



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 12:13 pm GMT

PDB ID : 5A1A  
EMDB ID: : EMD-2984  
Title : 2.2 Å resolution cryo-EM structure of beta-galactosidase in complex with a cell-permeant inhibitor  
Authors : Bartesaghi, A.; Merk, A.; Banerjee, S.; Matthies, D.; Wu, X.; Milne, J.; Subramaniam, S.  
Deposited on : 2015-04-29  
Resolution : 2.20 Å (reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc29047

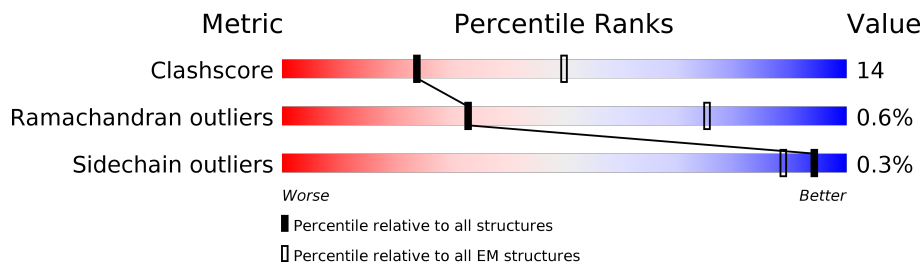
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.20 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	1022	72% 27% .
1	B	1022	71% 28% .
1	C	1022	72% 27% .
1	D	1022	71% 28% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PTQ	A	2001	-	-	X	-
2	PTQ	B	2001	-	-	X	-
2	PTQ	C	2001	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PTQ	D	2001	-	-	X	-

## 2 Entry composition [i](#)

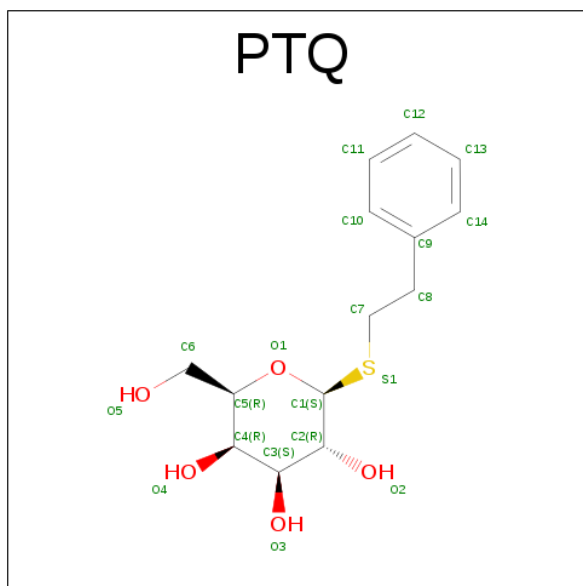
There are 5 unique types of molecules in this entry. The entry contains 33696 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 BETA-GALACTOSIDASE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1022	Total	C	N	O	S	0	0
			8206	5190	1452	1525	39		
1	B	1022	Total	C	N	O	S	0	0
			8206	5190	1452	1525	39		
1	C	1022	Total	C	N	O	S	0	0
			8206	5190	1452	1525	39		
1	D	1022	Total	C	N	O	S	0	0
			8206	5190	1452	1525	39		

- Molecule 2 is SUGAR (2-PHENYLETHYL 1-THIO-BETA-D-GALACTOPYRANOSIDE) (three-letter code: PTQ) (formula: C<sub>14</sub>H<sub>20</sub>O<sub>5</sub>S).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	O	S	0
			20	14	5	1	
2	B	1	Total	C	O	S	0
			20	14	5	1	

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Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total	C	O	S	0
			20	14	5	1	
2	D	1	Total	C	O	S	0
			20	14	5	1	

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

Mol	Chain	Residues	Atoms		AltConf
3	B	2	Total	Mg	0
			2	2	
3	A	2	Total	Mg	0
			2	2	
3	D	2	Total	Mg	0
			2	2	
3	C	2	Total	Mg	0
			2	2	

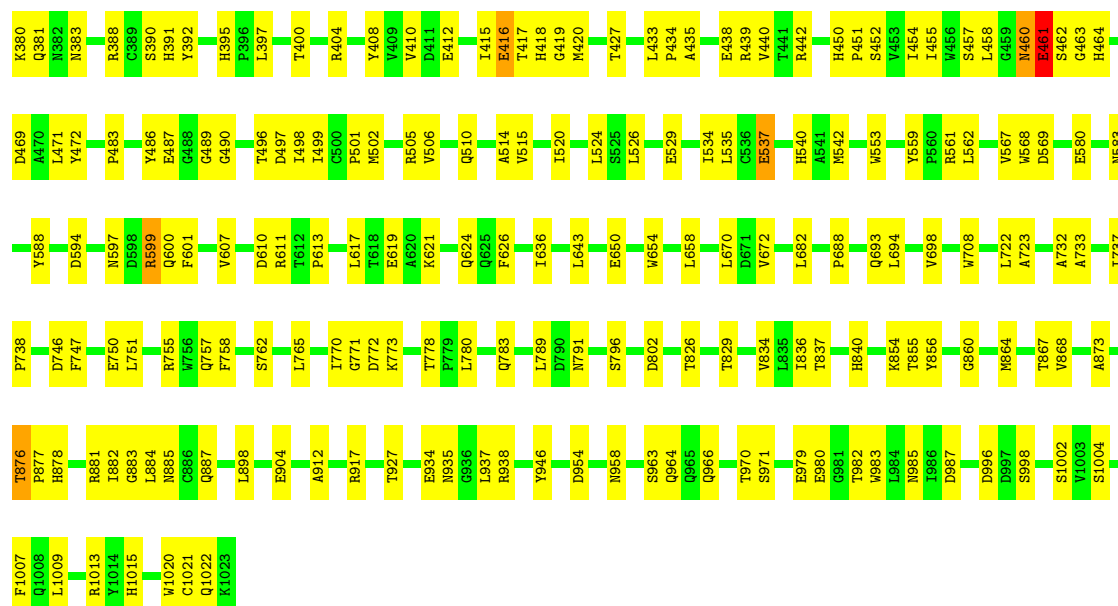
- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
4	B	2	Total	Na	0
			2	2	
4	A	2	Total	Na	0
			2	2	
4	D	2	Total	Na	0
			2	2	
4	C	2	Total	Na	0
			2	2	

- Molecule 5 is water.

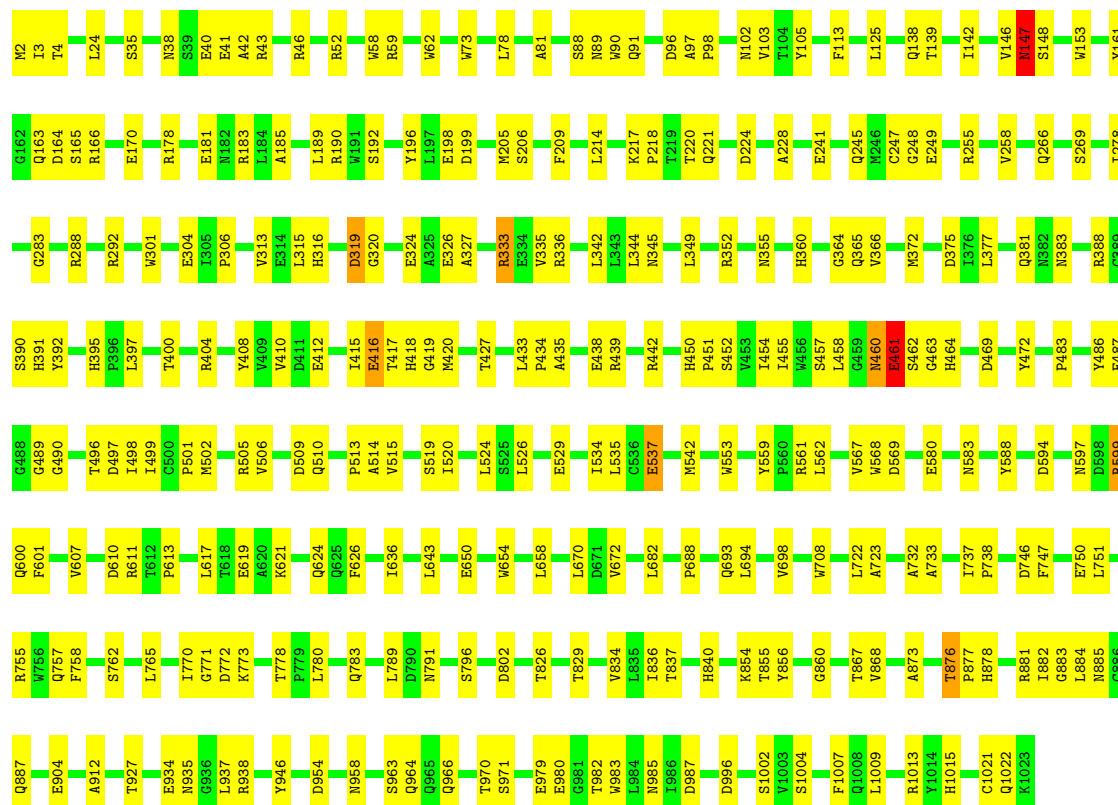
Mol	Chain	Residues	Atoms		AltConf
5	A	194	Total	O	0
			194	194	
5	B	194	Total	O	0
			194	194	
5	C	194	Total	O	0
			194	194	
5	D	194	Total	O	0
			194	194	





• Molecule 1: BETA-GALACTOSIDASE

Chain C: 72% 27%



• Molecule 1: BETA-GALACTOSIDASE

Chain D: 71% 28%

R1013	R881	F747	D594	L471	N392	S269	W153	W2
Y1014	I882	E750	N597	Y472	N393	S269	W153	I3
H1015	G883	L751	D598	P483	R388	L278	Y161	T4
	L884		R599		C389		G162	L24
W1020	N885	R755	Q600	E487	S390	G283	Q163	H30
C1021	C886	W756	F601	G488	H391	R288	S165	F31
Q1022	Q887	Q757	V607	G489	Y392		R166	
	L898	F758			H395	R292	E170	S35
	E904	S762	D610	T496	P396		R178	N38
	A912	L765	R611	D497	L397	W301		S39
	R917	I770	T612	T498	T400	E304	E181	E40
	T927	G771	P613	T499	R404	P305	N182	E41
		D772	L617	C500	M502	L306	R183	A42
		K773	T618	M502		Y313	L184	R43
			E619		Y408	E314	A185	
	E934	T778	A620	R505	W409	L315	L189	
	N935	P779	K621	V506	V410	H316	R190	R52
	G936	L780	Q624	Q610	D411		W191	
	L937		Q625	A514	E412	D319	S192	W58
	R938	Q783	F626	V515	I415	G320	D193	R59
					E416			
	Y946	L789	I636		T417	E324	Y196	W62
		D790	L643	T520	H418	A325	L197	
	D954	N791		L524	G419	E326	E198	W73
	N958	S796	E650	S525	M420	A327	D199	L78
				L526			M205	
	S963	D802	W654		T427	R333	S206	A81
	Q964		L658	E529	L433	E334	F209	S88
	Q966	T826		L534	P434	R336		N89
		T829	L670	L535	A435		L214	W90
	T970		D671	C536		L342	K217	Q91
	S971	V834	V672	E537	E438	L343	P218	
		L835			R439	L344	T219	D96
	E979	T836	L682	H540	W440	N345	T220	A97
	E980	T837		A541	T441	L349	Q221	P98
	G981		P688	M542	R442			
	T982	H840		W553	H450	R352	D224	N102
	L983		Q693	W559	P451			V103
	N985	K854	L694	Y559	S452	N355	A228	T104
	L986	T855	V698	P560	I453			Y105
	D987	Y856		R561	I455	H360	E241	F113
		G860	W708	L562	W456	G364	Q245	S124
	D996				S457	Q365	M246	L125
	D997	W664	L722	V667	L458	V366	C247	Q138
	S998	A723	A723	W568	G459		E249	T139
		T867	A732	D569	N460	N372		
	S1002	V868	A733	E580	S462	D375	R255	I142
	V1003		A873	N583	G463	L376		
	S1004				H464	L377	V258	
		T876	I737	Y588	D469	K380		V146
	F1007	Q877	P738		A470	Q381		N147
	Q1008	H878	D746					Q266
	L1009							



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	215000	Depositor
Image detector	GATAN K2 (4K X 4K)	Depositor

