



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:39 PM BST

PDB ID : 1GW8
EMDB ID: : EMD-1012
Title : quasi-atomic resolution model of bacteriophage PRD1 sus607 mutant, obtained by combined cryo-EM and X-ray crystallography.
Authors : San Martin, C.; Huiskonen, J.; Bamford, J.K.H.; Butcher, S.J.; Fuller, S.D.; Bamford, D.H.; Burnett, R.M.
Deposited on : 2002-03-08
Resolution : 13.30 Å(reported)
Based on PDB ID : 1HX6

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

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

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

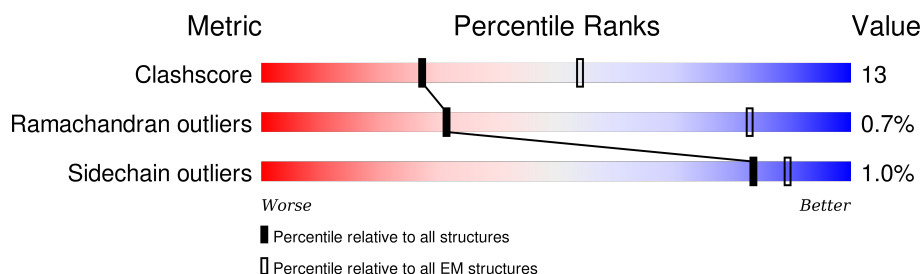
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 13.30 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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 ≥ 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	394	79% 14% • 6%
1	B	394	78% 15% • 5%
1	C	394	82% 11% • 6%
1	D	394	76% 17% • 6%
1	E	394	80% 14% • 5%
1	F	394	83% 10% • 6%
1	G	394	79% 14% • 6%
1	H	394	84% 10% • 5%
1	I	394	79% 14% • 6%

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Mol	Chain	Length	Quality of chain
1	J	394	<div><div></div><div>81%</div><div>13%</div><div>• 6%</div></div>
1	K	394	<div><div></div><div>81%</div><div>13%</div><div>• 5%</div></div>
1	L	394	<div><div></div><div>83%</div><div>10%</div><div>• 6%</div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 34170 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 MAJOR CAPSID PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	371	Total	C	N	O	S	0	1
			2837	1803	479	548	7		
1	B	373	Total	C	N	O	S	0	1
			2847	1804	485	551	7		
1	C	372	Total	C	N	O	S	0	1
			2861	1817	484	553	7		
1	D	371	Total	C	N	O	S	0	1
			2827	1795	478	547	7		
1	E	373	Total	C	N	O	S	0	1
			2847	1804	485	551	7		
1	F	372	Total	C	N	O	S	0	1
			2861	1817	484	553	7		
1	G	371	Total	C	N	O	S	0	1
			2837	1803	479	548	7		
1	H	373	Total	C	N	O	S	0	1
			2847	1804	485	551	7		
1	I	372	Total	C	N	O	S	0	1
			2861	1817	484	553	7		
1	J	371	Total	C	N	O	S	0	1
			2837	1803	479	548	7		
1	K	373	Total	C	N	O	S	0	1
			2847	1804	485	551	7		
1	L	372	Total	C	N	O	S	0	1
			2861	1817	484	553	7		

● Molecule 1: MAJOR CAPSID PROTEIN

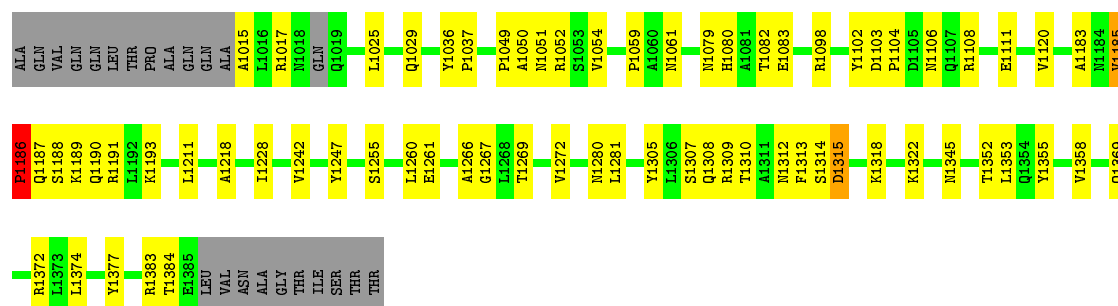
ILE	SER	THR	THR	V1242	ALA
				GLN	
				Y1247	VAL
				GLN	
				S1255	GLN
				LEU	
				L1260	THR
				PRO	
				T1269	ALA
				GLN	
				P1270	GLN
				GLN	
				M1271	LEU
				LEU	
				V1272	THR
				THR	
				D1273	ALA
				ALA	
				M1280	ALA
				ALA	
				L1281	ALA
				ALA	
				Y1305	ALA
				ALA	
				L1306	ALA
				ALA	
				S1307	ALA
				ALA	
				Q1308	ALA
				ALA	
				R1309	ALA
				ALA	
				T1310	ALA
				ALA	
				A1311	ALA
				ALA	
				M1312	ALA
				ALA	
				F1313	ALA
				ALA	
				S1314	ALA
				ALA	
				D1315	ALA
				ALA	
				K1318	ALA
				ALA	
				K1322	ALA
				ALA	
				M1345	ALA
				ALA	
				T1352	ALA
				ALA	
				L1353	ALA
				ALA	
				Q1354	ALA
				ALA	
				Y1355	ALA
				ALA	
				V1358	ALA
				ALA	
				M1363	ALA
				ALA	
				Q1369	ALA
				ALA	
				L1374	ALA
				ALA	
				Y1377	ALA
				ALA	
				R1383	ALA
				ALA	
				T1384	ALA
				ALA	
				E1385	ALA
				ALA	
				LEU	ALA
				ALA	
				VAL	ALA
				ALA	
				ASN	ALA
				ALA	
				GLY	ALA
				ALA	
				THR	ALA
				ALA	

[illegible]

N3245	G3246	Y3247	Y3275	A3279	N3280	L3281	Y3284	Q3308	R3309	T3310	A3311	N3312	N3345	Y3350	Y3351	T3352	L3353	Q3354	Y3355	Y3358	Y3361	Q3369	N3370	R3383	T3384	E3385	LEU	ASN	ASN	GLY	THR	ILE	SER	THR	THR						
ALA	GLN	VAL	GLN	GLN	LEU	PRO	ALA	GLN	GLN	ALA	A3014	R3015	R3016	L3025	Q3029	Q3033	T3044	Q3045	T3046	N3061	H3080	A3081	E3082	R3098	D3103	P3104	R3108	E3111	P3151	T3162	T3163	L3182	A3183	N3184	V3185	P3186	A3218	D3238	V3242	G3243	G3244

WORLDWIDE
PDB
PROTEIN DATA BANK

 **EMDataBank**
Unified Data Resource for 3DEM



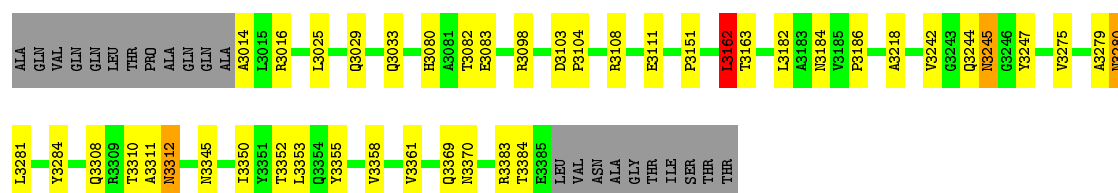
• Molecule 1: MAJOR CAPSID PROTEIN

Chain E: 80% 14% • 5%



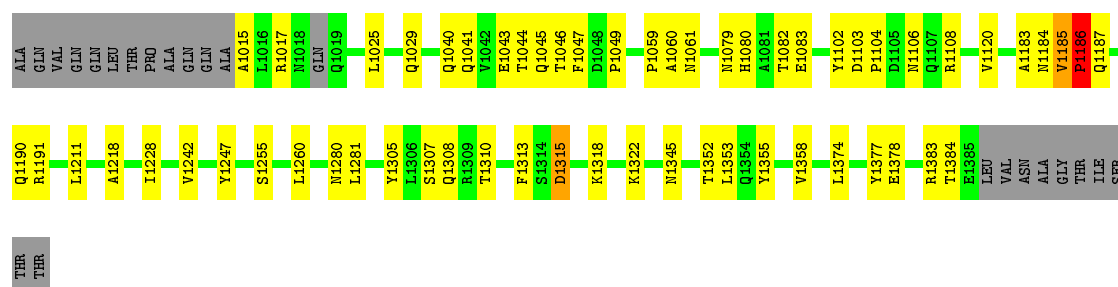
• Molecule 1: MAJOR CAPSID PROTEIN

Chain F: 83% 10% • 6%



• Molecule 1: MAJOR CAPSID PROTEIN

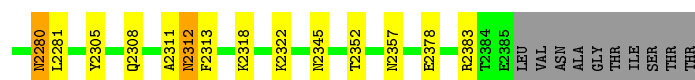
Chain G: 79% 14% • 6%



• Molecule 1: MAJOR CAPSID PROTEIN

Chain H: 84% 10% • 5%





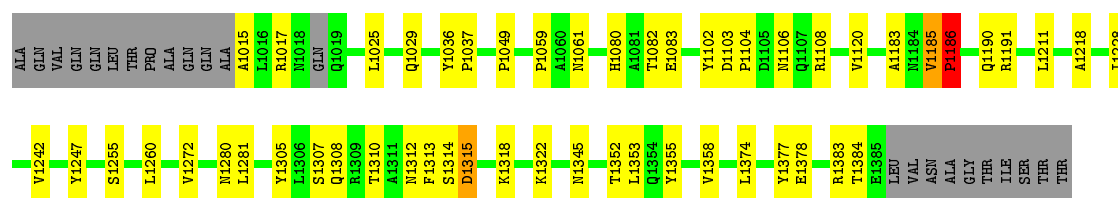
• Molecule 1: MAJOR CAPSID PROTEIN

Chain I: 79% 14% 6%



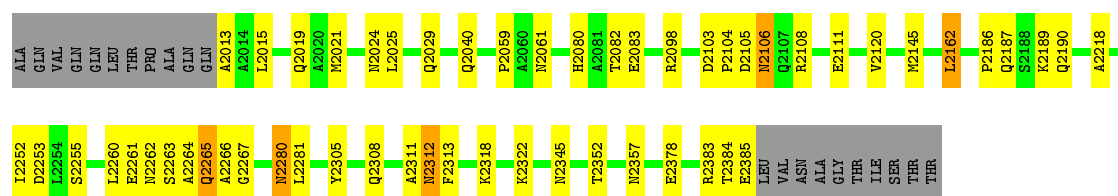
• Molecule 1: MAJOR CAPSID PROTEIN

Chain J: 81% 13% 6%



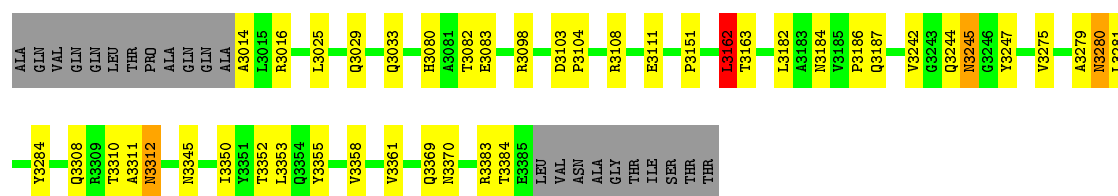
• Molecule 1: MAJOR CAPSID PROTEIN

Chain K: 81% 13% 5%



• Molecule 1: MAJOR CAPSID PROTEIN

Chain L: 83% 10% 6%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PHASE RESTORATION BY CTF- MULTIPLICATION OF IMAGES; AMPLITUDE RESTORATION BY COMPARISON WITH QUASI- ATOMIC MODEL	Depositor
Microscope	FEI CM200 FEG	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	4100	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor

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 >2	RMSZ	# Z >2
1	A	0.44	0/2902	0.72	0/3971
1	B	0.45	0/2910	0.73	1/3982 (0.0%)
1	C	0.44	0/2926	0.72	1/4003 (0.0%)
1	D	0.44	0/2888	0.72	0/3948
1	E	0.45	0/2910	0.73	1/3982 (0.0%)
1	F	0.43	0/2926	0.72	1/4003 (0.0%)
1	G	0.44	0/2902	0.72	0/3971
1	H	0.46	0/2910	0.73	1/3982 (0.0%)
1	I	0.43	0/2926	0.72	1/4003 (0.0%)
1	J	0.44	0/2902	0.72	0/3971
1	K	0.46	0/2910	0.73	1/3982 (0.0%)
1	L	0.44	0/2926	0.73	1/4003 (0.0%)
All	All	0.44	0/34938	0.72	8/47801 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	2162	LEU	CA-CB-CG	6.46	130.16	115.30
1	H	2162	LEU	CA-CB-CG	6.44	130.10	115.30
1	B	2162	LEU	CA-CB-CG	6.43	130.09	115.30
1	K	2162	LEU	CA-CB-CG	6.42	130.07	115.30
1	L	3162	LEU	CA-CB-CG	5.99	129.08	115.30
1	C	3162	LEU	CA-CB-CG	5.95	128.98	115.30
1	I	3162	LEU	CA-CB-CG	5.95	128.98	115.30
1	F	3162	LEU	CA-CB-CG	5.94	128.97	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2837	0	2713	110	0
1	B	2847	0	2723	225	0
1	C	2861	0	2751	60	0
1	D	2827	0	2697	206	0
1	E	2847	0	2721	162	0
1	F	2861	0	2752	35	0
1	G	2837	0	2713	117	0
1	H	2847	0	2729	34	0
1	I	2861	0	2742	158	0
1	J	2837	0	2714	57	0
1	K	2847	0	2728	130	0
1	L	2861	0	2752	34	0
All	All	34170	0	32735	863	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 13.

