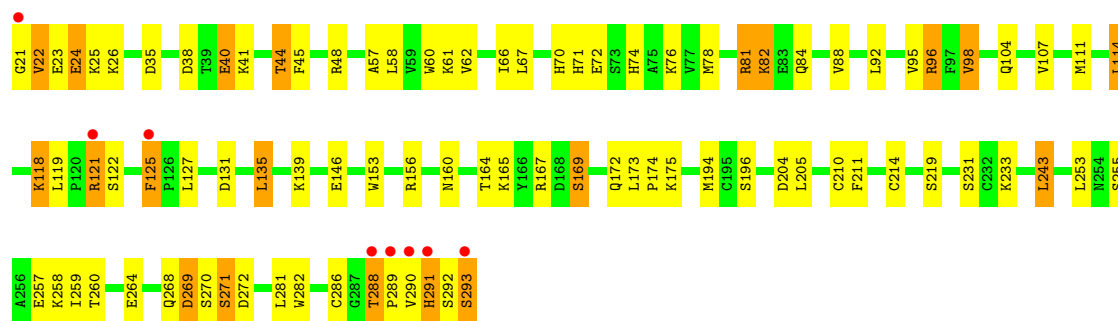


- Molecule 1: TBC1 domain family member 7





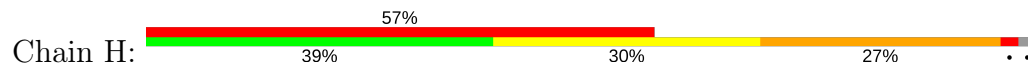
- Molecule 1: TBC1 domain family member 7



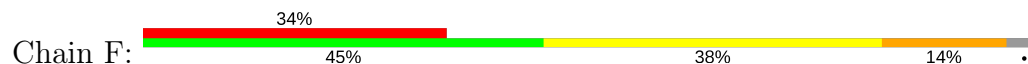
- Molecule 2: Hamartin



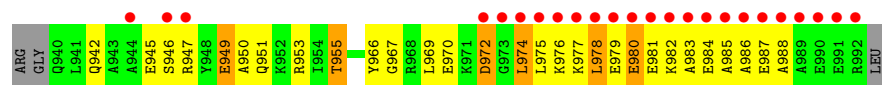
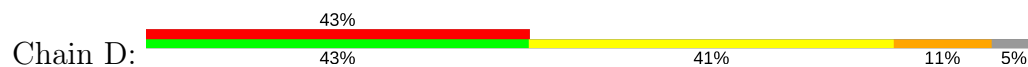
- Molecule 2: Hamartin



- Molecule 2: Hamartin



- Molecule 2: Hamartin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.99Å 145.69Å 114.76Å 90.00° 89.65° 90.00°	Depositor
Resolution (Å)	50.00 – 2.81 44.89 – 2.81	Depositor EDS
% Data completeness (in resolution range)	98.0 (50.00-2.81) 97.3 (44.89-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.206 , 0.255 0.206 , 0.253	Depositor DCC
R_{free} test set	2260 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	69.9	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 7.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.418 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10471	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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

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	0.78	2/2269 (0.1%)	0.86	2/3073 (0.1%)
1	B	0.78	2/2257 (0.1%)	0.88	1/3058 (0.0%)
1	E	0.79	3/2263 (0.1%)	0.88	0/3065
1	G	0.77	3/2263 (0.1%)	0.88	3/3065 (0.1%)
2	C	0.56	0/404	0.72	1/543 (0.2%)
2	D	0.59	0/404	0.72	0/543
2	F	0.58	0/409	0.75	0/550
2	H	0.54	0/417	0.72	0/560
All	All	0.75	10/10686 (0.1%)	0.85	7/14457 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	206	TRP	CD2-CE2	5.96	1.48	1.41
1	B	282	TRP	CD2-CE2	5.82	1.48	1.41
1	G	282	TRP	CD2-CE2	5.73	1.48	1.41
1	G	206	TRP	CD2-CE2	5.53	1.48	1.41
1	A	282	TRP	CD2-CE2	5.43	1.47	1.41
1	G	153	TRP	CD2-CE2	5.28	1.47	1.41
1	E	224	TRP	CD2-CE2	5.28	1.47	1.41
1	E	60	TRP	CD2-CE2	5.28	1.47	1.41
1	A	60	TRP	CD2-CE2	5.18	1.47	1.41
1	E	282	TRP	CD2-CE2	5.02	1.47	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	243	LEU	CA-CB-CG	-7.63	97.75	115.30
1	G	243	LEU	CA-CB-CG	-6.56	100.21	115.30
1	G	81	ARG	NE-CZ-NH1	-6.12	117.24	120.30
1	A	243	LEU	CA-CB-CG	-5.71	102.16	115.30
1	G	81	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	A	131	ASP	CB-CG-OD1	5.15	122.93	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	947	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2212	0	2253	103	1
1	B	2200	0	2237	58	1
1	E	2206	0	2248	71	2
1	G	2206	0	2248	100	2
2	C	402	0	382	64	0
2	D	402	0	383	87	0
2	F	407	0	385	81	0
2	H	415	0	392	92	0
3	A	1	0	0	1	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	2	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	6	0	0	0	0
3	H	2	0	0	0	0
All	All	10471	0	10528	644	3

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 31.