## 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: NA, MG, PTQ

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.40	6/8448 (0.1%)	0.52	14/11526 (0.1%)
1	B	0.40	6/8448 (0.1%)	0.52	14/11526 (0.1%)
1	C	0.40	6/8448 (0.1%)	0.52	14/11526 (0.1%)
1	D	0.40	6/8448 (0.1%)	0.52	14/11526 (0.1%)
All	All	0.40	24/33792 (0.1%)	0.52	56/46104 (0.1%)

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	3
1	B	0	3
1	C	0	3
1	D	0	3
All	All	0	12

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	146	VAL	C-N	-18.42	0.91	1.34
1	B	146	VAL	C-N	-18.42	0.91	1.34
1	C	146	VAL	C-N	-18.42	0.91	1.34
1	D	146	VAL	C-N	-18.42	0.91	1.34
1	A	461	GLU	C-N	-15.25	0.98	1.34
1	B	461	GLU	C-N	-15.25	0.98	1.34
1	C	461	GLU	C-N	-15.25	0.98	1.34
1	D	461	GLU	C-N	-15.25	0.98	1.34
1	A	139	THR	C-N	-12.93	1.04	1.34
1	B	139	THR	C-N	-12.93	1.04	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	139	THR	C-N	-12.93	1.04	1.34
1	D	139	THR	C-N	-12.93	1.04	1.34
1	A	138	GLN	C-N	10.66	1.58	1.34
1	B	138	GLN	C-N	10.66	1.58	1.34
1	C	138	GLN	C-N	10.66	1.58	1.34
1	D	138	GLN	C-N	10.66	1.58	1.34
1	A	877	PRO	N-CD	5.24	1.55	1.47
1	B	877	PRO	N-CD	5.24	1.55	1.47
1	C	877	PRO	N-CD	5.24	1.55	1.47
1	D	877	PRO	N-CD	5.24	1.55	1.47
1	A	98	PRO	N-CD	5.22	1.55	1.47
1	B	98	PRO	N-CD	5.22	1.55	1.47
1	C	98	PRO	N-CD	5.22	1.55	1.47
1	D	98	PRO	N-CD	5.22	1.55	1.47

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	461	GLU	O-C-N	19.17	153.38	122.70
1	B	461	GLU	O-C-N	19.17	153.38	122.70
1	C	461	GLU	O-C-N	19.17	153.38	122.70
1	D	461	GLU	O-C-N	19.17	153.38	122.70
1	A	147	ASN	O-C-N	-14.44	99.59	122.70
1	B	147	ASN	O-C-N	-14.44	99.59	122.70
1	C	147	ASN	O-C-N	-14.44	99.59	122.70
1	D	147	ASN	O-C-N	-14.44	99.59	122.70
1	A	461	GLU	CA-C-N	-14.05	86.30	117.20
1	B	461	GLU	CA-C-N	-14.05	86.30	117.20
1	C	461	GLU	CA-C-N	-14.05	86.30	117.20
1	D	461	GLU	CA-C-N	-14.05	86.30	117.20
1	A	146	VAL	C-N-CA	10.45	147.81	121.70
1	B	146	VAL	C-N-CA	10.45	147.81	121.70
1	C	146	VAL	C-N-CA	10.45	147.81	121.70
1	D	146	VAL	C-N-CA	10.45	147.81	121.70
1	A	147	ASN	CA-C-N	9.20	137.44	117.20
1	B	147	ASN	CA-C-N	9.20	137.44	117.20
1	C	147	ASN	CA-C-N	9.20	137.44	117.20
1	D	147	ASN	CA-C-N	9.20	137.44	117.20
1	A	146	VAL	O-C-N	-8.49	109.11	122.70
1	B	146	VAL	O-C-N	-8.49	109.11	122.70
1	C	146	VAL	O-C-N	-8.49	109.11	122.70
1	D	146	VAL	O-C-N	-8.49	109.11	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	ASN	O-C-N	-7.77	110.27	122.70
1	B	460	ASN	O-C-N	-7.77	110.27	122.70
1	C	460	ASN	O-C-N	-7.77	110.27	122.70
1	D	460	ASN	O-C-N	-7.77	110.27	122.70
1	A	139	THR	O-C-N	-7.67	110.43	122.70
1	B	139	THR	O-C-N	-7.67	110.43	122.70
1	C	139	THR	O-C-N	-7.67	110.43	122.70
1	D	139	THR	O-C-N	-7.67	110.43	122.70
1	A	461	GLU	C-N-CA	-6.67	105.02	121.70
1	B	461	GLU	C-N-CA	-6.67	105.02	121.70
1	C	461	GLU	C-N-CA	-6.67	105.02	121.70
1	D	461	GLU	C-N-CA	-6.67	105.02	121.70
1	A	147	ASN	C-N-CA	-6.42	105.66	121.70
1	B	147	ASN	C-N-CA	-6.42	105.66	121.70
1	C	147	ASN	C-N-CA	-6.42	105.66	121.70
1	D	147	ASN	C-N-CA	-6.42	105.66	121.70
1	A	146	VAL	CA-C-N	5.80	129.95	117.20
1	B	146	VAL	CA-C-N	5.80	129.95	117.20
1	C	146	VAL	CA-C-N	5.80	129.95	117.20
1	D	146	VAL	CA-C-N	5.80	129.95	117.20
1	A	97	ALA	C-N-CD	5.67	140.30	128.40
1	B	97	ALA	C-N-CD	5.67	140.30	128.40
1	C	97	ALA	C-N-CD	5.67	140.30	128.40
1	D	97	ALA	C-N-CD	5.67	140.30	128.40
1	A	876	THR	C-N-CD	5.50	139.94	128.40
1	B	876	THR	C-N-CD	5.50	139.94	128.40
1	C	876	THR	C-N-CD	5.50	139.94	128.40
1	D	876	THR	C-N-CD	5.50	139.94	128.40
1	A	139	THR	CA-C-N	5.20	128.64	117.20
1	B	139	THR	CA-C-N	5.20	128.64	117.20
1	C	139	THR	CA-C-N	5.20	128.64	117.20
1	D	139	THR	CA-C-N	5.20	128.64	117.20

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	147	ASN	Mainchain
1	A	460	ASN	Mainchain
1	A	882	ILE	Peptide
1	B	147	ASN	Mainchain
1	B	460	ASN	Mainchain

