



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:51 AM UTC

PDB ID : 6RUT / pdb_00006rut
Title : Mycoplasma Genitalium Heterodimer Nap Complex (P140-P110 globular)
Authors : Fita, I.; Aparicio, D.
Deposited on : 2019-05-29
Resolution : 2.65 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

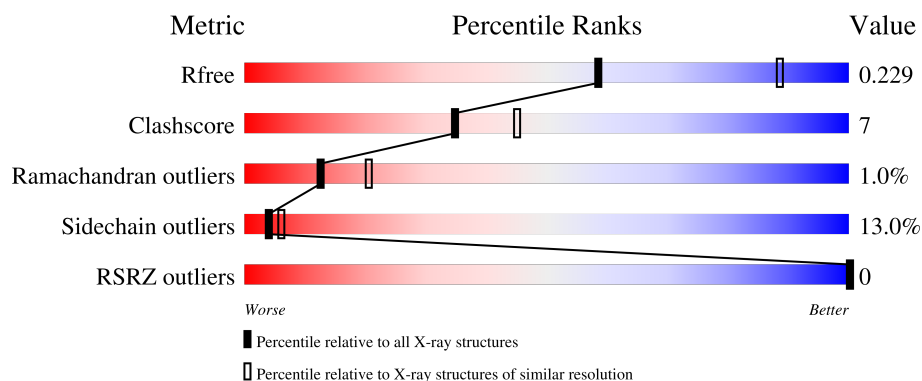
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

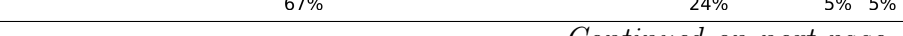
The reported resolution of this entry is 2.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	802	
1	C	802	
1	E	802	
1	G	802	
2	B	1334	

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Mol	Chain	Length	Quality of chain
2	D	1334	67%23%5%5%
2	F	1334	65%23%•6%
2	H	1334	65%24%5%7%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 64181 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Mgp-operon protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	781	Total	C	N	O	S	0	0	0
			6013	3758	1009	1240	6			
1	C	779	Total	C	N	O	S	0	0	0
			5999	3751	1006	1236	6			
1	E	783	Total	C	N	O	S	0	0	0
			6017	3760	1010	1241	6			
1	G	784	Total	C	N	O	S	0	0	0
			6023	3763	1011	1243	6			

- Molecule 2 is a protein called Adhesin P1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1268	Total	C	N	O	S	0	0	0
			9938	6303	1679	1942	14			
2	D	1265	Total	C	N	O	S	0	0	0
			9918	6293	1676	1935	14			
2	F	1250	Total	C	N	O	S	0	0	0
			9822	6242	1658	1909	13			
2	H	1247	Total	C	N	O	S	0	0	0
			9798	6228	1654	1903	13			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	62	Total	O	0	0
			62	62		
3	B	121	Total	O	0	0
			121	121		
3	C	87	Total	O	0	0
			87	87		
3	D	137	Total	O	0	0
			137	137		

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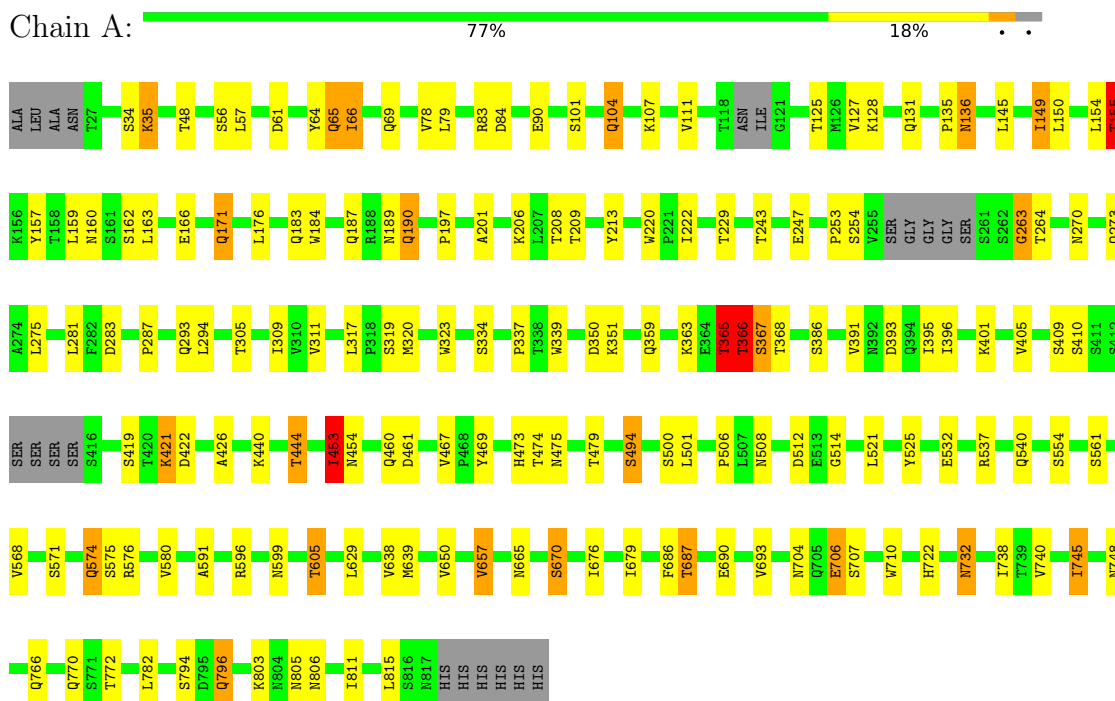
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	69	Total 69	O 69	0	0
3	F	70	Total 70	O 70	0	0
3	G	49	Total 49	O 49	0	0
3	H	58	Total 58	O 58	0	0

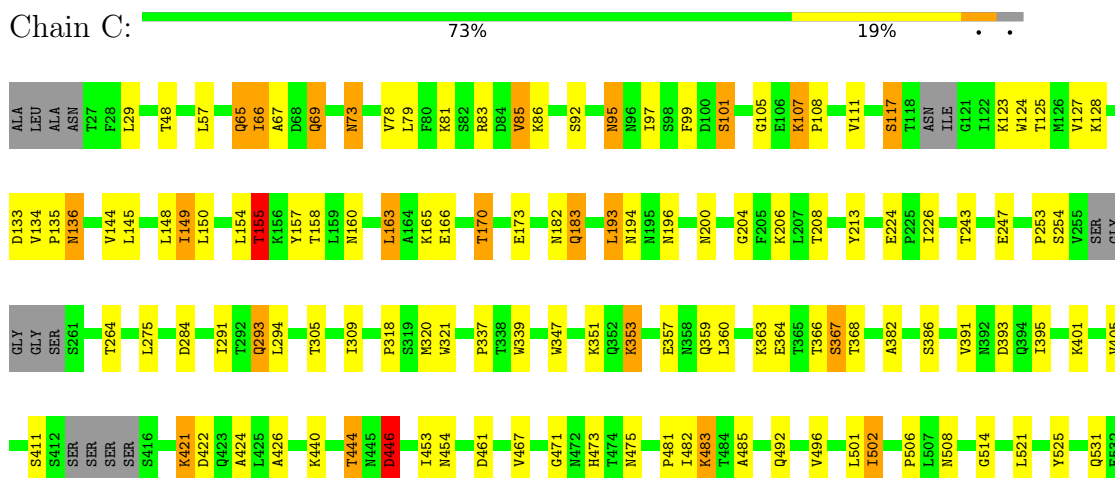
3 Residue-property plots

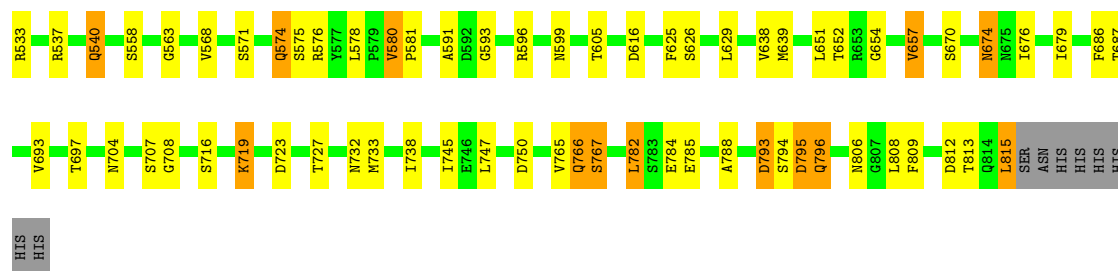
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Mgp-operon protein 3



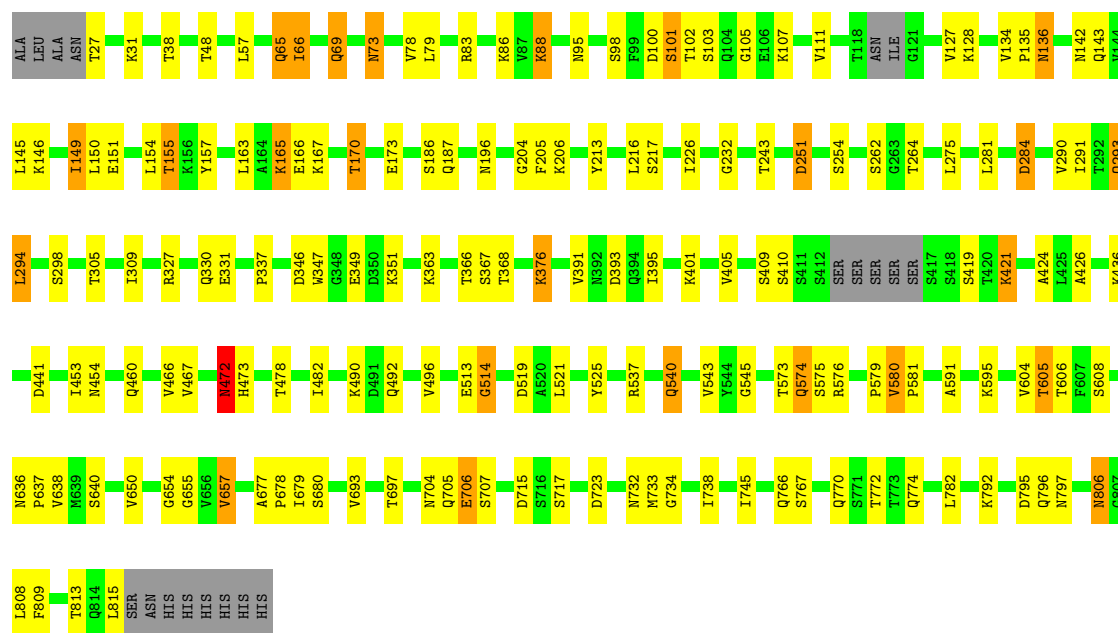
• Molecule 1: Mgp-operon protein 3

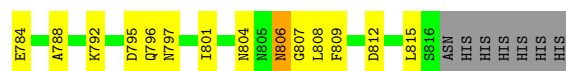




• Molecule 1: Mgp-operon protein 3

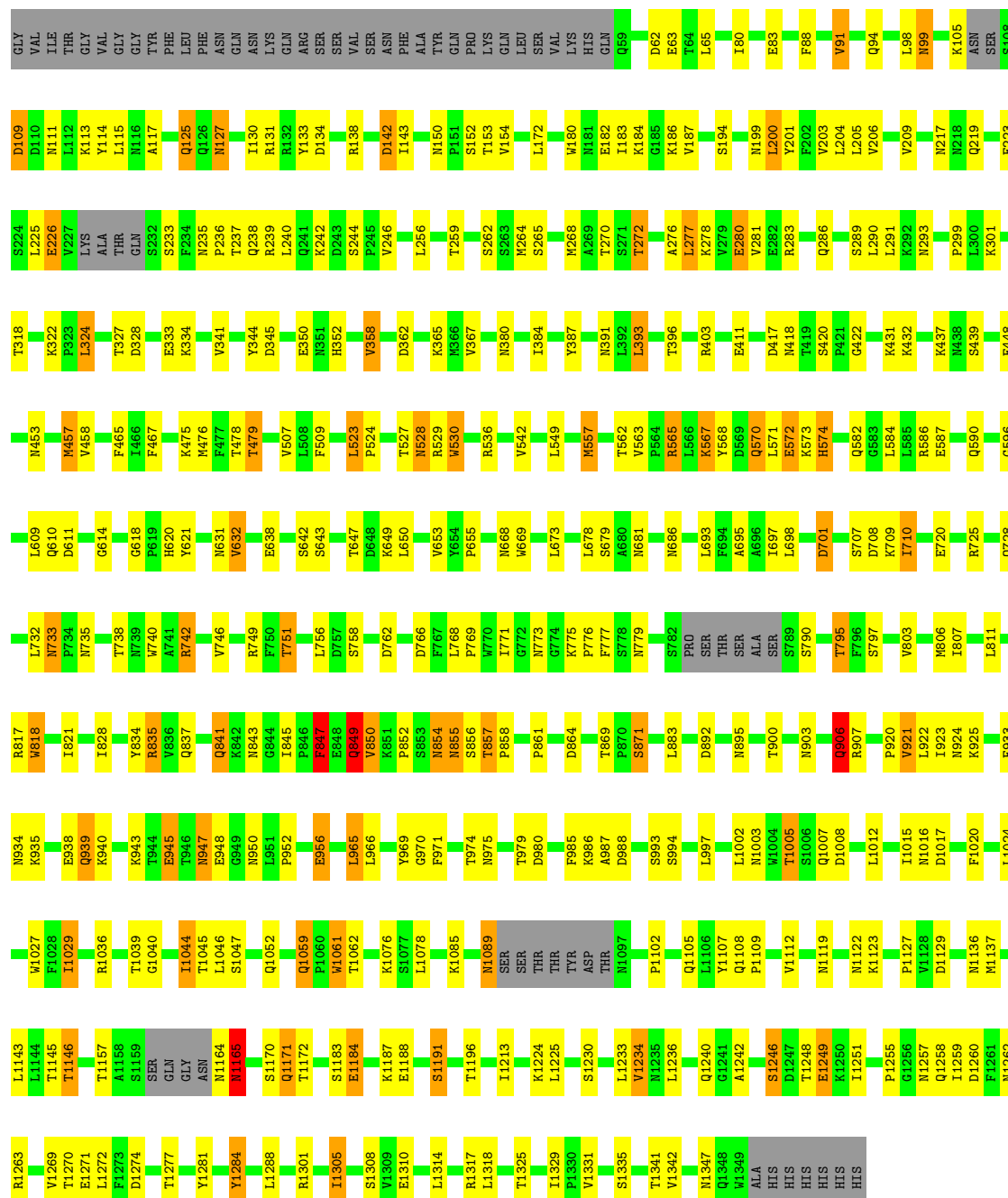
Chain E: 76% 18% . .