All (863) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2264:ALA:CB	1:D:1272:VAL:HG11	1.22	1.62
1:B:2189:LYS:CD	1:E:2061:ASN:H	1.15	1.60
1:B:2108:ARG:CD	1:D:1314:SER:HB2	1.19	1.58
1:B:2108:ARG:HD3	1:D:1314:SER:CB	1.12	1.58
1:B:2269:THR:CG2	1:I:3372:ARG:HD3	1.13	1.57
1:B:2264:ALA:CB	1:D:1272:VAL:CG1	1.81	1.57
1:D:1187:GLN:CB	1:G:1186:PRO:HA	1.27	1.56
1:B:2269:THR:HG21	1:I:3372:ARG:CD	1.12	1.55
1:B:2189:LYS:CG	1:E:2061:ASN:HB2	1.02	1.48
1:D:1051:ASN:CA	1:G:1046:THR:HB	1.43	1.46
1:E:2108:ARG:NH1	1:J:1314:SER:CA	1.78	1.46
1:B:2372:ARG:CD	1:D:1269:THR:HG21	1.44	1.46
1:B:2189:LYS:HD3	1:E:2061:ASN:N	1.16	1.45
1:D:1187:GLN:CB	1:G:1186:PRO:CA	1.94	1.42
1:A:1369:GLN:CD	1:K:2266:ALA:HB3	1.34	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2189:LYS:HG2	1:E:2061:ASN:CB	0.93	1.41
1:B:2272:VAL:HG11	1:I:3264:ALA:CB	1.50	1.39
1:B:2052:ARG:HD3	1:E:2045:GLN:NE2	1.38	1.39
1:A:1363:ASN:ND2	1:K:2108:ARG:HH22	1.18	1.37
1:A:1272:VAL:HA	1:K:2261:GLU:OE2	1.21	1.37
1:B:2264:ALA:HB2	1:D:1272:VAL:CG1	1.46	1.35
1:D:1266:ALA:HB3	1:I:3267:GLY:CA	1.59	1.33
1:B:2372:ARG:NE	1:D:1269:THR:HG21	1.43	1.32
1:E:2108:ARG:HH11	1:J:1314:SER:CB	1.43	1.32
1:B:2272:VAL:CG1	1:I:3264:ALA:HB2	1.59	1.32
1:D:1052:ARG:HD2	1:G:1045:GLN:CB	1.58	1.31
1:B:2061:ASN:OD1	1:E:2186:PRO:HB3	1.19	1.31
1:B:2372:ARG:HD3	1:D:1269:THR:CG2	1.60	1.30
1:B:2372:ARG:NH1	1:D:1272:VAL:CG2	1.93	1.30
1:A:1363:ASN:ND2	1:K:2108:ARG:NH2	1.76	1.29
1:E:2108:ARG:NH1	1:J:1314:SER:N	1.79	1.27
1:B:2185:VAL:O	1:E:2186:PRO:CG	1.82	1.26
1:B:2061:ASN:OD1	1:E:2186:PRO:CB	1.82	1.25
1:B:2052:ARG:HD3	1:E:2045:GLN:CD	1.54	1.25
1:B:2369:GLN:NE2	1:I:3369:GLN:NE2	1.83	1.25
1:D:1051:ASN:HA	1:G:1046:THR:CB	1.66	1.25
1:A:1369:GLN:OE1	1:K:2266:ALA:HB3	1.09	1.25
1:A:1271:ASN:ND2	1:K:2098:ARG:NH1	1.85	1.24
1:B:2051:ASN:CB	1:E:2046:THR:O	1.85	1.24
1:B:2369:GLN:CD	1:I:3369:GLN:CD	1.96	1.24
1:C:3186:PRO:CD	1:I:3188:SER:H	1.40	1.24
1:B:2369:GLN:OE1	1:I:3369:GLN:CD	1.77	1.24
1:B:2052:ARG:CD	1:E:2045:GLN:NE2	2.00	1.23
1:B:2052:ARG:HD3	1:E:2045:GLN:CG	1.70	1.20
1:B:2372:ARG:NH1	1:D:1272:VAL:HG23	1.54	1.20
1:B:2372:ARG:HD3	1:D:1269:THR:CB	1.70	1.20
1:B:2369:GLN:CD	1:I:3369:GLN:NE2	1.93	1.20
1:C:3186:PRO:HD3	1:I:3188:SER:N	1.22	1.19
1:B:2267:GLY:CA	1:I:3266:ALA:HB3	1.73	1.18
1:B:2269:THR:CB	1:I:3372:ARG:HD3	1.74	1.18
1:D:1187:GLN:CB	1:G:1186:PRO:C	2.11	1.18
1:D:1374:LEU:CD2	1:I:3272:VAL:HG21	1.74	1.18
1:B:2185:VAL:O	1:E:2186:PRO:HG2	1.39	1.17
1:E:2188:SER:C	1:K:2186:PRO:HG3	1.47	1.17
1:A:1369:GLN:NE2	1:K:2266:ALA:CB	2.07	1.17
1:B:2106:ASN:CG	1:E:2062:VAL:HG11	1.65	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2185:VAL:O	1:K:2186:PRO:HG2	1.46	1.15
1:D:1052:ARG:HB2	1:G:1045:GLN:HA	1.27	1.15
1:D:1051:ASN:C	1:G:1046:THR:HB	1.61	1.14
1:C:3186:PRO:CG	1:I:3188:SER:H	1.61	1.14
1:B:2269:THR:CB	1:I:3372:ARG:CD	2.26	1.14
1:E:2108:ARG:HH11	1:J:1314:SER:HB2	0.97	1.12
1:A:1369:GLN:CD	1:K:2266:ALA:CB	2.18	1.12
1:D:1372:ARG:CB	1:I:3269:THR:HG21	1.61	1.12
1:E:2191:ARG:NH2	1:K:2040:GLN:HE22	1.48	1.11
1:B:2269:THR:HG21	1:I:3372:ARG:HD2	1.21	1.11
1:E:2108:ARG:HH12	1:J:1314:SER:CA	1.48	1.11
1:B:2051:ASN:HB3	1:E:2046:THR:O	1.50	1.11
1:D:1372:ARG:HB3	1:I:3269:THR:CG2	1.80	1.10
1:B:2264:ALA:HB3	1:D:1272:VAL:CG1	1.71	1.10
1:B:2052:ARG:CD	1:E:2045:GLN:HE21	1.62	1.09
1:D:1191:ARG:HH11	1:G:1040:GLN:NE2	1.49	1.09
1:C:3186:PRO:CD	1:I:3188:SER:N	1.93	1.08
1:B:2372:ARG:CD	1:D:1269:THR:CG2	2.22	1.08
1:A:1363:ASN:HD22	1:K:2108:ARG:NH2	1.40	1.08
1:B:2106:ASN:OD1	1:E:2062:VAL:HG11	1.52	1.08
1:D:1052:ARG:CB	1:G:1045:GLN:HA	1.82	1.08
1:A:1271:ASN:ND2	1:K:2098:ARG:CZ	2.15	1.08
1:B:2264:ALA:HB1	1:D:1272:VAL:HG11	1.18	1.07
1:E:2108:ARG:HH12	1:J:1314:SER:HA	0.96	1.07
1:A:1271:ASN:CG	1:K:2098:ARG:NH1	2.09	1.06
1:D:1052:ARG:CD	1:G:1045:GLN:HB2	1.85	1.06
1:B:2264:ALA:HB2	1:D:1272:VAL:HG13	1.30	1.06
1:D:1051:ASN:C	1:G:1046:THR:CB	2.21	1.06
1:A:1369:GLN:NE2	1:K:2266:ALA:HB1	1.69	1.06
1:B:2056:ASP:OD1	1:E:2042:VAL:O	1.73	1.06
1:D:1189:LYS:HG2	1:G:1061:ASN:H	1.19	1.06
1:B:2372:ARG:HH12	1:D:1272:VAL:HG23	1.08	1.06
1:A:1369:GLN:OE1	1:K:2266:ALA:CB	2.03	1.06
1:B:2269:THR:CG2	1:I:3372:ARG:CD	1.88	1.05
1:D:1051:ASN:CA	1:G:1046:THR:CB	2.28	1.05
1:D:1266:ALA:HB3	1:I:3267:GLY:C	1.75	1.05
1:D:1374:LEU:HD21	1:I:3272:VAL:CG2	1.86	1.05
1:D:1372:ARG:NH1	1:I:3272:VAL:HG23	1.70	1.05
1:D:1374:LEU:CD2	1:I:3272:VAL:CG2	2.35	1.04
1:A:1305:TYR:CE2	1:K:2108:ARG:NH1	2.25	1.04
1:D:1189:LYS:CG	1:G:1061:ASN:H	1.69	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2369:GLN:HE22	1:I:3369:GLN:HG2	1.20	1.03
1:D:1189:LYS:NZ	1:G:1059:PRO:O	1.92	1.03
1:B:2372:ARG:NE	1:D:1269:THR:CG2	2.21	1.03
1:A:1363:ASN:ND2	1:K:2108:ARG:CZ	2.21	1.03
1:B:2061:ASN:OD1	1:E:2186:PRO:CG	2.07	1.02
1:B:2052:ARG:HD3	1:E:2045:GLN:HG2	1.35	1.02
1:B:2189:LYS:CG	1:E:2061:ASN:CA	2.38	1.02
1:B:2267:GLY:HA2	1:I:3266:ALA:HB3	1.38	1.02
1:B:2052:ARG:NE	1:E:2045:GLN:NE2	2.07	1.02
1:B:2189:LYS:HG2	1:E:2061:ASN:CA	1.91	1.01
1:D:1372:ARG:HB3	1:I:3269:THR:HG21	1.01	1.00
1:D:1051:ASN:HA	1:G:1046:THR:HB	1.03	1.00
1:D:1374:LEU:HD21	1:I:3272:VAL:HG21	1.01	1.00
1:D:1266:ALA:HB3	1:I:3267:GLY:HA2	1.38	1.00
1:B:2372:ARG:NH1	1:D:1272:VAL:HG21	1.77	0.99
1:B:2052:ARG:HB3	1:E:2045:GLN:HA	1.45	0.99
1:B:2264:ALA:HB3	1:D:1272:VAL:HG12	1.40	0.98
1:A:1270:PRO:HD2	1:K:2264:ALA:H	1.25	0.98
1:E:2108:ARG:NH1	1:J:1314:SER:CB	2.15	0.98
1:A:1270:PRO:O	1:K:2262:ASN:O	1.82	0.98
1:B:2052:ARG:CD	1:E:2045:GLN:HG2	1.93	0.97
1:B:2061:ASN:CG	1:E:2186:PRO:HB3	1.84	0.96
1:C:3044:THR:O	1:I:3052:ARG:HG3	1.64	0.96
1:E:2189:LYS:CG	1:K:2061:ASN:HB2	1.95	0.96
1:D:1052:ARG:HD2	1:G:1045:GLN:CA	1.96	0.96
1:D:1052:ARG:HH12	1:G:1043:GLU:CD	1.57	0.95
1:E:2108:ARG:NH1	1:J:1314:SER:HA	1.59	0.95
1:B:2267:GLY:HA3	1:I:3266:ALA:HB3	1.46	0.95
1:D:1052:ARG:HD2	1:G:1045:GLN:HB2	0.96	0.95
1:B:2267:GLY:HA2	1:I:3266:ALA:CB	1.96	0.95
1:A:1363:ASN:ND2	1:K:2108:ARG:NH1	2.14	0.95
1:C:3186:PRO:CB	1:I:3061:ASN:HD22	1.80	0.95
1:B:2269:THR:HG22	1:I:3372:ARG:HD3	1.48	0.94
1:B:2051:ASN:CA	1:E:2046:THR:O	2.15	0.94
1:B:2305:TYR:OH	1:I:3098:ARG:NH1	2.00	0.94
1:B:2272:VAL:CG1	1:I:3264:ALA:CB	2.29	0.94
1:A:1369:GLN:HE22	1:K:2266:ALA:CB	1.76	0.94
1:B:2187:GLN:CB	1:E:2185:VAL:CG2	2.44	0.94
1:B:2189:LYS:CG	1:E:2061:ASN:H	1.78	0.94
1:B:2189:LYS:CB	1:E:2061:ASN:HB2	1.97	0.93
1:D:1098:ARG:CZ	1:I:3318:LYS:HZ1	1.81	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1369:GLN:NE2	1:K:2266:ALA:HB3	1.76	0.93
1:B:2369:GLN:HE22	1:I:3369:GLN:CG	1.80	0.93
1:B:2369:GLN:NE2	1:I:3369:GLN:HE21	1.51	0.93
1:B:2052:ARG:HB3	1:E:2045:GLN:HG2	1.52	0.93
1:E:2108:ARG:NH1	1:J:1314:SER:H	1.53	0.92
1:C:3186:PRO:CB	1:I:3061:ASN:ND2	2.32	0.92
1:D:1189:LYS:HG2	1:G:1061:ASN:N	1.84	0.92
1:E:2282:TYR:OH	1:J:1312:ASN:CB	2.18	0.92
1:D:1052:ARG:CG	1:G:1045:GLN:HA	2.00	0.92
1:A:1314:SER:H	1:K:2384:THR:HA	1.34	0.91
1:C:3186:PRO:CG	1:I:3188:SER:N	2.28	0.91
1:B:2189:LYS:CG	1:E:2061:ASN:N	2.34	0.91
1:B:2189:LYS:CG	1:E:2061:ASN:CB	1.87	0.91
1:C:3186:PRO:CG	1:I:3061:ASN:ND2	2.33	0.91
1:D:1191:ARG:NH1	1:G:1040:GLN:OE1	2.04	0.91
1:B:2372:ARG:HD3	1:D:1269:THR:HG21	1.16	0.90
1:A:1363:ASN:CG	1:K:2108:ARG:HH12	1.74	0.90
1:B:2051:ASN:HA	1:E:2046:THR:HB	1.50	0.90
1:B:2372:ARG:CD	1:D:1269:THR:CB	2.49	0.90
1:B:2372:ARG:HD3	1:D:1269:THR:OG1	1.72	0.90
1:A:1363:ASN:ND2	1:K:2108:ARG:HH12	1.70	0.90
1:D:1189:LYS:NZ	1:G:1059:PRO:C	2.22	0.90
1:B:2043:GLU:HG3	1:K:2189:LYS:HD3	1.54	0.89
1:D:1191:ARG:HH11	1:G:1040:GLN:HE22	0.91	0.89
1:E:2191:ARG:HH22	1:K:2040:GLN:HE22	1.19	0.89
1:D:1372:ARG:NH1	1:I:3270:PRO:O	2.06	0.89
1:D:1191:ARG:NH1	1:G:1040:GLN:HE22	1.71	0.89
1:B:2108:ARG:HD3	1:D:1314:SER:CA	2.04	0.88
1:D:1372:ARG:NH1	1:I:3272:VAL:CG2	2.37	0.88
1:B:2189:LYS:HD3	1:E:2060:ALA:C	1.94	0.88
1:D:1189:LYS:CD	1:G:1061:ASN:H	1.79	0.88
1:A:1270:PRO:HD2	1:K:2264:ALA:N	1.88	0.87
1:B:2372:ARG:CZ	1:D:1269:THR:CG2	2.51	0.87
1:B:2264:ALA:HB2	1:D:1272:VAL:HG11	1.15	0.87
1:B:2052:ARG:CD	1:E:2045:GLN:CG	2.53	0.86
1:A:1305:TYR:HE2	1:K:2108:ARG:HH11	1.23	0.86
1:D:1266:ALA:CB	1:I:3267:GLY:HA2	2.05	0.86
1:C:3186:PRO:HB3	1:I:3061:ASN:ND2	1.90	0.86
1:D:1187:GLN:CB	1:G:1187:GLN:N	2.38	0.86
1:E:2108:ARG:NH1	1:J:1314:SER:HB2	1.82	0.86
1:B:2269:THR:HG21	1:I:3372:ARG:CG	2.06	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2052:ARG:CB	1:E:2045:GLN:HG2	2.04	0.86
1:C:3186:PRO:HG3	1:I:3188:SER:C	1.94	0.86
1:D:1266:ALA:CB	1:I:3267:GLY:CA	2.51	0.85
1:B:2369:GLN:NE2	1:I:3369:GLN:CG	2.37	0.85
1:A:1271:ASN:HB3	1:K:2111:GLU:CD	1.96	0.85
1:D:1052:ARG:HB2	1:G:1045:GLN:CA	2.04	0.85
1:B:2369:GLN:OE1	1:I:3369:GLN:CG	2.24	0.85
1:A:1272:VAL:CA	1:K:2261:GLU:OE2	2.17	0.85
1:D:1369:GLN:NE2	1:I:3369:GLN:OE1	2.10	0.85
1:B:2041:GLN:O	1:K:2106:ASN:HB2	1.78	0.84
1:B:2369:GLN:OE1	1:I:3369:GLN:OE1	1.94	0.84
1:A:1363:ASN:HD21	1:K:2108:ARG:NH2	1.70	0.84
1:B:2052:ARG:HD3	1:E:2045:GLN:HE21	1.21	0.83
1:B:2369:GLN:NE2	1:I:3369:GLN:CD	2.23	0.83
1:D:1098:ARG:NH1	1:I:3318:LYS:HZ1	1.76	0.83
1:D:1261:GLU:OE1	1:I:3313:PHE:CB	2.27	0.83
1:E:2108:ARG:CZ	1:J:1314:SER:H	1.91	0.82
1:D:1374:LEU:HD22	1:I:3272:VAL:HG22	1.61	0.82
1:B:2189:LYS:CD	1:E:2061:ASN:N	1.94	0.82
1:D:1098:ARG:NH2	1:I:3318:LYS:HZ2	1.76	0.82
1:B:2267:GLY:CA	1:I:3266:ALA:CB	2.55	0.82
1:B:2106:ASN:HB3	1:E:2238:ASP:OD1	1.80	0.81
1:D:1189:LYS:HZ3	1:G:1059:PRO:C	1.81	0.81
1:D:1098:ARG:CZ	1:I:3318:LYS:NZ	2.44	0.81
1:B:2185:VAL:O	1:E:2186:PRO:HG3	1.79	0.81
1:E:2191:ARG:HH22	1:K:2040:GLN:NE2	1.78	0.80
1:E:2188:SER:C	1:K:2186:PRO:CG	2.42	0.80
1:B:2106:ASN:OD1	1:E:2236:TYR:HE1	1.65	0.80
1:D:1191:ARG:NH1	1:G:1040:GLN:NE2	2.26	0.80
1:D:1052:ARG:CD	1:G:1045:GLN:CB	2.53	0.80
1:E:2061:ASN:OD1	1:K:2186:PRO:CB	2.29	0.80
1:D:1193:LYS:CE	1:G:1040:GLN:HE21	1.95	0.79
1:A:1305:TYR:HE2	1:K:2108:ARG:NH1	1.79	0.79
1:D:1266:ALA:HB3	1:I:3267:GLY:O	1.82	0.79
1:D:1266:ALA:CB	1:I:3267:GLY:O	2.31	0.79
1:D:1080:HIS:CD2	1:D:1083:GLU:H	2.01	0.79
1:D:1098:ARG:NH2	1:I:3318:LYS:NZ	2.31	0.79
1:B:2372:ARG:CZ	1:D:1269:THR:HG22	2.12	0.78
1:J:1080:HIS:CD2	1:J:1083:GLU:H	2.01	0.78