All (644) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ARG:HD2	1:A:125:PHE:CE2	1.20	1.73
1:A:121:ARG:CD	1:A:125:PHE:CE2	1.89	1.54
2:D:975:LEU:HA	2:D:978:LEU:CD1	1.29	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:975:LEU:CA	2:D:978:LEU:HD11	1.05	1.51
2:D:975:LEU:CA	2:D:978:LEU:CD1	1.86	1.50
1:G:22:VAL:C	1:G:24:GLU:HB2	1.34	1.45
1:A:121:ARG:HD2	1:A:125:PHE:CD2	1.57	1.36
1:A:21:GLY:C	1:A:24:GLU:HG2	1.43	1.36
2:F:975:LEU:HA	2:F:978:LEU:CD1	1.56	1.35
1:A:48:ARG:HD2	1:A:289:PRO:O	1.25	1.34
2:C:981:GLU:OE1	2:C:982:LYS:N	1.57	1.34
1:A:21:GLY:O	1:A:24:GLU:HG3	1.16	1.34
1:A:95:VAL:O	1:A:96:ARG:CG	1.76	1.32
1:A:21:GLY:O	1:A:24:GLU:CG	1.78	1.31
1:G:121:ARG:HG3	1:G:125:PHE:CE1	1.69	1.27
2:F:981:GLU:CD	2:F:982:LYS:N	1.88	1.27
2:D:975:LEU:O	2:D:978:LEU:HD22	1.38	1.24
1:A:21:GLY:C	1:A:24:GLU:CG	2.04	1.24
1:A:95:VAL:O	1:A:96:ARG:CD	1.86	1.23
2:D:981:GLU:OE1	2:D:982:LYS:N	1.68	1.23
2:D:983:ALA:O	2:D:986:ALA:HB3	1.39	1.23
2:D:975:LEU:CB	2:D:978:LEU:HD21	1.66	1.22
2:D:975:LEU:HA	2:D:978:LEU:CG	1.67	1.22
2:C:973:GLY:HA3	2:C:975:LEU:CD2	1.68	1.22
1:A:95:VAL:O	1:A:96:ARG:HG3	1.24	1.21
2:F:975:LEU:CA	2:F:978:LEU:HD11	1.69	1.21
1:A:21:GLY:CA	1:A:24:GLU:HG2	1.71	1.20
1:G:23:GLU:N	1:G:24:GLU:HB2	1.55	1.20
2:D:975:LEU:C	2:D:978:LEU:CD1	2.10	1.20
2:C:978:LEU:O	2:C:981:GLU:OE2	1.59	1.20
1:A:48:ARG:CD	1:A:289:PRO:O	1.89	1.19
2:C:976:LYS:CA	2:C:976:LYS:HE2	1.66	1.19
2:D:978:LEU:O	2:D:981:GLU:HB3	1.42	1.19
2:D:966:TYR:O	2:D:970:GLU:HG2	1.43	1.18
1:A:22:VAL:C	1:A:24:GLU:HB3	1.65	1.18
1:A:23:GLU:CB	1:A:26:LYS:HB2	1.72	1.18
1:E:48:ARG:HD3	1:E:289:PRO:O	1.42	1.17
2:F:966:TYR:O	2:F:970:GLU:HG2	1.46	1.16
1:G:45:PHE:HB2	1:G:291:HIS:CE1	1.80	1.16
1:A:121:ARG:NE	1:A:125:PHE:HE2	1.45	1.15
2:C:975:LEU:H	2:C:975:LEU:HD22	1.06	1.15
1:A:95:VAL:C	1:A:96:ARG:HG3	1.48	1.14
2:D:975:LEU:N	2:D:978:LEU:HD11	1.61	1.14
1:E:48:ARG:CD	1:E:289:PRO:O	1.96	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:GLU:N	1:A:24:GLU:HB3	1.61	1.13
2:D:983:ALA:O	2:D:986:ALA:CB	1.95	1.13
1:A:121:ARG:NE	1:A:125:PHE:CE2	2.13	1.13
2:H:976:LYS:CE	2:H:976:LYS:HA	1.77	1.12
2:H:942:GLN:O	2:H:945:GLU:HG3	1.49	1.12
2:H:981:GLU:CG	2:H:982:LYS:H	1.62	1.11
1:G:45:PHE:CB	1:G:291:HIS:HE1	1.64	1.10
2:H:966:TYR:O	2:H:970:GLU:HG2	1.50	1.10
2:C:981:GLU:OE1	2:C:982:LYS:CA	1.99	1.10
2:H:976:LYS:HE2	2:H:976:LYS:CA	1.82	1.09
2:C:973:GLY:C	2:C:975:LEU:HD22	1.72	1.09
2:C:966:TYR:O	2:C:970:GLU:HG2	1.51	1.09
2:D:978:LEU:H	2:D:978:LEU:HD13	0.94	1.09
2:F:978:LEU:H	2:F:978:LEU:HD13	0.99	1.07
2:H:942:GLN:HA	2:H:945:GLU:CG	1.84	1.07
1:G:95:VAL:HG11	1:G:97:PHE:HD2	1.10	1.07
2:D:975:LEU:O	2:D:978:LEU:CD2	2.01	1.07
2:C:973:GLY:HA3	2:C:975:LEU:HD21	1.07	1.06
2:D:978:LEU:CD1	2:D:978:LEU:H	1.69	1.06
2:D:975:LEU:HB3	2:D:978:LEU:HD21	1.13	1.06
1:E:233:LYS:NZ	1:E:286:CYS:SG	2.29	1.06
1:A:233:LYS:NZ	1:A:286:CYS:SG	2.30	1.05
2:H:939:GLY:C	2:H:942:GLN:HB3	1.77	1.05
1:A:24:GLU:OE2	1:A:24:GLU:HA	1.55	1.04
2:H:949:GLU:O	2:H:952:LYS:HG3	1.55	1.04
1:G:95:VAL:HG11	1:G:97:PHE:CD2	1.92	1.04
1:G:48:ARG:NH2	1:G:49:PHE:HE1	1.54	1.04
2:H:945:GLU:O	2:H:949:GLU:HG2	1.56	1.04
2:C:976:LYS:CE	2:C:976:LYS:HA	1.79	1.04
1:E:21:GLY:O	1:E:25:LYS:N	1.90	1.04
2:C:973:GLY:CA	2:C:975:LEU:CD2	2.36	1.03
2:D:975:LEU:C	2:D:978:LEU:HD13	1.77	1.03
1:A:121:ARG:HD2	1:A:125:PHE:CZ	1.92	1.03
1:G:45:PHE:CA	1:G:291:HIS:HE1	1.72	1.02
1:G:22:VAL:C	1:G:24:GLU:CB	2.28	1.01
1:G:95:VAL:CG1	1:G:97:PHE:HD2	1.74	1.01
2:C:975:LEU:HA	2:C:978:LEU:HD23	1.39	1.00
2:C:981:GLU:OE1	2:C:982:LYS:CB	2.10	1.00
1:A:121:ARG:CD	1:A:125:PHE:CD2	2.28	1.00
1:B:233:LYS:NZ	1:B:286:CYS:SG	2.34	0.99
2:D:975:LEU:CA	2:D:978:LEU:HD21	1.91	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:939:GLY:O	2:H:942:GLN:HB3	1.63	0.99
2:H:946:SER:HA	2:H:949:GLU:HG3	1.45	0.99
2:F:974:LEU:HD22	2:F:974:LEU:C	1.83	0.99
1:A:23:GLU:CB	1:A:26:LYS:CB	2.41	0.99
2:H:981:GLU:CD	2:H:982:LYS:H	1.67	0.98
1:G:121:ARG:CG	1:G:125:PHE:CE1	2.47	0.98
2:D:946:SER:O	2:D:949:GLU:HG3	1.62	0.98
2:C:985:ALA:O	2:C:988:ALA:CB	2.13	0.97
1:E:21:GLY:O	1:E:24:GLU:HB3	1.65	0.97
2:C:981:GLU:CD	2:C:982:LYS:N	2.16	0.97
2:D:974:LEU:HD13	2:D:974:LEU:H	1.30	0.96
2:F:946:SER:O	2:F:949:GLU:HG3	1.64	0.95
1:G:257:GLU:O	1:G:261:LYS:HG2	1.64	0.95
2:H:981:GLU:OE2	2:H:982:LYS:CB	2.14	0.95
2:D:978:LEU:HD13	2:D:978:LEU:N	1.79	0.95
2:D:975:LEU:CA	2:D:978:LEU:CD2	2.45	0.94
2:F:978:LEU:H	2:F:978:LEU:CD1	1.79	0.94
2:D:975:LEU:O	2:D:978:LEU:HD13	1.66	0.94
2:H:981:GLU:HG2	2:H:982:LYS:N	1.77	0.94
1:B:260:THR:O	1:B:264:GLU:HG3	1.67	0.93
1:A:121:ARG:HG2	1:A:125:PHE:CD2	2.03	0.93
2:D:969:LEU:CD2	2:D:974:LEU:HB3	1.99	0.93
2:C:973:GLY:CA	2:C:975:LEU:HD21	1.97	0.93
2:D:981:GLU:CD	2:D:982:LYS:N	2.21	0.92
2:F:978:LEU:N	2:F:978:LEU:HD13	1.83	0.92
2:D:983:ALA:O	2:D:986:ALA:N	2.02	0.92
2:C:976:LYS:CE	2:C:976:LYS:CA	2.44	0.92
2:F:975:LEU:HA	2:F:978:LEU:HD11	0.92	0.92
1:G:260:THR:O	1:G:264:GLU:HG3	1.68	0.92
2:F:969:LEU:CD2	2:F:974:LEU:HB3	2.00	0.92
1:G:45:PHE:HB2	1:G:291:HIS:HE1	1.18	0.92
1:A:23:GLU:CB	1:A:26:LYS:CG	2.48	0.91
2:C:985:ALA:O	2:C:988:ALA:HB2	1.70	0.91
1:B:288:THR:HG22	1:B:289:PRO:HD2	1.50	0.91
2:C:973:GLY:C	2:C:975:LEU:CD2	2.39	0.91
2:F:981:GLU:OE1	2:F:982:LYS:N	2.04	0.91
2:D:975:LEU:C	2:D:978:LEU:HD11	1.85	0.91
2:F:981:GLU:OE2	2:F:982:LYS:HA	1.71	0.90
1:E:121:ARG:HD2	1:E:125:PHE:CE1	2.05	0.90
1:A:22:VAL:C	1:A:24:GLU:CB	2.40	0.90
1:A:121:ARG:CG	1:A:125:PHE:CD2	2.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:942:GLN:HA	2:H:945:GLU:HG2	1.53	0.90
2:H:942:GLN:HA	2:H:945:GLU:CD	1.90	0.90
2:F:981:GLU:CD	2:F:981:GLU:C	2.29	0.90
1:A:104:GLN:HG2	3:A:301:HOH:O	1.71	0.89
2:C:976:LYS:HA	2:C:976:LYS:HE2	0.91	0.89
1:G:288:THR:HG22	1:G:289:PRO:HD2	1.53	0.89
2:F:981:GLU:OE2	2:F:982:LYS:CA	2.20	0.89
2:F:981:GLU:OE2	2:F:982:LYS:N	2.06	0.89
1:G:257:GLU:O	1:G:261:LYS:CG	2.22	0.87
2:H:981:GLU:CG	2:H:982:LYS:N	2.28	0.87
1:E:260:THR:O	1:E:264:GLU:HG3	1.74	0.87
1:G:24:GLU:OE2	1:G:24:GLU:HA	1.74	0.87
2:H:976:LYS:HE2	2:H:976:LYS:HA	0.90	0.86
1:G:22:VAL:CA	1:G:24:GLU:HB2	2.04	0.86
1:A:23:GLU:CB	1:A:26:LYS:CD	2.54	0.86
2:D:975:LEU:O	2:D:978:LEU:CD1	2.20	0.86
1:G:48:ARG:NE	1:G:49:PHE:CZ	2.42	0.86
2:F:975:LEU:HA	2:F:978:LEU:CG	1.97	0.85
2:F:988:ALA:O	2:F:992:ARG:N	2.09	0.85
1:G:45:PHE:CA	1:G:291:HIS:CE1	2.60	0.84
1:E:121:ARG:HD2	1:E:125:PHE:CZ	2.13	0.84
2:F:975:LEU:HB3	2:F:978:LEU:HD21	1.60	0.83
2:D:975:LEU:C	2:D:978:LEU:CD2	2.47	0.83
1:G:23:GLU:N	1:G:24:GLU:CB	2.39	0.83
1:G:233:LYS:HD2	1:G:233:LYS:H	1.41	0.83
1:E:25:LYS:HE3	1:E:29:GLU:OE1	1.79	0.82
2:F:975:LEU:CA	2:F:978:LEU:CD1	2.40	0.82
2:F:974:LEU:H	2:F:974:LEU:HD13	1.45	0.82
1:A:260:THR:O	1:A:264:GLU:HG3	1.80	0.82
1:G:45:PHE:CB	1:G:291:HIS:CE1	2.49	0.82
1:G:48:ARG:NH2	1:G:49:PHE:CE1	2.38	0.82
2:C:975:LEU:O	2:C:978:LEU:N	2.12	0.82
2:C:975:LEU:HD22	2:C:975:LEU:N	1.91	0.82