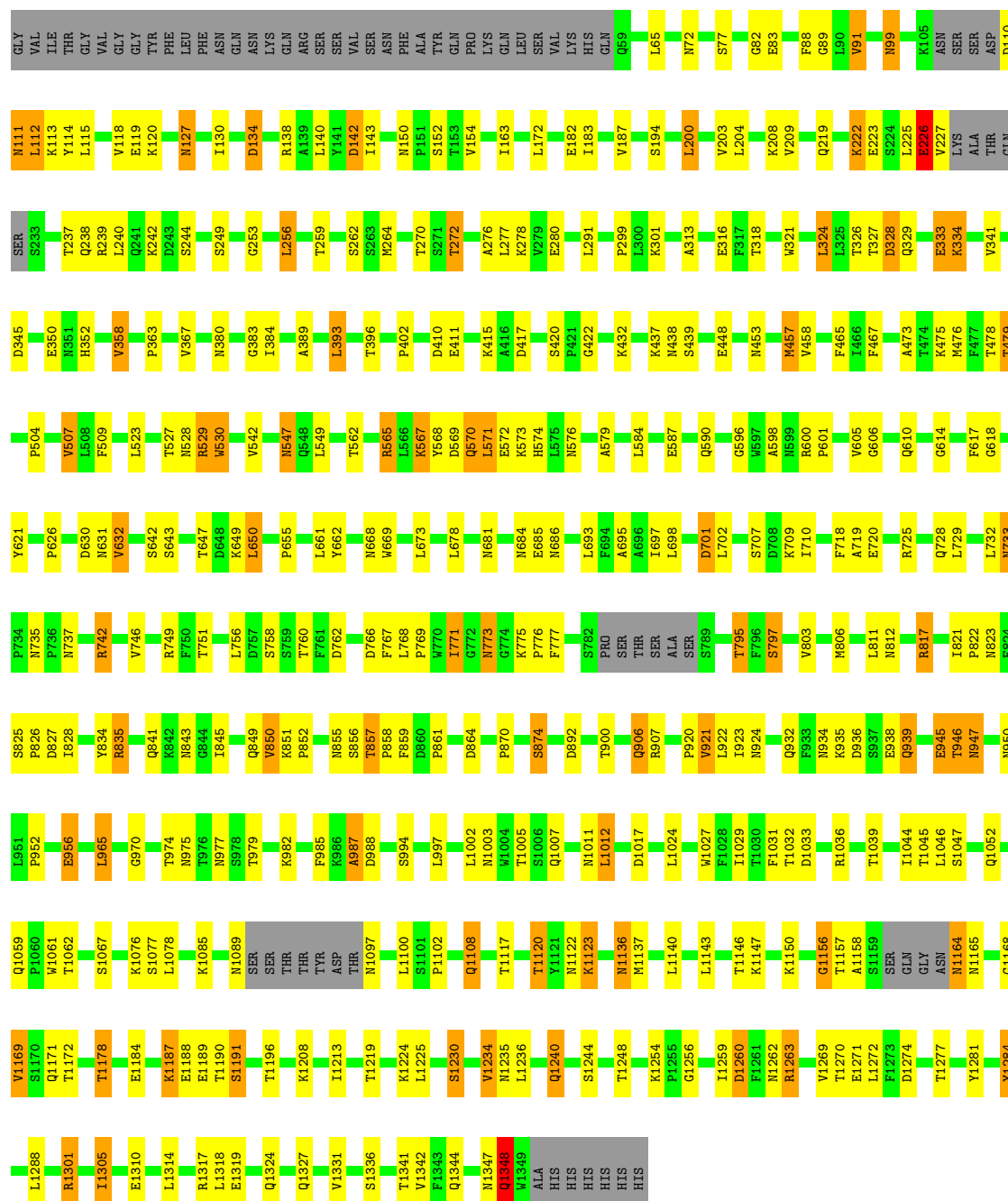
• Molecule 2: Adhesin P1

Chain B: 67% 24% 5% 5%



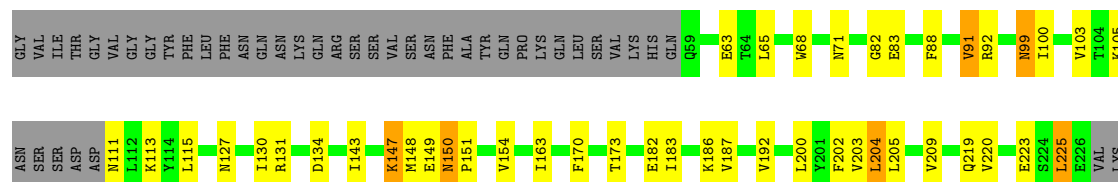
• Molecule 2: Adhesin P1

Chain D: 67% 23% 5% 5%



• Molecule 2: Adhesin P1

Chain F: 65% 23% 6%





F1343	Q1258	S1139	W1027	V921	V803	D701	L571	A416
Q1344	L1259	L1143	F1029	L922	M806	L702	E572	D417
P1345	D1260	F1261	I1029	I923	I807		K573	
F1346	F1261	T1146	T1030	N924	L811	S707	L584	S420
Q1347	N1262	K1150	F1031	F933	N812	D768	L585	P421
Q1348	R1263	G1156	T1032	N934	R817	K709	R586	G422
W1349	L1264	T1157	R1036	E938		I710	E587	K432
A1350	F1265	A1158	I1044	Q939	F820	E720	Q890	K436
HIS	L1267	T1157	T1045	E945	I821	R725	P594	K437
HIS	P1268	SER	L1046	T946	P822	Q728	N438	N438
HIS	V1269	SER	Q1050	N947	N823		S439	
HIS	T1270	GLN	Q1051	P952	P826	L732	E448	
HIS	E1271	GLY	Q1052		D827	N737	N453	
	L1272	ASN	Q1059	E956	I828	T738	Q610	
	F1273	ASN	F1060	V957		N739	Q618	
	D1274	G1156	W1061	N958	Y834	R742	P619	
	T1277	V1169	S1067	L965	R835	V746	H620	
	Y1281	Q1171	Y1068	H967	V836	R749	D630	
	Y1284	T1172	L1069	N975	Q841	F750	N631	
	L1288	I1173	T1074	T976	N843	T478	V632	
	S1293	N1174	F1088	N977	G844	T479	F477	
	R1301	E1184	ASN	D980	P846	D757	E638	
	I1305	K1187	SER	T983	G849	D762	T647	
	S1306	E1188	SER	G984	K850		D648	
	Y1307	T1190	THR	F985	K851	D766	K649	
	S1308	S1191	TYR	K986	P852	F767	L650	
	V1309	T1196	ASP	A987	S856	L768	L520	
	E1310	T1213	THR	D988	T857	P769	L523	
	N1311	M1221	N1097	S989		I770	V653	
Q1312	T1313	K1224	P1102	S990	D864	I771	Y654	
L1314	L1314	L1225	Q1105	S991	V868	N773	P655	
	R1317	L1225	L1106	S992	S874	K774	S659	
	L1318	S1230	Y1107	S993		K775	Y662	
	E1319		Q1108	S994	P864	P776		
	D1322	V1234	A1114	L997		F777	N668	
	Q1326	N1235	Y1115	L1002	D892	F781	L673	
	F1327	L1236	Q1116	M1003		SER	V542	
	F1328	I1237	T1117	W1004	N895	PRO	L551	
	I1329	N1238	T1120	T1005		SER	L678	
	P1330	G1239	Y1121	S1006	T900	THR	S679	
	V1331	Q1240	N1122	D1008	N901	ALA	A660	
	S1335	A1242	K1123	M1011	N903	SER	N651	
	S1336	D1245	L1124	L1012	Q906	S789	N654	
	T1337	T1248	M1136	D1017	L915	T795	E685	
	T1341	V1342	M1137	L1024		F796	N686	
			T1138			S797	A695	
							Y568	
							D669	
							Q570	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	151.00Å 157.28Å 192.37Å 90.00° 93.81° 90.00°	Depositor
Resolution (Å)	121.66 – 2.65 121.66 – 2.65	Depositor EDS
% Data completeness (in resolution range)	73.2 (121.66-2.65) 73.3 (121.66-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.187 , 0.224 0.199 , 0.229	Depositor DCC
R_{free} test set	9457 reflections (3.66%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 27.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	64181	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.83	0/6136	1.34	32/8340 (0.4%)
1	C	0.83	1/6122 (0.0%)	1.35	50/8321 (0.6%)
1	E	0.82	0/6141	1.34	26/8347 (0.3%)
1	G	0.82	0/6147	1.34	32/8355 (0.4%)
2	B	0.86	4/10187 (0.0%)	1.37	74/13863 (0.5%)
2	D	0.85	2/10167 (0.0%)	1.37	80/13836 (0.6%)
2	F	0.82	4/10069 (0.0%)	1.34	50/13701 (0.4%)
2	H	0.84	5/10044 (0.0%)	1.34	59/13668 (0.4%)
All	All	0.84	16/65013 (0.0%)	1.35	403/88431 (0.5%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1115	TYR	CA-C	15.31	1.72	1.52
2	B	557	MET	SD-CE	-7.65	1.60	1.79
2	F	557	MET	SD-CE	-7.48	1.60	1.79
2	D	150	ASN	CA-C	6.53	1.57	1.53
2	H	812	ASN	CG-ND2	-6.01	1.20	1.33
2	H	371	PRO	CA-C	5.88	1.55	1.51
2	B	1020	PHE	CA-C	5.86	1.59	1.52
2	F	457	MET	SD-CE	-5.79	1.65	1.79
2	D	457	MET	SD-CE	-5.78	1.65	1.79
2	F	857	THR	CA-C	5.72	1.60	1.52
2	H	1312	GLN	CD-NE2	-5.60	1.21	1.33
2	F	371	PRO	CA-C	5.41	1.54	1.51
2	B	457	MET	SD-CE	-5.26	1.66	1.79
2	B	206	VAL	CA-C	5.23	1.57	1.52
2	H	1259	ILE	CA-C	5.06	1.59	1.52
1	C	578	LEU	CA-C	5.00	1.57	1.52