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Mol	Chain	Res	Type	Group
1	B	882	ILE	Peptide
1	C	147	ASN	Mainchain
1	C	460	ASN	Mainchain
1	C	882	ILE	Peptide
1	D	147	ASN	Mainchain
1	D	460	ASN	Mainchain
1	D	882	ILE	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	8206	0	7802	218	0
1	B	8206	0	7802	221	0
1	C	8206	0	7802	218	0
1	D	8206	0	7802	218	0
2	A	20	0	18	20	0
2	B	20	0	18	20	0
2	C	20	0	18	20	0
2	D	20	0	18	19	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	194	0	0	19	0
5	B	194	0	0	19	0
5	C	194	0	0	19	0
5	D	194	0	0	19	0
All	All	33696	0	31280	878	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (878) 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:C:601:PHE:CG	2:C:2001:PTQ:H11	1.82	1.15
1:A:601:PHE:CG	2:A:2001:PTQ:H11	1.82	1.15
1:D:601:PHE:CG	2:D:2001:PTQ:H11	1.82	1.14
1:B:601:PHE:CG	2:B:2001:PTQ:H11	1.82	1.14
1:B:601:PHE:CD1	2:B:2001:PTQ:H11	1.97	1.00
1:D:601:PHE:CD1	2:D:2001:PTQ:H11	1.97	1.00
1:C:601:PHE:CD1	2:C:2001:PTQ:H11	1.97	0.98
1:A:601:PHE:CD1	2:A:2001:PTQ:H11	1.97	0.98
1:D:420:MET:HE3	5:D:5150:HOH:O	1.69	0.92
1:B:420:MET:HE3	5:B:5150:HOH:O	1.69	0.91
1:A:420:MET:HE3	5:A:5150:HOH:O	1.69	0.91
1:C:420:MET:HE3	5:C:5150:HOH:O	1.69	0.91
1:A:601:PHE:CD2	2:A:2001:PTQ:H11	2.07	0.90
1:C:601:PHE:CD2	2:C:2001:PTQ:H11	2.07	0.90
1:B:601:PHE:CD2	2:B:2001:PTQ:H11	2.07	0.89
1:D:601:PHE:CD2	2:D:2001:PTQ:H11	2.07	0.89
1:B:198:GLU:HG3	1:B:439:ARG:NH1	1.89	0.88
1:D:198:GLU:HG3	1:D:439:ARG:NH1	1.89	0.87
1:A:198:GLU:HG3	1:A:439:ARG:NH1	1.89	0.87
1:C:198:GLU:HG3	1:C:439:ARG:NH1	1.89	0.86
1:D:102:ASN:HD22	2:D:2001:PTQ:C14	1.89	0.85
1:B:102:ASN:HD22	2:B:2001:PTQ:C14	1.89	0.84
1:A:102:ASN:HD22	2:A:2001:PTQ:C14	1.89	0.84
1:C:102:ASN:HD22	2:C:2001:PTQ:C14	1.89	0.84
1:B:420:MET:CE	5:B:5150:HOH:O	2.25	0.81
1:D:420:MET:CE	5:D:5150:HOH:O	2.25	0.81
1:B:415:ILE:HD11	1:B:439:ARG:HB2	1.63	0.80
1:D:415:ILE:HD11	1:D:439:ARG:HB2	1.63	0.80
1:A:415:ILE:HD11	1:A:439:ARG:HB2	1.63	0.80
1:C:415:ILE:HD11	1:C:439:ARG:HB2	1.63	0.80
1:B:352:ARG:HD2	1:B:626:PHE:CZ	2.17	0.80
1:D:352:ARG:HD2	1:D:626:PHE:CZ	2.17	0.80
1:A:352:ARG:HD2	1:A:626:PHE:CZ	2.17	0.79
1:C:352:ARG:HD2	1:C:626:PHE:CZ	2.17	0.79
1:A:420:MET:CE	5:A:5150:HOH:O	2.25	0.77
1:C:420:MET:CE	5:C:5150:HOH:O	2.25	0.77
1:A:442:ARG:NH1	5:A:5095:HOH:O	2.19	0.76
1:C:198:GLU:HG3	1:C:439:ARG:HH12	1.48	0.76
1:C:442:ARG:NH1	5:C:5095:HOH:O	2.19	0.76
1:A:198:GLU:HG3	1:A:439:ARG:HH12	1.48	0.76
1:B:442:ARG:NH1	5:B:5095:HOH:O	2.19	0.74
1:D:442:ARG:NH1	5:D:5095:HOH:O	2.19	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:GLU:HG3	1:B:439:ARG:HH12	1.48	0.74
1:D:198:GLU:HG3	1:D:439:ARG:HH12	1.48	0.73
1:A:73:TRP:O	1:A:183:ARG:NH2	2.22	0.73
1:C:73:TRP:O	1:C:183:ARG:NH2	2.22	0.73
1:A:601:PHE:CD1	2:A:2001:PTQ:C11	2.72	0.73
1:B:73:TRP:O	1:B:183:ARG:NH2	2.22	0.73
1:D:73:TRP:O	1:D:183:ARG:NH2	2.22	0.73
1:C:601:PHE:CD1	2:C:2001:PTQ:C11	2.72	0.73
1:B:2:MET:O	1:B:4:THR:N	2.22	0.73
1:B:601:PHE:CD1	2:B:2001:PTQ:C11	2.72	0.72
1:D:2:MET:O	1:D:4:THR:N	2.22	0.72
1:D:601:PHE:CD1	2:D:2001:PTQ:C11	2.72	0.72
1:C:355:ASN:HD21	1:C:388:ARG:HH11	1.37	0.72
1:A:355:ASN:HD21	1:A:388:ARG:HH11	1.37	0.72
1:B:355:ASN:HD21	1:B:388:ARG:HH11	1.37	0.72
1:D:355:ASN:HD21	1:D:388:ARG:HH11	1.37	0.72
1:A:408:TYR:OH	5:A:5098:HOH:O	2.04	0.72
1:C:2:MET:O	1:C:4:THR:N	2.22	0.72
1:A:102:ASN:ND2	2:A:2001:PTQ:C14	2.53	0.71
1:A:2:MET:O	1:A:4:THR:N	2.22	0.71
1:C:102:ASN:ND2	2:C:2001:PTQ:C14	2.53	0.71
1:C:408:TYR:OH	5:C:5098:HOH:O	2.04	0.71
1:A:147:ASN:ND2	1:A:205:MET:O	2.24	0.70
1:C:147:ASN:ND2	1:C:205:MET:O	2.24	0.70
1:D:102:ASN:ND2	2:D:2001:PTQ:C14	2.53	0.70
1:B:102:ASN:ND2	2:B:2001:PTQ:C14	2.53	0.70
1:B:597:ASN:HD22	1:B:599:ARG:H	1.40	0.70
1:D:597:ASN:HD22	1:D:599:ARG:H	1.40	0.70
1:B:147:ASN:ND2	1:B:205:MET:O	2.24	0.69
1:D:147:ASN:ND2	1:D:205:MET:O	2.24	0.69
1:A:505:ARG:HH22	1:A:1002:SER:HA	1.57	0.69
1:C:505:ARG:HH22	1:C:1002:SER:HA	1.57	0.69
1:D:505:ARG:HH22	1:D:1002:SER:HA	1.57	0.69
1:B:505:ARG:HH22	1:B:1002:SER:HA	1.57	0.68
1:B:147:ASN:HB2	1:B:209:PHE:CE1	2.29	0.68
1:D:147:ASN:HB2	1:D:209:PHE:CE1	2.29	0.68
1:A:597:ASN:HD22	1:A:599:ARG:H	1.40	0.68
1:C:610:ASP:N	1:C:611:ARG:HA	2.09	0.68
1:A:610:ASP:N	1:A:611:ARG:HA	2.09	0.68
1:B:610:ASP:N	1:B:611:ARG:HA	2.09	0.68
1:C:597:ASN:HD22	1:C:599:ARG:H	1.40	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:610:ASP:N	1:D:611:ARG:HA	2.09	0.68
1:A:147:ASN:HB2	1:A:209:PHE:CE1	2.29	0.67
1:B:427:THR:HG21	1:B:462:SER:HB3	1.77	0.67
1:D:427:THR:HG21	1:D:462:SER:HB3	1.77	0.67
1:C:147:ASN:HB2	1:C:209:PHE:CE1	2.29	0.67
1:C:427:THR:HG21	1:C:462:SER:HB3	1.77	0.67
1:A:427:THR:HG21	1:A:462:SER:HB3	1.77	0.67
2:C:2001:PTQ:H8	2:C:2001:PTQ:O1	1.93	0.67
2:D:2001:PTQ:H8	2:D:2001:PTQ:O1	1.93	0.67
2:B:2001:PTQ:O1	2:B:2001:PTQ:H8	1.93	0.66
2:A:2001:PTQ:H8	2:A:2001:PTQ:O1	1.93	0.66
1:A:624:GLN:NE2	5:A:5017:HOH:O	2.27	0.66
1:C:624:GLN:NE2	5:C:5017:HOH:O	2.27	0.66
1:B:624:GLN:NE2	5:B:5017:HOH:O	2.27	0.66
1:D:624:GLN:NE2	5:D:5017:HOH:O	2.27	0.65
1:A:442:ARG:NH2	5:A:5095:HOH:O	2.29	0.65
1:C:442:ARG:NH2	5:C:5095:HOH:O	2.29	0.65
1:C:650:GLU:HB2	1:C:670:LEU:HB3	1.79	0.65
1:D:442:ARG:NH2	5:D:5095:HOH:O	2.29	0.65
1:A:650:GLU:HB2	1:A:670:LEU:HB3	1.79	0.65
1:B:38:ASN:HD22	1:B:41:GLU:HG3	1.62	0.65
1:B:442:ARG:NH2	5:B:5095:HOH:O	2.29	0.65
1:D:38:ASN:HD22	1:D:41:GLU:HG3	1.62	0.65
1:A:412:GLU:HA	1:A:457:SER:HB3	1.80	0.64
1:A:636:ILE:HD11	1:A:682:LEU:HD11	1.80	0.64
1:C:412:GLU:HA	1:C:457:SER:HB3	1.80	0.64
1:C:636:ILE:HD11	1:C:682:LEU:HD11	1.80	0.64
1:C:38:ASN:HD22	1:C:41:GLU:HG3	1.62	0.64
1:D:153:TRP:HB2	1:D:185:ALA:HB3	1.79	0.64
1:B:636:ILE:HD11	1:B:682:LEU:HD11	1.80	0.64
1:B:883:GLY:HA2	1:B:987:ASP:HA	1.79	0.64
1:A:38:ASN:HD22	1:A:41:GLU:HG3	1.62	0.64
1:B:153:TRP:HB2	1:B:185:ALA:HB3	1.79	0.64
1:B:658:LEU:HB2	1:B:694:LEU:HD23	1.79	0.64
1:D:636:ILE:HD11	1:D:682:LEU:HD11	1.80	0.64
1:D:658:LEU:HB2	1:D:694:LEU:HD23	1.79	0.64
1:A:658:LEU:HB2	1:A:694:LEU:HD23	1.79	0.64
1:C:658:LEU:HB2	1:C:694:LEU:HD23	1.79	0.64
1:D:883:GLY:HA2	1:D:987:ASP:HA	1.79	0.64
1:D:650:GLU:HB2	1:D:670:LEU:HB3	1.79	0.64
1:B:650:GLU:HB2	1:B:670:LEU:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:979:GLU:OE1	1:A:983:TRP:NE1	2.31	0.63
1:C:883:GLY:HA2	1:C:987:ASP:HA	1.79	0.63
1:B:979:GLU:OE1	1:B:983:TRP:NE1	2.31	0.63
1:C:979:GLU:OE1	1:C:983:TRP:NE1	2.31	0.63
1:A:883:GLY:HA2	1:A:987:ASP:HA	1.79	0.63
1:D:979:GLU:OE1	1:D:983:TRP:NE1	2.31	0.63
1:C:153:TRP:HB2	1:C:185:ALA:HB3	1.79	0.63
1:B:601:PHE:CE1	2:B:2001:PTQ:H11	2.34	0.63
1:D:601:PHE:CE1	2:D:2001:PTQ:H11	2.34	0.63
1:A:153:TRP:HB2	1:A:185:ALA:HB3	1.79	0.63
1:B:220:THR:HG22	1:B:315:LEU:HD21	1.81	0.63
1:D:220:THR:HG22	1:D:315:LEU:HD21	1.81	0.63
1:A:198:GLU:CG	1:A:439:ARG:NH1	2.63	0.62
1:B:412:GLU:HA	1:B:457:SER:HB3	1.80	0.62
1:C:198:GLU:CG	1:C:439:ARG:NH1	2.63	0.62
1:D:40:GLU:OE2	1:D:43:ARG:NH1	2.31	0.62
1:D:412:GLU:HA	1:D:457:SER:HB3	1.80	0.62
1:A:220:THR:HG22	1:A:315:LEU:HD21	1.81	0.62
1:C:220:THR:HG22	1:C:315:LEU:HD21	1.81	0.62
1:B:40:GLU:OE2	1:B:43:ARG:NH1	2.31	0.62
1:B:408:TYR:OH	5:B:5098:HOH:O	2.04	0.62
1:B:218:PRO:HG2	1:B:324:GLU:HB2	1.82	0.61
1:C:442:ARG:NH1	5:C:5094:HOH:O	2.25	0.61
1:C:601:PHE:CE1	2:C:2001:PTQ:H11	2.34	0.61
1:D:218:PRO:HG2	1:D:324:GLU:HB2	1.82	0.61
1:A:218:PRO:HG2	1:A:324:GLU:HB2	1.82	0.61
1:A:601:PHE:CE1	2:A:2001:PTQ:H11	2.34	0.61
1:D:408:TYR:OH	5:D:5098:HOH:O	2.04	0.61
1:A:442:ARG:NH1	5:A:5094:HOH:O	2.25	0.61
1:C:218:PRO:HG2	1:C:324:GLU:HB2	1.82	0.61
1:D:52:ARG:HG2	1:D:214:LEU:HB2	1.81	0.61
1:B:52:ARG:HG2	1:B:214:LEU:HB2	1.81	0.61
1:D:887:GLN:NE2	1:D:980:GLU:O	2.33	0.61
1:D:198:GLU:CG	1:D:439:ARG:NH1	2.63	0.61
1:B:198:GLU:CG	1:B:439:ARG:NH1	2.63	0.61
1:B:887:GLN:NE2	1:B:980:GLU:O	2.33	0.61
1:A:147:ASN:HA	1:A:165:SER:OG	2.02	0.60
1:C:147:ASN:HA	1:C:165:SER:OG	2.02	0.60
1:C:746:ASP:OD2	1:C:757:GLN:NE2	2.34	0.60