1:A:23:GLU:CB	1:A:26:LYS:HD2	2.11	0.80
1:G:48:ARG:NE	1:G:49:PHE:CE1	2.48	0.80
2:C:975:LEU:CD2	2:C:975:LEU:H	1.86	0.80
1:G:21:GLY:O	1:G:24:GLU:HB3	1.82	0.80
1:G:291:HIS:N	1:G:292:SER:C	2.35	0.80
1:G:291:HIS:H	1:G:292:SER:C	1.85	0.80
2:F:981:GLU:OE2	2:F:981:GLU:C	2.20	0.80
2:H:941:LEU:O	2:H:941:LEU:HD22	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:ARG:HD2	1:E:289:PRO:O	1.82	0.79
1:G:24:GLU:OE2	1:G:24:GLU:CA	2.30	0.79
2:H:978:LEU:HB3	2:H:981:GLU:OE1	1.83	0.79
2:F:974:LEU:HD22	2:F:978:LEU:HD11	1.65	0.79
2:H:942:GLN:HA	2:H:945:GLU:OE1	1.84	0.78
2:H:946:SER:HA	2:H:949:GLU:CG	2.14	0.78
2:F:974:LEU:CD2	2:F:974:LEU:C	2.49	0.78
1:A:95:VAL:O	1:A:96:ARG:HD3	1.80	0.78
1:A:23:GLU:N	1:A:24:GLU:CB	2.43	0.78
1:G:291:HIS:CA	1:G:292:SER:C	2.52	0.77
2:H:990:GLU:O	2:H:992:ARG:N	2.17	0.77
1:A:48:ARG:HD3	1:A:289:PRO:O	1.82	0.77
2:D:975:LEU:HB3	2:D:978:LEU:CD2	2.07	0.77
2:D:983:ALA:O	2:D:986:ALA:CA	2.32	0.77
1:G:95:VAL:CG1	1:G:97:PHE:CD2	2.60	0.77
2:F:975:LEU:CB	2:F:978:LEU:HD21	1.89	0.77
1:B:288:THR:HG22	1:B:289:PRO:CD	2.14	0.77
2:F:981:GLU:CD	2:F:982:LYS:CA	2.53	0.76
1:A:121:ARG:CZ	1:A:125:PHE:CE2	2.69	0.76
2:H:942:GLN:CA	2:H:945:GLU:CG	2.64	0.76
2:F:974:LEU:O	2:F:978:LEU:HD13	1.86	0.76
2:F:987:GLU:O	2:F:991:GLU:N	2.19	0.75
2:H:985:ALA:O	2:H:989:ALA:HB2	1.86	0.75
1:G:291:HIS:HB2	1:G:292:SER:C	2.06	0.75
1:A:24:GLU:CA	1:A:24:GLU:OE2	2.34	0.75
1:G:21:GLY:C	1:G:24:GLU:HB3	2.06	0.75
2:F:974:LEU:O	2:F:978:LEU:CD1	2.34	0.75
1:G:291:HIS:CB	1:G:292:SER:C	2.55	0.75
2:D:975:LEU:HD13	2:D:978:LEU:HG	1.67	0.74
2:D:975:LEU:HA	2:D:978:LEU:HD11	0.78	0.74
2:D:974:LEU:HD22	2:D:975:LEU:N	2.03	0.74
2:H:939:GLY:CA	2:H:942:GLN:HB3	2.17	0.74
2:D:974:LEU:O	2:D:978:LEU:CD1	2.35	0.74
2:D:979:GLU:O	2:D:981:GLU:N	2.21	0.74
1:A:290:VAL:HG12	1:A:291:HIS:H	1.51	0.73
2:D:981:GLU:OE1	2:D:982:LYS:CA	2.36	0.73
1:E:21:GLY:O	1:E:24:GLU:CB	2.36	0.73
2:C:955:THR:HG22	2:F:955:THR:HG22	1.71	0.73
2:F:981:GLU:O	2:F:984:GLU:N	2.21	0.73
1:A:23:GLU:HA	1:A:26:LYS:H	1.54	0.72
2:D:979:GLU:C	2:D:981:GLU:N	2.42	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:976:LYS:HE2	2:C:979:GLU:OE2	1.89	0.72
1:A:23:GLU:HA	1:A:26:LYS:N	2.05	0.72
1:A:121:ARG:HG2	1:A:125:PHE:HD2	1.49	0.72
2:H:940:GLN:CD	2:H:940:GLN:N	2.43	0.72
2:H:939:GLY:HA2	2:H:942:GLN:NE2	2.04	0.71
2:D:978:LEU:CD1	2:D:978:LEU:N	2.46	0.71
2:F:945:GLU:O	2:F:949:GLU:HG2	1.91	0.71
1:B:22:VAL:O	1:B:23:GLU:CB	2.37	0.71
2:D:975:LEU:O	2:D:978:LEU:CG	2.38	0.71
2:D:974:LEU:C	2:D:978:LEU:HD11	2.11	0.71
2:F:974:LEU:CD2	2:F:978:LEU:CD1	2.69	0.71
2:D:985:ALA:O	2:D:988:ALA:HB3	1.91	0.70
2:D:979:GLU:C	2:D:981:GLU:H	1.93	0.70
1:E:222:ARG:NH2	1:E:272:ASP:OD2	2.25	0.70
2:H:939:GLY:O	2:H:942:GLN:CB	2.39	0.70
1:A:22:VAL:CA	1:A:24:GLU:HB3	2.20	0.70
1:E:121:ARG:HD2	1:E:125:PHE:CD1	2.26	0.70
2:H:942:GLN:CB	2:H:945:GLU:OE1	2.40	0.70
1:A:121:ARG:CZ	1:A:125:PHE:HE2	2.04	0.70
2:D:945:GLU:O	2:D:949:GLU:HG2	1.92	0.70
2:D:969:LEU:O	2:D:972:ASP:O	2.10	0.70
2:C:983:ALA:O	2:C:986:ALA:HB3	1.92	0.70
1:E:48:ARG:HD2	1:E:288:THR:HG22	1.72	0.69
2:F:988:ALA:O	2:F:991:GLU:N	2.25	0.69
2:D:974:LEU:CD1	2:D:974:LEU:H	2.02	0.69
2:H:984:GLU:HA	2:H:987:GLU:HG3	1.74	0.69
2:C:985:ALA:O	2:C:988:ALA:HB3	1.91	0.69
1:G:45:PHE:HA	1:G:291:HIS:CE1	2.27	0.69
2:D:975:LEU:CA	2:D:978:LEU:CG	2.46	0.68
2:F:969:LEU:HD22	2:F:974:LEU:HB3	1.74	0.68
2:H:951:GLN:O	2:H:955:THR:HG23	1.93	0.68
1:A:23:GLU:CA	1:A:26:LYS:H	2.06	0.68
1:G:121:ARG:HG3	1:G:125:PHE:CD1	2.25	0.68
2:D:974:LEU:HD22	2:D:974:LEU:C	2.13	0.68
1:E:268:GLN:O	1:E:271:SER:OG	2.11	0.68
2:H:946:SER:CA	2:H:949:GLU:HG3	2.22	0.68
2:C:972:ASP:OD1	2:C:972:ASP:N	2.26	0.68
2:F:978:LEU:O	2:F:981:GLU:HB3	1.94	0.68
1:E:21:GLY:C	1:E:24:GLU:HB3	2.15	0.67
2:F:976:LYS:O	2:F:980:GLU:HG2	1.94	0.67
2:H:976:LYS:HE2	2:H:979:GLU:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:949:GLU:HG2	2:C:950:ALA:N	2.09	0.67
1:E:255:SER:OG	1:E:258:LYS:HE2	1.95	0.67
2:H:942:GLN:CA	2:H:945:GLU:OE1	2.42	0.67
1:A:95:VAL:O	1:A:95:VAL:CG1	2.42	0.66
2:C:981:GLU:CG	2:C:982:LYS:N	2.59	0.66
1:A:95:VAL:O	1:A:96:ARG:HD2	1.91	0.66
2:F:969:LEU:O	2:F:972:ASP:O	2.14	0.66
1:G:288:THR:HG22	1:G:289:PRO:CD	2.23	0.66
1:A:95:VAL:HG13	1:A:95:VAL:O	1.96	0.66
2:F:974:LEU:HD22	2:F:975:LEU:N	2.08	0.66
2:C:976:LYS:N	2:C:976:LYS:HE2	2.10	0.66
2:H:942:GLN:C	2:H:945:GLU:HG3	2.14	0.66
1:B:121:ARG:CB	1:B:125:PHE:HE2	2.09	0.65
2:H:942:GLN:CA	2:H:945:GLU:HG2	2.25	0.65
2:H:974:LEU:HD12	2:H:974:LEU:N	2.11	0.65
1:G:121:ARG:CG	1:G:125:PHE:HE1	2.07	0.65
2:H:966:TYR:OH	1:A:96:ARG:HG2	1.97	0.65
2:H:941:LEU:O	2:H:945:GLU:HG2	1.97	0.65
1:B:164:THR:OG1	1:B:165:LYS:N	2.29	0.65
2:H:955:THR:HG22	2:D:955:THR:HG22	1.78	0.65
1:G:48:ARG:CZ	1:G:49:PHE:CE1	2.80	0.65
2:F:981:GLU:OE1	2:F:982:LYS:CA	2.44	0.64
1:G:233:LYS:CD	1:G:233:LYS:H	2.10	0.64
1:A:121:ARG:NH1	1:A:125:PHE:CZ	2.65	0.64
1:B:121:ARG:CB	1:B:125:PHE:CE2	2.81	0.64
1:B:88:VAL:HG13	1:B:114:LEU:HD22	1.78	0.64
2:D:974:LEU:O	2:D:977:LYS:N	2.31	0.64
2:C:969:LEU:O	2:C:972:ASP:O	2.15	0.64
2:F:978:LEU:HD22	2:F:979:GLU:H	1.63	0.64
1:A:164:THR:OG1	1:A:165:LYS:N	2.31	0.64
2:F:981:GLU:O	2:F:983:ALA:N	2.31	0.64
2:H:940:GLN:H	2:H:940:GLN:CD	2.00	0.64
2:C:978:LEU:O	2:C:981:GLU:CD	2.36	0.63
2:D:969:LEU:CD2	2:D:974:LEU:CB	2.76	0.63
2:D:969:LEU:HD22	2:D:974:LEU:HB3	1.78	0.63
1:B:257:GLU:O	1:B:261:LYS:HG3	1.98	0.63
1:G:48:ARG:HH21	1:G:49:PHE:HE1	0.75	0.63
2:F:972:ASP:OD1	2:F:972:ASP:N	2.32	0.63
2:F:975:LEU:N	2:F:978:LEU:HD11	2.13	0.62
1:G:96:ARG:HD2	1:G:96:ARG:N	2.14	0.62
2:H:983:ALA:O	2:H:987:GLU:HG3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:974:LEU:CD2	2:F:974:LEU:O	2.48	0.62
1:G:38:ASP:HB3	1:G:41:LYS:HB2	1.82	0.62
2:C:974:LEU:HD23	2:C:974:LEU:C	2.20	0.62
2:C:978:LEU:C	2:C:981:GLU:OE2	2.38	0.61
1:A:292:SER:OG	1:A:293:SER:CB	2.48	0.61
2:H:948:TYR:CD1	2:H:948:TYR:C	2.74	0.61
2:F:988:ALA:HA	2:F:991:GLU:CB	2.31	0.61
2:H:974:LEU:HD12	2:H:974:LEU:H	1.64	0.61
1:G:24:GLU:OE2	1:G:24:GLU:N	2.34	0.61
2:F:987:GLU:O	2:F:991:GLU:CB	2.48	0.61
1:G:22:VAL:CA	1:G:24:GLU:CB	2.74	0.61
2:C:988:ALA:HA	1:E:126:PRO:HG2	1.83	0.61
1:A:21:GLY:HA3	1:A:24:GLU:HG2	1.75	0.61
1:E:21:GLY:O	1:E:24:GLU:CA	2.49	0.61
1:G:121:ARG:HB2	1:G:125:PHE:CE1	2.37	0.60
2:C:974:LEU:HD23	2:C:975:LEU:N	2.16	0.60
2:D:981:GLU:CD	2:D:981:GLU:C	2.59	0.60
1:E:164:THR:OG1	1:E:165:LYS:N	2.34	0.60
1:B:95:VAL:HG12	1:B:96:ARG:N	2.16	0.60
1:B:24:GLU:HA	1:B:24:GLU:OE2	2.01	0.60
1:B:38:ASP:HB3	1:B:41:LYS:HB2	1.84	0.60
2:H:990:GLU:O	2:H:991:GLU:C	2.40	0.60
1:B:283:HIS:O	1:B:287:GLY:N	2.32	0.60
2:C:973:GLY:CA	2:C:975:LEU:HD22	2.19	0.60
2:H:972:ASP:OD1	2:H:972:ASP:N	2.34	0.60
2:D:972:ASP:OD1	2:D:972:ASP:N	2.34	0.60
2:F:969:LEU:CD2	2:F:974:LEU:CB	2.76	0.60
1:G:96:ARG:O	1:G:96:ARG:HG2	2.01	0.60
2:H:976:LYS:CE	2:H:979:GLU:HB3	2.32	0.60
1:G:24:GLU:CD	1:G:24:GLU:N	2.55	0.59
1:A:84:GLN:HE21	2:D:950:ALA:HB2	1.65	0.59