All (403) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	99	ASN	CA-CB-CG	9.28	121.88	112.60
2	B	701	ASP	CA-CB-CG	9.28	121.88	112.60
1	G	261	SER	N-CA-C	9.16	124.40	113.23
2	H	1348	GLN	N-CA-C	-9.11	101.86	113.16
1	E	251	ASP	CA-CB-CG	8.41	121.01	112.60
2	B	987	ALA	CA-C-N	8.39	133.44	121.02
2	B	987	ALA	C-N-CA	8.39	133.44	121.02
2	D	1336	SER	CA-C-N	8.37	131.82	120.44
2	D	1336	SER	C-N-CA	8.37	131.82	120.44
2	F	1120	THR	CB-CA-C	-8.30	97.79	110.90
2	D	1165	ASN	CA-C-N	8.23	137.53	121.41
2	D	1165	ASN	C-N-CA	8.23	137.53	121.41
2	D	701	ASP	CA-CB-CG	8.13	120.73	112.60
2	D	530	TRP	N-CA-C	-8.06	95.43	108.41
2	H	989	SER	CA-CB-OG	-7.98	95.13	111.10
2	F	668	ASN	CA-CB-CG	7.82	120.42	112.60
2	D	1164	ASN	CA-CB-CG	7.75	120.35	112.60
1	G	367	SER	CA-C-N	7.62	136.09	121.54
1	G	367	SER	C-N-CA	7.62	136.09	121.54
2	B	1165	ASN	N-CA-C	7.54	117.95	108.45
2	H	990	SER	N-CA-C	-7.52	106.05	114.62
2	B	225	LEU	CA-C-N	7.50	131.84	120.82
2	B	225	LEU	C-N-CA	7.50	131.84	120.82
2	D	134	ASP	CA-CB-CG	7.42	120.02	112.60
2	B	849	GLN	CA-C-N	7.28	131.40	120.77
2	B	849	GLN	C-N-CA	7.28	131.40	120.77
2	D	647	THR	CA-C-N	7.27	130.75	120.28
2	D	647	THR	C-N-CA	7.27	130.75	120.28
1	C	73	ASN	CA-CB-CG	7.26	119.86	112.60
2	B	849	GLN	N-CA-C	-7.26	101.54	111.56
2	H	1115	TYR	N-CA-C	7.20	120.43	110.35
2	H	1115	TYR	CA-C-O	7.17	128.82	121.07
2	F	856	SER	N-CA-C	-7.17	103.20	112.23
2	D	226	GLU	CA-C-N	7.10	134.48	121.70
2	D	226	GLU	C-N-CA	7.10	134.48	121.70
2	F	82	GLY	CA-C-N	6.91	131.18	120.82
2	F	82	GLY	C-N-CA	6.91	131.18	120.82
2	D	225	LEU	CA-C-N	6.87	134.65	121.54
2	D	225	LEU	C-N-CA	6.87	134.65	121.54
2	B	647	THR	CA-C-N	6.84	129.75	120.38
2	B	647	THR	C-N-CA	6.84	129.75	120.38
2	D	1097	ASN	CA-CB-CG	6.83	119.43	112.60
2	D	719	ALA	CA-C-N	6.81	129.40	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	719	ALA	C-N-CA	6.81	129.40	120.28
1	C	183	GLN	N-CA-C	-6.79	104.74	113.16
1	E	73	ASN	CA-CB-CG	6.73	119.33	112.60
2	B	134	ASP	CA-CB-CG	6.70	119.30	112.60
2	B	530	TRP	N-CA-C	-6.68	97.83	108.73
2	B	632	VAL	N-CA-C	-6.64	106.04	112.29
2	F	71	ASN	CA-CB-CG	6.63	119.23	112.60
2	H	1115	TYR	O-C-N	-6.57	115.23	123.12
2	B	1347	ASN	CA-CB-CG	6.56	119.16	112.60
2	F	931	ASP	CA-CB-CG	6.54	119.14	112.60
1	E	513	GLU	CA-C-N	6.51	127.34	119.99
1	E	513	GLU	C-N-CA	6.51	127.34	119.99
1	C	95	ASN	CA-C-N	6.50	129.52	120.29
1	C	95	ASN	C-N-CA	6.50	129.52	120.29
1	A	162	SER	CA-C-N	6.46	128.94	120.28
1	A	162	SER	C-N-CA	6.46	128.94	120.28
2	D	208	LYS	CA-C-N	6.37	128.59	120.56
2	D	208	LYS	C-N-CA	6.37	128.59	120.56
1	A	160	ASN	CA-CB-CG	6.37	118.97	112.60
2	H	1312	GLN	OE1-CD-NE2	-6.35	116.25	122.60
2	B	563	VAL	N-CA-CB	6.33	115.39	110.45
1	A	365	THR	CA-C-O	-6.32	111.47	120.51
2	B	856	SER	N-CA-C	-6.31	102.96	111.54
1	A	155	THR	CA-C-N	6.30	129.36	120.28
1	A	155	THR	C-N-CA	6.30	129.36	120.28
2	H	1268	PRO	N-CA-C	6.30	120.34	111.33
1	E	608	SER	CA-C-N	6.29	126.92	119.94
1	E	608	SER	C-N-CA	6.29	126.92	119.94
1	G	686	PHE	CA-CB-CG	6.28	120.08	113.80
2	H	668	ASN	CA-CB-CG	6.27	118.87	112.60
2	B	1347	ASN	N-CA-C	-6.26	102.93	110.44
2	D	417	ASP	CA-CB-CG	6.26	118.86	112.60
2	D	1156	GLY	CA-C-N	6.25	133.48	121.54
2	D	1156	GLY	C-N-CA	6.25	133.48	121.54
2	H	82	GLY	CA-C-N	6.24	129.47	120.79
2	H	82	GLY	C-N-CA	6.24	129.47	120.79
2	H	1261	PHE	CB-CA-C	-6.24	109.39	116.63
2	D	507	VAL	CA-C-N	6.23	128.63	120.28
2	D	507	VAL	C-N-CA	6.23	128.63	120.28
1	G	731	ASP	CA-CB-CG	6.23	118.83	112.60
1	C	226	ILE	N-CA-C	-6.22	104.79	110.82
2	H	903	ASN	CA-C-N	6.19	127.82	120.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	903	ASN	C-N-CA	6.19	127.82	120.09
2	D	1031	PHE	CA-C-N	6.18	128.85	120.44
2	D	1031	PHE	C-N-CA	6.18	128.85	120.44
2	H	1347	ASN	CA-CB-CG	6.18	118.78	112.60
1	G	226	ILE	N-CA-C	-6.17	104.48	110.72
2	H	1346	PHE	CA-C-N	6.17	133.32	121.54
2	H	1346	PHE	C-N-CA	6.17	133.32	121.54
2	B	217	ASN	CA-CB-CG	6.16	118.76	112.60
2	H	71	ASN	CA-CB-CG	6.15	118.75	112.60
2	H	856	SER	N-CA-C	-6.15	103.44	111.74
2	H	1245	ASP	CA-C-N	6.15	129.14	120.28
2	H	1245	ASP	C-N-CA	6.15	129.14	120.28
1	C	674	ASN	CA-CB-CG	6.12	118.72	112.60
2	D	313	ALA	CA-C-N	6.12	128.73	120.65
2	D	313	ALA	C-N-CA	6.12	128.73	120.65
2	D	99	ASN	CA-CB-CG	6.11	118.71	112.60
1	A	772	THR	N-CA-C	-6.11	106.81	114.56
2	F	1284	TYR	CA-C-N	6.10	126.28	120.43
2	F	1284	TYR	C-N-CA	6.10	126.28	120.43
2	B	1284	TYR	CA-C-N	6.08	126.27	120.43
2	B	1284	TYR	C-N-CA	6.08	126.27	120.43
2	B	762	ASP	CA-C-N	6.08	128.43	120.28
2	B	762	ASP	C-N-CA	6.08	128.43	120.28
2	F	945	GLU	CB-CG-CD	6.08	122.93	112.60
2	D	1347	ASN	CA-CB-CG	6.07	118.67	112.60
2	F	857	THR	CB-CA-C	6.06	122.10	110.17
1	G	492	GLN	CA-C-N	6.06	128.72	120.54
1	G	492	GLN	C-N-CA	6.06	128.72	120.54
1	G	368	THR	N-CA-C	-6.05	97.91	110.80
1	A	183	GLN	CA-C-N	6.04	128.29	120.44
1	A	183	GLN	C-N-CA	6.04	128.29	120.44
2	B	507	VAL	CA-C-N	6.03	128.37	120.28
2	B	507	VAL	C-N-CA	6.03	128.37	120.28
1	C	183	GLN	CA-C-N	6.00	128.65	120.54
1	C	183	GLN	C-N-CA	6.00	128.65	120.54
2	H	980	ASP	CA-CB-CG	6.00	118.60	112.60
1	G	783	SER	CA-C-N	5.98	132.96	121.54
1	G	783	SER	C-N-CA	5.98	132.96	121.54
1	C	144	VAL	CA-C-N	5.97	128.56	120.38
1	C	144	VAL	C-N-CA	5.97	128.56	120.38
1	E	262	SER	CA-C-N	5.96	125.76	120.10
1	E	262	SER	C-N-CA	5.96	125.76	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	970	GLY	CA-C-N	5.95	128.85	120.28
2	B	970	GLY	C-N-CA	5.95	128.85	120.28
2	H	849	GLN	CA-C-N	5.91	132.61	121.97
2	H	849	GLN	C-N-CA	5.91	132.61	121.97
1	E	472	ASN	CA-C-N	5.90	129.22	120.90
1	E	472	ASN	C-N-CA	5.90	129.22	120.90
2	F	859	PHE	N-CA-C	-5.89	100.90	110.20
2	B	109	ASP	CA-CB-CG	5.88	118.48	112.60
1	C	160	ASN	CA-C-N	5.88	129.25	120.31
1	C	160	ASN	C-N-CA	5.88	129.25	120.31
2	B	818	TRP	CA-C-N	5.88	127.97	120.56
2	B	818	TRP	C-N-CA	5.88	127.97	120.56
2	D	509	PHE	CA-CB-CG	5.84	119.64	113.80
2	F	1156	GLY	CA-C-N	5.82	132.66	121.54
2	F	1156	GLY	C-N-CA	5.82	132.66	121.54
2	B	509	PHE	CA-CB-CG	5.82	119.62	113.80
2	D	987	ALA	CA-C-N	5.77	129.03	120.95
2	D	987	ALA	C-N-CA	5.77	129.03	120.95
2	D	817	ARG	N-CA-C	5.76	118.03	111.11
1	C	793	ASP	CA-CB-CG	5.76	118.36	112.60
1	A	283	ASP	N-CA-C	-5.74	100.96	109.11
2	B	574	HIS	CA-C-N	5.74	128.24	120.38
2	B	574	HIS	C-N-CA	5.74	128.24	120.38
2	B	856	SER	CA-C-N	5.74	135.79	121.80
2	B	856	SER	C-N-CA	5.74	135.79	121.80
1	A	101	SER	CA-C-N	5.72	129.40	120.82
1	A	101	SER	C-N-CA	5.72	129.40	120.82
2	D	598	ALA	N-CA-C	-5.71	102.03	110.48
2	H	1139	SER	CA-C-N	5.71	127.86	120.44
2	H	1139	SER	C-N-CA	5.71	127.86	120.44
1	G	732	ASN	CA-CB-CG	5.71	118.31	112.60
1	C	747	LEU	CA-C-N	5.69	130.45	122.08
1	C	747	LEU	C-N-CA	5.69	130.45	122.08
2	D	1284	TYR	CA-C-N	5.69	125.89	120.43
2	D	1284	TYR	C-N-CA	5.69	125.89	120.43
1	A	815	LEU	CA-C-N	5.69	130.34	121.76
1	A	815	LEU	C-N-CA	5.69	130.34	121.76
1	E	806	ASN	CA-CB-CG	5.68	118.28	112.60
2	H	631	ASN	CA-CB-CG	5.67	118.27	112.60
1	C	686	PHE	CA-CB-CG	5.65	119.45	113.80
2	D	1168	GLY	N-CA-C	5.62	118.02	110.43
2	F	845	ILE	CB-CA-C	5.62	116.76	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	99	ASN	CA-CB-CG	5.62	118.22	112.60
1	G	806	ASN	CA-CB-CG	5.60	118.20	112.60
1	C	293	GLN	CA-C-N	5.59	128.08	120.54
1	C	293	GLN	C-N-CA	5.59	128.08	120.54
2	H	892	ASP	CA-CB-CG	5.59	118.19	112.60
1	G	655	GLY	N-CA-C	5.58	118.74	110.42
1	G	513	GLU	CA-C-N	5.57	126.28	119.99
1	G	513	GLU	C-N-CA	5.57	126.28	119.99
2	H	1284	TYR	CA-C-N	5.57	125.78	120.43
2	H	1284	TYR	C-N-CA	5.57	125.78	120.43
2	B	631	ASN	CA-CB-CG	5.56	118.16	112.60
2	D	762	ASP	CA-CB-CG	5.56	118.16	112.60
2	B	246	VAL	CA-C-N	5.55	128.65	120.82
2	B	246	VAL	C-N-CA	5.55	128.65	120.82
2	B	183	ILE	CA-C-N	5.54	129.14	120.82
2	B	183	ILE	C-N-CA	5.54	129.14	120.82
2	B	947	ASN	CA-C-N	5.54	128.26	120.28
2	B	947	ASN	C-N-CA	5.54	128.26	120.28
2	D	226	GLU	CB-CG-CD	5.54	122.02	112.60
2	D	571	LEU	CA-C-N	5.54	127.96	120.38
2	D	571	LEU	C-N-CA	5.54	127.96	120.38
2	F	858	PRO	N-CA-C	5.54	119.90	111.15
2	H	383	GLY	CA-C-N	5.54	128.04	120.46
2	H	383	GLY	C-N-CA	5.54	128.04	120.46
2	B	62	ASP	CA-CB-CG	5.52	118.12	112.60
2	B	530	TRP	CA-C-N	-5.52	113.88	122.16
2	B	530	TRP	C-N-CA	-5.52	113.88	122.16
1	A	184	TRP	CA-C-N	5.52	127.94	120.38
1	A	184	TRP	C-N-CA	5.52	127.94	120.38
1	C	145	LEU	CA-C-N	5.51	127.93	120.38
1	C	145	LEU	C-N-CA	5.51	127.93	120.38
2	B	847	PHE	CA-C-N	5.50	131.34	121.15