1:A:746:ASP:OD2	1:A:757:GLN:NE2	2.34	0.60
1:D:442:ARG:NH1	5:D:5094:HOH:O	2.25	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:GLU:OE2	1:C:43:ARG:NH1	2.31	0.60
1:C:52:ARG:HG2	1:C:214:LEU:HB2	1.81	0.60
1:A:52:ARG:HG2	1:A:214:LEU:HB2	1.81	0.60
1:A:40:GLU:OE2	1:A:43:ARG:NH1	2.31	0.60
1:B:442:ARG:NH1	5:B:5094:HOH:O	2.25	0.60
1:B:746:ASP:OD2	1:B:757:GLN:NE2	2.34	0.59
1:C:381:GLN:NE2	1:C:708:TRP:O	2.35	0.59
1:A:381:GLN:NE2	1:A:708:TRP:O	2.35	0.59
1:B:524:LEU:O	1:B:561:ARG:NH1	2.36	0.59
1:D:524:LEU:O	1:D:561:ARG:NH1	2.36	0.59
1:D:746:ASP:OD2	1:D:757:GLN:NE2	2.34	0.59
1:D:147:ASN:HA	1:D:165:SER:OG	2.02	0.59
1:B:147:ASN:HA	1:B:165:SER:OG	2.02	0.59
1:A:442:ARG:CZ	5:A:5095:HOH:O	2.51	0.59
1:A:791:ASN:ND2	5:A:5065:HOH:O	2.23	0.59
1:B:758:PHE:HA	1:B:765:LEU:HA	1.84	0.59
1:C:442:ARG:CZ	5:C:5095:HOH:O	2.51	0.59
1:D:442:ARG:CZ	5:D:5095:HOH:O	2.51	0.59
1:D:758:PHE:HA	1:D:765:LEU:HA	1.84	0.59
1:B:442:ARG:CZ	5:B:5095:HOH:O	2.51	0.59
1:C:791:ASN:ND2	5:C:5065:HOH:O	2.23	0.59
1:A:166:ARG:HG3	1:A:392:TYR:HB2	1.85	0.58
1:C:166:ARG:HG3	1:C:392:TYR:HB2	1.85	0.58
1:A:524:LEU:O	1:A:561:ARG:NH1	2.36	0.58
1:A:758:PHE:HA	1:A:765:LEU:HA	1.84	0.58
1:C:887:GLN:NE2	1:C:980:GLU:O	2.33	0.58
1:A:887:GLN:NE2	1:A:980:GLU:O	2.33	0.58
1:C:524:LEU:O	1:C:561:ARG:NH1	2.36	0.58
1:C:758:PHE:HA	1:C:765:LEU:HA	1.84	0.58
1:D:166:ARG:HG3	1:D:392:TYR:HB2	1.85	0.58
1:B:166:ARG:HG3	1:B:392:TYR:HB2	1.85	0.58
1:A:499:ILE:HG22	1:A:501:PRO:HD3	1.87	0.57
1:C:499:ILE:HG22	1:C:501:PRO:HD3	1.87	0.57
1:A:105:TYR:CE1	1:A:419:GLY:HA3	2.40	0.57
1:C:105:TYR:CE1	1:C:419:GLY:HA3	2.40	0.57
1:C:487:GLU:HG3	1:C:502:MET:HG3	1.85	0.57
1:A:487:GLU:HG3	1:A:502:MET:HG3	1.85	0.57
1:D:487:GLU:HG3	1:D:502:MET:HG3	1.85	0.57
1:B:487:GLU:HG3	1:B:502:MET:HG3	1.85	0.57
1:A:885:ASN:HB2	1:A:985:ASN:HD22	1.70	0.57
1:B:224:ASP:HB3	1:B:245:GLN:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:TYR:OH	1:C:163:GLN:NE2	2.38	0.57
1:D:224:ASP:HB3	1:D:245:GLN:HB2	1.87	0.57
1:B:105:TYR:CE1	1:B:419:GLY:HA3	2.40	0.56
1:C:885:ASN:HB2	1:C:985:ASN:HD22	1.70	0.56
1:D:105:TYR:CE1	1:D:419:GLY:HA3	2.40	0.56
1:D:381:GLN:NE2	1:D:708:TRP:O	2.35	0.56
1:B:770:ILE:HB	1:B:773:LYS:HB3	1.87	0.56
1:B:499:ILE:HG22	1:B:501:PRO:HD3	1.87	0.56
1:D:499:ILE:HG22	1:D:501:PRO:HD3	1.87	0.56
1:D:770:ILE:HB	1:D:773:LYS:HB3	1.87	0.56
1:A:224:ASP:HB3	1:A:245:GLN:HB2	1.87	0.56
1:B:381:GLN:NE2	1:B:708:TRP:O	2.35	0.56
1:C:224:ASP:HB3	1:C:245:GLN:HB2	1.87	0.56
1:D:161:TYR:OH	1:D:163:GLN:NE2	2.38	0.56
1:D:472:TYR:OH	1:D:497:ASP:OD1	2.24	0.56
1:B:161:TYR:OH	1:B:163:GLN:NE2	2.38	0.56
1:B:472:TYR:OH	1:B:497:ASP:OD1	2.24	0.56
1:A:221:GLN:HG3	1:A:247:CYS:HB3	1.88	0.56
1:B:221:GLN:HG3	1:B:247:CYS:HB3	1.88	0.56
1:C:221:GLN:HG3	1:C:247:CYS:HB3	1.88	0.56
1:D:221:GLN:HG3	1:D:247:CYS:HB3	1.88	0.56
1:D:433:LEU:HB3	1:D:434:PRO:HD3	1.88	0.56
1:D:885:ASN:HB2	1:D:985:ASN:HD22	1.70	0.56
1:B:103:VAL:O	1:B:199:ASP:OD2	2.24	0.55
1:A:770:ILE:HB	1:A:773:LYS:HB3	1.87	0.55
1:B:433:LEU:HB3	1:B:434:PRO:HD3	1.88	0.55
1:B:885:ASN:HB2	1:B:985:ASN:HD22	1.70	0.55
1:C:770:ILE:HB	1:C:773:LYS:HB3	1.87	0.55
1:D:103:VAL:O	1:D:199:ASP:OD2	2.24	0.55
1:D:540:HIS:ND1	1:D:998:SER:OG	2.39	0.55
1:A:103:VAL:O	1:A:199:ASP:OD2	2.24	0.55
1:B:540:HIS:ND1	1:B:998:SER:OG	2.39	0.55
1:C:103:VAL:O	1:C:199:ASP:OD2	2.24	0.55
1:A:113:PHE:O	1:A:196:TYR:OH	2.22	0.55
1:C:113:PHE:O	1:C:196:TYR:OH	2.22	0.55
1:C:377:LEU:HD22	1:C:708:TRP:HA	1.88	0.55
1:A:377:LEU:HD22	1:A:708:TRP:HA	1.88	0.55
1:A:301:TRP:CH2	1:A:452:SER:HA	2.42	0.55
1:C:301:TRP:CH2	1:C:452:SER:HA	2.42	0.55
1:C:410:VAL:HG22	1:C:455:ILE:HB	1.89	0.55
1:D:410:VAL:HG22	1:D:455:ILE:HB	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:VAL:HG22	1:A:455:ILE:HB	1.89	0.55
1:B:410:VAL:HG22	1:B:455:ILE:HB	1.89	0.55
1:A:161:TYR:OH	1:A:163:GLN:NE2	2.38	0.54
1:A:737:ILE:HD12	1:A:738:PRO:HD2	1.89	0.54
1:C:737:ILE:HD12	1:C:738:PRO:HD2	1.89	0.54
1:B:737:ILE:HD12	1:B:738:PRO:HD2	1.89	0.54
1:C:433:LEU:HB3	1:C:434:PRO:HD3	1.88	0.54
1:A:433:LEU:HB3	1:A:434:PRO:HD3	1.88	0.54
1:B:791:ASN:ND2	5:B:5065:HOH:O	2.23	0.54
1:D:737:ILE:HD12	1:D:738:PRO:HD2	1.89	0.54
1:D:791:ASN:ND2	5:D:5065:HOH:O	2.23	0.54
1:A:747:PHE:HB2	1:A:758:PHE:HB2	1.90	0.54
1:C:747:PHE:HB2	1:C:758:PHE:HB2	1.90	0.54
1:D:747:PHE:HB2	1:D:758:PHE:HB2	1.90	0.54
1:A:636:ILE:HD13	1:A:698:VAL:HG11	1.90	0.54
1:B:747:PHE:HB2	1:B:758:PHE:HB2	1.90	0.54
1:C:636:ILE:HD13	1:C:698:VAL:HG11	1.90	0.54
1:D:352:ARG:NH1	1:D:626:PHE:CE2	2.76	0.54
1:D:198:GLU:CG	1:D:439:ARG:HH12	2.19	0.54
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.88	0.54
1:A:278:ILE:HG23	1:A:283:GLY:HA2	1.90	0.54
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.88	0.54
1:B:198:GLU:CG	1:B:439:ARG:HH12	2.19	0.54
1:B:352:ARG:NH1	1:B:626:PHE:CE2	2.76	0.54
1:C:278:ILE:HG23	1:C:283:GLY:HA2	1.90	0.54
1:B:636:ILE:HD13	1:B:698:VAL:HG11	1.90	0.54
1:D:301:TRP:CH2	1:D:452:SER:HA	2.42	0.54
1:D:636:ILE:HD13	1:D:698:VAL:HG11	1.90	0.54
1:B:301:TRP:CH2	1:B:452:SER:HA	2.42	0.53
1:A:954:ASP:HB3	1:C:1013:ARG:HH22	1.74	0.53
1:A:1013:ARG:HH22	1:C:954:ASP:HB3	1.74	0.53
1:A:601:PHE:CE2	2:A:2001:PTQ:H11	2.42	0.53
1:A:778:THR:HB	1:A:887:GLN:HB3	1.91	0.53
1:B:102:ASN:HD22	2:B:2001:PTQ:C13	2.21	0.53
1:C:198:GLU:CG	1:C:439:ARG:HH12	2.19	0.53
1:C:778:THR:HB	1:C:887:GLN:HB3	1.91	0.53
1:B:954:ASP:HB3	1:D:1013:ARG:HH22	1.74	0.53
1:D:102:ASN:HD22	2:D:2001:PTQ:C13	2.21	0.53
1:B:1013:ARG:HH22	1:D:954:ASP:HB3	1.74	0.53
1:C:601:PHE:CE2	2:C:2001:PTQ:H11	2.42	0.53
1:A:198:GLU:CG	1:A:439:ARG:HH12	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ARG:NH1	1:A:626:PHE:CE2	2.76	0.53
1:C:619:GLU:HA	1:C:912:ALA:HB2	1.91	0.53
1:A:619:GLU:HA	1:A:912:ALA:HB2	1.91	0.53
1:B:601:PHE:CE2	2:B:2001:PTQ:H11	2.42	0.53
1:C:352:ARG:NH1	1:C:626:PHE:CE2	2.76	0.53
1:B:278:ILE:HG23	1:B:283:GLY:HA2	1.90	0.53
1:B:619:GLU:HA	1:B:912:ALA:HB2	1.91	0.53
1:D:601:PHE:CE2	2:D:2001:PTQ:H11	2.42	0.53
1:D:278:ILE:HG23	1:D:283:GLY:HA2	1.90	0.53
1:C:102:ASN:HD22	2:C:2001:PTQ:C13	2.21	0.53
1:D:59:ARG:NH2	1:D:81:ALA:O	2.42	0.53
1:D:619:GLU:HA	1:D:912:ALA:HB2	1.91	0.53
1:B:59:ARG:NH2	1:B:81:ALA:O	2.42	0.53
1:A:102:ASN:HD22	2:A:2001:PTQ:C13	2.21	0.53
1:D:778:THR:HB	1:D:887:GLN:HB3	1.91	0.53
1:D:796:SER:HB2	1:D:802:ASP:HB3	1.91	0.53
1:A:59:ARG:NH2	1:A:81:ALA:O	2.42	0.52
1:B:526:LEU:HB2	1:B:529:GLU:HG3	1.91	0.52
1:B:778:THR:HB	1:B:887:GLN:HB3	1.91	0.52
1:B:796:SER:HB2	1:B:802:ASP:HB3	1.91	0.52
1:D:526:LEU:HB2	1:D:529:GLU:HG3	1.91	0.52
1:C:59:ARG:NH2	1:C:81:ALA:O	2.42	0.52
1:D:113:PHE:O	1:D:196:TYR:OH	2.22	0.52
1:D:496:THR:OG1	1:D:498:ILE:O	2.24	0.52
1:A:966:GLN:O	1:A:970:THR:OG1	2.25	0.52
1:C:105:TYR:CD1	1:C:419:GLY:HA3	2.45	0.52
1:A:105:TYR:CD1	1:A:419:GLY:HA3	2.45	0.52
1:A:607:VAL:HG12	1:A:613:PRO:HA	1.92	0.52
1:B:607:VAL:HG12	1:B:613:PRO:HA	1.92	0.52
1:C:607:VAL:HG12	1:C:613:PRO:HA	1.92	0.52
1:D:607:VAL:HG12	1:D:613:PRO:HA	1.92	0.52
1:B:496:THR:OG1	1:B:498:ILE:O	2.24	0.52
1:A:526:LEU:HB2	1:A:529:GLU:HG3	1.91	0.52
1:B:1021:CYS:SG	1:B:1022:GLN:N	2.83	0.52
1:B:113:PHE:O	1:B:196:TYR:OH	2.22	0.52
1:D:1021:CYS:SG	1:D:1022:GLN:N	2.83	0.52
1:D:553:TRP:CZ2	1:D:624:GLN:HG2	2.45	0.52
1:A:601:PHE:CE1	2:A:2001:PTQ:C11	2.93	0.52
1:B:553:TRP:CZ2	1:B:624:GLN:HG2	2.45	0.52
1:B:601:PHE:CG	2:B:2001:PTQ:C11	2.75	0.52
1:C:526:LEU:HB2	1:C:529:GLU:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:601:PHE:CE1	2:C:2001:PTQ:C11	2.93	0.52
1:D:105:TYR:CD1	1:D:419:GLY:HA3	2.45	0.52
1:A:553:TRP:CZ2	1:A:624:GLN:HG2	2.45	0.52
1:B:105:TYR:CD1	1:B:419:GLY:HA3	2.45	0.52
1:D:601:PHE:CG	2:D:2001:PTQ:C11	2.75	0.52
1:C:553:TRP:CZ2	1:C:624:GLN:HG2	2.45	0.52
1:B:313:VAL:N	1:B:326:GLU:O	2.40	0.52
1:A:416:GLU:CD	5:A:5078:HOH:O	2.48	0.51
1:B:349:LEU:HA	1:B:643:LEU:HD11	1.92	0.51
1:C:416:GLU:CD	5:C:5078:HOH:O	2.48	0.51
1:C:472:TYR:OH	1:C:497:ASP:OD1	2.24	0.51