1:A:121:ARG:CD	1:A:125:PHE:CZ	2.69	0.59
2:D:974:LEU:C	2:D:978:LEU:CD1	2.71	0.59
1:A:255:SER:HB2	1:A:258:LYS:H	1.68	0.59
2:D:974:LEU:N	2:D:974:LEU:HD13	2.09	0.59
2:F:975:LEU:HD12	2:F:978:LEU:HD11	1.84	0.59
1:A:292:SER:OG	1:A:293:SER:HB3	2.02	0.58
2:C:976:LYS:N	2:C:976:LYS:CE	2.66	0.58
1:G:121:ARG:HB2	1:G:125:PHE:HE1	1.66	0.58
1:G:222:ARG:NH2	1:G:272:ASP:OD1	2.36	0.58
1:G:255:SER:HB2	1:G:258:LYS:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:GLU:O	1:B:261:LYS:CG	2.50	0.58
2:C:984:GLU:O	2:C:987:GLU:CB	2.50	0.58
2:H:976:LYS:CE	2:H:976:LYS:CA	2.58	0.58
2:C:986:ALA:C	2:C:988:ALA:N	2.57	0.58
2:H:981:GLU:OE2	2:H:982:LYS:N	2.35	0.58
1:A:23:GLU:CB	1:A:26:LYS:HG3	2.30	0.58
1:E:84:GLN:HE21	2:F:950:ALA:HB2	1.67	0.58
2:C:986:ALA:C	2:C:988:ALA:H	2.05	0.58
2:F:974:LEU:CD1	2:F:974:LEU:H	2.14	0.58
1:B:40:GLU:O	1:B:44:THR:HG23	2.03	0.58
2:D:969:LEU:HD23	2:D:969:LEU:O	2.04	0.58
1:G:195:CYS:O	1:G:256:ALA:HB2	2.04	0.58
2:H:942:GLN:O	2:H:945:GLU:CG	2.39	0.57
1:E:95:VAL:CG1	1:E:95:VAL:O	2.52	0.57
2:H:939:GLY:O	2:H:942:GLN:CD	2.43	0.57
2:D:974:LEU:O	2:D:978:LEU:HD13	2.05	0.57
2:F:974:LEU:CD2	2:F:978:LEU:HD12	2.34	0.57
2:F:974:LEU:N	2:F:974:LEU:HD13	2.18	0.57
1:E:88:VAL:HG13	1:E:114:LEU:HD22	1.86	0.57
2:H:981:GLU:O	2:H:982:LYS:C	2.42	0.57
1:B:93:LYS:O	1:B:95:VAL:O	2.23	0.57
2:H:942:GLN:CG	2:H:945:GLU:OE1	2.53	0.57
1:E:121:ARG:HD2	1:E:125:PHE:CE2	2.39	0.56
1:E:255:SER:HB2	1:E:258:LYS:H	1.71	0.56
1:G:121:ARG:CB	1:G:125:PHE:CE1	2.88	0.56
2:H:945:GLU:O	2:H:949:GLU:CG	2.45	0.56
2:F:969:LEU:O	2:F:969:LEU:HD23	2.05	0.56
2:H:983:ALA:O	2:H:987:GLU:CG	2.54	0.56
1:G:21:GLY:C	1:G:24:GLU:CB	2.73	0.56
1:A:57:ALA:O	1:A:61:LYS:HG3	2.06	0.56
2:C:949:GLU:O	2:C:952:LYS:HG2	2.05	0.56
2:D:975:LEU:HA	2:D:978:LEU:CD2	2.14	0.56
1:G:67:LEU:HD21	1:G:78:MET:HG2	1.87	0.56
2:C:974:LEU:O	2:C:977:LYS:N	2.35	0.56
2:C:982:LYS:O	2:C:986:ALA:N	2.33	0.56
1:E:271:SER:O	1:E:272:ASP:C	2.43	0.56
2:H:939:GLY:HA2	2:H:942:GLN:HB3	1.88	0.55
1:G:121:ARG:CB	1:G:125:PHE:HE1	2.19	0.55
2:F:981:GLU:CD	2:F:982:LYS:HA	2.23	0.55
2:D:975:LEU:HA	2:D:978:LEU:HG	1.80	0.55
1:A:21:GLY:C	1:A:24:GLU:CB	2.75	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:22:VAL:C	1:E:24:GLU:H	2.10	0.55
1:E:22:VAL:O	1:E:23:GLU:CB	2.54	0.55
1:B:255:SER:OG	1:B:258:LYS:HE2	2.06	0.55
1:B:268:GLN:O	1:B:271:SER:OG	2.22	0.55
1:E:67:LEU:HD21	1:E:78:MET:HG2	1.89	0.55
2:D:984:GLU:C	2:D:986:ALA:N	2.60	0.55
1:E:57:ALA:O	1:E:61:LYS:HG3	2.07	0.54
2:F:970:GLU:OE2	2:F:974:LEU:HD12	2.06	0.54
1:G:258:LYS:HA	1:G:261:LYS:HG3	1.87	0.54
2:H:978:LEU:CB	2:H:981:GLU:OE1	2.55	0.54
1:G:93:LYS:O	1:G:96:ARG:HB3	2.07	0.54
2:H:981:GLU:O	2:H:983:ALA:N	2.41	0.54
1:E:114:LEU:HD12	1:E:119:LEU:HD22	1.90	0.54
1:E:40:GLU:O	1:E:44:THR:HG23	2.07	0.54
1:E:95:VAL:HG12	1:E:97:PHE:HD2	1.72	0.54
2:F:974:LEU:HD22	2:F:978:LEU:CD1	2.32	0.54
2:H:979:GLU:O	2:H:983:ALA:HB2	2.07	0.54
2:C:974:LEU:O	2:C:977:LYS:CB	2.55	0.54
1:A:268:GLN:O	1:A:271:SER:OG	2.19	0.53
1:A:67:LEU:HD21	1:A:78:MET:HG2	1.89	0.53
1:G:164:THR:OG1	1:G:165:LYS:N	2.41	0.53
1:G:291:HIS:HB2	1:G:292:SER:O	2.07	0.53
1:A:255:SER:HB3	1:A:257:GLU:HB2	1.90	0.53
2:D:980:GLU:OE2	2:D:980:GLU:HA	2.09	0.52
1:E:21:GLY:O	1:E:24:GLU:N	2.41	0.52
1:G:95:VAL:HG12	1:G:96:ARG:CA	2.40	0.52
1:E:38:ASP:HB3	1:E:41:LYS:HB2	1.91	0.52
1:A:22:VAL:O	1:A:22:VAL:CG2	2.57	0.52
2:D:951:GLN:O	2:D:955:THR:HG23	2.09	0.52
1:B:195:CYS:O	1:B:256:ALA:HB2	2.10	0.52
2:H:942:GLN:C	2:H:945:GLU:CG	2.78	0.52
1:B:255:SER:H	1:B:258:LYS:CE	2.23	0.52
2:D:974:LEU:C	2:D:974:LEU:CD2	2.78	0.52
2:H:981:GLU:HG2	2:H:982:LYS:H	1.39	0.52
1:A:40:GLU:O	1:A:44:THR:HG23	2.09	0.52
1:B:112:TYR:CD1	1:B:156:ARG:HD3	2.44	0.52
2:H:976:LYS:NZ	2:H:979:GLU:CB	2.73	0.52
2:F:981:GLU:C	2:F:983:ALA:N	2.62	0.51
2:C:973:GLY:C	2:C:975:LEU:H	2.13	0.51
2:F:974:LEU:HD22	2:F:974:LEU:O	2.08	0.51
1:B:57:ALA:O	1:B:61:LYS:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:LEU:HD12	1:E:120:PRO:HD2	1.92	0.51
1:B:84:GLN:HB2	2:C:947:ARG:HG3	1.92	0.51
1:E:66:ILE:O	1:E:81:ARG:NH2	2.44	0.51
2:C:951:GLN:O	2:C:955:THR:HG23	2.10	0.51
1:E:257:GLU:OE1	1:E:261:LYS:NZ	2.42	0.50
2:F:988:ALA:O	2:F:991:GLU:CA	2.59	0.50
2:C:990:GLU:O	2:C:991:GLU:C	2.50	0.50
1:E:210:CYS:O	1:E:211:PHE:HB2	2.12	0.50
1:G:112:TYR:HD1	1:G:156:ARG:HG2	1.76	0.50
1:G:97:PHE:HA	1:G:123:PRO:HG3	1.93	0.50
2:H:967:GLY:HA2	2:H:970:GLU:HG3	1.94	0.50
2:C:973:GLY:O	2:C:975:LEU:CD2	2.59	0.50
1:E:21:GLY:O	1:E:24:GLU:C	2.48	0.50
1:E:254:ASN:HB2	1:E:258:LYS:NZ	2.26	0.50
1:A:38:ASP:HB3	1:A:41:LYS:HB2	1.93	0.50
2:D:978:LEU:O	2:D:981:GLU:CB	2.36	0.50
1:G:45:PHE:N	1:G:291:HIS:CE1	2.80	0.50
2:H:975:LEU:N	2:H:975:LEU:HD12	2.26	0.50
1:B:97:PHE:HA	1:B:123:PRO:HG3	1.94	0.50
2:H:978:LEU:H	2:H:978:LEU:HD12	1.77	0.50
1:G:116:SER:O	1:G:118:LYS:HG2	2.12	0.50
2:C:991:GLU:O	2:C:992:ARG:C	2.49	0.50
1:G:22:VAL:N	1:G:24:GLU:CB	2.75	0.50
1:A:107:VAL:O	1:A:111:MET:HG3	2.12	0.49
1:A:23:GLU:H	1:A:25:LYS:N	2.10	0.49
1:A:88:VAL:HG13	1:A:114:LEU:HD22	1.93	0.49
1:A:288:THR:HG22	1:A:289:PRO:HD2	1.93	0.49
1:G:23:GLU:H	1:G:25:LYS:N	2.10	0.49
2:F:974:LEU:HD23	2:F:978:LEU:CD1	2.43	0.49
2:H:980:GLU:O	2:H:981:GLU:O	2.29	0.49
1:A:121:ARG:NH1	1:A:125:PHE:HZ	2.09	0.49
1:B:24:GLU:CA	1:B:24:GLU:OE2	2.56	0.49
1:G:96:ARG:NH1	2:D:966:TYR:CE1	2.80	0.49
1:E:97:PHE:HA	1:E:123:PRO:HG3	1.94	0.49
2:H:940:GLN:OE1	2:H:940:GLN:N	2.46	0.49
1:A:269:ASP:N	1:A:269:ASP:OD1	2.39	0.49
1:B:291:HIS:O	1:B:292:SER:C	2.50	0.49
2:F:974:LEU:C	2:F:978:LEU:HD11	2.32	0.49
1:E:121:ARG:CD	1:E:125:PHE:CZ	2.93	0.49
2:H:981:GLU:OE2	2:H:982:LYS:CA	2.61	0.48
2:F:988:ALA:O	2:F:991:GLU:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:GLU:N	1:A:26:LYS:H	2.11	0.48
2:C:969:LEU:HD23	2:C:969:LEU:O	2.13	0.48
1:G:23:GLU:N	1:G:24:GLU:CA	2.77	0.48
1:A:66:ILE:O	1:A:81:ARG:NH2	2.46	0.48
2:D:974:LEU:O	2:D:975:LEU:C	2.52	0.48
1:E:48:ARG:HG2	1:E:288:THR:CG2	2.43	0.48
1:A:121:ARG:HE	1:A:121:ARG:HB3	1.50	0.48
1:A:92:LEU:HB3	1:A:98:VAL:HG13	1.95	0.48
1:B:260:THR:O	1:B:264:GLU:CG	2.53	0.48
1:G:175:LYS:HD3	1:G:175:LYS:HA	1.67	0.48
1:G:188:LEU:HD22	1:G:247:LYS:HG3	1.95	0.48
1:G:233:LYS:N	1:G:233:LYS:HD2	2.21	0.47
2:H:982:LYS:O	2:H:983:ALA:C	2.52	0.47
1:A:21:GLY:CA	1:A:24:GLU:CG	2.64	0.47
2:F:974:LEU:O	2:F:978:LEU:HD11	2.13	0.47
1:G:102:THR:HG22	1:G:107:VAL:HG23	1.96	0.47
1:G:88:VAL:HG13	1:G:114:LEU:HD22	1.96	0.47
1:A:169:SER:HA	1:A:172:GLN:HE21	1.79	0.47
1:G:107:VAL:O	1:G:111:MET:HG3	2.15	0.47
2:H:975:LEU:N	2:H:975:LEU:CD1	2.77	0.47
1:G:168:ASP:O	1:G:171:PRO:HD2	2.15	0.47
1:G:66:ILE:O	1:G:81:ARG:NH2	2.47	0.47
2:H:978:LEU:CA	2:H:981:GLU:OE1	2.63	0.47
2:D:983:ALA:C	2:D:986:ALA:H	2.14	0.47
2:F:951:GLN:O	2:F:955:THR:HG23	2.15	0.47
2:H:976:LYS:NZ	2:H:979:GLU:HB3	2.29	0.46
2:H:938:ARG:O	2:H:942:GLN:HB2	2.15	0.46
2:D:969:LEU:HD21	2:D:974:LEU:CB	2.45	0.46
2:F:974:LEU:HD23	2:F:974:LEU:O	2.15	0.46