1:B:2372:ARG:HH11	1:D:1269:THR:HB	1.46	0.78
1:D:1266:ALA:CB	1:I:3267:GLY:C	2.51	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2185:VAL:C	1:E:2186:PRO:HG2	2.04	0.78
1:D:1372:ARG:CB	1:I:3269:THR:CG2	2.51	0.78
1:D:1261:GLU:CD	1:I:3313:PHE:CB	2.52	0.78
1:G:1080:HIS:CD2	1:G:1083:GLU:H	2.01	0.78
1:D:1051:ASN:CG	1:G:1047:PHE:HA	2.04	0.78
1:B:2189:LYS:HE3	1:B:2190:GLN:O	1.84	0.77
1:H:2189:LYS:HE3	1:H:2190:GLN:O	1.84	0.77
1:A:1080:HIS:CD2	1:A:1083:GLU:H	2.01	0.77
1:B:2051:ASN:CG	1:E:2046:THR:O	2.23	0.77
1:D:1106:ASN:ND2	1:D:1191:ARG:HH22	1.83	0.77
1:C:3238:ASP:OD2	1:I:3106:ASN:HB3	1.85	0.77
1:E:2108:ARG:HD3	1:J:1314:SER:HB2	1.65	0.77
1:A:1106:ASN:ND2	1:A:1191:ARG:HH22	1.83	0.77
1:J:1106:ASN:ND2	1:J:1191:ARG:HH22	1.83	0.77
1:G:1106:ASN:ND2	1:G:1191:ARG:HH22	1.83	0.77
1:A:1270:PRO:CD	1:K:2264:ALA:H	1.98	0.76
1:E:2189:LYS:HE3	1:E:2190:GLN:O	1.85	0.76
1:B:2052:ARG:CD	1:E:2045:GLN:CD	2.43	0.76
1:D:1108:ARG:CZ	1:I:3313:PHE:O	2.26	0.76
1:A:1308:GLN:HE22	1:A:1345:ASN:HD21	1.34	0.76
1:C:3186:PRO:HG2	1:I:3061:ASN:ND2	1.99	0.76
1:B:2369:GLN:NE2	1:I:3369:GLN:HG2	1.98	0.76
1:D:1374:LEU:HD22	1:I:3272:VAL:CG2	2.13	0.76
1:G:1308:GLN:HE22	1:G:1345:ASN:HD21	1.34	0.76
1:K:2189:LYS:HE3	1:K:2190:GLN:O	1.84	0.75
1:J:1308:GLN:HE22	1:J:1345:ASN:HD21	1.34	0.75
1:C:3186:PRO:CG	1:I:3061:ASN:HD22	1.95	0.75
1:A:1271:ASN:O	1:K:2111:GLU:OE1	2.04	0.75
1:D:1193:LYS:CE	1:G:1040:GLN:NE2	2.49	0.74
1:D:1054:VAL:HG11	1:G:1041:GLN:HE21	1.52	0.74
1:B:2108:ARG:CG	1:D:1314:SER:HB2	2.13	0.74
1:A:1271:ASN:CB	1:K:2111:GLU:OE2	2.35	0.74
1:B:2106:ASN:OD1	1:E:2236:TYR:CE1	2.40	0.74
1:A:1305:TYR:OH	1:K:2108:ARG:CZ	2.35	0.74
1:B:2051:ASN:HA	1:E:2046:THR:O	1.85	0.74
1:E:2189:LYS:HG2	1:K:2061:ASN:HB2	1.68	0.74
1:C:3186:PRO:HG3	1:I:3188:SER:N	2.00	0.74
1:A:1271:ASN:HB3	1:K:2111:GLU:OE2	1.86	0.74
1:D:1280:ASN:HD22	1:D:1355:TYR:N	1.86	0.74
1:E:2188:SER:O	1:K:2186:PRO:HG3	1.86	0.73
1:D:1051:ASN:HA	1:G:1046:THR:CG2	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1051:ASN:OD1	1:G:1047:PHE:HA	1.89	0.73
1:A:1280:ASN:HD22	1:A:1355:TYR:N	1.87	0.73
1:J:1280:ASN:HD22	1:J:1355:TYR:N	1.86	0.73
1:A:1314:SER:N	1:K:2384:THR:HA	2.04	0.73
1:G:1280:ASN:HD22	1:G:1355:TYR:N	1.86	0.73
1:B:2269:THR:HB	1:I:3372:ARG:CD	2.19	0.72
1:A:1272:VAL:HG22	1:K:2261:GLU:HB3	1.70	0.72
1:A:1369:GLN:HE22	1:K:2266:ALA:HB1	1.37	0.72
1:D:1052:ARG:NH2	1:G:1044:THR:N	2.37	0.72
1:E:2191:ARG:NH2	1:K:2040:GLN:NE2	2.29	0.72
1:I:3029:GLN:O	1:I:3033:GLN:HG3	1.90	0.72
1:D:1191:ARG:NH1	1:G:1040:GLN:CD	2.43	0.72
1:B:2106:ASN:CG	1:E:2062:VAL:CG1	2.52	0.71
1:D:1308:GLN:HE22	1:D:1345:ASN:HD21	1.34	0.71
1:B:2187:GLN:CB	1:E:2185:VAL:HG23	2.20	0.71
1:E:2108:ARG:CZ	1:J:1314:SER:N	2.51	0.71
1:C:3186:PRO:HG2	1:I:3185:VAL:O	1.90	0.71
1:A:1280:ASN:O	1:A:1281:LEU:HB3	1.91	0.71
1:K:2080:HIS:CD2	1:K:2083:GLU:H	2.09	0.71
1:K:2322:LYS:HD3	1:L:3163:THR:HG21	1.73	0.70
1:C:3186:PRO:HD3	1:I:3188:SER:H	1.00	0.70
1:H:2322:LYS:HD3	1:I:3163:THR:HG21	1.73	0.70
1:B:2080:HIS:CD2	1:B:2083:GLU:H	2.09	0.70
1:L:3029:GLN:O	1:L:3033:GLN:HG3	1.90	0.70
1:B:2269:THR:HB	1:I:3372:ARG:NE	2.03	0.70
1:D:1052:ARG:CD	1:G:1045:GLN:CA	2.70	0.70
1:B:2106:ASN:OD1	1:E:2062:VAL:CG1	2.36	0.70
1:C:3045:GLN:HG3	1:I:3052:ARG:HB2	1.74	0.70
1:J:1280:ASN:O	1:J:1281:LEU:HB3	1.91	0.70
1:E:2322:LYS:HD3	1:F:3163:THR:HG21	1.73	0.70
1:C:3029:GLN:O	1:C:3033:GLN:HG3	1.90	0.70
1:E:2080:HIS:CD2	1:E:2083:GLU:H	2.09	0.70
1:F:3029:GLN:O	1:F:3033:GLN:HG3	1.90	0.70
1:B:2187:GLN:CB	1:E:2184:ASN:OD1	2.40	0.70
1:I:3098:ARG:NH2	1:I:3111:GLU:OE2	2.25	0.70
1:D:1052:ARG:NH1	1:G:1043:GLU:CD	2.35	0.70
1:H:2080:HIS:CD2	1:H:2083:GLU:H	2.09	0.70
1:C:3080:HIS:CD2	1:C:3083:GLU:H	2.10	0.70
1:D:1054:VAL:HG11	1:G:1041:GLN:NE2	2.07	0.69
1:D:1280:ASN:O	1:D:1281:LEU:HB3	1.91	0.69
1:B:2369:GLN:CD	1:I:3369:GLN:CG	2.60	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1280:ASN:O	1:G:1281:LEU:HB3	1.91	0.69
1:L:3098:ARG:NH2	1:L:3111:GLU:OE2	2.25	0.69
1:D:1310:THR:HG22	1:D:1358:VAL:HG22	1.75	0.69
1:F:3080:HIS:CD2	1:F:3083:GLU:H	2.10	0.69
1:L:3080:HIS:CD2	1:L:3083:GLU:H	2.11	0.69
1:A:1305:TYR:CZ	1:K:2108:ARG:NH1	2.59	0.69
1:D:1191:ARG:HD3	1:G:1060:ALA:CB	2.22	0.69
1:D:1080:HIS:HD2	1:D:1083:GLU:H	1.39	0.69
1:G:1310:THR:HG22	1:G:1358:VAL:HG22	1.75	0.69
1:B:2322:LYS:HD3	1:C:3163:THR:HG21	1.73	0.69
1:F:3098:ARG:NH2	1:F:3111:GLU:OE2	2.25	0.69
1:B:2269:THR:HB	1:I:3372:ARG:HD3	1.74	0.69
1:C:3098:ARG:NH2	1:C:3111:GLU:OE2	2.25	0.68
1:A:1310:THR:HG22	1:A:1358:VAL:HG22	1.75	0.68
1:D:1189:LYS:CD	1:G:1061:ASN:N	2.55	0.68
1:A:1080:HIS:HD2	1:A:1082:THR:H	1.41	0.68
1:I:3080:HIS:CD2	1:I:3083:GLU:H	2.10	0.68
1:E:2061:ASN:OD1	1:K:2186:PRO:HB3	1.92	0.68
1:B:2108:ARG:CD	1:D:1314:SER:CB	2.06	0.68
1:B:2051:ASN:CA	1:E:2046:THR:HB	2.22	0.68
1:B:2189:LYS:HG2	1:E:2061:ASN:CG	2.06	0.67
1:J:1080:HIS:HD2	1:J:1082:THR:H	1.41	0.67
1:D:1052:ARG:NH1	1:G:1043:GLU:OE2	2.24	0.67
1:J:1106:ASN:HD22	1:J:1191:ARG:HH22	1.42	0.67
1:B:2369:GLN:OE1	1:I:3369:GLN:HG3	1.93	0.67
1:D:1098:ARG:NH1	1:I:3305:TYR:CE2	2.63	0.67
1:J:1310:THR:HG22	1:J:1358:VAL:HG22	1.74	0.67
1:A:1318:LYS:NZ	1:K:2108:ARG:HB2	2.10	0.67
1:B:2318:LYS:HZ2	1:I:3098:ARG:NH2	1.92	0.67
1:D:1280:ASN:HD22	1:D:1355:TYR:H	1.43	0.67
1:J:1080:HIS:HD2	1:J:1083:GLU:H	1.39	0.67
1:D:1080:HIS:HD2	1:D:1082:THR:H	1.42	0.67
1:H:2308:GLN:HE22	1:H:2345:ASN:HD21	1.43	0.67
1:E:2108:ARG:HH12	1:J:1314:SER:N	1.67	0.66
1:A:1271:ASN:CG	1:K:2098:ARG:HH11	1.94	0.66
1:E:2308:GLN:HE22	1:E:2345:ASN:HD21	1.43	0.66
1:G:1106:ASN:HD22	1:G:1191:ARG:HH22	1.42	0.66
1:F:3080:HIS:HD2	1:F:3083:GLU:H	1.43	0.66
1:B:2272:VAL:CG1	1:I:3264:ALA:HB3	2.25	0.66
1:D:1111:GLU:OE1	1:I:3313:PHE:O	2.14	0.66
1:G:1080:HIS:HD2	1:G:1082:THR:H	1.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1280:ASN:HD22	1:G:1355:TYR:H	1.43	0.66
1:C:3061:ASN:HB2	1:I:3189:LYS:HG2	1.77	0.66
1:L:3308:GLN:HE22	1:L:3345:ASN:HD21	1.44	0.66
1:G:1080:HIS:HD2	1:G:1083:GLU:H	1.39	0.66
1:C:3238:ASP:OD2	1:I:3106:ASN:ND2	2.26	0.66
1:A:1106:ASN:HD22	1:A:1191:ARG:HH22	1.42	0.66
1:I:3080:HIS:HD2	1:I:3083:GLU:H	1.43	0.65
1:B:2187:GLN:CB	1:E:2184:ASN:CG	2.65	0.65
1:D:1106:ASN:HD22	1:D:1191:ARG:HH22	1.42	0.65
1:C:3080:HIS:HD2	1:C:3083:GLU:H	1.43	0.65
1:B:2308:GLN:HE22	1:B:2345:ASN:HD21	1.43	0.65
1:L:3080:HIS:HD2	1:L:3083:GLU:H	1.43	0.65
1:H:2184:ASN:O	1:H:2186:PRO:HD3	1.97	0.65
1:A:1080:HIS:HD2	1:A:1083:GLU:H	1.39	0.65
1:B:2372:ARG:CZ	1:D:1272:VAL:CG2	2.74	0.65
1:B:2051:ASN:HA	1:E:2046:THR:CB	2.25	0.65
1:J:1280:ASN:HD22	1:J:1355:TYR:H	1.43	0.65
1:K:2080:HIS:HD2	1:K:2083:GLU:H	1.44	0.65
1:C:3308:GLN:HE22	1:C:3345:ASN:HD21	1.44	0.65
1:C:3080:HIS:HD2	1:C:3082:THR:H	1.45	0.65
1:B:2184:ASN:O	1:B:2186:PRO:HD3	1.97	0.64
1:L:3080:HIS:HD2	1:L:3082:THR:H	1.45	0.64
1:I:3308:GLN:HE22	1:I:3345:ASN:HD21	1.44	0.64
1:F:3308:GLN:HE22	1:F:3345:ASN:HD21	1.44	0.64
1:E:2080:HIS:HD2	1:E:2083:GLU:H	1.44	0.64
1:E:2024:ASN:HD21	1:E:2253:ASP:H	1.46	0.64
1:B:2189:LYS:HG3	1:E:2061:ASN:CA	2.27	0.64
1:B:2080:HIS:HD2	1:B:2083:GLU:H	1.44	0.64
1:B:2185:VAL:O	1:E:2186:PRO:CD	2.46	0.64
1:D:1193:LYS:HE3	1:G:1040:GLN:NE2	2.13	0.64
1:B:2024:ASN:HD21	1:B:2253:ASP:H	1.46	0.64
1:B:2269:THR:CG2	1:I:3372:ARG:HD2	1.94	0.64
1:A:1280:ASN:HD22	1:A:1355:TYR:H	1.43	0.64
1:H:2080:HIS:HD2	1:H:2083:GLU:H	1.44	0.64
1:F:3080:HIS:HD2	1:F:3082:THR:H	1.45	0.63
1:I:3080:HIS:HD2	1:I:3082:THR:H	1.45	0.63
1:K:2308:GLN:HE22	1:K:2345:ASN:HD21	1.43	0.63
1:D:1191:ARG:HH11	1:G:1040:GLN:CD	2.00	0.63
1:B:2187:GLN:CB	1:E:2185:VAL:HG22	2.26	0.63
1:H:2024:ASN:HD21	1:H:2253:ASP:H	1.46	0.63
1:A:1269:THR:HG23	1:K:2265:GLN:HE22	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2372:ARG:CZ	1:D:1272:VAL:HG21	2.29	0.63
1:A:1369:GLN:HE22	1:K:2267:GLY:N	1.97	0.63
1:C:3186:PRO:HG2	1:I:3061:ASN:HD22	1.60	0.63
1:K:2024:ASN:HD21	1:K:2253:ASP:H	1.46	0.63
1:A:1363:ASN:HD22	1:K:2108:ARG:HH22	0.65	0.62
1:A:1106:ASN:HD22	1:A:1191:ARG:NH2	1.98	0.62
1:J:1308:GLN:HE22	1:J:1345:ASN:ND2	1.97	0.62
1:A:1271:ASN:CB	1:K:2098:ARG:NH1	2.62	0.62
1:B:2061:ASN:OD1	1:E:2186:PRO:HG3	1.98	0.62
1:D:1106:ASN:HD22	1:D:1191:ARG:NH2	1.98	0.62
1:A:1308:GLN:HE22	1:A:1345:ASN:ND2	1.98	0.62
1:B:2106:ASN:HB3	1:E:2238:ASP:CG	2.20	0.61
1:J:1106:ASN:HD22	1:J:1191:ARG:NH2	1.98	0.61
1:D:1052:ARG:HB2	1:G:1045:GLN:HG3	1.82	0.61
1:B:2189:LYS:CD	1:E:2061:ASN:HB2	2.17	0.61
1:D:1050:ALA:O	1:G:1046:THR:HG21	2.01	0.61
1:G:1308:GLN:HE22	1:G:1345:ASN:ND2	1.97	0.61
1:G:1185:VAL:CB	1:G:1186:PRO:CD	2.79	0.61
1:H:2255:SER:HA	1:H:2383:ARG:HD2	1.83	0.61
1:E:2255:SER:HA	1:E:2383:ARG:HD2	1.83	0.61
1:B:2052:ARG:HB3	1:E:2045:GLN:CA	2.26	0.61
1:A:1185:VAL:CB	1:A:1186:PRO:CD	2.79	0.61
1:G:1025:LEU:O	1:G:1029:GLN:HG3	2.01	0.60
1:D:1187:GLN:CB	1:G:1186:PRO:N	2.63	0.60
1:G:1106:ASN:HD22	1:G:1191:ARG:NH2	1.98	0.60
1:E:2189:LYS:CD	1:K:2061:ASN:HB2	2.31	0.60
1:H:2080:HIS:HD2	1:H:2082:THR:H	1.49	0.60
1:B:2255:SER:HA	1:B:2383:ARG:HD2	1.83	0.60
1:D:1185:VAL:CB	1:D:1186:PRO:CD	2.79	0.60
1:K:2080:HIS:HD2	1:K:2082:THR:H	1.49	0.60
1:J:1025:LEU:O	1:J:1029:GLN:HG3	2.01	0.60
1:J:1185:VAL:CB	1:J:1186:PRO:CD	2.79	0.60
1:B:2372:ARG:NH1	1:D:1269:THR:HB	2.15	0.60
1:B:2272:VAL:HG11	1:I:3264:ALA:HB2	0.67	0.60
1:B:2059:PRO:HG2	1:B:2190:GLN:HB2	1.84	0.60
1:D:1266:ALA:HB3	1:I:3267:GLY:HA3	1.73	0.60
1:B:2318:LYS:HZ2	1:I:3098:ARG:HH22	1.50	0.60
1:D:1308:GLN:HE22	1:D:1345:ASN:ND2	1.98	0.60
1:B:2052:ARG:CZ	1:E:2045:GLN:NE2	2.64	0.59
1:K:2255:SER:HA	1:K:2383:ARG:HD2	1.83	0.59
1:D:1188:SER:HB2	1:G:1184:ASN:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1052:ARG:NH2	1:G:1044:THR:H	2.00	0.59
1:E:2080:HIS:HD2	1:E:2082:THR:H	1.49	0.59
1:A:1025:LEU:O	1:A:1029:GLN:HG3	2.01	0.59
1:A:1271:ASN:ND2	1:K:2098:ARG:HH12	1.96	0.59
1:D:1372:ARG:NH2	1:I:3270:PRO:O	2.35	0.59
1:B:2052:ARG:CG	1:E:2045:GLN:HG2	2.31	0.59
1:D:1025:LEU:O	1:D:1029:GLN:HG3	2.01	0.59
1:A:1271:ASN:HD21	1:K:2098:ARG:CZ	2.09	0.59
1:B:2189:LYS:HG3	1:E:2061:ASN:CB	2.20	0.59
1:E:2059:PRO:HG2	1:E:2190:GLN:HB2	1.84	0.59
1:B:2106:ASN:CB	1:E:2238:ASP:OD1	2.51	0.59
1:A:1080:HIS:CD2	1:A:1082:THR:H	2.21	0.59