1:D:313:VAL:N	1:D:326:GLU:O	2.40	0.51
1:D:349:LEU:H	1:D:349:LEU:HD23	1.75	0.51
1:A:796:SER:HB2	1:A:802:ASP:HB3	1.91	0.51
1:C:796:SER:HB2	1:C:802:ASP:HB3	1.91	0.51
1:D:349:LEU:HA	1:D:643:LEU:HD11	1.92	0.51
1:A:472:TYR:OH	1:A:497:ASP:OD1	2.24	0.51
1:B:349:LEU:HD23	1:B:349:LEU:H	1.75	0.51
1:B:395:HIS:HD2	1:B:397:LEU:H	1.58	0.51
1:D:395:HIS:HD2	1:D:397:LEU:H	1.58	0.51
1:A:1021:CYS:SG	1:A:1022:GLN:N	2.83	0.51
1:D:694:LEU:HD12	1:D:723:ALA:HB3	1.93	0.51
1:A:496:THR:OG1	1:A:498:ILE:O	2.24	0.51
1:B:245:GLN:HG2	1:B:288:ARG:HG2	1.93	0.51
1:B:694:LEU:HD12	1:B:723:ALA:HB3	1.93	0.51
1:D:245:GLN:HG2	1:D:288:ARG:HG2	1.93	0.51
1:B:416:GLU:CD	5:B:5078:HOH:O	2.48	0.51
1:B:966:GLN:O	1:B:970:THR:OG1	2.25	0.51
1:C:1021:CYS:SG	1:C:1022:GLN:N	2.83	0.51
1:C:496:THR:OG1	1:C:498:ILE:O	2.24	0.51
1:A:349:LEU:HA	1:A:643:LEU:HD11	1.92	0.51
1:C:349:LEU:HA	1:C:643:LEU:HD11	1.92	0.51
1:D:416:GLU:CD	5:D:5078:HOH:O	2.48	0.51
1:A:738:PRO:HG3	1:A:751:LEU:HD22	1.93	0.51
1:A:937:LEU:HA	1:A:958:ASN:HB3	1.93	0.51
1:B:693:GLN:NE2	1:B:694:LEU:O	2.37	0.51
1:C:458:LEU:HD11	1:C:472:TYR:HB2	1.93	0.51
1:C:738:PRO:HG3	1:C:751:LEU:HD22	1.93	0.51
1:A:455:ILE:HG12	1:A:483:PRO:HG2	1.93	0.51
1:A:458:LEU:HD11	1:A:472:TYR:HB2	1.93	0.51
1:C:349:LEU:HD23	1:C:349:LEU:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:ILE:HG12	1:C:483:PRO:HG2	1.93	0.51
1:C:937:LEU:HA	1:C:958:ASN:HB3	1.93	0.51
1:A:245:GLN:HG2	1:A:288:ARG:HG2	1.93	0.50
1:A:349:LEU:H	1:A:349:LEU:HD23	1.75	0.50
1:B:490:GLY:HA2	1:B:515:VAL:HG13	1.93	0.50
1:B:937:LEU:HA	1:B:958:ASN:HB3	1.93	0.50
1:D:490:GLY:HA2	1:D:515:VAL:HG13	1.93	0.50
1:D:937:LEU:HA	1:D:958:ASN:HB3	1.93	0.50
1:A:524:LEU:HD11	1:A:562:LEU:HG	1.93	0.50
1:C:245:GLN:HG2	1:C:288:ARG:HG2	1.93	0.50
1:C:524:LEU:HD11	1:C:562:LEU:HG	1.93	0.50
1:D:693:GLN:NE2	1:D:694:LEU:O	2.37	0.50
1:B:88:SER:HA	1:B:366:VAL:HG21	1.92	0.50
1:C:178:ARG:NH1	1:C:181:GLU:O	2.45	0.50
1:C:345:ASN:ND2	5:C:5124:HOH:O	2.39	0.50
1:D:458:LEU:HD11	1:D:472:TYR:HB2	1.93	0.50
1:A:178:ARG:NH1	1:A:181:GLU:O	2.45	0.50
1:A:490:GLY:HA2	1:A:515:VAL:HG13	1.93	0.50
1:B:1004:SER:HB3	1:B:1007:PHE:HD2	1.77	0.50
1:B:458:LEU:HD11	1:B:472:TYR:HB2	1.93	0.50
1:C:490:GLY:HA2	1:C:515:VAL:HG13	1.93	0.50
1:D:1004:SER:HB3	1:D:1007:PHE:HD2	1.77	0.50
1:D:836:ILE:HG23	1:D:856:TYR:HB2	1.93	0.50
1:A:1004:SER:HB3	1:A:1007:PHE:HD2	1.77	0.50
1:A:313:VAL:N	1:A:326:GLU:O	2.40	0.50
1:A:88:SER:HA	1:A:366:VAL:HG21	1.92	0.50
1:A:694:LEU:HD12	1:A:723:ALA:HB3	1.93	0.50
1:B:601:PHE:CE1	2:B:2001:PTQ:C11	2.93	0.50
1:B:524:LEU:HD11	1:B:562:LEU:HG	1.93	0.50
1:B:836:ILE:HG23	1:B:856:TYR:HB2	1.93	0.50
1:C:395:HIS:HD2	1:C:397:LEU:H	1.58	0.50
1:D:88:SER:HA	1:D:366:VAL:HG21	1.92	0.50
1:D:524:LEU:HD11	1:D:562:LEU:HG	1.93	0.50
1:A:395:HIS:HD2	1:A:397:LEU:H	1.58	0.50
1:A:836:ILE:HG23	1:A:856:TYR:HB2	1.93	0.50
1:C:1004:SER:HB3	1:C:1007:PHE:HD2	1.77	0.50
1:C:313:VAL:N	1:C:326:GLU:O	2.40	0.50
1:C:694:LEU:HD12	1:C:723:ALA:HB3	1.93	0.50
1:A:345:ASN:ND2	5:A:5124:HOH:O	2.39	0.50
1:B:738:PRO:HD3	1:B:860:GLY:HA2	1.93	0.50
1:C:88:SER:HA	1:C:366:VAL:HG21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:383:ASN:ND2	1:C:621:LYS:O	2.38	0.50
1:C:836:ILE:HG23	1:C:856:TYR:HB2	1.93	0.50
1:D:601:PHE:CE1	2:D:2001:PTQ:C11	2.93	0.50
1:D:738:PRO:HD3	1:D:860:GLY:HA2	1.93	0.50
1:A:738:PRO:HD3	1:A:860:GLY:HA2	1.93	0.50
1:B:30:HIS:ND1	1:B:31:PRO:O	2.31	0.50
1:C:738:PRO:HD3	1:C:860:GLY:HA2	1.93	0.50
1:A:383:ASN:ND2	1:A:621:LYS:O	2.38	0.49
1:B:96:ASP:OD2	1:B:190:ARG:NH1	2.45	0.49
1:B:455:ILE:HG12	1:B:483:PRO:HG2	1.93	0.49
1:A:643:LEU:HD11	5:A:5099:HOH:O	2.12	0.49
1:C:643:LEU:HD11	5:C:5099:HOH:O	2.12	0.49
1:D:455:ILE:HG12	1:D:483:PRO:HG2	1.93	0.49
1:D:96:ASP:OD2	1:D:190:ARG:NH1	2.45	0.49
1:D:30:HIS:ND1	1:D:31:PRO:O	2.31	0.49
1:D:345:ASN:ND2	5:D:5124:HOH:O	2.39	0.49
1:C:62:TRP:NE1	1:C:96:ASP:HB2	2.28	0.49
1:C:96:ASP:OD2	1:C:190:ARG:NH1	2.45	0.49
1:D:103:VAL:HG22	1:D:418:HIS:CE1	2.48	0.49
1:A:62:TRP:NE1	1:A:96:ASP:HB2	2.28	0.49
1:A:96:ASP:OD2	1:A:190:ARG:NH1	2.45	0.49
1:B:103:VAL:HG22	1:B:418:HIS:CE1	2.48	0.49
1:B:738:PRO:HG3	1:B:751:LEU:HD22	1.93	0.49
1:D:738:PRO:HG3	1:D:751:LEU:HD22	1.93	0.49
1:A:228:ALA:HB3	1:A:241:GLU:HG2	1.95	0.49
1:B:345:ASN:ND2	5:B:5124:HOH:O	2.39	0.49
1:C:228:ALA:HB3	1:C:241:GLU:HG2	1.95	0.49
1:B:62:TRP:NE1	1:B:96:ASP:HB2	2.28	0.49
1:D:62:TRP:NE1	1:D:96:ASP:HB2	2.28	0.49
1:A:601:PHE:CG	2:A:2001:PTQ:C11	2.75	0.48
1:B:372:MET:HE2	1:B:372:MET:HB2	1.66	0.48
1:C:601:PHE:CG	2:C:2001:PTQ:C11	2.75	0.48
1:D:178:ARG:NH1	1:D:181:GLU:O	2.45	0.48
1:A:41:GLU:HG2	1:A:46:ARG:HD2	1.95	0.48
1:B:178:ARG:NH1	1:B:181:GLU:O	2.45	0.48
1:C:41:GLU:HG2	1:C:46:ARG:HD2	1.95	0.48
1:D:966:GLN:O	1:D:970:THR:OG1	2.25	0.48
1:B:643:LEU:HD11	5:B:5099:HOH:O	2.12	0.48
1:B:771:GLY:HA3	1:B:772:ASP:C	2.34	0.48
1:D:771:GLY:HA3	1:D:772:ASP:C	2.34	0.48
1:B:383:ASN:ND2	1:B:621:LYS:O	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:GLU:O	5:C:5105:HOH:O	2.20	0.48
1:D:643:LEU:HD11	5:D:5099:HOH:O	2.12	0.48
1:B:780:LEU:HD11	1:B:884:LEU:HB3	1.96	0.48
1:D:780:LEU:HD11	1:D:884:LEU:HB3	1.96	0.48
1:A:304:GLU:O	5:A:5105:HOH:O	2.20	0.48
1:A:103:VAL:HG22	1:A:418:HIS:CE1	2.48	0.48
1:B:568:TRP:HA	1:B:569:ASP:HA	1.57	0.48
1:C:750:GLU:HG2	1:C:755:ARG:HG2	1.96	0.48
1:D:228:ALA:HB3	1:D:241:GLU:HG2	1.95	0.48
1:D:583:ASN:OD1	1:D:583:ASN:N	2.41	0.48
1:D:383:ASN:ND2	1:D:621:LYS:O	2.38	0.48
1:A:750:GLU:HG2	1:A:755:ARG:HG2	1.96	0.48
1:A:762:SER:O	1:A:840:HIS:NE2	2.34	0.48
1:A:771:GLY:HA3	1:A:772:ASP:C	2.34	0.48
1:B:228:ALA:HB3	1:B:241:GLU:HG2	1.95	0.48
1:B:583:ASN:N	1:B:583:ASN:OD1	2.41	0.48
1:B:750:GLU:HG2	1:B:755:ARG:HG2	1.96	0.48
1:C:103:VAL:HG22	1:C:418:HIS:CE1	2.48	0.48
1:C:771:GLY:HA3	1:C:772:ASP:C	2.34	0.48
1:D:372:MET:HB2	1:D:372:MET:HE2	1.66	0.48
1:D:750:GLU:HG2	1:D:755:ARG:HG2	1.96	0.48
1:A:583:ASN:N	1:A:583:ASN:OD1	2.41	0.48
1:C:583:ASN:OD1	1:C:583:ASN:N	2.41	0.48
1:D:304:GLU:O	5:D:5105:HOH:O	2.20	0.48
1:A:780:LEU:HD11	1:A:884:LEU:HB3	1.96	0.47
1:B:762:SER:O	1:B:840:HIS:NE2	2.34	0.47
1:B:78:LEU:CB	5:B:5049:HOH:O	2.62	0.47
1:C:762:SER:O	1:C:840:HIS:NE2	2.34	0.47
1:C:780:LEU:HD11	1:C:884:LEU:HB3	1.96	0.47
1:D:762:SER:O	1:D:840:HIS:NE2	2.34	0.47
1:D:78:LEU:CB	5:D:5049:HOH:O	2.62	0.47
2:B:2001:PTQ:H2	5:B:5037:HOH:O	2.13	0.47
1:B:304:GLU:O	5:B:5105:HOH:O	2.20	0.47
2:D:2001:PTQ:H2	5:D:5037:HOH:O	2.13	0.47
1:D:41:GLU:HG2	1:D:46:ARG:HD2	1.95	0.47
1:B:41:GLU:HG2	1:B:46:ARG:HD2	1.95	0.47
1:A:783:GLN:HE22	1:A:964:GLN:HG3	1.80	0.47
2:C:2001:PTQ:H2	5:C:5037:HOH:O	2.13	0.47
1:C:783:GLN:HE22	1:C:964:GLN:HG3	1.80	0.47
2:A:2001:PTQ:H2	5:A:5037:HOH:O	2.13	0.47
1:D:837:THR:HG23	1:D:855:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:837:THR:HG23	1:B:855:THR:HG22	1.96	0.47
1:A:881:ARG:NH2	1:A:934:GLU:OE1	2.48	0.47
1:B:390:SER:HB2	1:B:391:HIS:CD2	2.50	0.47
1:D:390:SER:HB2	1:D:391:HIS:CD2	2.50	0.47
1:C:881:ARG:NH2	1:C:934:GLU:OE1	2.48	0.47
1:A:878:HIS:HB3	1:A:1009:LEU:O	2.15	0.46
1:A:588:TYR:OH	1:A:971:SER:O	2.29	0.46
1:C:878:HIS:HB3	1:C:1009:LEU:O	2.15	0.46
1:C:24:LEU:HB2	1:C:161:TYR:HB3	1.97	0.46
1:C:390:SER:HA	1:C:391:HIS:HA	1.52	0.46
1:A:390:SER:HB2	1:A:391:HIS:CD2	2.50	0.46
1:A:78:LEU:CB	5:A:5049:HOH:O	2.62	0.46
1:B:450:HIS:HA	1:B:451:PRO:HD2	1.76	0.46
1:B:878:HIS:HB3	1:B:1009:LEU:O	2.15	0.46
1:C:390:SER:HB2	1:C:391:HIS:CD2	2.50	0.46
1:C:613:PRO:HB3	1:C:617:LEU:CD2	2.46	0.46
1:C:78:LEU:CB	5:C:5049:HOH:O	2.62	0.46
1:C:588:TYR:OH	1:C:971:SER:O	2.29	0.46
1:D:450:HIS:HA	1:D:451:PRO:HD2	1.76	0.46
1:D:878:HIS:HB3	1:D:1009:LEU:O	2.15	0.46
1:A:24:LEU:HB2	1:A:161:TYR:HB3	1.97	0.46
1:A:613:PRO:HB3	1:A:617:LEU:CD2	2.46	0.46
1:B:502:MET:HE3	1:B:537:GLU:OE1	2.15	0.46
1:A:196:TYR:O	1:A:417:THR:HG22	2.15	0.46
1:A:506:VAL:HA	1:A:520:ILE:HG12	1.96	0.46
1:C:506:VAL:HA	1:C:520:ILE:HG12	1.96	0.46
1:D:24:LEU:HB2	1:D:161:TYR:HB3	1.97	0.46