2:H:974:LEU:HD12	2:H:975:LEU:HD12	1.98	0.46
1:A:58:LEU:O	1:A:62:VAL:HG23	2.16	0.46
1:G:40:GLU:O	1:G:44:THR:HG23	2.16	0.46
2:H:974:LEU:CD1	2:H:974:LEU:H	2.25	0.46
2:H:980:GLU:HG3	2:H:981:GLU:N	2.31	0.46
2:F:969:LEU:HD21	2:F:974:LEU:CB	2.44	0.46
2:C:948:TYR:CD1	2:C:948:TYR:C	2.89	0.46
2:D:975:LEU:C	2:D:978:LEU:HD21	2.26	0.46
1:E:255:SER:HB3	1:E:257:GLU:HB2	1.97	0.46
1:A:121:ARG:CZ	1:A:125:PHE:CZ	2.99	0.45
1:A:210:CYS:O	1:A:211:PHE:HB2	2.16	0.45
2:H:974:LEU:O	2:H:978:LEU:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:VAL:CG1	1:B:96:ARG:N	2.79	0.45
1:B:48:ARG:HG3	1:B:289:PRO:O	2.16	0.45
1:E:269:ASP:OD1	1:E:269:ASP:N	2.46	0.45
1:E:66:ILE:HD13	1:E:153:TRP:HB3	1.97	0.45
2:F:974:LEU:HD23	2:F:978:LEU:HD12	1.97	0.45
1:G:118:LYS:HE2	1:G:118:LYS:HB3	1.70	0.45
2:H:976:LYS:NZ	2:H:979:GLU:HB2	2.30	0.45
1:B:21:GLY:CA	1:B:24:GLU:HG2	2.46	0.45
2:C:973:GLY:O	2:C:975:LEU:HD22	2.11	0.45
2:C:983:ALA:O	2:C:987:GLU:N	2.49	0.45
2:C:989:ALA:O	2:C:990:GLU:C	2.53	0.45
1:A:114:LEU:HD12	1:A:119:LEU:HD22	1.99	0.45
1:A:292:SER:HA	1:A:293:SER:HA	1.71	0.45
1:A:24:GLU:HG3	1:A:25:LYS:H	1.81	0.45
2:F:976:LYS:HD3	2:F:976:LYS:HA	1.80	0.45
2:F:980:GLU:O	2:F:983:ALA:HB3	2.15	0.45
1:G:95:VAL:HG12	1:G:97:PHE:N	2.32	0.45
2:C:974:LEU:N	2:C:975:LEU:HD22	2.28	0.45
1:E:95:VAL:HG13	1:E:95:VAL:O	2.17	0.45
1:G:112:TYR:CD1	1:G:156:ARG:HD3	2.52	0.45
1:A:22:VAL:O	1:A:22:VAL:HG23	2.17	0.45
2:F:947:ARG:HE	2:F:947:ARG:HB3	1.51	0.45
2:F:974:LEU:O	2:F:977:LYS:CB	2.65	0.45
2:F:981:GLU:OE2	2:F:981:GLU:O	2.35	0.45
1:E:67:LEU:HB3	1:E:74:HIS:CD2	2.51	0.45
1:B:188:LEU:HD22	1:B:247:LYS:HG3	1.98	0.44
1:G:233:LYS:O	1:G:234:ILE:C	2.55	0.44
1:B:45:PHE:CD2	1:B:45:PHE:C	2.91	0.44
2:D:984:GLU:O	2:D:987:GLU:N	2.50	0.44
1:G:23:GLU:CB	1:G:26:LYS:HB2	2.47	0.44
1:G:45:PHE:C	1:G:45:PHE:CD2	2.90	0.44
1:E:254:ASN:HB2	1:E:258:LYS:HZ3	1.81	0.44
1:G:257:GLU:OE1	1:G:261:LYS:HE3	2.17	0.44
1:B:206:TRP:CD1	1:B:211:PHE:CE1	3.06	0.44
1:A:281:LEU:HA	1:A:281:LEU:HD12	1.85	0.44
1:B:255:SER:H	1:B:258:LYS:HE2	1.82	0.44
2:C:968:ARG:HG2	2:F:969:LEU:HD11	1.99	0.44
2:C:984:GLU:O	2:C:987:GLU:N	2.50	0.44
1:A:23:GLU:CA	1:A:24:GLU:C	2.86	0.44
1:B:112:TYR:HD1	1:B:156:ARG:HG2	1.83	0.44
2:F:981:GLU:C	2:F:983:ALA:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:976:LYS:HA	2:H:979:GLU:HB3	1.99	0.44
1:B:246:PHE:CE1	1:B:267:PRO:HG2	2.52	0.44
1:A:67:LEU:HB3	1:A:74:HIS:CD2	2.53	0.44
1:B:118:LYS:HB3	1:B:118:LYS:HE2	1.61	0.44
1:G:268:GLN:O	1:G:271:SER:OG	2.26	0.44
1:E:143:GLU:HB2	1:E:217:GLU:HG2	2.00	0.44
1:E:107:VAL:O	1:E:111:MET:HG3	2.18	0.43
2:F:950:ALA:O	2:F:953:ARG:HB2	2.18	0.43
2:H:974:LEU:CD1	2:H:975:LEU:HD12	2.48	0.43
1:B:175:LYS:HD3	1:B:175:LYS:HA	1.77	0.43
1:B:48:ARG:HD3	1:B:49:PHE:CZ	2.53	0.43
2:D:981:GLU:O	2:D:982:LYS:C	2.55	0.43
1:E:205:LEU:HD21	1:E:214:CYS:HB2	2.00	0.43
1:E:21:GLY:CA	1:E:24:GLU:HB3	2.47	0.43
1:A:82:LYS:HB2	1:A:82:LYS:HE3	1.77	0.43
1:B:23:GLU:HA	1:B:26:LYS:HB2	2.00	0.43
1:A:23:GLU:HA	1:A:24:GLU:C	2.38	0.43
1:B:288:THR:CG2	1:B:289:PRO:CD	2.93	0.43
1:G:55:TYR:O	1:G:59:VAL:HG23	2.18	0.43
1:E:102:THR:HG22	1:E:107:VAL:HG23	2.01	0.43
2:F:981:GLU:O	2:F:982:LYS:C	2.57	0.43
2:H:949:GLU:O	2:H:952:LYS:CG	2.46	0.43
1:A:21:GLY:HA2	1:A:24:GLU:HG2	1.83	0.43
1:B:168:ASP:O	1:B:171:PRO:HD2	2.18	0.43
2:D:977:LYS:O	2:D:980:GLU:HB3	2.18	0.43
2:H:978:LEU:N	2:H:978:LEU:HD12	2.33	0.43
1:B:114:LEU:CD1	2:C:957:VAL:HG21	2.49	0.43
1:E:121:ARG:HD2	1:E:125:PHE:CG	2.54	0.43
1:E:48:ARG:HG2	1:E:288:THR:HG21	2.00	0.43
1:E:290:VAL:HG12	1:E:291:HIS:H	1.84	0.43
1:B:79:MET:O	1:B:80:TYR:C	2.54	0.43
2:D:975:LEU:HD22	2:D:975:LEU:H	1.84	0.43
1:E:121:ARG:NH1	1:E:125:PHE:CZ	2.87	0.43
1:E:22:VAL:HG13	1:E:26:LYS:HE2	2.00	0.43
1:B:79:MET:CE	1:B:82:LYS:NZ	2.81	0.43
2:F:981:GLU:CD	2:F:982:LYS:H	1.97	0.43
1:B:139:LYS:HA	1:B:142:GLU:HG3	2.00	0.43
1:G:96:ARG:HD2	1:G:96:ARG:H	1.84	0.43
1:A:24:GLU:CG	1:A:25:LYS:H	2.32	0.42
1:E:255:SER:H	1:E:258:LYS:CE	2.31	0.42
1:A:290:VAL:HG12	1:A:291:HIS:N	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:22:VAL:O	1:G:24:GLU:HG2	2.19	0.42
1:B:269:ASP:N	1:B:269:ASP:OD1	2.52	0.42
2:D:975:LEU:CD1	2:D:978:LEU:HG	2.44	0.42
2:D:975:LEU:O	2:D:978:LEU:N	2.53	0.42
1:E:206:TRP:CD1	1:E:211:PHE:CE1	3.08	0.42
1:B:204:ASP:OD2	1:B:204:ASP:N	2.47	0.42
1:G:173:LEU:N	1:G:174:PRO:CD	2.83	0.42
1:G:258:LYS:CA	1:G:261:LYS:HG3	2.49	0.42
2:H:939:GLY:HA2	2:H:942:GLN:CB	2.49	0.42
2:H:975:LEU:H	2:H:975:LEU:CD1	2.33	0.42
2:D:946:SER:C	2:D:949:GLU:HG3	2.36	0.42
2:F:976:LYS:O	2:F:979:GLU:HB3	2.18	0.42
1:E:194:MET:CE	1:E:194:MET:HA	2.50	0.42
1:G:119:LEU:HD12	1:G:120:PRO:CD	2.50	0.42
1:E:195:CYS:O	1:E:256:ALA:HB2	2.20	0.42
2:H:946:SER:CA	2:H:949:GLU:CG	2.90	0.41
1:A:23:GLU:N	1:A:25:LYS:N	2.69	0.41
2:D:947:ARG:HE	2:D:947:ARG:HB3	1.62	0.41
2:D:967:GLY:HA2	2:D:970:GLU:HG3	2.01	0.41
1:E:45:PHE:CD2	1:E:45:PHE:C	2.93	0.41
1:E:64:LEU:O	1:E:157:ARG:NH1	2.53	0.41
1:G:246:PHE:CE1	1:G:267:PRO:HG2	2.56	0.41
1:A:66:ILE:HD13	1:A:153:TRP:HB3	2.01	0.41
1:B:257:GLU:O	1:B:261:LYS:HG2	2.20	0.41
1:B:82:LYS:HB2	1:B:82:LYS:HE3	1.62	0.41
1:E:82:LYS:HE3	1:E:82:LYS:HB2	1.74	0.41
1:A:23:GLU:N	1:A:24:GLU:CA	2.83	0.41
1:B:192:LEU:HD11	1:B:243:LEU:HD22	2.03	0.41
1:B:64:LEU:O	1:B:157:ARG:NH1	2.53	0.41
1:B:205:LEU:HD21	1:B:214:CYS:HB2	2.03	0.41
1:B:255:SER:HB2	1:B:258:LYS:H	1.86	0.41
1:E:112:TYR:HD1	1:E:156:ARG:HG2	1.85	0.41
1:A:173:LEU:N	1:A:174:PRO:CD	2.83	0.41
2:C:975:LEU:C	2:C:977:LYS:N	2.74	0.41
1:G:58:LEU:O	1:G:62:VAL:HG23	2.21	0.41
2:H:939:GLY:CA	2:H:942:GLN:NE2	2.81	0.41
1:B:257:GLU:HA	1:B:257:GLU:OE1	2.21	0.41
2:D:969:LEU:HD23	2:D:974:LEU:HB3	1.94	0.41
2:H:979:GLU:HG2	2:H:980:GLU:N	2.35	0.41
1:B:84:GLN:HE21	2:C:950:ALA:HB2	1.86	0.41
2:D:974:LEU:O	2:D:976:LYS:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:975:LEU:CD2	2:D:975:LEU:H	2.34	0.41
2:D:974:LEU:C	2:D:976:LYS:N	2.72	0.41
2:F:975:LEU:HD12	2:F:978:LEU:CD1	2.50	0.41
2:H:940:GLN:C	2:H:942:GLN:N	2.68	0.41
2:H:948:TYR:O	2:H:948:TYR:CD1	2.74	0.41
1:A:45:PHE:CD2	1:A:45:PHE:C	2.95	0.41
1:B:114:LEU:HD12	2:C:957:VAL:HG21	2.03	0.41
1:E:95:VAL:CG1	1:E:97:PHE:HD2	2.34	0.41
1:G:82:LYS:HB2	1:G:82:LYS:HE3	1.62	0.41
1:A:205:LEU:HD21	1:A:214:CYS:HB2	2.02	0.40
2:H:954:ILE:HG22	2:H:955:THR:N	2.35	0.40
1:A:135:LEU:O	1:A:139:LYS:HG3	2.21	0.40
1:A:288:THR:HA	1:A:289:PRO:HD3	1.90	0.40
2:F:978:LEU:HD22	2:F:979:GLU:N	2.33	0.40
1:A:22:VAL:C	1:A:24:GLU:HB2	2.36	0.40
1:A:253:LEU:HD22	1:A:258:LYS:HB3	2.02	0.40
1:A:23:GLU:H	1:A:26:LYS:H	1.69	0.40
1:E:169:SER:HA	1:E:172:GLN:HE21	1.86	0.40
1:E:34:ASP:HB3	1:E:36:ARG:O	2.21	0.40
1:G:23:GLU:H	1:G:26:LYS:H	1.69	0.40
2:H:978:LEU:HA	2:H:981:GLU:HB3	2.03	0.40
2:D:950:ALA:O	2:D:953:ARG:HB2	2.21	0.40
2:D:975:LEU:O	2:D:979:GLU:N	2.51	0.40
1:G:119:LEU:HD12	1:G:119:LEU:HA	1.86	0.40
1:G:173:LEU:HD22	1:G:236:VAL:CG2	2.51	0.40
1:G:192:LEU:HD11	1:G:243:LEU:HD22	2.02	0.40