1:B:2052:ARG:NE	1:E:2045:GLN:HE21	1.85	0.58
1:E:2189:LYS:HG2	1:K:2061:ASN:CB	2.34	0.58
1:B:2058:THR:HG21	1:K:2186:PRO:C	2.16	0.58
1:K:2025:LEU:O	1:K:2029:GLN:HG3	2.04	0.58
1:B:2080:HIS:HD2	1:B:2082:THR:H	1.49	0.58
1:C:3186:PRO:CG	1:I:3061:ASN:HD21	2.14	0.58
1:K:2059:PRO:HG2	1:K:2190:GLN:HB2	1.84	0.58
1:E:2025:LEU:O	1:E:2029:GLN:HG3	2.04	0.58
1:B:2372:ARG:NH1	1:D:1272:VAL:CB	2.65	0.58
1:D:1189:LYS:HG2	1:G:1061:ASN:CA	2.34	0.58
1:H:2059:PRO:HG2	1:H:2190:GLN:HB2	1.84	0.58
1:L:3103:ASP:HB2	1:L:3104:PRO:CD	2.34	0.58
1:A:1273:ASP:OD2	1:K:2108:ARG:NH2	2.37	0.58
1:D:1266:ALA:HB2	1:I:3267:GLY:O	2.03	0.58
1:C:3103:ASP:HB2	1:C:3104:PRO:CD	2.34	0.57
1:D:1191:ARG:HD3	1:G:1060:ALA:HB2	1.85	0.57
1:C:3279:ALA:O	1:C:3280:ASN:O	2.22	0.57
1:B:2189:LYS:HD3	1:E:2061:ASN:H	0.63	0.57
1:D:1187:GLN:CB	1:G:1185:VAL:O	2.52	0.57
1:B:2050:ALA:O	1:E:2046:THR:HB	2.04	0.57
1:F:3279:ALA:O	1:F:3280:ASN:O	2.22	0.57
1:D:1193:LYS:NZ	1:G:1040:GLN:HE21	2.02	0.57
1:F:3103:ASP:HB2	1:F:3104:PRO:CD	2.34	0.57
1:D:1052:ARG:HH21	1:G:1044:THR:H	1.52	0.57
1:B:2056:ASP:OD1	1:E:2042:VAL:C	2.40	0.57
1:A:1314:SER:H	1:K:2384:THR:CA	2.10	0.57
1:D:1052:ARG:CD	1:G:1045:GLN:HA	2.34	0.57
1:D:1372:ARG:HH12	1:I:3272:VAL:HG23	1.62	0.57
1:B:2052:ARG:HB3	1:E:2045:GLN:CG	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1080:HIS:CD2	1:D:1082:THR:H	2.21	0.57
1:I:3279:ALA:O	1:I:3280:ASN:O	2.22	0.57
1:H:2025:LEU:O	1:H:2029:GLN:HG3	2.04	0.57
1:B:2025:LEU:O	1:B:2029:GLN:HG3	2.04	0.57
1:D:1189:LYS:HG2	1:G:1061:ASN:HB2	1.86	0.57
1:I:3103:ASP:HB2	1:I:3104:PRO:CD	2.34	0.57
1:D:1372:ARG:CZ	1:I:3270:PRO:O	2.52	0.57
1:L:3279:ALA:O	1:L:3280:ASN:O	2.22	0.57
1:B:2189:LYS:HD3	1:E:2060:ALA:CA	2.34	0.56
1:A:1271:ASN:OD1	1:K:2111:GLU:OE2	2.23	0.56
1:A:1314:SER:HA	1:K:2383:ARG:O	2.04	0.56
1:L:3308:GLN:HE22	1:L:3345:ASN:ND2	2.03	0.56
1:B:2189:LYS:HG3	1:E:2061:ASN:O	2.05	0.56
1:J:1080:HIS:CD2	1:J:1082:THR:H	2.21	0.56
1:F:3308:GLN:HE22	1:F:3345:ASN:ND2	2.03	0.56
1:C:3046:THR:N	1:I:3051:ASN:O	2.30	0.56
1:L:3383:ARG:HG2	1:L:3384:THR:N	2.21	0.56
1:F:3383:ARG:HG2	1:F:3384:THR:N	2.21	0.56
1:B:2051:ASN:OD1	1:E:2046:THR:O	2.24	0.56
1:C:3280:ASN:O	1:C:3281:LEU:HB2	2.06	0.56
1:I:3280:ASN:O	1:I:3281:LEU:HB2	2.06	0.56
1:G:1080:HIS:CD2	1:G:1082:THR:H	2.21	0.56
1:A:1318:LYS:HZ1	1:K:2108:ARG:HB2	1.69	0.56
1:I:3308:GLN:HE22	1:I:3345:ASN:ND2	2.03	0.56
1:L:3280:ASN:O	1:L:3281:LEU:HB2	2.06	0.56
1:I:3383:ARG:HG2	1:I:3384:THR:N	2.21	0.55
1:E:2185:VAL:O	1:K:2186:PRO:CG	2.37	0.55
1:D:1372:ARG:NH1	1:I:3269:THR:C	2.60	0.55
1:J:1185:VAL:CB	1:J:1186:PRO:HD2	2.36	0.55
1:F:3280:ASN:O	1:F:3281:LEU:HB2	2.06	0.55
1:L:3352:THR:O	1:L:3353:LEU:HB2	2.06	0.55
1:I:3352:THR:O	1:I:3353:LEU:HB2	2.06	0.55
1:B:2372:ARG:HH11	1:D:1272:VAL:CG2	2.08	0.55
1:D:1098:ARG:NH1	1:I:3318:LYS:NZ	2.52	0.55
1:C:3352:THR:O	1:C:3353:LEU:HB2	2.06	0.55
1:C:3383:ARG:HG2	1:C:3384:THR:N	2.21	0.55
1:F:3080:HIS:CD2	1:F:3082:THR:H	2.25	0.55
1:D:1185:VAL:CB	1:D:1186:PRO:HD2	2.37	0.55
1:L:3352:THR:O	1:L:3353:LEU:CB	2.54	0.55
1:F:3352:THR:O	1:F:3353:LEU:CB	2.54	0.55
1:F:3352:THR:O	1:F:3353:LEU:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:3352:THR:O	1:I:3353:LEU:CB	2.54	0.55
1:D:1372:ARG:CZ	1:I:3272:VAL:HG23	2.34	0.55
1:B:2369:GLN:CG	1:I:3369:GLN:NE2	2.70	0.55
1:C:3308:GLN:HE22	1:C:3345:ASN:ND2	2.03	0.54
1:E:2189:LYS:HG3	1:K:2061:ASN:HB2	1.83	0.54
1:C:3352:THR:O	1:C:3353:LEU:CB	2.54	0.54
1:E:2264:ALA:CB	1:J:1272:VAL:CG1	2.85	0.54
1:A:1270:PRO:HD2	1:K:2263:SER:CA	2.37	0.54
1:B:2266:ALA:HB3	1:D:1267:GLY:CA	2.38	0.54
1:A:1271:ASN:HD22	1:K:2098:ARG:NH1	1.94	0.54
1:C:3080:HIS:CD2	1:C:3082:THR:H	2.25	0.54
1:A:1369:GLN:HE22	1:K:2266:ALA:C	2.11	0.54
1:A:1271:ASN:O	1:K:2261:GLU:OE2	2.25	0.54
1:L:3080:HIS:CD2	1:L:3082:THR:H	2.25	0.54
1:D:1191:ARG:HD2	1:G:1040:GLN:HE22	1.72	0.54
1:B:2189:LYS:HG3	1:E:2061:ASN:C	2.28	0.54
1:E:2189:LYS:HD3	1:K:2061:ASN:HB2	1.90	0.54
1:I:3025:LEU:O	1:I:3029:GLN:HG3	2.08	0.54
1:L:3025:LEU:O	1:L:3029:GLN:HG3	2.08	0.54
1:A:1185:VAL:CB	1:A:1186:PRO:HD2	2.37	0.54
1:B:2106:ASN:HB3	1:E:2238:ASP:OD2	2.08	0.54
1:F:3025:LEU:O	1:F:3029:GLN:HG3	2.08	0.54
1:I:3080:HIS:CD2	1:I:3082:THR:H	2.25	0.54
1:A:1015:ALA:C	1:A:1017:ARG:H	2.12	0.54
1:G:1185:VAL:CB	1:G:1186:PRO:HD2	2.36	0.53
1:H:2080:HIS:CD2	1:H:2082:THR:H	2.27	0.53
1:L:3244:GLN:O	1:L:3245:ASN:CB	2.56	0.53
1:C:3244:GLN:O	1:C:3245:ASN:CB	2.56	0.53
1:D:1098:ARG:NH1	1:I:3305:TYR:CZ	2.77	0.53
1:K:2080:HIS:CD2	1:K:2082:THR:H	2.27	0.53
1:K:2120:VAL:HG21	1:K:2260:LEU:HD13	1.91	0.53
1:B:2106:ASN:HB2	1:E:2062:VAL:HG13	1.91	0.53
1:H:2120:VAL:HG21	1:H:2260:LEU:HD13	1.91	0.53
1:D:1052:ARG:CG	1:G:1045:GLN:CA	2.79	0.53
1:D:1052:ARG:HH21	1:G:1044:THR:N	2.05	0.53
1:F:3244:GLN:O	1:F:3245:ASN:CB	2.56	0.53
1:D:1015:ALA:C	1:D:1017:ARG:H	2.12	0.53
1:A:1270:PRO:HD2	1:K:2263:SER:HA	1.91	0.53
1:E:2120:VAL:HG21	1:E:2260:LEU:HD13	1.91	0.53
1:B:2269:THR:HG21	1:I:3372:ARG:CB	2.37	0.53
1:G:1015:ALA:C	1:G:1017:ARG:H	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2108:ARG:CD	1:J:1314:SER:HB2	2.39	0.52
1:I:3244:GLN:O	1:I:3245:ASN:CB	2.56	0.52
1:B:2305:TYR:CZ	1:I:3098:ARG:NH1	2.77	0.52
1:D:1052:ARG:NH2	1:G:1043:GLU:C	2.59	0.52
1:G:1305:TYR:CZ	1:G:1318:LYS:HE3	2.45	0.52
1:A:1305:TYR:CZ	1:A:1318:LYS:HE3	2.45	0.52
1:D:1372:ARG:HH12	1:I:3270:PRO:C	2.09	0.52
1:B:2041:GLN:O	1:K:2106:ASN:CB	2.53	0.52
1:J:1305:TYR:CZ	1:J:1318:LYS:HE3	2.45	0.52
1:C:3025:LEU:O	1:C:3029:GLN:HG3	2.08	0.52
1:E:2080:HIS:CD2	1:E:2082:THR:H	2.27	0.52
1:H:2308:GLN:HE22	1:H:2345:ASN:ND2	2.08	0.52
1:K:2308:GLN:HE22	1:K:2345:ASN:ND2	2.08	0.52
1:J:1307:SER:OG	1:J:1315:ASP:HB3	2.10	0.52
1:E:2280:ASN:O	1:E:2281:LEU:HB2	2.10	0.52
1:E:2184:ASN:O	1:E:2186:PRO:HD3	1.97	0.52
1:H:2280:ASN:O	1:H:2281:LEU:HB2	2.10	0.52
1:B:2080:HIS:CD2	1:B:2082:THR:H	2.27	0.51
1:A:1363:ASN:CG	1:K:2108:ARG:NH1	2.50	0.51
1:B:2120:VAL:HG21	1:B:2260:LEU:HD13	1.91	0.51
1:C:3186:PRO:HG3	1:I:3188:SER:O	2.08	0.51
1:D:1305:TYR:CZ	1:D:1318:LYS:HE3	2.45	0.51
1:D:1188:SER:N	1:G:1184:ASN:O	2.43	0.51
1:G:1307:SER:OG	1:G:1315:ASP:HB3	2.10	0.51
1:K:2280:ASN:O	1:K:2281:LEU:HB2	2.10	0.51
1:J:1015:ALA:C	1:J:1017:ARG:H	2.12	0.51
1:B:2372:ARG:NH1	1:D:1269:THR:CG2	2.74	0.51
1:B:2372:ARG:HH12	1:D:1272:VAL:CG2	1.81	0.51
1:A:1310:THR:O	1:K:2385:GLU:N	2.44	0.51
1:D:1307:SER:OG	1:D:1315:ASP:HB3	2.10	0.51
1:A:1271:ASN:CG	1:K:2111:GLU:OE2	2.50	0.50
1:B:2308:GLN:HE22	1:B:2345:ASN:ND2	2.08	0.50
1:B:2280:ASN:O	1:B:2281:LEU:HB2	2.10	0.50
1:B:2189:LYS:CD	1:E:2061:ASN:CB	2.79	0.50
1:D:1255:SER:HA	1:D:1383:ARG:HD2	1.94	0.50
1:B:2106:ASN:HB2	1:E:2062:VAL:CG1	2.42	0.50
1:A:1307:SER:OG	1:A:1315:ASP:HB3	2.11	0.50
1:J:1049:PRO:HG3	1:J:1228:ILE:HD12	1.93	0.50
1:B:2189:LYS:HD3	1:E:2060:ALA:HA	1.93	0.50
1:I:3108:ARG:HD2	1:I:3111:GLU:OE1	2.12	0.50
1:D:1308:GLN:NE2	1:D:1345:ASN:HD21	2.07	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1280:ASN:ND2	1:J:1355:TYR:HB2	2.27	0.50
1:G:1280:ASN:ND2	1:G:1355:TYR:HB2	2.27	0.50
1:D:1049:PRO:HG3	1:D:1228:ILE:HD12	1.93	0.50
1:A:1049:PRO:HG3	1:A:1228:ILE:HD12	1.93	0.50
1:G:1255:SER:HA	1:G:1383:ARG:HD2	1.94	0.49
1:A:1269:THR:CG2	1:K:2265:GLN:HE22	2.25	0.49
1:J:1308:GLN:NE2	1:J:1345:ASN:HD21	2.07	0.49
1:A:1280:ASN:ND2	1:A:1355:TYR:HB2	2.27	0.49
1:K:2322:LYS:CD	1:L:3163:THR:HG21	2.42	0.49
1:F:3108:ARG:HD2	1:F:3111:GLU:OE1	2.12	0.49
1:D:1189:LYS:HB3	1:G:1061:ASN:HB2	1.95	0.49
1:L:3108:ARG:HD2	1:L:3111:GLU:OE1	2.12	0.49
1:A:1255:SER:HA	1:A:1383:ARG:HD2	1.94	0.49
1:A:1318:LYS:NZ	1:K:2108:ARG:H	2.09	0.49
1:J:1255:SER:HA	1:J:1383:ARG:HD2	1.94	0.49
1:E:2188:SER:O	1:K:2186:PRO:CG	2.56	0.49
1:D:1280:ASN:ND2	1:D:1355:TYR:HB2	2.27	0.49
1:E:2322:LYS:CD	1:F:3163:THR:HG21	2.42	0.49
1:E:2264:ALA:CB	1:J:1272:VAL:HG13	2.43	0.49
1:G:1049:PRO:HG3	1:G:1228:ILE:HD12	1.93	0.49
1:E:2015:LEU:O	1:E:2019:GLN:HG3	2.13	0.49
1:D:1193:LYS:HE2	1:G:1040:GLN:NE2	2.26	0.49
1:A:1103:ASP:HB2	1:A:1104:PRO:CD	2.43	0.49
1:C:3108:ARG:HD2	1:C:3111:GLU:OE1	2.12	0.49
1:E:2308:GLN:HE22	1:E:2345:ASN:ND2	2.08	0.49
1:G:1103:ASP:HB2	1:G:1104:PRO:CD	2.43	0.49
1:K:2015:LEU:O	1:K:2019:GLN:HG3	2.13	0.49
1:B:2272:VAL:HG12	1:I:3264:ALA:HB3	1.94	0.48
1:D:1050:ALA:O	1:G:1046:THR:CG2	2.61	0.48
1:D:1372:ARG:NH1	1:I:3269:THR:O	2.46	0.48
1:J:1103:ASP:HB2	1:J:1104:PRO:CD	2.43	0.48
1:B:2040:GLN:NE2	1:K:2105:ASP:HA	2.28	0.48
1:B:2269:THR:OG1	1:I:3372:ARG:CD	2.54	0.48
1:D:1052:ARG:HG3	1:G:1045:GLN:HA	1.92	0.48
1:B:2015:LEU:O	1:B:2019:GLN:HG3	2.13	0.48
1:J:1120:VAL:HG21	1:J:1260:LEU:HD13	1.96	0.48
1:H:2103:ASP:HB2	1:H:2104:PRO:CD	2.44	0.48
1:B:2372:ARG:CD	1:D:1269:THR:HB	2.39	0.48
1:B:2051:ASN:HA	1:E:2046:THR:C	2.33	0.48
1:D:1051:ASN:OD1	1:G:1047:PHE:CA	2.60	0.48
1:D:1052:ARG:CZ	1:G:1044:THR:N	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2103:ASP:HB2	1:E:2104:PRO:CD	2.44	0.48
1:D:1103:ASP:HB2	1:D:1104:PRO:CD	2.43	0.48
1:A:1318:LYS:HZ1	1:K:2108:ARG:CB	2.27	0.48
1:H:2015:LEU:O	1:H:2019:GLN:HG3	2.13	0.48
1:B:2106:ASN:CB	1:E:2238:ASP:OD2	2.62	0.48
1:J:1102:TYR:CE2	1:J:1108:ARG:HG3	2.49	0.48
1:C:3308:GLN:NE2	1:C:3345:ASN:HD21	2.11	0.48
1:A:1102:TYR:CE2	1:A:1108:ARG:HG3	2.49	0.47
1:A:1120:VAL:HG21	1:A:1260:LEU:HD13	1.96	0.47
1:K:2103:ASP:HB2	1:K:2104:PRO:CD	2.44	0.47
1:B:2103:ASP:HB2	1:B:2104:PRO:CD	2.44	0.47
1:E:2191:ARG:CZ	1:K:2040:GLN:HE22	2.21	0.47
1:L:3281:LEU:HD12	1:L:3281:LEU:N	2.29	0.47
1:B:2106:ASN:CB	1:E:2062:VAL:CG1	2.93	0.47
1:C:3061:ASN:HB2	1:I:3189:LYS:CG	2.42	0.47
1:E:2061:ASN:OD1	1:K:2186:PRO:HB2	2.13	0.47
1:C:3281:LEU:HD12	1:C:3281:LEU:N	2.29	0.47
1:D:1120:VAL:HG21	1:D:1260:LEU:HD13	1.96	0.47
1:G:1102:TYR:CE2	1:G:1108:ARG:HG3	2.49	0.47
1:F:3281:LEU:N	1:F:3281:LEU:HD12	2.30	0.47
1:D:1102:TYR:CE2	1:D:1108:ARG:HG3	2.49	0.47
1:B:2312:ASN:O	1:I:3108:ARG:HB3	2.15	0.47
1:C:3238:ASP:OD2	1:I:3106:ASN:CB	2.61	0.47
1:A:1308:GLN:NE2	1:A:1345:ASN:HD21	2.07	0.47
1:F:3308:GLN:NE2	1:F:3345:ASN:HD21	2.11	0.47
1:I:3308:GLN:NE2	1:I:3345:ASN:HD21	2.11	0.47
1:G:1352:THR:O	1:G:1353:LEU:CB	2.62	0.47
1:J:1352:THR:O	1:J:1353:LEU:CB	2.63	0.47