2	B	847	PHE	C-N-CA	5.50	131.34	121.15
1	E	101	SER	CA-C-N	5.50	127.92	120.38
1	E	101	SER	C-N-CA	5.50	127.92	120.38
2	F	183	ILE	CA-C-N	5.50	129.07	120.82
2	F	183	ILE	C-N-CA	5.50	129.07	120.82
1	A	422	ASP	CA-CB-CG	5.49	118.09	112.60
1	C	766	GLN	CA-C-N	5.49	127.95	120.54
1	C	766	GLN	C-N-CA	5.49	127.95	120.54
1	A	263	GLY	N-CA-C	5.48	118.36	112.33
2	F	1139	SER	CA-C-N	5.48	127.89	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1139	SER	C-N-CA	5.48	127.89	120.44
1	E	145	LEU	CA-C-N	5.48	127.88	120.38
1	E	145	LEU	C-N-CA	5.48	127.88	120.38
1	C	367	SER	CA-C-N	5.47	131.98	121.54
1	C	367	SER	C-N-CA	5.47	131.98	121.54
1	A	554	SER	CA-C-N	5.46	127.60	120.28
1	A	554	SER	C-N-CA	5.46	127.60	120.28
1	C	750	ASP	CA-C-N	5.46	127.86	120.38
1	C	750	ASP	C-N-CA	5.46	127.86	120.38
1	C	708	GLY	N-CA-C	-5.46	106.12	115.08
1	E	293	GLN	CA-C-N	5.46	127.60	120.28
1	E	293	GLN	C-N-CA	5.46	127.60	120.28
2	H	1331	VAL	CA-C-N	5.46	128.14	120.28
2	H	1331	VAL	C-N-CA	5.46	128.14	120.28
2	F	103	VAL	CA-C-N	5.46	128.84	120.82
2	F	103	VAL	C-N-CA	5.46	128.84	120.82
2	H	856	SER	CA-C-N	5.45	135.10	121.80
2	H	856	SER	C-N-CA	5.45	135.10	121.80
2	D	1256	GLY	CA-C-N	5.45	127.52	120.44
2	D	1256	GLY	C-N-CA	5.45	127.52	120.44
1	C	101	SER	CA-C-N	5.42	127.55	120.28
1	C	101	SER	C-N-CA	5.42	127.55	120.28
2	H	632	VAL	N-CA-C	-5.42	107.19	112.29
1	G	634	ASP	CA-CB-CG	5.41	118.01	112.60
2	D	576	ASN	CA-C-N	5.40	127.52	120.28
2	D	576	ASN	C-N-CA	5.40	127.52	120.28
1	A	805	ASN	CA-C-N	5.39	130.06	122.46
1	A	805	ASN	C-N-CA	5.39	130.06	122.46
2	D	855	ASN	CA-CB-CG	5.39	117.99	112.60
2	H	849	GLN	N-CA-C	-5.39	106.38	113.17
2	B	571	LEU	CA-C-N	5.39	127.76	120.38
2	B	571	LEU	C-N-CA	5.39	127.76	120.38
2	B	980	ASP	CA-CB-CG	5.39	117.99	112.60
2	F	134	ASP	CA-CB-CG	5.39	117.99	112.60
2	H	630	ASP	CA-CB-CG	5.39	117.99	112.60
2	B	1119	ASN	CA-C-N	5.38	127.43	120.44
2	B	1119	ASN	C-N-CA	5.38	127.43	120.44
1	C	795	ASP	CA-C-N	5.37	130.04	122.09
1	C	795	ASP	C-N-CA	5.37	130.04	122.09
2	D	142	ASP	N-CA-C	5.37	119.53	111.96
1	G	184	TRP	CA-C-N	5.37	127.73	120.38
1	G	184	TRP	C-N-CA	5.37	127.73	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	632	VAL	N-CA-C	-5.36	107.52	112.83
2	H	417	ASP	CA-CB-CG	5.36	117.96	112.60
2	F	316	GLU	N-CA-C	5.35	118.03	111.82
1	A	732	ASN	CA-CB-CG	5.33	117.92	112.60
2	F	980	ASP	CA-CB-CG	5.32	117.92	112.60
2	B	142	ASP	N-CA-C	5.32	119.46	111.96
2	D	253	GLY	N-CA-C	-5.32	108.07	114.66
1	E	473	HIS	N-CA-C	5.31	117.73	110.24
2	F	1031	PHE	CA-C-N	5.31	127.66	120.44
2	F	1031	PHE	C-N-CA	5.31	127.66	120.44
2	F	903	ASN	CA-C-N	5.31	127.58	120.58
2	F	903	ASN	C-N-CA	5.31	127.58	120.58
1	A	473	HIS	N-CA-C	5.30	118.00	110.10
2	D	333	GLU	CA-C-N	5.30	129.07	120.60
2	D	333	GLU	C-N-CA	5.30	129.07	120.60
1	E	492	GLN	CA-C-N	5.29	127.69	120.54
1	E	492	GLN	C-N-CA	5.29	127.69	120.54
2	D	1348	GLN	N-CA-C	-5.29	105.05	112.25
1	G	781	PRO	CA-C-N	5.29	131.64	121.54
1	G	781	PRO	C-N-CA	5.29	131.64	121.54
1	A	686	PHE	CA-CB-CG	5.29	119.08	113.80
2	D	569	ASP	CA-CB-CG	5.28	117.88	112.60
2	F	1169	VAL	N-CA-C	5.28	115.45	107.80
2	D	856	SER	N-CA-C	-5.28	104.36	111.54
2	B	80	ILE	N-CA-CB	5.28	116.47	110.72
2	B	217	ASN	CA-C-N	5.26	128.07	120.38
2	B	217	ASN	C-N-CA	5.26	128.07	120.38
2	D	760	THR	CA-C-N	5.26	127.33	120.28
2	D	760	THR	C-N-CA	5.26	127.33	120.28
1	G	73	ASN	N-CA-C	-5.26	99.61	110.80
2	F	817	ARG	N-CA-C	5.25	117.41	111.11
1	C	473	HIS	N-CA-C	5.25	117.92	110.10
2	D	1136	ASN	CA-CB-CG	5.24	117.84	112.60
2	H	1115	TYR	CA-C-N	-5.24	112.69	121.39
2	H	1115	TYR	C-N-CA	-5.24	112.69	121.39
1	A	745	ILE	N-CA-CB	5.23	116.80	110.95
2	D	82	GLY	CA-C-N	5.23	129.50	121.19
2	D	82	GLY	C-N-CA	5.23	129.50	121.19
2	D	946	THR	CA-C-N	5.23	127.81	120.28
2	D	946	THR	C-N-CA	5.23	127.81	120.28
2	D	861	PRO	N-CA-C	-5.22	103.00	111.19
2	H	1017	ASP	CA-CB-CG	5.21	117.81	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1265	PHE	CA-CB-CG	5.21	119.02	113.80
2	D	614	GLY	CA-C-N	5.21	127.26	120.28
2	D	614	GLY	C-N-CA	5.21	127.26	120.28
2	F	857	THR	CA-C-O	-5.20	113.03	120.16
2	D	858	PRO	N-CA-C	5.20	119.37	111.15
2	B	1089	ASN	CA-CB-CG	5.20	117.80	112.60
1	E	655	GLY	N-CA-C	5.19	118.28	110.18
2	B	847	PHE	CA-CB-CG	5.19	118.99	113.80
2	D	977	ASN	CA-CB-CG	5.19	117.79	112.60
1	A	61	ASP	CA-C-N	5.19	127.95	120.38
1	A	61	ASP	C-N-CA	5.19	127.95	120.38
2	D	631	ASN	CA-CB-CG	5.19	117.79	112.60
2	B	417	ASP	CA-CB-CG	5.19	117.79	112.60
1	G	314	ASN	CA-CB-CG	5.18	117.78	112.60
2	F	509	PHE	CA-CB-CG	5.18	118.98	113.80
2	D	812	ASN	CA-CB-CG	5.18	117.78	112.60
2	B	779	ASN	CA-C-N	5.17	127.19	120.26
2	B	779	ASN	C-N-CA	5.17	127.19	120.26
2	D	383	GLY	CA-C-N	5.17	127.54	120.46
2	D	383	GLY	C-N-CA	5.17	127.54	120.46
2	H	1239	GLY	CA-C-N	5.16	128.18	120.95
2	H	1239	GLY	C-N-CA	5.16	128.18	120.95
2	B	861	PRO	N-CA-C	-5.16	103.17	111.38
1	E	723	ASP	CA-CB-CG	5.16	117.76	112.60
1	C	687	THR	N-CA-C	-5.15	102.56	110.14
1	C	353	LYS	CA-C-N	5.15	127.18	120.28
1	C	353	LYS	C-N-CA	5.15	127.18	120.28
2	D	617	PHE	CA-C-N	5.15	129.96	121.87
2	D	617	PHE	C-N-CA	5.15	129.96	121.87
2	F	246	VAL	CA-C-N	5.15	128.09	120.82
2	F	246	VAL	C-N-CA	5.15	128.09	120.82
2	D	970	GLY	CA-C-N	5.14	127.69	120.28
2	D	970	GLY	C-N-CA	5.14	127.69	120.28
1	G	376	LYS	CA-C-N	5.14	129.86	122.35
1	G	376	LYS	C-N-CA	5.14	129.86	122.35
1	C	625	PHE	CA-CB-CG	5.14	118.94	113.80
1	G	207	LEU	CA-C-N	5.14	129.37	120.58
1	G	207	LEU	C-N-CA	5.14	129.37	120.58
1	G	691	SER	CA-C-N	5.13	128.11	120.31
1	G	691	SER	C-N-CA	5.13	128.11	120.31
2	H	1156	GLY	CA-C-N	5.13	131.33	121.54
2	H	1156	GLY	C-N-CA	5.13	131.33	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	762	ASP	CA-C-N	5.12	127.66	120.28
2	H	762	ASP	C-N-CA	5.12	127.66	120.28
2	B	1129	ASP	CA-CB-CG	5.12	117.72	112.60
2	B	854	ASN	CA-CB-CG	5.12	117.72	112.60
1	G	409	SER	CA-C-N	5.12	128.50	120.82
1	G	409	SER	C-N-CA	5.12	128.50	120.82
2	B	380	ASN	CA-CB-CG	5.12	117.72	112.60
1	C	364	GLU	CA-C-N	5.11	129.40	122.19
1	C	364	GLU	C-N-CA	5.11	129.40	122.19
2	H	647	THR	CA-C-N	5.11	127.64	120.28
2	H	647	THR	C-N-CA	5.11	127.64	120.28
1	C	767	SER	N-CA-C	5.09	117.22	111.11
2	F	647	THR	CA-C-N	5.09	127.11	120.28
2	F	647	THR	C-N-CA	5.09	127.11	120.28
2	D	579	ALA	CA-C-N	5.09	127.10	120.28
2	D	579	ALA	C-N-CA	5.09	127.10	120.28
2	F	967	HIS	CA-C-N	5.09	127.10	120.28
2	F	967	HIS	C-N-CA	5.09	127.10	120.28
2	F	1337	THR	N-CA-C	-5.09	107.01	114.39
1	C	616	ASP	CA-CB-CG	5.08	117.69	112.60
2	F	762	ASP	CA-C-N	5.08	127.09	120.28
2	F	762	ASP	C-N-CA	5.08	127.09	120.28
2	F	1157	THR	CA-C-N	5.08	131.25	121.54
2	F	1157	THR	C-N-CA	5.08	131.25	121.54
2	B	858	PRO	N-CA-C	5.07	119.16	111.15
2	F	774	GLY	N-CA-C	-5.07	108.33	115.32
2	H	977	ASN	CA-C-N	5.06	127.32	120.38
2	H	977	ASN	C-N-CA	5.06	127.32	120.38
1	E	376	LYS	CA-C-N	5.06	129.92	122.63
1	E	376	LYS	C-N-CA	5.06	129.92	122.63
2	B	906	GLN	CB-CG-CD	5.06	121.20	112.60
2	D	630	ASP	CA-CB-CG	5.06	117.66	112.60
2	D	183	ILE	CA-C-N	5.05	127.36	120.54
2	D	183	ILE	C-N-CA	5.05	127.36	120.54
2	H	1189	GLU	CA-C-N	5.05	127.05	120.28
2	H	1189	GLU	C-N-CA	5.05	127.05	120.28
2	H	967	HIS	CA-C-N	5.05	127.05	120.28
2	H	967	HIS	C-N-CA	5.05	127.05	120.28
1	C	422	ASP	CA-CB-CG	5.05	117.65	112.60
2	B	1145	THR	CA-C-N	5.04	127.34	120.54
2	B	1145	THR	C-N-CA	5.04	127.34	120.54
1	E	519	ASP	CA-CB-CG	5.03	117.63	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	602	ASP	CA-CB-CG	5.03	117.63	112.60
1	C	492	GLN	CA-C-N	5.03	126.97	120.44
1	C	492	GLN	C-N-CA	5.03	126.97	120.44
1	A	145	LEU	CA-C-N	5.02	127.32	120.54
1	A	145	LEU	C-N-CA	5.02	127.32	120.54
1	C	155	THR	CA-C-N	5.02	127.50	120.28
1	C	155	THR	C-N-CA	5.02	127.50	120.28
1	C	193	LEU	N-CA-C	-5.02	104.42	110.44
1	E	514	GLY	N-CA-C	5.02	118.71	112.64
2	F	1346	PHE	CA-C-N	-5.02	114.91	122.24
2	F	1346	PHE	C-N-CA	-5.02	114.91	122.24
2	F	538	ALA	N-CA-C	-5.02	96.66	107.49
1	G	532	GLU	CB-CG-CD	5.02	121.13	112.60
2	B	1146	THR	CA-C-N	5.01	127.70	120.38
2	B	1146	THR	C-N-CA	5.01	127.70	120.38
1	A	409	SER	CA-C-N	5.01	131.11	121.54
1	A	409	SER	C-N-CA	5.01	131.11	121.54
1	C	558	SER	CA-C-N	5.01	127.00	120.28
1	C	558	SER	C-N-CA	5.01	127.00	120.28
2	B	1016	ASN	CA-C-N	5.01	127.49	120.28
2	B	1016	ASN	C-N-CA	5.01	127.49	120.28
1	C	95	ASN	CA-CB-CG	5.01	117.61	112.60
1	C	446	ASP	CA-CB-CG	5.01	117.61	112.60
2	H	774	GLY	N-CA-C	-5.00	108.22	115.27