All (3) 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:G:24:GLU:OE1	1:E:290:VAL:N[1_655]	1.80	0.40
1:G:23:GLU:O	1:E:288:THR:O[1_655]	1.88	0.32
1:B:290:VAL:CG2	1:A:40:GLU:OE2[1_655]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	272/273 (100%)	253 (93%)	18 (7%)	1 (0%)	38	70
1	B	271/273 (99%)	254 (94%)	16 (6%)	1 (0%)	38	70
1	E	271/273 (99%)	254 (94%)	17 (6%)	0	100	100
1	G	271/273 (99%)	255 (94%)	16 (6%)	0	100	100
2	C	51/56 (91%)	43 (84%)	6 (12%)	2 (4%)	3	11
2	D	51/56 (91%)	39 (76%)	11 (22%)	1 (2%)	9	27
2	F	52/56 (93%)	48 (92%)	3 (6%)	1 (2%)	9	29
2	H	53/56 (95%)	47 (89%)	2 (4%)	4 (8%)	1	2
All	All	1292/1316 (98%)	1193 (92%)	89 (7%)	10 (1%)	22	53

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	981	GLU
2	H	991	GLU
2	F	982	LYS
2	D	980	GLU
1	B	23	GLU
2	C	990	GLU
2	H	982	LYS
2	H	990	GLU
1	A	118	LYS
2	C	991	GLU