1:D:1352:THR:O	1:D:1353:LEU:CB	2.63	0.47
1:D:1098:ARG:HH12	1:I:3318:LYS:HE3	1.80	0.47
1:G:1120:VAL:HG21	1:G:1260:LEU:HD13	1.96	0.47
1:A:1269:THR:HG23	1:K:2264:ALA:N	2.30	0.47
1:B:2107:GLN:OE1	1:D:1312:ASN:O	2.33	0.47
1:A:1352:THR:O	1:A:1353:LEU:CB	2.62	0.46
1:I:3184:ASN:O	1:I:3186:PRO:HD3	2.16	0.46
1:B:2313:PHE:CB	1:I:3111:GLU:HB3	2.45	0.46
1:E:2264:ALA:HB3	1:J:1272:VAL:CG1	2.46	0.46
1:A:1318:LYS:HZ3	1:K:2108:ARG:HB2	1.79	0.46
1:D:1189:LYS:CG	1:G:1061:ASN:HB2	2.44	0.46
1:L:3308:GLN:NE2	1:L:3345:ASN:HD21	2.11	0.46
1:I:3281:LEU:HD12	1:I:3281:LEU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2185:VAL:C	1:E:2186:PRO:CG	2.73	0.46
1:A:1271:ASN:CB	1:K:2098:ARG:HH12	2.27	0.46
1:G:1308:GLN:NE2	1:G:1345:ASN:HD21	2.07	0.46
1:J:1059:PRO:HD2	1:J:1190:GLN:HB2	1.98	0.46
1:A:1059:PRO:HD2	1:A:1190:GLN:HB2	1.98	0.46
1:B:2058:THR:HG22	1:K:2186:PRO:O	2.16	0.46
1:B:2186:PRO:C	1:E:2184:ASN:O	2.47	0.46
1:B:2191:ARG:HD3	1:E:2060:ALA:HB2	1.98	0.46
1:H:2059:PRO:CG	1:H:2190:GLN:HB2	2.46	0.46
1:B:2322:LYS:CD	1:C:3163:THR:HG21	2.42	0.45
1:E:2186:PRO:O	1:E:2187:GLN:CB	2.65	0.45
1:D:1189:LYS:CB	1:G:1061:ASN:HB2	2.45	0.45
1:E:2024:ASN:HD22	1:E:2252:ILE:H	1.64	0.45
1:E:2013:ALA:C	1:E:2015:LEU:H	2.20	0.45
1:B:2013:ALA:C	1:B:2015:LEU:H	2.20	0.45
1:B:2374:LEU:HD21	1:D:1272:VAL:HG21	1.99	0.45
1:D:1189:LYS:HG2	1:G:1061:ASN:CB	2.46	0.45
1:K:2024:ASN:HD22	1:K:2252:ILE:H	1.64	0.45
1:H:2083:GLU:HB3	1:H:2218:ALA:HB3	1.99	0.45
1:I:3311:ALA:O	1:I:3312:ASN:CB	2.65	0.45
1:D:1059:PRO:HD2	1:D:1190:GLN:HB2	1.98	0.45
1:G:1059:PRO:HD2	1:G:1190:GLN:HB2	1.98	0.45
1:L:3184:ASN:O	1:L:3186:PRO:HD3	2.16	0.45
1:C:3186:PRO:HG3	1:I:3188:SER:CA	2.46	0.45
1:G:1106:ASN:ND2	1:G:1191:ARG:NH2	2.56	0.45
1:E:2083:GLU:HB3	1:E:2218:ALA:HB3	1.99	0.45
1:H:2305:TYR:CZ	1:H:2318:LYS:HE3	2.51	0.45
1:B:2305:TYR:CZ	1:B:2318:LYS:HE3	2.51	0.45
1:H:2186:PRO:O	1:H:2187:GLN:CB	2.64	0.45
1:K:2305:TYR:CZ	1:K:2318:LYS:HE3	2.51	0.45
1:I:3310:THR:HG22	1:I:3358:VAL:HG22	1.99	0.45
1:F:3310:THR:HG22	1:F:3358:VAL:HG22	1.99	0.45
1:B:2061:ASN:CB	1:E:2186:PRO:HB3	2.45	0.45
1:K:2013:ALA:C	1:K:2015:LEU:H	2.20	0.45
1:I:3103:ASP:HB2	1:I:3104:PRO:HD2	1.99	0.45
1:C:3311:ALA:O	1:C:3312:ASN:CB	2.65	0.45
1:J:1211:LEU:HD21	1:J:1374:LEU:HD13	1.99	0.45
1:F:3311:ALA:O	1:F:3312:ASN:CB	2.65	0.45
1:A:1363:ASN:HD21	1:K:2108:ARG:CZ	2.15	0.45
1:F:3184:ASN:O	1:F:3186:PRO:HD3	2.16	0.45
1:L:3310:THR:HG22	1:L:3358:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1083:GLU:HB3	1:J:1218:ALA:HB3	1.99	0.44
1:B:2083:GLU:HB3	1:B:2218:ALA:HB3	1.99	0.44
1:H:2280:ASN:HA	1:H:2352:THR:OG1	2.18	0.44
1:L:3311:ALA:O	1:L:3312:ASN:CB	2.65	0.44
1:B:2308:GLN:NE2	1:B:2345:ASN:HD21	2.14	0.44
1:E:2305:TYR:CZ	1:E:2318:LYS:HE3	2.51	0.44
1:D:1187:GLN:CB	1:G:1185:VAL:C	2.85	0.44
1:A:1312:ASN:HA	1:K:2384:THR:H	1.43	0.44
1:G:1083:GLU:HB3	1:G:1218:ALA:HB3	1.99	0.44
1:B:2186:PRO:O	1:B:2187:GLN:CB	2.65	0.44
1:E:2059:PRO:CG	1:E:2190:GLN:HB2	2.46	0.44
1:K:2059:PRO:CG	1:K:2190:GLN:HB2	2.46	0.44
1:H:2322:LYS:CD	1:I:3163:THR:HG21	2.42	0.44
1:B:2024:ASN:HD22	1:B:2252:ILE:H	1.64	0.44
1:J:1307:SER:HB2	1:J:1318:LYS:HA	2.00	0.44
1:J:1322:LYS:HE2	1:K:2145:MET:O	2.17	0.44
1:E:2280:ASN:HA	1:E:2352:THR:OG1	2.18	0.44
1:H:2013:ALA:C	1:H:2015:LEU:H	2.19	0.44
1:D:1061:ASN:HB3	1:D:1183:ALA:O	2.18	0.44
1:B:2059:PRO:CG	1:B:2190:GLN:HB2	2.46	0.44
1:B:2051:ASN:OD1	1:E:2047:PHE:HA	2.17	0.44
1:K:2083:GLU:HB3	1:K:2218:ALA:HB3	1.99	0.44
1:D:1036:TYR:HA	1:D:1037:PRO:HD3	1.83	0.44
1:A:1307:SER:HB2	1:A:1318:LYS:HA	2.00	0.44
1:D:1193:LYS:HE3	1:G:1040:GLN:HE21	1.72	0.44
1:C:3103:ASP:HB2	1:C:3104:PRO:HD2	2.00	0.44
1:F:3103:ASP:HB2	1:F:3104:PRO:HD2	2.00	0.44
1:D:1307:SER:HB2	1:D:1318:LYS:HA	2.00	0.44
1:B:2280:ASN:HA	1:B:2352:THR:OG1	2.18	0.44
1:A:1322:LYS:HE2	1:B:2145:MET:O	2.18	0.44
1:B:2052:ARG:CB	1:E:2045:GLN:HA	2.30	0.44
1:D:1211:LEU:HD21	1:D:1374:LEU:HD13	1.99	0.44
1:A:1083:GLU:HB3	1:A:1218:ALA:HB3	1.99	0.44
1:C:3310:THR:HG22	1:C:3358:VAL:HG22	1.99	0.44
1:B:2106:ASN:CG	1:E:2238:ASP:OD1	2.56	0.44
1:G:1322:LYS:HE2	1:H:2145:MET:O	2.18	0.44
1:D:1191:ARG:HD3	1:G:1060:ALA:HB1	1.97	0.43
1:G:1061:ASN:HB3	1:G:1183:ALA:O	2.18	0.43
1:H:2024:ASN:HD22	1:H:2252:ILE:H	1.64	0.43
1:L:3103:ASP:HB2	1:L:3104:PRO:HD2	1.99	0.43
1:D:1322:LYS:HE2	1:E:2145:MET:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1036:TYR:HA	1:A:1037:PRO:HD3	1.83	0.43
1:B:2314:SER:HA	1:I:3108:ARG:HD3	1.76	0.43
1:A:1102:TYR:HB2	1:A:1191:ARG:HB2	2.01	0.43
1:B:2024:ASN:ND2	1:B:2252:ILE:H	2.16	0.43
1:A:1211:LEU:HD21	1:A:1374:LEU:HD13	1.99	0.43
1:H:2311:ALA:O	1:H:2312:ASN:C	2.57	0.43
1:K:2186:PRO:O	1:K:2187:GLN:CB	2.64	0.43
1:D:1083:GLU:HB3	1:D:1218:ALA:HB3	2.00	0.43
1:G:1307:SER:HB2	1:G:1318:LYS:HA	2.00	0.43
1:K:2280:ASN:HA	1:K:2352:THR:OG1	2.18	0.43
1:A:1260:LEU:HA	1:A:1377:TYR:O	2.19	0.43
1:B:2188:SER:HA	1:E:2184:ASN:HA	1.71	0.43
1:J:1102:TYR:HB2	1:J:1191:ARG:HB2	2.01	0.43
1:G:1260:LEU:HA	1:G:1377:TYR:O	2.19	0.43
1:B:2108:ARG:HH12	1:D:1309:ARG:HG3	1.83	0.43
1:D:1102:TYR:HB2	1:D:1191:ARG:HB2	2.01	0.43
1:C:3182:LEU:HD11	1:C:3184:ASN:ND2	2.34	0.43
1:E:2024:ASN:ND2	1:E:2252:ILE:H	2.16	0.43
1:K:2260:LEU:HD22	1:K:2378:GLU:HG3	2.01	0.43
1:H:2260:LEU:HD22	1:H:2378:GLU:HG3	2.01	0.43
1:L:3182:LEU:HD11	1:L:3184:ASN:ND2	2.34	0.43
1:L:3151:PRO:HD2	1:L:3162:LEU:HD22	2.00	0.43
1:I:3151:PRO:HD2	1:I:3162:LEU:HD22	2.00	0.43
1:B:2260:LEU:HD22	1:B:2378:GLU:HG3	2.01	0.43
1:A:1061:ASN:HB3	1:A:1183:ALA:O	2.18	0.43
1:B:2269:THR:OG1	1:I:3372:ARG:HD2	2.18	0.43
1:E:2260:LEU:HD22	1:E:2378:GLU:HG3	2.01	0.43
1:H:2311:ALA:O	1:H:2313:PHE:N	2.52	0.43
1:C:3151:PRO:HD2	1:C:3162:LEU:HD22	2.00	0.43
1:K:2024:ASN:ND2	1:K:2252:ILE:H	2.16	0.42
1:G:1211:LEU:HD21	1:G:1374:LEU:HD13	1.99	0.42
1:J:1061:ASN:HB3	1:J:1183:ALA:O	2.18	0.42
1:B:2108:ARG:NE	1:D:1314:SER:N	2.58	0.42
1:D:1098:ARG:HH22	1:I:3318:LYS:HZ2	1.63	0.42
1:F:3182:LEU:HD11	1:F:3184:ASN:ND2	2.34	0.42
1:I:3284:TYR:HB2	1:I:3350:ILE:HB	2.01	0.42
1:B:2372:ARG:NH1	1:D:1269:THR:CB	2.81	0.42
1:H:2024:ASN:ND2	1:H:2252:ILE:H	2.16	0.42
1:C:3284:TYR:HB2	1:C:3350:ILE:HB	2.01	0.42
1:E:2311:ALA:O	1:E:2312:ASN:C	2.57	0.42
1:F:3151:PRO:HD2	1:F:3162:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3284:TYR:HB2	1:F:3350:ILE:HB	2.01	0.42
1:B:2311:ALA:O	1:B:2312:ASN:C	2.57	0.42
1:A:1106:ASN:ND2	1:A:1191:ARG:NH2	2.56	0.42
1:G:1102:TYR:HB2	1:G:1191:ARG:HB2	2.01	0.42
1:J:1242:VAL:HG22	1:J:1247:TYR:CD2	2.55	0.42
1:G:1242:VAL:HG22	1:G:1247:TYR:CD2	2.55	0.42
1:C:3369:GLN:O	1:C:3370:ASN:HB2	2.20	0.42
1:I:3182:LEU:HD11	1:I:3184:ASN:ND2	2.34	0.42
1:F:3369:GLN:O	1:F:3370:ASN:HB2	2.20	0.42
1:A:1305:TYR:OH	1:K:2108:ARG:NH1	2.52	0.42
1:D:1260:LEU:HA	1:D:1377:TYR:O	2.19	0.42
1:I:3014:ALA:C	1:I:3016:ARG:H	2.23	0.42
1:D:1242:VAL:HG22	1:D:1247:TYR:CD2	2.55	0.42
1:C:3242:VAL:HG22	1:C:3247:TYR:CD2	2.55	0.42
1:B:2372:ARG:CZ	1:D:1272:VAL:HG23	2.35	0.42
1:B:2311:ALA:O	1:B:2313:PHE:N	2.52	0.42
1:B:2024:ASN:ND2	1:B:2253:ASP:H	2.17	0.42
1:J:1260:LEU:HA	1:J:1377:TYR:O	2.19	0.42
1:F:3242:VAL:HG22	1:F:3247:TYR:CD2	2.55	0.42
1:F:3014:ALA:C	1:F:3016:ARG:H	2.23	0.42
1:A:1242:VAL:HG22	1:A:1247:TYR:CD2	2.55	0.42
1:C:3275:VAL:HG22	1:C:3361:VAL:HG22	2.02	0.42
1:E:2308:GLN:NE2	1:E:2345:ASN:HD21	2.14	0.42
1:H:2021:MET:HE3	1:H:2252:ILE:CD1	2.50	0.42
1:E:2311:ALA:O	1:E:2313:PHE:N	2.52	0.42
1:K:2311:ALA:O	1:K:2312:ASN:C	2.57	0.42
1:K:2311:ALA:O	1:K:2313:PHE:N	2.52	0.42
1:A:1272:VAL:HG22	1:K:2261:GLU:CB	2.46	0.41
1:L:3369:GLN:O	1:L:3370:ASN:HB2	2.20	0.41
1:B:2272:VAL:CG2	1:I:3372:ARG:NH1	2.84	0.41
1:B:2021:MET:HE3	1:B:2252:ILE:CD1	2.50	0.41
1:K:2021:MET:HE3	1:K:2252:ILE:CD1	2.51	0.41
1:C:3014:ALA:C	1:C:3016:ARG:H	2.23	0.41
1:I:3275:VAL:HG22	1:I:3361:VAL:HG22	2.02	0.41
1:I:3242:VAL:HG22	1:I:3247:TYR:CD2	2.55	0.41
1:L:3284:TYR:HB2	1:L:3350:ILE:HB	2.01	0.41
1:C:3098:ARG:HE	1:C:3098:ARG:HB3	1.69	0.41
1:I:3369:GLN:O	1:I:3370:ASN:HB2	2.20	0.41
1:F:3275:VAL:HG22	1:F:3361:VAL:HG22	2.02	0.41
1:K:2189:LYS:HE3	1:K:2189:LYS:HB2	1.86	0.41
1:J:1260:LEU:HD22	1:J:1378:GLU:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1363:ASN:CB	1:K:2108:ARG:HH12	2.32	0.41
1:J:1036:TYR:HA	1:J:1037:PRO:HD3	1.83	0.41
1:D:1079:ASN:O	1:D:1079:ASN:CG	2.59	0.41
1:A:1314:SER:CA	1:K:2383:ARG:O	2.69	0.41
1:K:2106:ASN:HD22	1:K:2106:ASN:HA	1.68	0.41
1:C:3083:GLU:HB3	1:C:3218:ALA:HB3	2.03	0.41
1:H:2308:GLN:NE2	1:H:2345:ASN:HD21	2.14	0.41
1:G:1260:LEU:HD22	1:G:1378:GLU:HG2	2.03	0.41
1:L:3275:VAL:HG22	1:L:3361:VAL:HG22	2.02	0.41
1:L:3242:VAL:HG22	1:L:3247:TYR:CD2	2.55	0.41
1:A:1318:LYS:HZ2	1:K:2108:ARG:H	1.69	0.41
1:E:2021:MET:HE3	1:E:2252:ILE:CD1	2.51	0.41
1:I:3162:LEU:N	1:I:3162:LEU:HD23	2.36	0.41
1:B:2103:ASP:HB2	1:B:2104:PRO:HD2	2.04	0.40
1:L:3014:ALA:C	1:L:3016:ARG:H	2.23	0.40
1:G:1079:ASN:CG	1:G:1079:ASN:O	2.60	0.40
1:F:3083:GLU:HB3	1:F:3218:ALA:HB3	2.03	0.40
1:I:3083:GLU:HB3	1:I:3218:ALA:HB3	2.03	0.40
1:H:2013:ALA:O	1:H:2014:ALA:HB3	2.22	0.40
1:L:3186:PRO:O	1:L:3187:GLN:CB	2.69	0.40
1:F:3162:LEU:N	1:F:3162:LEU:HD23	2.36	0.40
1:B:2318:LYS:NZ	1:I:3098:ARG:NH2	2.65	0.40
1:I:3352:THR:O	1:I:3353:LEU:HG	2.21	0.40
1:F:3352:THR:O	1:F:3353:LEU:HG	2.22	0.40
1:H:2103:ASP:HB2	1:H:2104:PRO:HD2	2.03	0.40
1:D:1189:LYS:HZ1	1:G:1059:PRO:C	1.91	0.40
1:D:1098:ARG:NH1	1:I:3305:TYR:OH	2.54	0.40
1:L:3281:LEU:CD1	1:L:3281:LEU:N	2.85	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	369/394 (94%)	349 (95%)	16 (4%)	4 (1%)	17	63
1	B	371/394 (94%)	349 (94%)	21 (6%)	1 (0%)	46	83
1	C	370/394 (94%)	348 (94%)	19 (5%)	3 (1%)	24	69
1	D	367/394 (93%)	347 (95%)	16 (4%)	4 (1%)	17	63
1	E	371/394 (94%)	349 (94%)	21 (6%)	1 (0%)	46	83
1	F	370/394 (94%)	348 (94%)	19 (5%)	3 (1%)	24	69
1	G	369/394 (94%)	349 (95%)	16 (4%)	4 (1%)	17	63
1	H	371/394 (94%)	349 (94%)	21 (6%)	1 (0%)	46	83
1	I	370/394 (94%)	348 (94%)	19 (5%)	3 (1%)	24	69
1	J	369/394 (94%)	349 (95%)	16 (4%)	4 (1%)	17	63
1	K	371/394 (94%)	349 (94%)	21 (6%)	1 (0%)	46	83
1	L	370/394 (94%)	348 (94%)	19 (5%)	3 (1%)	24	69
All	All	4438/4728 (94%)	4182 (94%)	224 (5%)	32 (1%)	31	71