1:D:502:MET:HE3	1:D:537:GLU:OE1	2.15	0.46
1:B:559:TYR:HB2	1:B:562:LEU:HD12	1.98	0.46
1:C:196:TYR:O	1:C:417:THR:HG22	2.15	0.46
1:C:502:MET:HE3	1:C:537:GLU:OE1	2.15	0.46
1:D:559:TYR:HB2	1:D:562:LEU:HD12	1.98	0.46
1:D:568:TRP:HA	1:D:569:ASP:HA	1.57	0.46
1:A:688:PRO:HG3	1:A:694:LEU:HD21	1.98	0.46
1:B:24:LEU:HB2	1:B:161:TYR:HB3	1.97	0.46
1:B:601:PHE:CD1	2:B:2001:PTQ:C10	2.99	0.46
1:B:510:GLN:N	1:B:510:GLN:OE1	2.49	0.46
1:B:506:VAL:HA	1:B:520:ILE:HG12	1.96	0.46
1:B:783:GLN:HE22	1:B:964:GLN:HG3	1.80	0.46
1:C:688:PRO:HG3	1:C:694:LEU:HD21	1.98	0.46
1:D:510:GLN:N	1:D:510:GLN:OE1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:601:PHE:CD1	2:D:2001:PTQ:C10	2.99	0.46
1:A:390:SER:HA	1:A:391:HIS:HA	1.52	0.46
1:A:502:MET:HE3	1:A:537:GLU:OE1	2.16	0.46
1:A:837:THR:HG23	1:A:855:THR:HG22	1.96	0.46
1:C:837:THR:HG23	1:C:855:THR:HG22	1.96	0.46
1:D:506:VAL:HA	1:D:520:ILE:HG12	1.96	0.46
1:D:613:PRO:HB3	1:D:617:LEU:CD2	2.46	0.46
1:B:613:PRO:HB3	1:B:617:LEU:CD2	2.46	0.46
1:B:881:ARG:NH2	1:B:934:GLU:OE1	2.48	0.46
1:D:196:TYR:O	1:D:417:THR:HG22	2.15	0.46
1:D:783:GLN:HE22	1:D:964:GLN:HG3	1.80	0.46
1:A:601:PHE:CD1	2:A:2001:PTQ:C10	2.99	0.46
1:A:501:PRO:HG2	1:A:535:LEU:HD23	1.98	0.46
1:B:196:TYR:O	1:B:417:THR:HG22	2.15	0.46
1:B:873:ALA:O	1:B:876:THR:HG22	2.16	0.46
1:C:501:PRO:HG2	1:C:535:LEU:HD23	1.98	0.46
1:C:610:ASP:N	1:C:610:ASP:OD1	2.41	0.46
1:D:873:ALA:O	1:D:876:THR:HG22	2.16	0.46
1:B:501:PRO:HG2	1:B:535:LEU:HD23	1.98	0.45
1:C:601:PHE:CD1	2:C:2001:PTQ:C10	2.99	0.45
1:D:881:ARG:NH2	1:D:934:GLU:OE1	2.48	0.45
1:B:688:PRO:HG3	1:B:694:LEU:HD21	1.98	0.45
1:D:501:PRO:HG2	1:D:535:LEU:HD23	1.98	0.45
1:A:360:HIS:N	1:A:364:GLY:O	2.40	0.45
1:D:688:PRO:HG3	1:D:694:LEU:HD21	1.98	0.45
1:A:610:ASP:N	1:A:610:ASP:OD1	2.41	0.45
1:A:163:GLN:NE2	1:A:192:SER:OG	2.50	0.45
1:A:248:GLY:HA2	1:A:249:GLU:HB2	1.99	0.45
1:C:163:GLN:NE2	1:C:192:SER:OG	2.50	0.45
1:C:248:GLY:HA2	1:C:249:GLU:HB2	1.99	0.45
1:C:360:HIS:N	1:C:364:GLY:O	2.40	0.45
1:C:510:GLN:N	1:C:510:GLN:OE1	2.49	0.45
1:A:510:GLN:N	1:A:510:GLN:OE1	2.49	0.45
1:A:694:LEU:HB2	1:A:722:LEU:O	2.16	0.45
1:A:464:HIS:HB2	1:A:489:GLY:HA3	1.99	0.45
1:C:464:HIS:HB2	1:C:489:GLY:HA3	1.99	0.45
1:C:694:LEU:HB2	1:C:722:LEU:O	2.16	0.45
1:C:873:ALA:O	1:C:876:THR:HG22	2.16	0.45
1:D:163:GLN:NE2	1:D:192:SER:OG	2.50	0.45
1:D:142:ILE:HG12	1:D:170:GLU:HG2	1.98	0.45
1:A:829:THR:HG22	1:A:834:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:GLN:NE2	1:B:192:SER:OG	2.50	0.45
1:B:829:THR:HG22	1:B:834:VAL:HG22	1.99	0.45
1:B:958:ASN:OD1	1:B:985:ASN:HB2	2.17	0.45
1:C:829:THR:HG22	1:C:834:VAL:HG22	1.99	0.45
1:D:829:THR:HG22	1:D:834:VAL:HG22	1.99	0.45
1:D:958:ASN:OD1	1:D:985:ASN:HB2	2.17	0.45
1:A:854:LYS:HG2	1:A:868:VAL:HG22	1.99	0.45
1:A:873:ALA:O	1:A:876:THR:HG22	2.16	0.45
1:B:142:ILE:HG12	1:B:170:GLU:HG2	1.98	0.45
1:B:91:GLN:HG3	1:B:96:ASP:O	2.17	0.45
1:C:854:LYS:HG2	1:C:868:VAL:HG22	1.99	0.45
1:C:91:GLN:NE2	1:C:206:SER:OG	2.50	0.45
1:D:91:GLN:HG3	1:D:96:ASP:O	2.17	0.45
1:A:418:HIS:ND1	1:A:461:GLU:OE1	2.50	0.45
1:A:91:GLN:NE2	1:A:206:SER:OG	2.50	0.45
1:B:464:HIS:HB2	1:B:489:GLY:HA3	1.99	0.45
1:B:732:ALA:HA	1:B:733:ALA:HA	1.71	0.45
1:C:198:GLU:HG3	1:C:439:ARG:HH11	1.80	0.45
1:C:418:HIS:ND1	1:C:461:GLU:OE1	2.50	0.45
1:D:355:ASN:HD21	1:D:388:ARG:HD3	1.82	0.45
1:D:464:HIS:HB2	1:D:489:GLY:HA3	1.99	0.45
1:A:91:GLN:HG3	1:A:96:ASP:O	2.17	0.44
1:B:189:LEU:HD12	1:B:189:LEU:N	2.32	0.44
1:C:199:ASP:C	1:C:416:GLU:HG2	2.38	0.44
1:C:91:GLN:HG3	1:C:96:ASP:O	2.17	0.44
1:D:189:LEU:HD12	1:D:189:LEU:N	2.32	0.44
1:A:199:ASP:C	1:A:416:GLU:HG2	2.38	0.44
1:A:559:TYR:HB2	1:A:562:LEU:HD12	1.98	0.44
1:A:958:ASN:OD1	1:A:985:ASN:HB2	2.17	0.44
1:B:355:ASN:HD21	1:B:388:ARG:HD3	1.82	0.44
1:B:694:LEU:HB2	1:B:722:LEU:O	2.16	0.44
1:B:854:LYS:HG2	1:B:868:VAL:HG22	1.99	0.44
1:C:147:ASN:HA	1:C:148:SER:HA	1.69	0.44
1:C:142:ILE:HG12	1:C:170:GLU:HG2	1.98	0.44
1:C:559:TYR:HB2	1:C:562:LEU:HD12	1.98	0.44
1:B:418:HIS:ND1	1:B:461:GLU:OE1	2.50	0.44
1:C:258:VAL:HG22	1:C:313:VAL:HG22	1.99	0.44
1:C:355:ASN:HD21	1:C:388:ARG:HD3	1.82	0.44
1:C:958:ASN:OD1	1:C:985:ASN:HB2	2.17	0.44
1:D:418:HIS:ND1	1:D:461:GLU:OE1	2.50	0.44
1:D:854:LYS:HG2	1:D:868:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ILE:HG12	1:A:170:GLU:HG2	1.98	0.44
1:A:198:GLU:HG3	1:A:439:ARG:HH11	1.80	0.44
1:A:355:ASN:HD21	1:A:388:ARG:HD3	1.82	0.44
1:A:670:LEU:HG	1:A:672:VAL:HG23	2.00	0.44
1:C:670:LEU:HG	1:C:672:VAL:HG23	2.00	0.44
1:D:694:LEU:HB2	1:D:722:LEU:O	2.16	0.44
1:D:864:MET:O	1:D:1020:TRP:N	2.43	0.44
1:A:258:VAL:HG22	1:A:313:VAL:HG22	1.99	0.44
1:B:258:VAL:HG22	1:B:313:VAL:HG22	1.99	0.44
1:B:770:ILE:HG22	1:B:771:GLY:H	1.82	0.44
1:C:732:ALA:HA	1:C:733:ALA:HA	1.71	0.44
1:A:147:ASN:HA	1:A:148:SER:HA	1.69	0.44
1:D:35:SER:HB2	1:D:217:LYS:HD3	1.99	0.44
1:A:464:HIS:NE2	1:A:469:ASP:OD1	2.51	0.44
1:A:963:SER:HB3	1:A:983:TRP:CE2	2.53	0.44
1:B:91:GLN:NE2	1:B:206:SER:OG	2.50	0.44
1:B:35:SER:HB2	1:B:217:LYS:HD3	1.99	0.44
1:B:864:MET:O	1:B:1020:TRP:N	2.43	0.44
1:C:464:HIS:NE2	1:C:469:ASP:OD1	2.51	0.44
1:C:963:SER:HB3	1:C:983:TRP:CE2	2.53	0.44
1:D:258:VAL:HG22	1:D:313:VAL:HG22	1.99	0.44
1:D:400:THR:HG22	1:D:404:ARG:HH11	1.83	0.44
1:D:770:ILE:HG22	1:D:771:GLY:H	1.82	0.44
1:B:400:THR:HG22	1:B:404:ARG:HH11	1.83	0.44
1:C:336:ARG:O	1:C:336:ARG:HG3	2.18	0.44
1:D:380:LYS:HE3	1:D:380:LYS:HB3	1.80	0.44
1:A:336:ARG:HG3	1:A:336:ARG:O	2.18	0.44
1:B:248:GLY:HA2	1:B:249:GLU:HB2	1.99	0.44
1:B:336:ARG:HG3	1:B:336:ARG:O	2.18	0.44
1:B:963:SER:HB3	1:B:983:TRP:CE2	2.53	0.44
1:C:996:ASP:H	1:C:1002:SER:HB2	1.83	0.44
1:C:189:LEU:HD12	1:C:189:LEU:N	2.32	0.44
1:D:248:GLY:HA2	1:D:249:GLU:HB2	1.99	0.44
1:D:336:ARG:O	1:D:336:ARG:HG3	2.18	0.44
1:D:610:ASP:OD1	1:D:610:ASP:N	2.41	0.44
1:D:91:GLN:NE2	1:D:206:SER:OG	2.50	0.44
1:D:963:SER:HB3	1:D:983:TRP:CE2	2.53	0.44
1:A:996:ASP:H	1:A:1002:SER:HB2	1.83	0.43
1:A:189:LEU:HD12	1:A:189:LEU:N	2.32	0.43
1:B:996:ASP:H	1:B:1002:SER:HB2	1.83	0.43
1:C:335:VAL:HG21	1:C:454:ILE:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:THR:HG22	1:A:404:ARG:HH11	1.83	0.43
1:A:335:VAL:HG21	1:A:454:ILE:HG22	2.01	0.43
1:B:463:GLY:O	1:B:486:TYR:OH	2.28	0.43
1:B:464:HIS:NE2	1:B:469:ASP:OD1	2.51	0.43
1:B:773:LYS:HA	1:B:773:LYS:HD2	1.82	0.43
1:B:90:TRP:HE1	1:B:96:ASP:HB3	1.83	0.43
1:C:400:THR:HG22	1:C:404:ARG:HH11	1.83	0.43
1:C:946:TYR:OH	1:C:982:THR:HG21	2.17	0.43
1:D:996:ASP:H	1:D:1002:SER:HB2	1.83	0.43
1:D:946:TYR:OH	1:D:982:THR:HG21	2.17	0.43
1:A:105:TYR:CE2	1:A:196:TYR:HA	2.54	0.43
1:A:732:ALA:HA	1:A:733:ALA:HA	1.71	0.43
1:B:610:ASP:N	1:B:610:ASP:OD1	2.41	0.43
1:C:105:TYR:CE2	1:C:196:TYR:HA	2.54	0.43
1:C:461:GLU:OE2	1:C:502:MET:HE1	2.19	0.43
1:D:464:HIS:NE2	1:D:469:ASP:OD1	2.51	0.43
1:A:770:ILE:HG22	1:A:771:GLY:H	1.82	0.43
1:A:946:TYR:OH	1:A:982:THR:HG21	2.17	0.43
1:B:380:LYS:HE3	1:B:380:LYS:HB3	1.80	0.43
1:B:461:GLU:OE2	1:B:502:MET:HE1	2.18	0.43
1:B:588:TYR:OH	1:B:971:SER:O	2.29	0.43
1:B:946:TYR:OH	1:B:982:THR:HG21	2.17	0.43
1:C:42:ALA:HB1	1:C:327:ALA:HB2	2.01	0.43
1:C:90:TRP:HE1	1:C:96:ASP:HB3	1.83	0.43
1:D:461:GLU:OE2	1:D:502:MET:HE1	2.18	0.43
1:D:90:TRP:HE1	1:D:96:ASP:HB3	1.83	0.43
1:A:42:ALA:HB1	1:A:327:ALA:HB2	2.01	0.43
1:B:105:TYR:CE2	1:B:196:TYR:HA	2.54	0.43
1:B:514:ALA:HB2	1:C:278:ILE:O	2.19	0.43
1:C:770:ILE:HG22	1:C:771:GLY:H	1.82	0.43
1:D:105:TYR:CE2	1:D:196:TYR:HA	2.54	0.43
1:D:198:GLU:HG3	1:D:439:ARG:HH11	1.80	0.43
1:A:278:ILE:O	1:D:514:ALA:HB2	2.19	0.43
1:A:333:ARG:HB2	1:A:344:LEU:HD11	2.00	0.43
1:A:90:TRP:HE1	1:A:96:ASP:HB3	1.83	0.43
1:B:199:ASP:C	1:B:416:GLU:HG2	2.38	0.43
1:B:78:LEU:HB2	5:B:5049:HOH:O	2.19	0.43
1:C:568:TRP:HA	1:C:569:ASP:HA	1.57	0.43
1:D:773:LYS:HA	1:D:773:LYS:HD2	1.82	0.43
1:A:375:ASP:OD2	1:A:611:ARG:NH1	2.52	0.43
1:B:670:LEU:HG	1:B:672:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:ARG:HB2	1:C:344:LEU:HD11	2.00	0.43