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	249/249 (100%)	209 (84%)	40 (16%)	3	8
1	B	247/249 (99%)	212 (86%)	35 (14%)	4	11
1	E	248/249 (100%)	208 (84%)	40 (16%)	3	8
1	G	248/249 (100%)	207 (84%)	41 (16%)	2	7
2	C	36/45 (80%)	26 (72%)	10 (28%)	0	1
2	D	36/45 (80%)	30 (83%)	6 (17%)	2	7
2	F	36/45 (80%)	27 (75%)	9 (25%)	1	2
2	H	37/45 (82%)	24 (65%)	13 (35%)	0	0
All	All	1137/1176 (97%)	943 (83%)	194 (17%)	2	6

All (194) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	22	VAL
1	B	39[A]	THR
1	B	39[B]	THR
1	B	44	THR
1	B	48	ARG
1	B	53	SER
1	B	54	MET
1	B	70	HIS
1	B	71	HIS
1	B	76	LYS
1	B	79	MET
1	B	81	ARG
1	B	82	LYS
1	B	100	ASP
1	B	118	LYS
1	B	122	SER
1	B	125	PHE
1	B	127	LEU
1	B	135	LEU
1	B	156	ARG
1	B	165	LYS
1	B	169	SER
1	B	175	LYS
1	B	194	MET