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1185	VAL
1	C	3245	ASN
1	C	3280	ASN
1	C	3312	ASN
1	D	1185	VAL
1	F	3245	ASN
1	F	3280	ASN
1	F	3312	ASN
1	G	1185	VAL
1	I	3245	ASN
1	I	3280	ASN
1	I	3312	ASN
1	J	1185	VAL
1	L	3245	ASN
1	L	3280	ASN
1	L	3312	ASN
1	A	1186	PRO
1	A	1313	PHE
1	D	1186	PRO
1	D	1313	PHE
1	G	1186	PRO
1	G	1313	PHE

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Mol	Chain	Res	Type
1	J	1186	PRO
1	J	1313	PHE
1	B	2312	ASN
1	D	1384	THR
1	E	2312	ASN
1	H	2312	ASN
1	K	2312	ASN
1	A	1384	THR
1	G	1384	THR
1	J	1384	THR

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	292/325 (90%)	290 (99%)	2 (1%)	88	94
1	B	294/325 (90%)	289 (98%)	5 (2%)	68	87
1	C	298/325 (92%)	296 (99%)	2 (1%)	88	94
1	D	291/325 (90%)	289 (99%)	2 (1%)	88	94
1	E	294/325 (90%)	289 (98%)	5 (2%)	68	87
1	F	298/325 (92%)	296 (99%)	2 (1%)	88	94
1	G	292/325 (90%)	290 (99%)	2 (1%)	88	94
1	H	294/325 (90%)	289 (98%)	5 (2%)	68	87
1	I	298/325 (92%)	296 (99%)	2 (1%)	88	94
1	J	292/325 (90%)	290 (99%)	2 (1%)	88	94
1	K	294/325 (90%)	289 (98%)	5 (2%)	68	87
1	L	298/325 (92%)	296 (99%)	2 (1%)	88	94
All	All	3535/3900 (91%)	3499 (99%)	36 (1%)	83	92