1:C:375:ASP:OD2	1:C:611:ARG:NH1	2.52	0.43
1:D:670:LEU:HG	1:D:672:VAL:HG23	2.00	0.43
1:D:78:LEU:HB2	5:D:5049:HOH:O	2.19	0.43
1:D:588:TYR:OH	1:D:971:SER:O	2.29	0.43
1:A:450:HIS:HA	1:A:451:PRO:HD2	1.76	0.43
1:D:199:ASP:C	1:D:416:GLU:HG2	2.38	0.43
1:A:594:ASP:N	1:A:594:ASP:OD1	2.52	0.43
1:A:732:ALA:HB1	1:A:733:ALA:HB2	2.01	0.43
1:B:198:GLU:HG3	1:B:439:ARG:HH11	1.80	0.43
1:B:567:VAL:HG23	5:B:5017:HOH:O	2.19	0.43
1:B:904:GLU:HA	1:B:938:ARG:HD3	2.00	0.43
1:C:35:SER:HB2	1:C:217:LYS:HD3	1.99	0.43
1:C:594:ASP:OD1	1:C:594:ASP:N	2.52	0.43
1:C:732:ALA:HB1	1:C:733:ALA:HB2	2.01	0.43
1:D:567:VAL:HG23	5:D:5017:HOH:O	2.19	0.43
1:A:35:SER:HB2	1:A:217:LYS:HD3	1.99	0.42
1:A:461:GLU:OE2	1:A:502:MET:HE1	2.19	0.42
1:B:319:ASP:H	1:B:320:GLY:CA	2.32	0.42
1:B:335:VAL:HG21	1:B:454:ILE:HG22	2.01	0.42
1:D:319:ASP:H	1:D:320:GLY:CA	2.32	0.42
1:D:335:VAL:HG21	1:D:454:ILE:HG22	2.01	0.42
1:D:333:ARG:HB2	1:D:344:LEU:HD11	2.00	0.42
1:D:904:GLU:HA	1:D:938:ARG:HD3	2.00	0.42
1:A:102:ASN:ND2	2:A:2001:PTQ:C9	2.82	0.42
1:B:102:ASN:ND2	2:B:2001:PTQ:C9	2.82	0.42
1:B:333:ARG:HB2	1:B:344:LEU:HD11	2.00	0.42
1:B:360:HIS:N	1:B:364:GLY:O	2.40	0.42
1:D:102:ASN:ND2	2:D:2001:PTQ:C9	2.82	0.42
1:D:867:THR:HG23	1:D:1015:HIS:HE1	1.83	0.42
1:A:568:TRP:HA	1:A:569:ASP:HA	1.57	0.42
1:A:904:GLU:HA	1:A:938:ARG:HD3	2.00	0.42
1:B:601:PHE:CZ	2:B:2001:PTQ:H11	2.54	0.42
1:B:375:ASP:OD2	1:B:611:ARG:NH1	2.52	0.42
1:C:102:ASN:ND2	2:C:2001:PTQ:C9	2.82	0.42
1:C:450:HIS:HA	1:C:451:PRO:HD2	1.76	0.42
1:C:580:GLU:N	1:C:580:GLU:OE1	2.46	0.42
1:C:904:GLU:HA	1:C:938:ARG:HD3	2.00	0.42
1:D:601:PHE:CZ	2:D:2001:PTQ:H11	2.54	0.42
1:A:514:ALA:HB2	1:D:278:ILE:O	2.19	0.42
1:D:375:ASP:OD2	1:D:611:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:THR:HG23	1:A:1015:HIS:HE1	1.83	0.42
1:A:319:ASP:H	1:A:320:GLY:CA	2.32	0.42
1:B:42:ALA:HB1	1:B:327:ALA:HB2	2.01	0.42
1:B:867:THR:HG23	1:B:1015:HIS:HE1	1.83	0.42
1:C:867:THR:HG23	1:C:1015:HIS:HE1	1.83	0.42
2:C:2001:PTQ:H7A	2:C:2001:PTQ:H14	1.47	0.42
1:C:319:ASP:H	1:C:320:GLY:CA	2.32	0.42
1:D:42:ALA:HB1	1:D:327:ALA:HB2	2.01	0.42
1:B:278:ILE:O	1:C:514:ALA:HB2	2.19	0.42
1:B:435:ALA:O	1:B:439:ARG:HG2	2.19	0.42
1:D:58:TRP:CZ2	1:D:125:LEU:HD22	2.55	0.42
1:A:58:TRP:CZ2	1:A:125:LEU:HD22	2.55	0.42
1:A:567:VAL:HG23	5:A:5017:HOH:O	2.19	0.42
1:B:58:TRP:CZ2	1:B:125:LEU:HD22	2.55	0.42
1:B:732:ALA:HB1	1:B:733:ALA:HB2	2.01	0.42
1:C:355:ASN:ND2	1:C:388:ARG:HH11	2.11	0.42
1:C:567:VAL:HG23	5:C:5017:HOH:O	2.19	0.42
1:C:58:TRP:CZ2	1:C:125:LEU:HD22	2.55	0.42
5:A:5052:HOH:O	1:D:438:GLU:CD	2.58	0.42
1:D:435:ALA:O	1:D:439:ARG:HG2	2.19	0.42
1:D:732:ALA:HB1	1:D:733:ALA:HB2	2.01	0.42
1:A:241:GLU:HA	1:A:292:ARG:HA	2.02	0.42
1:C:241:GLU:HA	1:C:292:ARG:HA	2.02	0.42
1:C:463:GLY:O	1:C:486:TYR:OH	2.28	0.42
1:D:360:HIS:N	1:D:364:GLY:O	2.40	0.42
1:D:613:PRO:HB3	1:D:617:LEU:HD22	2.02	0.42
2:A:2001:PTQ:H14	2:A:2001:PTQ:H7A	1.47	0.42
1:B:438:GLU:CD	5:C:5052:HOH:O	2.58	0.42
1:B:613:PRO:HB3	1:B:617:LEU:HD22	2.02	0.42
1:A:355:ASN:ND2	1:A:388:ARG:HH11	2.11	0.42
1:B:534:ILE:HG22	5:B:5168:HOH:O	2.19	0.42
1:B:357:HIS:HE2	1:B:568:TRP:HH2	1.66	0.42
1:A:255:ARG:HB2	1:A:316:HIS:CE1	2.55	0.42
1:A:613:PRO:HB3	1:A:617:LEU:HD22	2.02	0.42
1:A:78:LEU:HB2	5:A:5049:HOH:O	2.19	0.42
1:B:352:ARG:HB3	1:B:553:TRP:CH2	2.55	0.42
1:B:927:THR:H	1:B:935:ASN:ND2	2.18	0.42
1:C:255:ARG:HB2	1:C:316:HIS:CE1	2.55	0.42
1:C:78:LEU:HB2	5:C:5049:HOH:O	2.19	0.42
1:D:534:ILE:HG22	5:D:5168:HOH:O	2.19	0.42
1:D:352:ARG:HB3	1:D:553:TRP:CH2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:594:ASP:OD1	1:D:594:ASP:N	2.52	0.42
1:D:927:THR:H	1:D:935:ASN:ND2	2.18	0.42
1:A:463:GLY:O	1:A:486:TYR:OH	2.28	0.41
1:A:927:THR:H	1:A:935:ASN:ND2	2.18	0.41
1:B:390:SER:HA	1:B:391:HIS:HA	1.52	0.41
1:B:594:ASP:OD1	1:B:594:ASP:N	2.52	0.41
1:C:613:PRO:HB3	1:C:617:LEU:HD22	2.02	0.41
1:A:435:ALA:O	1:A:439:ARG:HG2	2.19	0.41
1:A:580:GLU:OE1	1:A:580:GLU:N	2.46	0.41
1:B:601:PHE:CE1	2:B:2001:PTQ:C10	3.03	0.41
1:C:927:THR:H	1:C:935:ASN:ND2	2.18	0.41
1:A:352:ARG:HB3	1:A:553:TRP:CH2	2.55	0.41
1:A:826:THR:O	1:A:836:ILE:HG13	2.21	0.41
1:B:89:ASN:ND2	1:B:365:GLN:H	2.18	0.41
1:C:826:THR:O	1:C:836:ILE:HG13	2.21	0.41
1:D:601:PHE:CE1	2:D:2001:PTQ:C10	3.03	0.41
1:D:89:ASN:ND2	1:D:365:GLN:H	2.18	0.41
1:A:420:MET:HB3	1:A:420:MET:HE2	1.88	0.41
1:A:601:PHE:CE1	2:A:2001:PTQ:C10	3.03	0.41
1:A:693:GLN:NE2	1:A:694:LEU:O	2.37	0.41
1:C:89:ASN:ND2	1:C:365:GLN:H	2.18	0.41
1:C:435:ALA:O	1:C:439:ARG:HG2	2.19	0.41
1:C:352:ARG:HB3	1:C:553:TRP:CH2	2.55	0.41
1:C:601:PHE:CE1	2:C:2001:PTQ:C10	3.03	0.41
1:A:542:MET:HE3	1:A:600:GLN:HG2	2.02	0.41
1:B:255:ARG:HB2	1:B:316:HIS:CE1	2.55	0.41
1:B:420:MET:HB3	1:B:420:MET:HE2	1.88	0.41
1:C:601:PHE:CZ	2:C:2001:PTQ:H11	2.54	0.41
1:C:542:MET:HE3	1:C:600:GLN:HG2	2.02	0.41
1:D:241:GLU:HA	1:D:292:ARG:HA	2.02	0.41
1:D:342:LEU:HG	1:D:349:LEU:HD21	2.03	0.41
1:A:601:PHE:CZ	2:A:2001:PTQ:H11	2.54	0.41
1:A:89:ASN:ND2	1:A:365:GLN:H	2.18	0.41
1:B:342:LEU:HG	1:B:349:LEU:HD21	2.03	0.41
1:B:542:MET:HE3	1:B:600:GLN:HG2	2.02	0.41
1:C:693:GLN:NE2	1:C:694:LEU:O	2.37	0.41
1:D:255:ARG:HB2	1:D:316:HIS:CE1	2.55	0.41
1:B:601:PHE:CE1	2:B:2001:PTQ:H10	2.56	0.41
1:B:241:GLU:HA	1:B:292:ARG:HA	2.02	0.41
1:B:601:PHE:CD1	2:B:2001:PTQ:H10	2.56	0.41
1:C:534:ILE:HG22	5:C:5168:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:601:PHE:CE1	2:D:2001:PTQ:H10	2.56	0.41
1:D:542:MET:HE3	1:D:600:GLN:HG2	2.02	0.41
1:D:601:PHE:CD1	2:D:2001:PTQ:H10	2.56	0.41
1:A:342:LEU:HG	1:A:349:LEU:HD21	2.03	0.41
1:A:372:MET:HB2	1:A:372:MET:HE2	1.66	0.41
1:A:534:ILE:HG22	5:A:5168:HOH:O	2.19	0.41
1:A:783:GLN:NE2	1:A:964:GLN:HG3	2.36	0.41
1:B:580:GLU:N	1:B:580:GLU:OE1	2.46	0.41
1:D:390:SER:HA	1:D:391:HIS:HA	1.52	0.41
1:A:601:PHE:CD1	2:A:2001:PTQ:H10	2.56	0.41
1:B:898:LEU:HB2	1:B:917:ARG:HE	1.86	0.41
1:C:601:PHE:CD1	2:C:2001:PTQ:H10	2.56	0.41
1:C:342:LEU:HG	1:C:349:LEU:HD21	2.03	0.41
1:C:783:GLN:NE2	1:C:964:GLN:HG3	2.36	0.41
1:B:193:ASP:N	1:B:193:ASP:OD1	2.54	0.41
1:B:654:TRP:CE2	1:B:682:LEU:HD22	2.56	0.41
5:B:5052:HOH:O	1:C:438:GLU:CD	2.58	0.41
1:D:193:ASP:OD1	1:D:193:ASP:N	2.54	0.41
1:D:898:LEU:HB2	1:D:917:ARG:HE	1.86	0.41
1:A:266:GLN:NE2	1:A:269:SER:HB2	2.36	0.41
1:B:440:VAL:HG21	1:B:471:LEU:HD23	2.02	0.41
1:B:826:THR:O	1:B:836:ILE:HG13	2.21	0.41
1:D:440:VAL:HG21	1:D:471:LEU:HD23	2.02	0.41
1:D:580:GLU:N	1:D:580:GLU:OE1	2.46	0.41
1:A:438:GLU:CD	5:D:5052:HOH:O	2.58	0.40
1:C:266:GLN:NE2	1:C:269:SER:HB2	2.36	0.40
1:C:773:LYS:HD2	1:C:773:LYS:HA	1.82	0.40
1:D:654:TRP:CE2	1:D:682:LEU:HD22	2.56	0.40
1:D:826:THR:O	1:D:836:ILE:HG13	2.21	0.40
1:A:654:TRP:CE2	1:A:682:LEU:HD22	2.56	0.40
1:C:966:GLN:O	1:C:970:THR:OG1	2.25	0.40
1:A:105:TYR:HE2	1:A:196:TYR:HA	1.85	0.40
1:A:601:PHE:CE1	2:A:2001:PTQ:H10	2.56	0.40
1:A:498:ILE:HG21	1:A:534:ILE:HD12	2.03	0.40
1:A:513:PRO:O	1:A:515:VAL:N	2.51	0.40
1:B:124:SER:HA	1:B:184:LEU:O	2.22	0.40
1:B:789:LEU:HD21	1:B:934:GLU:HB3	2.04	0.40
1:B:927:THR:H	1:B:935:ASN:HD22	1.69	0.40
1:C:105:TYR:HE2	1:C:196:TYR:HA	1.85	0.40
1:C:601:PHE:CE1	2:C:2001:PTQ:H10	2.56	0.40
1:C:372:MET:HE2	1:C:372:MET:HB2	1.66	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:498:ILE:HG21	1:C:534:ILE:HD12	2.03	0.40
1:C:513:PRO:O	1:C:515:VAL:N	2.51	0.40
1:C:654:TRP:CE2	1:C:682:LEU:HD22	2.56	0.40
1:D:789:LEU:HD21	1:D:934:GLU:HB3	2.04	0.40
1:D:927:THR:H	1:D:935:ASN:HD22	1.69	0.40
1:A:103:VAL:HG13	1:A:418:HIS:CG	2.57	0.40
1:A:509:ASP:HB3	1:A:519:SER:N	2.37	0.40
1:A:789:LEU:HD21	1:A:934:GLU:HB3	2.04	0.40
2:B:2001:PTQ:H7A	2:B:2001:PTQ:H14	1.47	0.40
1:B:266:GLN:NE2	1:B:269:SER:HB2	2.36	0.40
1:C:103:VAL:HG13	1:C:418:HIS:CG	2.57	0.40
1:C:509:ASP:HB3	1:C:519:SER:N	2.37	0.40
1:C:789:LEU:HD21	1:C:934:GLU:HB3	2.04	0.40
1:D:124:SER:HA	1:D:184:LEU:O	2.22	0.40
1:D:266:GLN:NE2	1:D:269:SER:HB2	2.36	0.40
1:D:355:ASN:ND2	1:D:388:ARG:HH11	2.11	0.40