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Mol	Chain	Res	Type
1	B	196	SER
1	B	204	ASP
1	B	219	SER
1	B	243	LEU
1	B	270	SER
1	B	271	SER
1	B	272	ASP
1	B	288	THR
1	B	290	VAL
1	B	291	HIS
1	B	292	SER
2	C	941	LEU
2	C	942	GLN
2	C	949	GLU
2	C	955	THR
2	C	972	ASP
2	C	974	LEU
2	C	975	LEU
2	C	976	LYS
2	C	980	GLU
2	C	981	GLU
1	G	22	VAL
1	G	24	GLU
1	G	39[A]	THR
1	G	39[B]	THR
1	G	44	THR
1	G	48	ARG
1	G	53	SER
1	G	54	MET
1	G	70	HIS
1	G	71	HIS
1	G	76	LYS
1	G	79	MET
1	G	81	ARG
1	G	82	LYS
1	G	95	VAL
1	G	96	ARG
1	G	98	VAL
1	G	114	LEU
1	G	118	LYS
1	G	121	ARG
1	G	122	SER

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Mol	Chain	Res	Type
1	G	125	PHE
1	G	127	LEU
1	G	135	LEU
1	G	146	GLU
1	G	156	ARG
1	G	165	LYS
1	G	169	SER
1	G	175	LYS
1	G	194	MET
1	G	196	SER
1	G	204	ASP
1	G	214	CYS
1	G	219	SER
1	G	233	LYS
1	G	243	LEU
1	G	259	ILE
1	G	261	LYS
1	G	271	SER
1	G	288	THR
1	G	290	VAL
2	H	940	GLN
2	H	941	LEU
2	H	942	GLN
2	H	945	GLU
2	H	946	SER
2	H	948	TYR
2	H	949	GLU
2	H	966	TYR
2	H	972	ASP
2	H	974	LEU
2	H	976	LYS
2	H	980	GLU
2	H	981	GLU
1	E	22	VAL
1	E	35	ASP
1	E	40	GLU
1	E	44	THR
1	E	48	ARG
1	E	53	SER
1	E	54	MET
1	E	70	HIS
1	E	71	HIS

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Mol	Chain	Res	Type
1	E	72	GLU
1	E	81	ARG
1	E	82	LYS
1	E	98	VAL
1	E	114	LEU
1	E	122	SER
1	E	125	PHE
1	E	127	LEU
1	E	132	GLU
1	E	135	LEU
1	E	146	GLU
1	E	156	ARG
1	E	160	ASN
1	E	167	ARG
1	E	169	SER
1	E	175	LYS
1	E	194	MET
1	E	196	SER
1	E	204	ASP
1	E	219	SER
1	E	231	SER
1	E	243	LEU
1	E	257	GLU
1	E	259	ILE
1	E	261	LYS
1	E	269	ASP
1	E	270	SER
1	E	271	SER
1	E	290	VAL
1	E	291	HIS
1	E	292	SER
2	F	941	LEU
2	F	942	GLN
2	F	949	GLU
2	F	955	THR
2	F	972	ASP
2	F	974	LEU
2	F	975	LEU
2	F	978	LEU
2	F	981	GLU
1	A	22	VAL
1	A	24	GLU

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Mol	Chain	Res	Type
1	A	35	ASP
1	A	40	GLU
1	A	44	THR
1	A	70	HIS
1	A	71	HIS
1	A	72	GLU
1	A	76	LYS
1	A	81	ARG
1	A	82	LYS
1	A	96	ARG
1	A	98	VAL
1	A	114	LEU
1	A	118	LYS
1	A	121	ARG
1	A	122	SER
1	A	125	PHE
1	A	127	LEU
1	A	135	LEU
1	A	146	GLU
1	A	156	ARG
1	A	160	ASN
1	A	167	ARG
1	A	169	SER
1	A	175	LYS
1	A	194	MET
1	A	196	SER
1	A	204	ASP
1	A	219	SER
1	A	231	SER
1	A	243	LEU
1	A	259	ILE
1	A	269	ASP
1	A	270	SER
1	A	271	SER
1	A	272	ASP
1	A	288	THR
1	A	291	HIS
1	A	293	SER
2	D	942	GLN
2	D	949	GLU
2	D	955	THR
2	D	972	ASP

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Mol	Chain	Res	Type
2	D	974	LEU
2	D	978	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	172	GLN
1	B	283	HIS
2	C	940	GLN
2	C	942	GLN
1	G	172	GLN
1	G	291	HIS
2	H	942	GLN
1	E	84	GLN
1	E	172	GLN
2	F	940	GLN
2	F	942	GLN
1	A	84	GLN
1	A	172	GLN
2	D	940	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 ⓘ

There are no ligands in this entry.

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	273/273 (100%)	-0.24	8 (2%)	52	41	38, 59, 109, 198	0
1	B	272/273 (99%)	-0.36	5 (1%)	69	60	39, 60, 99, 165	0
1	E	272/273 (99%)	-0.26	8 (2%)	52	41	39, 59, 105, 185	0
1	G	272/273 (99%)	-0.27	5 (1%)	69	60	40, 60, 103, 170	0
2	C	53/56 (94%)	3.00	28 (52%)	0	0	36, 72, 150, 155	21 (39%)
2	D	53/56 (94%)	2.30	24 (45%)	0	0	34, 71, 125, 160	25 (47%)
2	F	54/56 (96%)	1.78	19 (35%)	0	0	51, 70, 126, 149	21 (38%)
2	H	55/56 (98%)	3.27	32 (58%)	0	0	38, 75, 195, 213	22 (40%)
All	All	1304/1316 (99%)	0.19	129 (9%)	8	4	34, 61, 121, 213	89 (6%)

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	985	ALA	12.6
2	C	985	ALA	11.6
1	A	290	VAL	10.5
2	F	989	ALA	9.8
2	C	980	GLU	9.7
2	H	974	LEU	9.6
2	C	988	ALA	9.5
2	C	978	LEU	9.0
2	F	993	LEU	8.9
1	A	291	HIS	8.9
2	D	989	ALA	8.8
2	D	988	ALA	8.7
2	H	980	GLU	8.7
2	H	983	ALA	8.7
2	H	975	LEU	8.3
1	B	290	VAL	8.3

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Mol	Chain	Res	Type	RSRZ
2	H	987	GLU	8.2
2	C	989	ALA	8.1
2	F	988	ALA	7.9
2	H	986	ALA	7.8
2	H	978	LEU	7.6
2	D	984	GLU	7.6
2	F	986	ALA	7.4
1	G	290	VAL	7.3
2	C	942	GLN	7.3
2	C	941	LEU	7.3
2	C	990	GLU	7.3
2	H	941	LEU	7.2
1	E	291	HIS	7.0
1	E	290	VAL	7.0
2	H	989	ALA	7.0
2	C	973	GLY	6.9
2	F	980	GLU	6.7
2	C	946	SER	6.7
2	H	946	SER	6.7
2	D	991	GLU	6.6
2	C	975	LEU	6.6
2	H	988	ALA	6.4
2	H	982	LYS	6.2
2	D	990	GLU	6.2
2	D	992	ARG	6.1
2	D	980	GLU	6.1
2	F	990	GLU	5.9
2	H	940	GLN	5.8
2	H	979	GLU	5.8
2	C	986	ALA	5.7
2	H	992	ARG	5.6
2	D	975	LEU	5.6
2	H	976	LYS	5.6
1	A	288	THR	5.5
2	C	983	ALA	5.5
2	D	973	GLY	5.4
2	H	947	ARG	5.4
1	G	288	THR	5.4
2	D	979	GLU	5.3
1	E	292	SER	5.3
2	C	987	GLU	5.3
2	H	942	GLN	5.3

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Mol	Chain	Res	Type	RSRZ
2	C	984	GLU	5.1
2	D	976	LYS	5.1
1	A	289	PRO	5.1
2	F	981	GLU	5.0
2	F	984	GLU	5.0
2	F	983	ALA	4.9
2	D	974	LEU	4.9
2	F	991	GLU	4.9
2	D	983	ALA	4.8
2	D	977	LYS	4.7
2	H	984	GLU	4.7
2	C	982	LYS	4.7
2	F	992	ARG	4.6
2	F	987	GLU	4.6
2	D	978	LEU	4.6
2	D	987	GLU	4.6
2	D	985	ALA	4.5
2	C	947	ARG	4.5
1	A	293	SER	4.5
2	C	976	LYS	4.5
2	F	979	GLU	4.3
2	H	943	ALA	4.2
1	G	291	HIS	4.2
2	H	973	GLY	4.2
1	E	121	ARG	4.0
2	D	986	ALA	3.9
1	B	289	PRO	3.9
2	H	944	ALA	3.9
2	H	981	GLU	3.8
2	C	940	GLN	3.8
2	C	945	GLU	3.8
2	C	981	GLU	3.8
2	C	944	ALA	3.8
2	F	985	ALA	3.6
2	F	982	LYS	3.6
2	C	943	ALA	3.6
1	A	121	ARG	3.5
2	C	979	GLU	3.5
1	A	21	GLY	3.5
1	E	289	PRO	3.4
2	C	991	GLU	3.4
1	G	289	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
2	H	977	LYS	3.3
2	H	972	ASP	3.3
2	C	977	LYS	3.2
2	D	981	GLU	3.2
2	D	946	SER	3.1
2	H	938	ARG	3.1
2	F	944	ALA	3.0
2	D	944	ALA	3.0
1	E	168	ASP	3.0
2	D	972	ASP	3.0
1	A	125	PHE	2.9
1	B	288	THR	2.9
2	H	991	GLU	2.9
2	H	945	GLU	2.9
2	C	972	ASP	2.9
2	H	939	GLY	2.8
2	F	946	SER	2.6
2	F	978	LEU	2.6
1	E	125	PHE	2.5
2	C	974	LEU	2.5
2	H	990	GLU	2.4
2	D	947	ARG	2.4
1	E	164	THR	2.2
2	D	982	LYS	2.1
1	G	36	ARG	2.1
2	F	941	LEU	2.1
2	H	949	GLU	2.1
1	B	291	HIS	2.0
1	B	21	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.