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	6013	0	5805	62	0
1	C	5999	0	5794	73	0
1	E	6017	0	5809	63	0
1	G	6023	0	5814	90	0
2	B	9938	0	9645	149	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	9918	0	9631	163	0
2	F	9822	0	9548	159	0
2	H	9798	0	9529	206	0
3	A	62	0	0	0	0
3	B	121	0	0	2	0
3	C	87	0	0	0	0
3	D	137	0	0	5	0
3	E	69	0	0	0	0
3	F	70	0	0	1	0
3	G	49	0	0	0	0
3	H	58	0	0	2	0
All	All	64181	0	61575	933	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 7.

All (933) 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:G:812:ASP:OD2	1:G:815:LEU:CD1	1.72	1.35
2:B:524:PRO:HD2	2:B:557:MET:HE2	1.31	1.12
1:G:255:VAL:HG23	1:G:726:GLN:HB3	1.19	1.11
1:G:812:ASP:OD2	1:G:815:LEU:HD13	1.36	1.09
1:G:812:ASP:OD2	1:G:815:LEU:HD12	1.54	1.06
1:G:460:GLN:CA	2:H:812:ASN:HD21	1.68	1.05
1:E:73:ASN:HD21	1:E:327:ARG:HH22	1.05	1.01
1:G:460:GLN:N	2:H:812:ASN:HD21	1.57	1.01
2:H:989:SER:OG	2:H:1115:TYR:CA	2.08	1.01
1:C:66:ILE:HD11	1:C:69:GLN:HG3	1.43	0.99
2:B:527:THR:HG23	2:B:678:LEU:HD23	1.46	0.97
2:H:989:SER:CB	2:H:1115:TYR:O	2.13	0.97
2:H:994:SER:OG	2:H:1137:MET:HE2	1.65	0.96
2:B:611:ASP:OD1	2:B:614:GLY:HA2	1.66	0.96
1:G:255:VAL:HG22	1:G:261:SER:HB2	1.49	0.95
1:C:440:LYS:O	1:C:444:THR:HG23	1.72	0.90
1:E:66:ILE:HD11	1:E:69:GLN:HG3	1.53	0.90
2:B:280:GLU:HG3	2:B:650:LEU:HD12	1.55	0.89
2:D:685:GLU:HG3	2:D:686:ASN:H	1.37	0.88
1:G:460:GLN:HA	2:H:812:ASN:HD21	1.38	0.87
1:G:460:GLN:CA	2:H:812:ASN:ND2	2.37	0.87
2:H:1265:PHE:HA	2:H:1312:GLN:NE2	1.89	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1344:GLN:HG3	2:F:1348:GLN:HB3	1.57	0.86
2:H:989:SER:OG	2:H:1115:TYR:C	2.18	0.86
2:D:852:PRO:HB2	2:D:857:THR:HG22	1.57	0.84
2:H:527:THR:HG23	2:H:678:LEU:HD23	1.59	0.84
2:H:1301:ARG:HH21	2:H:1301:ARG:HG3	1.39	0.84
1:E:540:GLN:HG2	1:E:579:PRO:HA	1.58	0.84
1:G:460:GLN:HA	2:H:812:ASN:ND2	1.93	0.83
2:H:1265:PHE:HB3	2:H:1312:GLN:HE21	1.44	0.83
2:H:318:THR:HG23	2:H:319:GLU:H	1.42	0.82
1:A:440:LYS:O	1:A:444:THR:HG23	1.80	0.82
1:G:66:ILE:HD11	1:G:69:GLN:HG3	1.62	0.82
2:H:1267:LEU:H	2:H:1267:LEU:HD12	1.44	0.82
1:G:749:GLN:HE21	1:G:749:GLN:HA	1.46	0.81
1:G:540:GLN:HG2	1:G:579:PRO:HA	1.63	0.81
2:D:1344:GLN:HG3	2:D:1348:GLN:HB3	1.63	0.80
1:G:652:THR:HG21	1:G:657:VAL:CG1	2.11	0.80
2:D:1301:ARG:HH21	2:D:1301:ARG:HG3	1.45	0.79
2:H:1265:PHE:CA	2:H:1312:GLN:NE2	2.45	0.78
2:F:1005:THR:HG22	2:F:1007:GLN:H	1.49	0.78
1:G:255:VAL:CG2	1:G:261:SER:HB2	2.12	0.78
2:F:524:PRO:HD2	2:F:557:MET:HE2	1.66	0.78
2:B:766:ASP:OD2	2:B:797:SER:HB3	1.84	0.78
2:H:989:SER:HB3	2:H:1115:TYR:O	1.84	0.77
2:D:527:THR:HG23	2:D:678:LEU:HD23	1.66	0.77
2:F:988:ASP:OD2	2:F:993:SER:HB2	1.85	0.77
2:F:527:THR:HG23	2:F:678:LEU:HD23	1.67	0.76
1:G:255:VAL:CG2	1:G:726:GLN:HB3	2.10	0.76
2:B:1305:ILE:HD11	2:B:1317:ARG:HB3	1.68	0.76
2:F:1301:ARG:HH21	2:F:1301:ARG:HG3	1.49	0.76
2:D:766:ASP:OD2	2:D:797:SER:HB3	1.86	0.76
1:A:66:ILE:HD12	1:A:78:VAL:HG13	1.67	0.75
2:F:845:ILE:HG23	2:F:849:GLN:OE1	1.85	0.75
1:A:596:ARG:HB2	1:A:599:ASN:ND2	2.01	0.75
2:H:852:PRO:HB2	2:H:857:THR:HG22	1.67	0.75
1:A:366:THR:HG22	1:A:494:SER:HA	1.65	0.75
2:B:524:PRO:HD2	2:B:557:MET:CE	2.14	0.75
1:G:460:GLN:N	2:H:812:ASN:ND2	2.35	0.75
2:H:845:ILE:HG21	2:H:849:GLN:OE1	1.85	0.75
2:B:924:ASN:HB2	2:B:985:PHE:HA	1.69	0.75
2:D:1254:LYS:HB3	2:D:1259:ILE:CD1	2.16	0.74
2:D:695:ALA:HB3	2:D:751:THR:HG22	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:989:SER:OG	2:H:1115:TYR:CB	2.36	0.74
1:A:596:ARG:HB2	1:A:599:ASN:HD22	1.53	0.74
2:B:988:ASP:OD1	2:B:993:SER:HB2	1.88	0.74
2:D:1005:THR:HG22	2:D:1007:GLN:H	1.51	0.74
1:E:65:GLN:HE22	1:E:83:ARG:HG3	1.51	0.74
2:B:65:LEU:HB3	2:B:91:VAL:HG13	1.70	0.73
2:H:989:SER:OG	2:H:1115:TYR:O	2.04	0.73
1:G:66:ILE:HD11	1:G:69:GLN:CG	2.18	0.73
1:C:66:ILE:HD11	1:C:69:GLN:CG	2.16	0.73
1:G:652:THR:HG21	1:G:657:VAL:HG12	1.71	0.73
2:F:773:ASN:HD22	2:F:775:LYS:HB2	1.52	0.72
1:G:652:THR:CG2	1:G:657:VAL:CG1	2.66	0.72
1:A:136:ASN:H	1:A:136:ASN:HD22	1.36	0.72
2:H:989:SER:OG	2:H:1115:TYR:HB2	1.90	0.72
2:H:1265:PHE:CB	2:H:1312:GLN:HE21	2.03	0.72
1:G:73:ASN:HD21	1:G:327:ARG:HH22	1.37	0.72
1:G:66:ILE:HD12	1:G:78:VAL:HG13	1.72	0.71
2:H:989:SER:OG	2:H:1115:TYR:N	2.22	0.71
1:A:65:GLN:HE22	1:A:83:ARG:HG3	1.55	0.71
2:F:763:GLN:HE22	2:F:799:ILE:HD13	1.56	0.71
2:B:1269:VAL:HA	2:B:1272:LEU:HD12	1.73	0.71
2:H:100:ILE:O	2:H:103:VAL:HG22	1.91	0.71
2:F:1305:ILE:HD11	2:F:1317:ARG:HB3	1.73	0.71
2:F:857:THR:HG23	2:F:858:PRO:HD2	1.72	0.71
2:H:65:LEU:HB3	2:H:91:VAL:HG13	1.71	0.71
2:F:150:ASN:H	2:F:151:PRO:HD3	1.54	0.70
2:H:138:ARG:HG2	2:H:1242:ALA:HB1	1.73	0.70
2:D:773:ASN:HD21	2:D:975:ASN:HB3	1.55	0.70
2:D:850:VAL:CG2	2:D:859:PHE:HB3	2.20	0.70
2:D:773:ASN:HD22	2:D:775:LYS:HB2	1.55	0.70
2:D:685:GLU:HG3	2:D:686:ASN:N	2.07	0.70
2:F:278:LYS:HB2	2:F:650:LEU:HD11	1.73	0.70
2:F:773:ASN:HD21	2:F:975:ASN:HB3	1.57	0.69
2:D:1254:LYS:HB3	2:D:1259:ILE:HD11	1.75	0.69
2:B:773:ASN:HD22	2:B:775:LYS:HB2	1.56	0.69
1:C:454:ASN:ND2	1:C:467:VAL:H	1.91	0.69
1:C:65:GLN:HE22	1:C:83:ARG:HG3	1.58	0.69
2:H:1005:THR:HG22	2:H:1007:GLN:H	1.57	0.68
2:H:845:ILE:HG23	2:H:849:GLN:NE2	2.09	0.68
1:E:410:SER:HB2	1:E:421:LYS:HG3	1.75	0.68
2:F:362:ASP:HB3	2:F:365:LYS:HG2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:845:ILE:CG2	2:H:849:GLN:HE22	2.06	0.68
2:H:1265:PHE:CA	2:H:1312:GLN:HE21	2.04	0.68
1:C:808:LEU:HD11	2:D:702:LEU:HD12	1.76	0.67
2:D:835:ARG:HD3	2:D:845:ILE:HG21	1.75	0.67
2:D:946:THR:HA	2:D:1120:THR:CG2	2.24	0.67
1:G:410:SER:HB2	1:G:421:LYS:HG3	1.75	0.67
2:F:1230:SER:HB3	2:F:1235:ASN:ND2	2.09	0.67
2:H:103:VAL:HG21	2:H:118:VAL:HG22	1.75	0.67
1:A:155:THR:HG22	1:A:157:TYR:H	1.58	0.67
2:B:262:SER:HB2	2:B:643:SER:HB3	1.77	0.67
2:B:1246:SER:O	2:B:1249:GLU:OE2	2.12	0.67
1:E:73:ASN:ND2	1:E:327:ARG:HH22	1.85	0.67
2:F:127:ASN:HD21	2:F:147:LYS:HE3	1.60	0.67
1:G:704:ASN:HB3	1:G:707:SER:HB2	1.76	0.67
2:B:994:SER:HB2	2:B:1137:MET:HE2	1.77	0.66
1:C:596:ARG:HB2	1:C:599:ASN:ND2	2.10	0.66
2:D:226:GLU:HG2	2:D:239:ARG:HH21	1.59	0.66
2:H:1265:PHE:HA	2:H:1312:GLN:HE22	1.58	0.66
1:C:454:ASN:HD22	1:C:467:VAL:H	1.42	0.66
2:D:65:LEU:HB3	2:D:91:VAL:HG13	1.78	0.66
1:G:766:GLN:O	2:H:742:ARG:HD2	1.95	0.65
2:F:424:LYS:HG2	2:F:433:ASP:HA	1.76	0.65
2:F:1003:ASN:HB3	2:F:1102:PRO:HG2	1.77	0.65
2:D:226:GLU:HG2	2:D:239:ARG:NH2	2.11	0.65
2:H:422:GLY:HA2	2:H:439:SER:OG	1.97	0.65
2:F:857:THR:HG23	2:F:858:PRO:CD	2.27	0.65
2:H:1305:ILE:HD11	2:H:1317:ARG:HB3	1.78	0.64
2:B:527:THR:HG23	2:B:678:LEU:CD2	2.24	0.64
2:B:835:ARG:HD3	2:B:845:ILE:HG21	1.80	0.64
2:H:131:ARG:HB2	2:H:142:ASP:OD1	1.96	0.64
2:F:924:ASN:HB2	2:F:985:PHE:HA	1.78	0.64
1:G:347:TRP:HH2	1:G:401:LYS:HG3	1.61	0.64
2:H:1265:PHE:HB3	2:H:1312:GLN:NE2	2.10	0.64
2:D:590:GLN:CD	2:D:906:GLN:HG2	2.23	0.64
2:D:822:PRO:HB2	2:D:1189:GLU:HB2	1.80	0.64
2:F:341:VAL:HG22	2:F:358:VAL:HB	1.80	0.64
2:H:366:MET:HG3	2:H:370:TYR:HE1	1.61	0.63
2:H:845:ILE:CG2	2:H:849:GLN:NE2	2.61	0.63
1:G:652:THR:CG2	1:G:657:VAL:HG12	2.28	0.63
1:A:687:THR:HG23	1:A:690:GLU:OE1	1.98	0.63
2:D:223:GLU:HG3	2:D:478:THR:OG1	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:280:GLU:HG3	2:H:650:LEU:HD12	1.79	0.63
2:H:114:TYR:CE2	2:H:217:ASN:ND2	2.67	0.62
1:E:574:GLN:HE21	1:E:575:SER:H	1.46	0.62
1:C:411:SER:H	1:C:421:LYS:HE3	1.63	0.62
2:B:341:VAL:HG22	2:B:358:VAL:HB	1.82	0.62
2:F:766:ASP:OD2	2:F:797:SER:HB3	1.99	0.62
2:B:921:VAL:HG13	2:B:965:LEU:HD13	1.81	0.62
1:A:104:GLN:OE1	1:A:104:GLN:HA	2.00	0.62
2:D:326:THR:OG1	2:D:329:GLN:HG3	1.99	0.62
1:G:661:PHE:CE1	1:G:668:LEU:HD23	2.35	0.62
2:D:65:LEU:HD21	2:D:127:ASN:HB3	1.82	0.62
2:F:244:SER:HB2	2:F:568:TYR:O	2.00	0.62
1:A:794:SER:H	1:A:796:GLN:HE22	1.48	0.61
2:H:366:MET:HG3	2:H:370:TYR:CE1	2.35	0.61
2:H:1268:PRO:HB3	2:H:1309:VAL:HG13	1.80	0.61
2:D:280:GLU:HG3	2:D:650:LEU:HD12	1.82	0.61
1:E:155:THR:HG23	1:E:157:TYR:H	1.64	0.61
2:F:1011:ASN:HD22	2:F:1067:SER:H	1.46	0.61
1:C:596:ARG:HB2	1:C:599:ASN:HD22	1.65	0.61
2:D:1269:VAL:HA	2:D:1272:LEU:HD12	1.83	0.61
2:F:280:GLU:HG3	2:F:650:LEU:HD12	1.81	0.61
2:F:901:ASN:HB3	2:F:958:ASN:HD21	1.66	0.61
2:H:773:ASN:HD22	2:H:775:LYS:HB2	1.64	0.61
2:B:934:ASN:O	2:B:938:GLU:HB2	2.00	0.61
2:B:1005:THR:HG22	2:B:1007:GLN:H	1.65	0.61
2:B:1248:THR:HB	2:B:1331:VAL:HG13	1.82	0.61
2:D:823:ASN:HD22	2:D:825:SER:H	1.48	0.61
2:H:822:PRO:HB2	2:H:1189:GLU:HB2	1.82	0.61
2:F:537:MET:HE1	2:F:551:LEU:HD21	1.82	0.61
2:B:278:LYS:HB2	2:B:650:LEU:HD11	1.83	0.61
2:F:837:GLN:HG3	2:F:846:PRO:HD2	1.83	0.61
2:F:1269:VAL:HA	2:F:1272:LEU:HD12	1.82	0.61
2:H:1301:ARG:HH21	2:H:1301:ARG:CG	2.10	0.61
1:A:365:THR:O	1:A:367:SER:N	2.34	0.60
1:C:66:ILE:HD12	1:C:78:VAL:HG13	1.83	0.60
2:D:226:GLU:HG3	2:D:239:ARG:NE	2.15	0.60
2:F:318:THR:HG23	2:F:319:GLU:H	1.65	0.60
2:H:114:TYR:HE2	2:H:217:ASN:ND2	1.98	0.60
2:H:924:ASN:HB2	2:H:985:PHE:HA	1.82	0.60
1:A:460:GLN:HG3	2:B:895:ASN:HB2	1.83	0.60