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1186	PRO
1	A	1315	ASP
1	B	2106	ASN
1	B	2162	LEU
1	B	2265	GLN
1	B	2280	ASN
1	B	2357	ASN
1	C	3162	LEU
1	C	3355	TYR
1	D	1186	PRO
1	D	1315	ASP
1	E	2106	ASN
1	E	2162	LEU
1	E	2265	GLN
1	E	2280	ASN
1	E	2357	ASN
1	F	3162	LEU
1	F	3355	TYR
1	G	1186	PRO
1	G	1315	ASP
1	H	2106	ASN
1	H	2162	LEU
1	H	2265	GLN
1	H	2280	ASN
1	H	2357	ASN
1	I	3162	LEU
1	I	3355	TYR
1	J	1186	PRO
1	J	1315	ASP
1	K	2106	ASN
1	K	2162	LEU
1	K	2265	GLN
1	K	2280	ASN
1	K	2357	ASN
1	L	3162	LEU
1	L	3355	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (111) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1041	GLN
1	A	1061	ASN
1	A	1079	ASN

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Mol	Chain	Res	Type
1	A	1080	HIS
1	A	1106	ASN
1	A	1190	GLN
1	A	1200	ASN
1	A	1271	ASN
1	A	1280	ASN
1	A	1304	ASN
1	A	1345	ASN
1	A	1363	ASN
1	B	2024	ASN
1	B	2033	GLN
1	B	2041	GLN
1	B	2080	HIS
1	B	2107	GLN
1	B	2190	GLN
1	B	2200	ASN
1	B	2265	GLN
1	B	2345	ASN
1	B	2357	ASN
1	B	2369	GLN
1	C	3041	GLN
1	C	3080	HIS
1	C	3271	ASN
1	C	3345	ASN
1	C	3354	GLN
1	D	1041	GLN
1	D	1061	ASN
1	D	1079	ASN
1	D	1080	HIS
1	D	1106	ASN
1	D	1190	GLN
1	D	1200	ASN
1	D	1280	ASN
1	D	1345	ASN
1	D	1369	GLN
1	E	2024	ASN
1	E	2033	GLN
1	E	2041	GLN
1	E	2045	GLN
1	E	2080	HIS
1	E	2106	ASN
1	E	2107	GLN