There are no symmetry-related clashes.

## 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 PDB entries followed by that with respect to all EM entries.

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	1020/1022 (100%)	974 (96%)	40 (4%)	6 (1%)	28	29
1	B	1020/1022 (100%)	974 (96%)	40 (4%)	6 (1%)	28	29
1	C	1020/1022 (100%)	974 (96%)	40 (4%)	6 (1%)	28	29
1	D	1020/1022 (100%)	974 (96%)	40 (4%)	6 (1%)	28	29
All	All	4080/4088 (100%)	3896 (96%)	160 (4%)	24 (1%)	33	29

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	461	GLU
1	B	3	ILE
1	B	461	GLU
1	C	3	ILE
1	C	461	GLU
1	D	3	ILE
1	D	461	GLU
1	A	164	ASP
1	B	164	ASP
1	C	164	ASP
1	D	164	ASP
1	A	319	ASP
1	B	319	ASP
1	C	319	ASP
1	D	319	ASP
1	A	306	PRO
1	A	599	ARG
1	B	306	PRO
1	B	599	ARG
1	C	306	PRO
1	C	599	ARG
1	D	306	PRO
1	D	599	ARG

### 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 PDB entries followed by that with respect to all EM entries.

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	874/874 (100%)	871 (100%)	3 (0%)	94	97
1	B	874/874 (100%)	871 (100%)	3 (0%)	94	97
1	C	874/874 (100%)	871 (100%)	3 (0%)	94	97
1	D	874/874 (100%)	871 (100%)	3 (0%)	94	97
All	All	3496/3496 (100%)	3484 (100%)	12 (0%)	94	97

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	333	ARG
1	A	416	GLU
1	A	537	GLU
1	B	333	ARG
1	B	416	GLU
1	B	537	GLU
1	C	333	ARG
1	C	416	GLU
1	C	537	GLU
1	D	333	ARG
1	D	416	GLU
1	D	537	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	38	ASN
1	A	89	ASN
1	A	102	ASN
1	A	163	GLN
1	A	262	GLN
1	A	266	GLN
1	A	355	ASN
1	A	391	HIS
1	A	395	HIS
1	A	573	GLN
1	A	597	ASN
1	A	624	GLN
1	A	653	HIS
1	A	767	GLN
1	A	775	GLN
1	A	935	ASN
1	A	985	ASN
1	A	1015	HIS
1	B	25	ASN
1	B	38	ASN
1	B	89	ASN
1	B	102	ASN
1	B	163	GLN
1	B	262	GLN
1	B	266	GLN
1	B	355	ASN

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Mol	Chain	Res	Type
1	B	391	HIS
1	B	395	HIS
1	B	573	GLN
1	B	597	ASN
1	B	624	GLN
1	B	653	HIS
1	B	767	GLN
1	B	775	GLN
1	B	935	ASN
1	B	985	ASN
1	B	1015	HIS
1	C	25	ASN
1	C	38	ASN
1	C	89	ASN
1	C	102	ASN
1	C	163	GLN
1	C	262	GLN
1	C	266	GLN
1	C	355	ASN
1	C	391	HIS
1	C	395	HIS
1	C	573	GLN
1	C	597	ASN
1	C	624	GLN
1	C	653	HIS
1	C	767	GLN
1	C	775	GLN
1	C	935	ASN
1	C	985	ASN
1	C	1015	HIS
1	D	25	ASN
1	D	38	ASN
1	D	89	ASN
1	D	102	ASN
1	D	163	GLN
1	D	262	GLN
1	D	266	GLN
1	D	355	ASN
1	D	391	HIS
1	D	395	HIS
1	D	573	GLN
1	D	597	ASN

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Mol	Chain	Res	Type
1	D	624	GLN
1	D	653	HIS
1	D	767	GLN
1	D	775	GLN
1	D	935	ASN
1	D	985	ASN
1	D	1015	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 16 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	PTQ	A	2001	4	21,21,21	2.59	4 (19%)	26,28,28	1.51	2 (7%)
2	PTQ	B	2001	4	21,21,21	2.59	4 (19%)	26,28,28	1.51	2 (7%)
2	PTQ	C	2001	4	21,21,21	2.59	4 (19%)	26,28,28	1.51	2 (7%)
2	PTQ	D	2001	4	21,21,21	2.59	4 (19%)	26,28,28	1.51	2 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PTQ	A	2001	4	-	0/8/28/28	0/2/2/2
2	PTQ	B	2001	4	-	0/8/28/28	0/2/2/2
2	PTQ	C	2001	4	-	0/8/28/28	0/2/2/2
2	PTQ	D	2001	4	-	0/8/28/28	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	PTQ	C7-S1	-2.83	1.77	1.81
2	C	2001	PTQ	C7-S1	-2.83	1.77	1.81
2	B	2001	PTQ	C7-S1	-2.83	1.77	1.81
2	D	2001	PTQ	C7-S1	-2.83	1.77	1.81
2	A	2001	PTQ	C12-C11	5.66	1.51	1.38
2	C	2001	PTQ	C12-C11	5.66	1.51	1.38
2	B	2001	PTQ	C12-C11	5.66	1.51	1.38
2	D	2001	PTQ	C12-C11	5.66	1.51	1.38
2	A	2001	PTQ	C10-C9	6.24	1.51	1.38
2	C	2001	PTQ	C10-C9	6.24	1.51	1.38
2	B	2001	PTQ	C10-C9	6.24	1.51	1.38
2	D	2001	PTQ	C10-C9	6.24	1.51	1.38
2	A	2001	PTQ	C13-C14	6.63	1.51	1.38
2	C	2001	PTQ	C13-C14	6.63	1.51	1.38
2	B	2001	PTQ	C13-C14	6.63	1.51	1.38
2	D	2001	PTQ	C13-C14	6.63	1.51	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	PTQ	C7-C8-C9	-3.27	108.41	114.05
2	C	2001	PTQ	C7-C8-C9	-3.27	108.41	114.05
2	B	2001	PTQ	C7-C8-C9	-3.27	108.41	114.05
2	D	2001	PTQ	C7-C8-C9	-3.27	108.41	114.05
2	A	2001	PTQ	C7-S1-C1	6.24	109.54	100.28
2	C	2001	PTQ	C7-S1-C1	6.24	109.54	100.28
2	B	2001	PTQ	C7-S1-C1	6.24	109.54	100.28
2	D	2001	PTQ	C7-S1-C1	6.24	109.54	100.28

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

4 monomers are involved in 79 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	PTQ	20	0
2	B	2001	PTQ	20	0
2	C	2001	PTQ	20	0
2	D	2001	PTQ	19	0

## 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.