1:G:460:GLN:H	2:H:812:ASN:HD21	1.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:460:GLN:HA	2:F:812:ASN:OD1	2.01	0.60
1:C:405:VAL:HG11	1:C:426:ALA:HB2	1.84	0.60
1:C:766:GLN:O	2:D:742:ARG:HD2	2.02	0.60
1:A:187:GLN:O	1:A:190:GLN:HG2	2.02	0.59
1:E:346:ASP:HB3	1:E:573:THR:O	2.02	0.59
2:H:110:ASP:HA	2:H:220:VAL:HG13	1.83	0.59
2:D:262:SER:HB2	2:D:643:SER:HB3	1.84	0.59
1:C:318:PRO:HB3	1:C:382:ALA:HB1	1.84	0.59
2:F:276:ALA:HB2	2:F:655:PRO:HD3	1.85	0.59
2:H:845:ILE:HG23	2:H:849:GLN:HE22	1.65	0.59
2:H:989:SER:HA	2:H:1114:ALA:HB1	1.84	0.59
2:D:570:GLN:HG3	2:D:573:LYS:HE3	1.83	0.59
1:A:135:PRO:HB3	1:A:337:PRO:HG2	1.85	0.59
1:E:66:ILE:HD12	1:E:78:VAL:HG13	1.83	0.59
1:A:670:SER:HA	1:A:679:ILE:HG22	1.85	0.59
1:C:531:GLN:HE22	1:C:593:GLY:H	1.50	0.59
2:B:807:ILE:HG21	2:B:828:ILE:HD12	1.85	0.59
1:G:460:GLN:HG3	2:H:895:ASN:HB2	1.84	0.59
1:A:166:GLU:HG3	1:A:206:LYS:HB2	1.85	0.59
2:B:237:THR:HG22	2:B:1108:GLN:HG3	1.85	0.59
2:F:115:LEU:HD11	2:F:324:LEU:HD22	1.83	0.59
2:D:341:VAL:HG22	2:D:358:VAL:HB	1.85	0.58
1:C:704:ASN:HB3	1:C:707:SER:HB2	1.84	0.58
2:F:994:SER:HB2	2:F:1137:MET:HE2	1.84	0.58
1:G:386:SER:HB3	1:G:626:SER:OG	2.03	0.58
2:F:777:PHE:HB3	2:F:795:THR:CG2	2.33	0.58
1:C:525:TYR:CE1	1:C:591:ALA:HB1	2.39	0.58
2:D:1011:ASN:HD22	2:D:1067:SER:H	1.52	0.58
2:H:773:ASN:HD21	2:H:975:ASN:HB3	1.68	0.58
1:C:574:GLN:HE21	1:C:575:SER:H	1.51	0.58
2:D:1301:ARG:HG3	2:D:1301:ARG:NH2	2.18	0.58
2:F:1259:ILE:HG12	2:F:1260:ASP:H	1.69	0.58
2:F:65:LEU:HB3	2:F:91:VAL:HG13	1.86	0.58
2:H:537:MET:HE1	2:H:551:LEU:HD21	1.86	0.58
2:H:115:LEU:HD11	2:H:324:LEU:HD22	1.86	0.58
2:B:1255:PRO:HB2	2:B:1257:ASN:OD1	2.04	0.57
2:F:620:HIS:H	2:F:620:HIS:CD2	2.20	0.57
2:B:1260:ASP:OD2	2:B:1263:ARG:HB2	2.04	0.57
1:C:521:LEU:HD23	1:C:580:VAL:HG23	1.87	0.57
2:D:1305:ILE:HD11	2:D:1317:ARG:HB3	1.86	0.57
2:F:988:ASP:OD1	2:F:1114:ALA:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:525:TYR:HE1	1:E:591:ALA:HB1	1.69	0.57
2:D:924:ASN:HB2	2:D:985:PHE:HA	1.85	0.57
2:H:742:ARG:HH11	2:H:742:ARG:HG2	1.70	0.57
2:D:244:SER:HB2	2:D:568:TYR:O	2.04	0.57
2:B:268:MET:HB2	2:B:871:SER:OG	2.04	0.57
1:G:308:HIS:CD2	1:G:326:GLU:OE2	2.58	0.57
1:A:561:SER:HB3	2:D:1178:THR:HG21	1.87	0.56
2:B:590:GLN:CD	2:B:906:GLN:HG2	2.29	0.56
2:D:1248:THR:HB	2:D:1331:VAL:HG13	1.85	0.56
2:B:226:GLU:HB2	2:B:239:ARG:CZ	2.35	0.56
2:F:1305:ILE:HD11	2:F:1317:ARG:CB	2.35	0.56
2:D:1027:TRP:CE3	2:D:1046:LEU:HB3	2.40	0.56
2:F:186:LYS:HB3	2:F:205:LEU:HB3	1.87	0.56
2:F:1029:ILE:HD11	2:F:1044:ILE:HG12	1.86	0.56
2:H:151:PRO:HG3	2:H:180:TRP:CE2	2.40	0.56
2:B:235:ASN:HD22	2:B:236:PRO:HD2	1.70	0.56
2:H:299:PRO:HD2	2:H:605:VAL:HG12	1.87	0.56
1:C:514:GLY:HA2	1:C:605:THR:O	2.05	0.56
2:D:240:LEU:HB2	2:D:584:LEU:HD22	1.87	0.56
2:F:742:ARG:HH11	2:F:742:ARG:HG2	1.71	0.56
1:C:347:TRP:HH2	1:C:401:LYS:HG3	1.71	0.56
2:D:892:ASP:HA	2:D:900:THR:HG23	1.88	0.56
2:D:1254:LYS:HB3	2:D:1259:ILE:HD13	1.85	0.56
2:D:934:ASN:O	2:D:938:GLU:HB2	2.05	0.56
2:F:68:TRP:CD1	2:F:92:ARG:HB2	2.41	0.56
2:B:115:LEU:HD11	2:B:324:LEU:HD22	1.87	0.56
2:H:1268:PRO:HB3	2:H:1309:VAL:CG1	2.35	0.56
2:D:334:LYS:HE3	3:D:1414:HOH:O	2.05	0.55
1:E:66:ILE:HD11	1:E:69:GLN:CG	2.32	0.55
2:F:845:ILE:CG2	2:F:849:GLN:OE1	2.53	0.55
1:G:369:ASN:HA	1:G:371:HIS:CD2	2.41	0.55
2:H:892:ASP:HA	2:H:900:THR:HG23	1.87	0.55
2:B:773:ASN:HB3	2:B:775:LYS:H	1.71	0.55
1:A:111:VAL:HG11	1:A:309:ILE:HG21	1.88	0.55
2:B:528:ASN:ND2	2:B:530:TRP:HE3	2.04	0.55
2:H:1003:ASN:HB3	2:H:1102:PRO:HG2	1.88	0.55
2:B:611:ASP:OD1	2:B:614:GLY:CA	2.47	0.55
2:D:693:LEU:HD21	2:D:1024:LEU:HD22	1.89	0.55
2:F:476:MET:H	2:F:479:THR:HG22	1.72	0.55
2:H:528:ASN:OD1	2:H:530:TRP:O	2.24	0.55
2:B:1046:LEU:HD12	2:B:1213:ILE:HD12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:114:TYR:HE2	2:H:217:ASN:HD21	1.54	0.55
2:H:527:THR:HG23	2:H:678:LEU:CD2	2.35	0.55
2:D:278:LYS:HB2	2:D:650:LEU:HD11	1.88	0.55
1:E:525:TYR:CE1	1:E:591:ALA:HB1	2.42	0.55
2:F:739:ASN:O	2:F:742:ARG:HB2	2.06	0.55
2:H:393:LEU:HD12	2:H:571:LEU:HD11	1.88	0.55
2:H:695:ALA:HB3	2:H:751:THR:HG22	1.88	0.55
2:H:807:ILE:HG21	2:H:828:ILE:HD12	1.88	0.55
2:H:835:ARG:NE	2:H:849:GLN:OE1	2.40	0.55
2:H:1237:ILE:O	2:H:1240:GLN:HB2	2.06	0.55
2:B:777:PHE:O	2:B:795:THR:HG22	2.06	0.55
2:B:849:GLN:HE22	2:B:883:LEU:HD12	1.72	0.55
2:D:476:MET:H	2:D:479:THR:HG22	1.71	0.55
2:D:806:MET:HG3	2:D:827:ASP:OD1	2.05	0.55
2:H:849:GLN:HG2	2:H:1122:ASN:O	2.07	0.55
2:B:590:GLN:OE1	2:B:906:GLN:HG2	2.06	0.55
2:H:989:SER:HG	2:H:1115:TYR:N	2.03	0.55
1:C:135:PRO:HB3	1:C:337:PRO:HG2	1.88	0.55
2:F:150:ASN:H	2:F:151:PRO:CD	2.20	0.54
1:C:29:LEU:HD21	1:C:124:TRP:HZ2	1.72	0.54
1:C:149:ILE:HG23	1:C:213:TYR:HB3	1.90	0.54
1:C:697:THR:HG21	1:C:719:LYS:HD2	1.88	0.54
2:D:946:THR:HA	2:D:1120:THR:HG21	1.88	0.54
1:G:155:THR:HG23	1:G:157:TYR:H	1.73	0.54
2:B:240:LEU:HB2	2:B:584:LEU:HD22	1.88	0.54
2:H:946:THR:HA	2:H:1120:THR:CG2	2.38	0.54
2:D:777:PHE:O	2:D:795:THR:HG22	2.06	0.54
2:F:590:GLN:CD	2:F:906:GLN:HG2	2.32	0.54
2:H:1230:SER:HB3	2:H:1235:ASN:ND2	2.21	0.54
2:B:391:ASN:HD22	2:B:418:ASN:HD22	1.56	0.54
1:C:320:MET:HE3	1:C:339:TRP:HZ3	1.71	0.54
2:D:773:ASN:HB3	2:D:775:LYS:H	1.72	0.54
2:H:835:ARG:NH2	2:H:884:PRO:O	2.40	0.54
2:H:1029:ILE:HD11	2:H:1044:ILE:HG12	1.90	0.54
1:E:460:GLN:HG3	2:F:895:ASN:HB2	1.89	0.54
2:B:773:ASN:HD21	2:B:975:ASN:HB3	1.71	0.54
2:H:1046:LEU:HD12	2:H:1213:ILE:HD12	1.90	0.54
1:A:66:ILE:HD12	1:A:78:VAL:CG1	2.37	0.54
2:B:695:ALA:HB3	2:B:751:THR:HG22	1.90	0.54
1:E:149:ILE:HG23	1:E:213:TYR:HB3	1.90	0.54
2:F:769:PRO:HA	2:F:776:PRO:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:652:THR:HG21	1:C:657:VAL:HG12	1.90	0.54
1:G:369:ASN:HB3	1:G:497:LYS:HE2	1.90	0.54
1:A:66:ILE:HD11	1:A:69:GLN:HB3	1.90	0.53
2:F:714:LYS:HA	2:F:717:GLU:HG3	1.90	0.53
2:F:777:PHE:O	2:F:795:THR:HG22	2.08	0.53
2:H:777:PHE:O	2:H:795:THR:HG22	2.08	0.53
2:H:422:GLY:CA	2:H:439:SER:OG	2.57	0.53
1:G:804:ASN:HD21	1:G:807:GLY:H	1.55	0.53
2:H:114:TYR:CD1	2:H:114:TYR:C	2.86	0.53
2:F:773:ASN:HB3	2:F:775:LYS:H	1.73	0.53
1:G:582:TYR:HB2	1:G:588:ILE:HG21	1.91	0.53
2:H:1259:ILE:HG12	2:H:1260:ASP:H	1.73	0.53
2:F:271:SER:HB2	2:F:868:VAL:HG22	1.90	0.53
2:F:570:GLN:HG3	2:F:573:LYS:HE3	1.90	0.53
2:D:272:THR:HG21	2:D:864:ASP:HB3	1.89	0.53
1:E:151:GLU:HB2	1:E:213:TYR:CE1	2.43	0.53
1:E:574:GLN:NE2	1:E:575:SER:H	2.07	0.53
2:H:476:MET:HB2	2:H:479:THR:HB	1.91	0.53
2:B:194:SER:HB2	2:B:200:LEU:HB3	1.91	0.53
2:B:1003:ASN:HB3	2:B:1102:PRO:HG2	1.91	0.53
1:C:794:SER:H	1:C:796:GLN:HE22	1.57	0.53
2:F:150:ASN:N	2:F:151:PRO:HD3	2.24	0.53
2:H:1011:ASN:HD22	2:H:1067:SER:H	1.56	0.53
2:H:1313:THR:HG22	2:H:1344:GLN:HB3	1.91	0.53
2:B:1008:ASP:HB3	2:B:1061:TRP:CD1	2.44	0.53
2:F:952:PRO:HG2	2:F:956:GLU:HG2	1.91	0.53
2:F:1046:LEU:HD12	2:F:1213:ILE:HD12	1.90	0.53
2:H:1263:ARG:O	2:H:1267:LEU:HD11	2.10	0.53
2:B:1301:ARG:HH21	2:B:1301:ARG:HG3	1.73	0.52
1:C:117:SER:OG	1:C:125:THR:HG22	2.10	0.52
2:F:1301:ARG:HG3	2:F:1301:ARG:NH2	2.23	0.52
1:G:460:GLN:O	2:H:812:ASN:ND2	2.42	0.52
2:D:870:PRO:HD2	2:D:874:SER:O	2.09	0.52
2:D:920:PRO:HB2	2:D:997:LEU:HG	1.92	0.52
2:D:1062:THR:HG21	2:D:1085:LYS:HB2	1.91	0.52
2:B:1234:VAL:HG13	2:B:1236:LEU:HG	1.91	0.52
2:B:476:MET:H	2:B:479:THR:HG22	1.73	0.52
1:C:475:ASN:O	2:D:817:ARG:HD2	2.10	0.52
2:D:822:PRO:HB2	2:D:1189:GLU:CB	2.40	0.52
2:D:1305:ILE:HD11	2:D:1317:ARG:CB	2.40	0.52
2:D:222:LYS:HE2	2:D:321:TRP:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:523:LEU:HG	2:F:557:MET:HE1	1.92	0.52
1:G:66:ILE:HD12	1:G:78:VAL:CG1	2.38	0.52
2:H:766:ASP:OD2	2:H:797:SER:HB3	2.10	0.52
2:B:1260:ASP:CG	2:B:1263:ARG:HB2	2.35	0.52
2:H:131:ARG:HD2	2:H:139:ALA:HB1	1.92	0.52
2:H:244:SER:HB2	2:H:568:TYR:O	2.10	0.52
2:H:989:SER:HG	2:H:1115:TYR:HB2	1.73	0.52
1:A:281:LEU:H	1:A:293:GLN:HE22	1.57	0.52
1:G:272:LYS:HE3	1:G:285:GLN:NE2	2.25	0.52
1:C:155:THR:HG23	1:C:157:TYR:H	1.74	0.52
2:D:226:GLU:HG3	2:D:239:ARG:HE	1.74	0.52
2:D:845:ILE:HG23	2:D:849:GLN:HE22	1.75	0.52
2:D:821:ILE:HD11	2:D:828:ILE:HD11	1.91	0.52
1:E:767:SER:HB2	1:E:809:PHE:CD1	2.45	0.52
2:F:903:ASN:HB2	2:F:905:PRO:HD2	1.91	0.52
2:B:769:PRO:HA	2:B:776:PRO:HA	1.92	0.51
1:G:514:GLY:HA2	1:G:605:THR:O	2.10	0.51
2:H:277:LEU:HB2	2:H:653:VAL:HB	1.92	0.51
2:H:1105:GLN:HB3	2:H:1107:TYR:CE2	2.45	0.51
2:B:903:ASN:O	2:B:907:ARG:HG3	2.10	0.51
1:C:85:VAL:HG23	1:C:107:LYS:O	2.11	0.51
2:D:1046:LEU:HD12	2:D:1213:ILE:HD12	1.92	0.51
2:H:457:MET:HA	2:H:465:PHE:O	2.09	0.51
1:C:166:GLU:HG3	1:C:206:LYS:HB2	1.92	0.51
2:D:237:THR:HG22	2:D:1108:GLN:HG3	1.90	0.51
1:E:521:LEU:HD23	1:E:580:VAL:HG23	1.92	0.51
1:G:347:TRP:CH2	1:G:401:LYS:HG3	2.43	0.51
2:D:112:LEU:HB3	3:D:1515:HOH:O	2.11	0.51
2:H:590:GLN:CD	2:H:906:GLN:HG2	2.36	0.51
1:A:197:PRO:HD2	1:A:453:ILE:HD11	1.92	0.51
2:B:920:PRO:HB2	2:B:997:LEU:HG	1.93	0.51
1:E:767:SER:HB2	1:E:809:PHE:HD1	1.76	0.51
2:F:549:LEU:HD23	2:F:698:LEU:HB2	1.91	0.51
2:H:820:PHE:CE2	2:H:895:ASN:HA	2.46	0.51
1:E:293:GLN:HA	1:E:293:GLN:NE2	2.25	0.51