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Mol	Chain	Res	Type
1	E	2190	GLN
1	E	2200	ASN
1	E	2265	GLN
1	E	2345	ASN
1	E	2357	ASN
1	F	3041	GLN
1	F	3080	HIS
1	F	3271	ASN
1	F	3345	ASN
1	F	3354	GLN
1	G	1040	GLN
1	G	1041	GLN
1	G	1061	ASN
1	G	1079	ASN
1	G	1080	HIS
1	G	1106	ASN
1	G	1190	GLN
1	G	1200	ASN
1	G	1280	ASN
1	G	1345	ASN
1	H	2024	ASN
1	H	2033	GLN
1	H	2041	GLN
1	H	2061	ASN
1	H	2080	HIS
1	H	2106	ASN
1	H	2107	GLN
1	H	2190	GLN
1	H	2200	ASN
1	H	2265	GLN
1	H	2345	ASN
1	H	2357	ASN
1	I	3041	GLN
1	I	3061	ASN
1	I	3080	HIS
1	I	3190	GLN
1	I	3271	ASN
1	I	3345	ASN
1	I	3354	GLN
1	I	3370	ASN
1	J	1041	GLN
1	J	1061	ASN

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Mol	Chain	Res	Type
1	J	1079	ASN
1	J	1080	HIS
1	J	1106	ASN
1	J	1190	GLN
1	J	1200	ASN
1	J	1280	ASN
1	J	1345	ASN
1	K	2024	ASN
1	K	2033	GLN
1	K	2040	GLN
1	K	2041	GLN
1	K	2061	ASN
1	K	2080	HIS
1	K	2107	GLN
1	K	2190	GLN
1	K	2200	ASN
1	K	2265	GLN
1	K	2345	ASN
1	K	2357	ASN
1	L	3041	GLN
1	L	3080	HIS
1	L	3271	ASN
1	L	3345	ASN
1	L	3354	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.