2:F:127:ASN:HD21	2:F:147:LYS:CE	2.24	0.51
2:H:278:LYS:HB2	2:H:650:LEU:HD11	1.92	0.51
2:H:341:VAL:HG22	2:H:358:VAL:HB	1.92	0.51
2:B:1005:THR:HG23	3:B:1422:HOH:O	2.10	0.51
1:C:357:GLU:HA	1:C:360:LEU:HD12	1.93	0.51
1:E:545:GLY:HA3	1:E:573:THR:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:299:PRO:HD2	2:F:605:VAL:HG12	1.93	0.51
1:G:454:ASN:ND2	1:G:467:VAL:H	2.09	0.51
1:G:101:SER:HB3	1:G:106:GLU:OE1	2.11	0.51
1:G:194:ASN:HB2	1:G:483:LYS:HD2	1.92	0.51
1:A:514:GLY:HA2	1:A:605:THR:HG23	1.93	0.50
1:A:766:GLN:O	2:B:742:ARG:HD2	2.11	0.50
2:D:758:SER:HA	2:D:907:ARG:NH1	2.26	0.50
1:E:196:ASN:HA	1:E:482:ILE:HG23	1.93	0.50
2:F:807:ILE:HG21	2:F:828:ILE:HD12	1.93	0.50
1:G:175:HIS:HB3	1:G:191:HIS:CD2	2.45	0.50
2:F:574:HIS:CE1	2:F:596:GLY:HA3	2.46	0.50
1:G:782:LEU:HD22	1:G:788:ALA:HB2	1.93	0.50
2:H:296:ALA:HA	2:H:384:ILE:HG21	1.92	0.50
2:H:934:ASN:O	2:H:938:GLU:HB2	2.11	0.50
2:B:283:ARG:HD2	2:B:290:LEU:HD23	1.92	0.50
1:C:148:LEU:HD11	1:C:502:ILE:HG13	1.93	0.50
1:E:734:GLY:HA2	1:E:774:GLN:O	2.11	0.50
2:F:664:TRP:CD1	2:F:898:THR:HG22	2.46	0.50
2:F:1050:GLN:HG3	3:F:1444:HOH:O	2.10	0.50
2:B:244:SER:HB2	2:B:568:TYR:O	2.12	0.50
2:D:134:ASP:HB3	2:D:140:LEU:HD21	1.92	0.50
2:B:362:ASP:HB3	2:B:365:LYS:HG2	1.92	0.50
1:C:767:SER:HB2	1:C:809:PHE:HD1	1.76	0.50
2:H:296:ALA:HA	2:H:384:ILE:CG2	2.42	0.50
2:H:476:MET:H	2:H:479:THR:HG22	1.76	0.50
2:B:268:MET:HG3	2:B:638:GLU:OE1	2.11	0.50
2:D:921:VAL:HG13	2:D:965:LEU:HD13	1.94	0.50
2:D:1076:LYS:HB3	2:D:1169:VAL:CG1	2.42	0.50
2:H:585:LEU:HD12	2:H:1105:GLN:HG3	1.94	0.50
2:B:286:GLN:OE1	2:B:289:SER:HB3	2.10	0.50
2:B:1109:PRO:HB3	2:B:1137:MET:HE1	1.93	0.50
1:G:808:LEU:HD11	2:H:702:LEU:HD12	1.93	0.50
1:C:693:VAL:HG21	1:C:738:ILE:HD11	1.93	0.50
2:D:110:ASP:HB3	3:D:1515:HOH:O	2.11	0.50
2:H:952:PRO:HG2	2:H:956:GLU:HG2	1.93	0.50
2:D:1230:SER:HB3	2:D:1235:ASN:ND2	2.27	0.50
2:F:1008:ASP:HB3	2:F:1061:TRP:CD1	2.46	0.50
2:H:387:TYR:O	2:H:391:ASN:HB2	2.12	0.50
1:A:475:ASN:O	2:B:817:ARG:HD2	2.12	0.49
1:A:693:VAL:HG21	1:A:738:ILE:HD11	1.94	0.49
2:B:111:ASN:O	2:B:115:LEU:HG	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:ARG:HG2	2:B:1242:ALA:HB1	1.94	0.49
2:D:528:ASN:OD1	2:D:530:TRP:O	2.29	0.49
2:D:1003:ASN:HB3	2:D:1102:PRO:HG2	1.93	0.49
2:D:1301:ARG:HH22	2:D:1319:GLU:CD	2.20	0.49
2:D:851:LYS:HD3	2:D:1123:LYS:HZ2	1.77	0.49
2:F:994:SER:HB2	2:F:1137:MET:CE	2.43	0.49
1:G:65:GLN:HE22	1:G:83:ARG:HG2	1.76	0.49
2:H:362:ASP:HB3	2:H:365:LYS:HG2	1.93	0.49
2:H:852:PRO:HB2	2:H:857:THR:CG2	2.40	0.49
1:G:149:ILE:HG23	1:G:213:TYR:HB3	1.94	0.49
2:H:769:PRO:HA	2:H:776:PRO:HA	1.94	0.49
1:C:525:TYR:HE1	1:C:591:ALA:HB1	1.76	0.49
2:D:823:ASN:ND2	2:D:825:SER:H	2.11	0.49
1:E:454:ASN:ND2	1:E:467:VAL:H	2.10	0.49
2:H:821:ILE:HG22	2:H:823:ASN:H	1.77	0.49
2:H:1150:LYS:HE2	2:H:1156:GLY:HA2	1.95	0.49
2:D:402:PRO:HG2	2:D:415:LYS:O	2.12	0.49
1:E:127:VAL:HG12	1:E:128:LYS:HG3	1.94	0.49
2:H:240:LEU:HB2	2:H:584:LEU:HD22	1.95	0.49
2:H:1008:ASP:HB3	2:H:1061:TRP:CD1	2.48	0.49
2:B:277:LEU:HB2	2:B:653:VAL:HB	1.94	0.49
2:B:952:PRO:HG2	2:B:956:GLU:HG2	1.94	0.49
2:B:1233:LEU:HD21	2:B:1329:ILE:HG21	1.94	0.49
1:C:767:SER:HB2	1:C:809:PHE:CD1	2.47	0.49
2:D:806:MET:HG2	2:D:826:PRO:HG2	1.95	0.49
2:H:115:LEU:HD22	2:H:209:VAL:HG11	1.94	0.49
1:A:474:THR:HG21	1:A:479:THR:CG2	2.42	0.49
2:F:65:LEU:HD21	2:F:127:ASN:HB3	1.95	0.49
2:B:693:LEU:HD21	2:B:1024:LEU:HD22	1.95	0.49
2:B:1305:ILE:HD11	2:B:1317:ARG:CB	2.40	0.49
2:D:850:VAL:HG23	2:D:859:PHE:HB3	1.92	0.49
2:D:936:ASP:HB2	3:D:1520:HOH:O	2.12	0.49
2:H:295:PHE:HB3	3:H:1407:HOH:O	2.11	0.49
2:H:920:PRO:HB2	2:H:997:LEU:HG	1.95	0.49
1:C:117:SER:OG	1:C:125:THR:CG2	2.60	0.48
2:B:1029:ILE:HD11	2:B:1044:ILE:HG12	1.93	0.48
2:D:697:ILE:HD12	2:D:749:ARG:HB2	1.94	0.48
2:F:806:MET:HG3	2:F:827:ASP:OD1	2.13	0.48
2:F:821:ILE:HG22	2:F:823:ASN:H	1.77	0.48
2:H:68:TRP:CD1	2:H:92:ARG:HB2	2.48	0.48
1:A:127:VAL:HG12	1:A:128:LYS:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:969:TYR:HB3	2:B:971:PHE:CD1	2.48	0.48
1:C:133:ASP:O	1:C:337:PRO:HD3	2.13	0.48
2:D:852:PRO:HB2	2:D:857:THR:CG2	2.35	0.48
2:F:742:ARG:HG2	2:F:742:ARG:NH1	2.29	0.48
2:B:98:LEU:HD12	2:B:125:GLN:HG2	1.94	0.48
1:C:359:GLN:HG2	1:C:405:VAL:HG12	1.96	0.48
2:D:475:LYS:HD2	2:D:479:THR:O	2.13	0.48
1:E:86:LYS:HB2	1:E:105:GLY:HA3	1.95	0.48
2:F:240:LEU:HB2	2:F:584:LEU:HD22	1.95	0.48
2:B:742:ARG:HG2	2:B:742:ARG:HH11	1.79	0.48
1:C:111:VAL:HG11	1:C:309:ILE:HG21	1.96	0.48
2:D:946:THR:HA	2:D:1120:THR:HG23	1.94	0.48
2:D:1240:GLN:HA	2:D:1240:GLN:OE1	2.13	0.48
2:F:327:THR:HG22	2:F:410:ASP:OD2	2.13	0.48
1:G:767:SER:HB2	1:G:809:PHE:CD1	2.48	0.48
1:E:693:VAL:HG21	1:E:738:ILE:HD11	1.96	0.48
2:H:821:ILE:HD13	2:H:826:PRO:HA	1.96	0.48
1:A:521:LEU:HD23	1:A:580:VAL:HG23	1.96	0.48
2:H:845:ILE:HG21	2:H:849:GLN:CD	2.39	0.48
2:H:191:VAL:HG22	2:H:203:VAL:HG12	1.96	0.48
2:B:259:THR:HG22	2:B:278:LYS:HD3	1.94	0.48
1:G:767:SER:HB2	1:G:809:PHE:HD1	1.77	0.48
2:H:235:ASN:HD22	2:H:236:PRO:HD2	1.79	0.48
2:H:1281:TYR:HB2	2:H:1284:TYR:HD2	1.79	0.48
2:B:180:TRP:O	2:B:184:LYS:HB2	2.14	0.48
2:D:328:ASP:HB2	3:D:1424:HOH:O	2.13	0.48
1:E:293:GLN:HA	1:E:293:GLN:HE21	1.79	0.48
1:E:581:PRO:HG3	1:E:654:GLY:HA3	1.96	0.48
2:D:1254:LYS:CB	2:D:1259:ILE:HD11	2.43	0.47
1:E:136:ASN:H	1:E:136:ASN:HD22	1.61	0.47
2:H:504:PRO:HG2	2:H:507:VAL:HG23	1.96	0.47
2:H:1003:ASN:ND2	2:H:1146:THR:HG21	2.29	0.47
2:H:1305:ILE:HD11	2:H:1317:ARG:CB	2.43	0.47
2:D:299:PRO:HD2	2:D:605:VAL:HG12	1.96	0.47
2:D:393:LEU:HD23	2:D:565:ARG:HD2	1.95	0.47
2:D:947:ASN:HD22	2:D:947:ASN:H	1.63	0.47
2:F:277:LEU:HB2	2:F:653:VAL:HB	1.96	0.47
2:F:467:PHE:CG	2:F:542:VAL:HG21	2.49	0.47
2:F:1067:SER:HB3	2:F:1077:SER:OG	2.15	0.47
2:F:1187:LYS:O	2:F:1196:THR:HG21	2.14	0.47
1:G:792:LYS:HE3	1:G:797:ASN:HD21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:773:ASN:HB3	2:H:775:LYS:H	1.79	0.47
1:A:474:THR:HG21	1:A:479:THR:HG21	1.97	0.47
2:D:327:THR:HG22	2:D:410:ASP:OD2	2.13	0.47
2:D:1076:LYS:HB3	2:D:1169:VAL:HG12	1.96	0.47
2:F:847:PHE:CD2	2:F:850:VAL:HB	2.50	0.47
2:B:393:LEU:HD23	2:B:565:ARG:HD2	1.96	0.47
2:D:457:MET:HA	2:D:465:PHE:O	2.14	0.47
1:E:460:GLN:CA	2:F:812:ASN:OD1	2.63	0.47
2:F:422:GLY:HA2	2:F:439:SER:HB2	1.97	0.47
2:F:693:LEU:HD21	2:F:1024:LEU:HD22	1.97	0.47
2:H:78:LEU:O	2:H:87:SER:HA	2.14	0.47
1:A:710:TRP:HB2	1:A:740:VAL:HB	1.96	0.47
1:E:294:LEU:O	1:E:298:SER:HB2	2.15	0.47
2:F:947:ASN:HD22	2:F:947:ASN:H	1.61	0.47
1:G:281:LEU:H	1:G:293:GLN:HE22	1.62	0.47
2:H:851:LYS:HD3	2:H:1123:LYS:HZ2	1.79	0.47
2:H:1265:PHE:O	2:H:1312:GLN:NE2	2.47	0.47
2:D:111:ASN:O	2:D:115:LEU:HG	2.14	0.47
2:D:411:GLU:HB3	2:D:415:LYS:HD3	1.97	0.47
2:D:1032:THR:HG22	2:D:1033:ASP:OD1	2.14	0.47
1:E:281:LEU:H	1:E:293:GLN:HE22	1.62	0.47
1:E:514:GLY:HA2	1:E:605:THR:O	2.15	0.47
2:H:114:TYR:HE1	2:H:118:VAL:HG21	1.79	0.47
2:B:65:LEU:HD21	2:B:127:ASN:HB3	1.96	0.47
1:C:293:GLN:OE1	1:C:293:GLN:HA	2.14	0.47
2:D:835:ARG:HB2	2:D:845:ILE:HD13	1.97	0.47
2:F:457:MET:HA	2:F:465:PHE:O	2.14	0.47
2:F:1229:VAL:HG22	2:F:1239:GLY:HA2	1.96	0.47
2:H:237:THR:HG22	2:H:1108:GLN:HG3	1.97	0.47
1:A:410:SER:HB2	1:A:421:LYS:HG3	1.96	0.47
1:A:650:VAL:HG13	1:A:657:VAL:HG13	1.96	0.47
2:B:570:GLN:HG3	2:B:573:LYS:HE3	1.97	0.47
2:B:735:ASN:HB2	2:B:738:THR:HG23	1.97	0.47
2:F:834:TYR:CZ	2:F:945:GLU:HG3	2.49	0.47
2:F:934:ASN:O	2:F:938:GLU:HB2	2.15	0.47
1:A:273:GLN:HG2	1:A:722:HIS:HD2	1.79	0.47
2:B:1191:SER:HB3	2:B:1196:THR:HG23	1.97	0.47
2:D:1067:SER:HB3	2:D:1077:SER:OG	2.15	0.47
1:G:151:GLU:HB2	1:G:213:TYR:CE1	2.50	0.47
2:H:520:LEU:HD23	2:H:757:ASP:HA	1.95	0.47
2:H:697:ILE:HD12	2:H:749:ARG:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:901:ASN:HB3	2:H:958:ASN:HD21	1.80	0.47
1:A:706:GLU:H	1:A:706:GLU:HG2	1.48	0.46
1:C:66:ILE:HD12	1:C:78:VAL:CG1	2.46	0.46
1:C:723:ASP:OD2	1:C:727:THR:HB	2.15	0.46
2:F:429:ASP:HB3	2:F:432:LYS:HD3	1.96	0.46
1:A:171:GLN:NE2	1:A:201:ALA:HB3	2.29	0.46
2:F:835:ARG:HD3	2:F:845:ILE:HG21	1.96	0.46
2:F:943:LYS:HB3	2:F:948:GLU:HB2	1.97	0.46
1:A:405:VAL:HG11	1:A:426:ALA:HB2	1.98	0.46
1:C:471:GLY:O	1:C:481:PRO:HA	2.15	0.46
1:E:216:LEU:HA	1:E:290:VAL:HB	1.96	0.46
1:G:652:THR:CG2	1:G:657:VAL:HG13	2.44	0.46
2:H:946:THR:HA	2:H:1120:THR:HG21	1.98	0.46
1:A:135:PRO:HA	1:A:337:PRO:HD2	1.97	0.46
1:A:363:LYS:O	1:A:363:LYS:HG2	2.15	0.46
2:B:387:TYR:O	2:B:391:ASN:HB2	2.15	0.46
2:D:226:GLU:CG	2:D:239:ARG:NE	2.78	0.46
2:D:1191:SER:HB3	2:D:1196:THR:HG23	1.97	0.46
2:F:1188:GLU:HG2	2:F:1189:GLU:HG2	1.96	0.46
1:G:735:PHE:CD1	1:G:776:LEU:HB2	2.51	0.46
2:B:939:GLN:HE21	2:B:950:ASN:HB2	1.80	0.46
2:B:1027:TRP:CE3	2:B:1046:LEU:HB3	2.50	0.46
1:C:204:GLY:HA3	1:C:424:ALA:O	2.16	0.46
1:C:808:LEU:HD23	2:D:742:ARG:HG2	1.96	0.46
2:D:574:HIS:CE1	2:D:596:GLY:HA3	2.50	0.46
2:D:685:GLU:CG	2:D:686:ASN:H	2.18	0.46
1:E:704:ASN:HB3	1:E:707:SER:HB2	1.97	0.46
2:H:143:ILE:HG23	2:H:148:MET:HE3	1.97	0.46
2:B:777:PHE:HB3	2:B:795:THR:CG2	2.46	0.46
2:D:567:LYS:HD3	2:D:621:TYR:CE2	2.51	0.46
1:E:472:ASN:HD22	1:E:478:THR:HB	1.79	0.46
1:E:574:GLN:HE21	1:E:575:SER:N	2.12	0.46
2:H:271:SER:HB2	2:H:868:VAL:HG22	1.97	0.46
2:H:1274:ASP:HB3	2:H:1277:THR:HG22	1.98	0.46
1:A:704:ASN:HB3	1:A:707:SER:HB2	1.97	0.46
2:H:61:VAL:HG13	2:H:131:ARG:NH1	2.31	0.46
2:H:634:ASN:O	2:H:638:GLU:HB2	2.15	0.46
1:A:506:PRO:HB2	1:A:540:GLN:HA	1.97	0.46
1:A:525:TYR:CE1	1:A:591:ALA:HB1	2.50	0.46
2:F:634:ASN:O	2:F:638:GLU:HB2	2.16	0.46
2:H:203:VAL:HG13	2:H:343:PHE:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:345:ASP:HA	2:D:352:HIS:O	2.16	0.46
2:D:733:ASN:HD22	2:D:733:ASN:H	1.64	0.46
2:D:821:ILE:HG22	2:D:823:ASN:H	1.80	0.46
1:G:363:LYS:HG3	1:G:374:HIS:CE1	2.50	0.46
1:C:170:THR:HG22	1:C:173:GLU:H	1.81	0.46
2:D:547:ASN:HD22	2:D:547:ASN:H	1.62	0.46
2:D:626:PRO:HG3	2:D:661:LEU:HG	1.98	0.46
1:G:671:THR:HG21	1:G:676:ILE:HG12	1.97	0.46
1:G:801:ILE:HD13	1:G:815:LEU:O	2.15	0.46
2:H:318:THR:CG2	2:H:319:GLU:H	2.18	0.46
2:H:777:PHE:HB3	2:H:795:THR:CG2	2.46	0.46
2:H:1261:PHE:CD2	2:H:1265:PHE:HE2	2.34	0.46
2:D:111:ASN:HA	2:D:114:TYR:HB3	1.97	0.45
2:D:422:GLY:HA2	2:D:439:SER:HB2	1.98	0.45
1:E:766:GLN:O	2:F:742:ARG:HD2	2.16	0.45
2:F:390:ARG:HD3	2:F:396:THR:O	2.16	0.45
1:G:135:PRO:HB3	1:G:337:PRO:HG2	1.96	0.45
2:B:892:ASP:HA	2:B:900:THR:HG23	1.97	0.45
2:B:1059:GLN:HG2	3:B:1521:HOH:O	2.16	0.45
1:G:368:THR:O	1:G:369:ASN:HB2	2.16	0.45
2:H:806:MET:HG2	2:H:826:PRO:HG2	1.98	0.45
2:B:523:LEU:HG	2:B:557:MET:HE1	1.98	0.45
1:A:366:THR:HG22	1:A:494:SER:CA	2.42	0.45
2:B:697:ILE:HD12	2:B:749:ARG:HB2	1.98	0.45
1:C:196:ASN:HA	1:C:482:ILE:HG23	1.98	0.45
2:D:259:THR:HG22	2:D:278:LYS:HD3	1.99	0.45
2:F:1234:VAL:HG13	2:F:1236:LEU:HG	1.98	0.45
2:F:1274:ASP:HB3	2:F:1277:THR:HG22	1.97	0.45
2:B:272:THR:HG21	2:B:864:ASP:HB3	1.99	0.45
2:B:852:PRO:HB2	2:B:857:THR:HG22	1.99	0.45
2:B:1112:VAL:HA	2:B:1127:PRO:HA	1.97	0.45
2:D:1147:LYS:HA	2:D:1150:LYS:HD3	1.97	0.45
2:F:501:THR:HG21	2:F:708:ASP:C	2.41	0.45
2:F:806:MET:HG2	2:F:826:PRO:HG2	1.98	0.45
2:F:892:ASP:HA	2:F:900:THR:HG23	1.99	0.45
2:H:276:ALA:HB2	2:H:655:PRO:HD3	1.99	0.45
2:H:570:GLN:HG3	2:H:573:LYS:HE3	1.99	0.45
1:C:386:SER:HB3	1:C:626:SER:OG	2.16	0.45
2:D:1078:LEU:HD22	2:D:1225:LEU:HD23	1.99	0.45
2:H:91:VAL:HG12	2:H:129:ALA:HB3	1.99	0.45
2:H:203:VAL:HG13	2:H:343:PHE:HE1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ILE:HG22	1:A:629:LEU:HD21	1.99	0.45
2:B:1274:ASP:HB3	2:B:1277:THR:HG22	1.99	0.45
1:C:506:PRO:HB2	1:C:540:GLN:HA	1.99	0.45
2:D:939:GLN:NE2	2:D:950:ASN:HB2	2.32	0.45
2:D:1234:VAL:HG13	2:D:1236:LEU:HG	1.99	0.45
1:E:405:VAL:HG11	1:E:426:ALA:HB2	1.99	0.45
2:B:668:ASN:HB2	2:B:669:TRP:CE3	2.51	0.45
2:D:72:ASN:HB2	2:D:473:ALA:HB2	1.98	0.45
2:D:223:GLU:HG2	2:D:1100:LEU:HD23	1.98	0.45
2:F:1003:ASN:ND2	2:F:1146:THR:HG21	2.31	0.45
2:H:244:SER:HB3	2:H:571:LEU:HB2	1.97	0.45
2:H:1269:VAL:HG11	2:H:1307:TYR:HB2	1.99	0.45
2:D:529:ARG:NH2	2:D:729:LEU:O	2.50	0.45
2:D:600:ARG:HG2	2:D:669:TRP:CH2	2.52	0.45
2:D:952:PRO:HG2	2:D:956:GLU:HG2	1.98	0.45
2:F:272:THR:HG21	2:F:864:ASP:HB3	1.99	0.45
1:G:184:TRP:CD2	1:G:199:PRO:HB3	2.51	0.45
2:H:114:TYR:CE1	2:H:118:VAL:HG21	2.52	0.45
2:H:1269:VAL:HA	2:H:1272:LEU:HD12	1.98	0.45
1:A:320:MET:HE3	1:A:339:TRP:HZ3	1.82	0.45
1:A:574:GLN:HE21	1:A:575:SER:H	1.64	0.45
2:B:834:TYR:OH	2:B:945:GLU:HG2	2.17	0.45
1:C:193:LEU:HD21	1:C:485:ALA:HB3	1.98	0.45
2:F:225:LEU:O	2:F:225:LEU:HG	2.17	0.45
2:F:1265:PHE:CZ	2:F:1288:LEU:HD21	2.52	0.45
1:G:521:LEU:HD23	1:G:580:VAL:HG23	1.98	0.45
1:C:194:ASN:HB2	1:C:483:LYS:HD3	1.99	0.44
2:D:767:PHE:CZ	2:D:1208:LYS:HG2	2.52	0.44
2:H:1265:PHE:CB	2:H:1312:GLN:NE2	2.70	0.44
1:C:136:ASN:H	1:C:136:ASN:HD22	1.66	0.44
2:F:557:MET:SD	2:F:692:SER:HB2	2.58	0.44
2:B:152:SER:HB2	2:B:172:LEU:HD22	1.99	0.44
2:D:363:PRO:O	2:D:367:VAL:HG23	2.17	0.44
2:F:244:SER:HB3	2:F:571:LEU:HB2	1.98	0.44
1:A:469:TYR:CE1	2:B:818:TRP:HD1	2.34	0.44
1:C:170:THR:OG1	1:C:200:ASN:HA	2.17	0.44
2:D:467:PHE:CD1	2:D:542:VAL:HG21	2.52	0.44
2:D:504:PRO:HG2	2:D:507:VAL:HG23	1.99	0.44
2:D:565:ARG:HG3	2:D:601:PRO:HB3	1.99	0.44
2:F:834:TYR:HE1	2:F:944:THR:HG23	1.83	0.44
2:B:299:PRO:HB2	2:B:609:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:226:GLU:CG	2:D:239:ARG:HE	2.30	0.44
2:D:256:LEU:HD13	2:D:606:GLY:HA3	1.99	0.44
2:H:739:ASN:O	2:H:742:ARG:HB2	2.16	0.44
2:H:915:LEU:O	2:H:1027:TRP:CD1	2.71	0.44
2:H:1265:PHE:C	2:H:1312:GLN:NE2	2.76	0.44
1:C:67:ALA:HB2	1:C:81:LYS:HG2	2.00	0.44
2:F:1029:ILE:HD12	2:F:1046:LEU:HD21	2.00	0.44
2:F:1178:THR:HG22	1:G:566:THR:HG21	1.99	0.44
2:F:1301:ARG:HH22	2:F:1319:GLU:CD	2.26	0.44
1:A:34:SER:HB2	1:A:65:GLN:HB2	1.99	0.44
2:F:529:ARG:CZ	2:F:732:LEU:HD23	2.48	0.44
1:G:434:ASP:OD1	1:G:469:TYR:HA	2.18	0.44
2:B:186:LYS:HB3	2:B:205:LEU:HB3	1.99	0.44
2:B:933:PHE:HZ	2:B:939:GLN:HG2	1.81	0.44
2:B:1040:GLY:HA3	2:B:1183:SER:HB3	2.00	0.44
2:D:467:PHE:CG	2:D:542:VAL:HG21	2.53	0.44
2:F:363:PRO:O	2:F:367:VAL:HG23	2.16	0.44
2:F:476:MET:HB2	2:F:479:THR:HB	1.99	0.44
1:G:73:ASN:HD21	1:G:327:ARG:NH2	2.08	0.44
2:H:806:MET:HG3	2:H:827:ASP:OD1	2.18	0.44
2:B:223:GLU:HG3	2:B:478:THR:OG1	2.18	0.44
2:D:1274:ASP:HB3	2:D:1277:THR:HG22	2.00	0.44
2:F:706:LEU:HD13	2:F:743:TYR:CD2	2.53	0.44
2:H:822:PRO:HB2	2:H:1189:GLU:CB	2.47	0.44
2:B:536:ARG:NH1	2:B:686:ASN:HB3	2.33	0.43
2:B:758:SER:HA	2:B:907:ARG:NH1	2.33	0.43
2:B:956:GLU:H	2:B:956:GLU:HG3	1.56	0.43
2:D:194:SER:HB2	2:D:200:LEU:HB3	1.99	0.43
2:F:1233:LEU:HD21	2:F:1329:ILE:HG21	2.00	0.43
1:G:261:SER:CB	1:G:726:GLN:HB2	2.47	0.43
1:G:406:GLY:HA2	1:G:499:ASN:O	2.18	0.43
2:H:152:SER:HB2	2:H:172:LEU:HD22	2.00	0.43
2:H:585:LEU:CD1	2:H:1105:GLN:HG3	2.48	0.43
2:B:834:TYR:CZ	2:B:945:GLU:HG2	2.53	0.43
2:D:380:ASN:HA	2:D:718:PHE:CZ	2.53	0.43
1:G:171:GLN:HG2	1:G:184:TRP:HH2	1.83	0.43
2:B:939:GLN:HE21	2:B:950:ASN:HD22	1.66	0.43
2:D:549:LEU:HD23	2:D:698:LEU:HB2	1.99	0.43
2:H:1191:SER:HB3	2:H:1196:THR:HG23	2.01	0.43
2:B:115:LEU:HD22	2:B:209:VAL:HG11	2.01	0.43
2:B:1078:LEU:HD22	2:B:1225:LEU:HD23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1184:GLU:CD	2:B:1184:GLU:H	2.26	0.43
2:H:732:LEU:HD13	2:H:732:LEU:HA	1.92	0.43
2:H:850:VAL:C	2:H:1123:LYS:HZ1	2.26	0.43
2:H:1335:SER:C	2:H:1337:THR:H	2.27	0.43
1:A:35:LYS:HE2	1:A:64:TYR:O	2.19	0.43
1:A:222:ILE:HD12	1:A:270:ASN:HD21	1.82	0.43
1:A:461:ASP:HB3	2:B:811:LEU:HD13	2.01	0.43
1:C:461:ASP:HB3	2:D:811:LEU:HD13	2.01	0.43
2:F:695:ALA:HB3	2:F:751:THR:HG22	1.99	0.43
2:F:770:TRP:HE3	2:F:773:ASN:HB2	1.83	0.43
1:G:460:GLN:C	2:H:812:ASN:ND2	2.75	0.43
2:H:223:GLU:HG3	2:H:478:THR:OG1	2.19	0.43
2:H:327:THR:HG22	2:H:410:ASP:OD2	2.18	0.43
2:B:567:LYS:HD3	2:B:621:TYR:CE2	2.53	0.43
2:B:574:HIS:CE1	2:B:596:GLY:HA3	2.54	0.43
2:B:1281:TYR:HB2	2:B:1284:TYR:CD2	2.53	0.43
2:F:299:PRO:HB2	2:F:609:LEU:HD12	2.01	0.43
1:G:489:LYS:HE2	1:G:491:ASP:HB2	1.99	0.43
2:H:1281:TYR:HD2	2:H:1284:TYR:HE2	1.67	0.43
2:D:932:GLN:HB2	2:D:982:LYS:HB3	1.99	0.43
2:F:527:THR:HG23	2:F:678:LEU:CD2	2.44	0.43
2:H:921:VAL:HG13	2:H:965:LEU:HD13	2.00	0.43
2:H:1032:THR:HG21	3:H:1401:HOH:O	2.17	0.43
1:C:127:VAL:HG12	1:C:128:LYS:HG3	2.01	0.43
2:D:769:PRO:HA	2:D:776:PRO:HA	2.01	0.43
2:F:923:ILE:HD12	2:F:983:ILE:HG22	2.00	0.43
2:F:1105:GLN:HB2	2:F:1107:TYR:CE2	2.54	0.43
2:H:371:PRO:HD2	2:H:374:TRP:CD2	2.54	0.43
2:B:114:TYR:O	2:B:117:ALA:HB3	2.19	0.43
2:B:467:PHE:CG	2:B:542:VAL:HG21	2.54	0.43
1:C:320:MET:HB2	1:C:321:TRP:CE3	2.54	0.43
2:D:119:GLU:HG2	2:D:209:VAL:HG23	2.00	0.43
2:D:389:ALA:O	2:D:393:LEU:HB2	2.18	0.43
2:F:411:GLU:HB3	2:F:415:LYS:HD3	2.00	0.43
1:G:351:LYS:HG2	1:G:355:PHE:HE2	1.84	0.43
1:G:475:ASN:O	2:H:817:ARG:HD2	2.18	0.43
2:H:272:THR:HG21	2:H:864:ASP:HB3	2.01	0.43
2:H:1322:ASP:HB2	2:H:1329:ILE:HG12	2.00	0.43
1:C:99:PHE:CZ	1:C:108:PRO:HB3	2.54	0.43
2:F:192:VAL:HG12	2:F:202:PHE:HB2	2.00	0.43
2:F:921:VAL:HG13	2:F:965:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:115:LEU:HD22	2:D:209:VAL:HG11	2.01	0.42
1:E:88:LYS:HE3	1:E:100:ASP:HA	2.01	0.42
1:E:166:GLU:HG3	1:E:206:LYS:HB2	2.01	0.42
2:F:520:LEU:HD23	2:F:757:ASP:HA	2.01	0.42
2:F:860:ASP:O	2:F:863:SER:HB3	2.19	0.42
2:H:114:TYR:C	2:H:114:TYR:HD1	2.26	0.42
2:H:467:PHE:CG	2:H:542:VAL:HG21	2.54	0.42
2:B:549:LEU:HD23	2:B:698:LEU:HB2	1.99	0.42
2:F:523:LEU:HG	2:F:557:MET:CE	2.49	0.42
2:F:697:ILE:HD12	2:F:749:ARG:HB2	2.00	0.42
1:G:545:GLY:HA3	1:G:573:THR:HG22	2.01	0.42
2:D:835:ARG:HB3	2:D:1122:ASN:HA	2.02	0.42
1:E:636:ASN:HA	1:E:637:PRO:HD3	1.96	0.42
1:G:66:ILE:HD11	1:G:69:GLN:HG2	1.98	0.42
2:B:281:VAL:HG22	2:B:293:ASN:HA	2.00	0.42
2:D:945:GLU:H	2:D:945:GLU:HG3	1.40	0.42
1:G:167:LYS:HE2	1:G:202:SER:HB2	2.01	0.42
2:H:536:ARG:NH1	2:H:686:ASN:HB3	2.35	0.42
2:H:1261:PHE:O	2:H:1263:ARG:N	2.53	0.42
1:A:149:ILE:HG23	1:A:213:TYR:HB3	2.02	0.42
1:A:155:THR:CG2	1:A:157:TYR:H	2.28	0.42
1:A:454:ASN:ND2	1:A:467:VAL:H	2.17	0.42
2:B:131:ARG:HD2	2:B:133:TYR:CE1	2.54	0.42
2:B:1062:THR:HG21	2:B:1085:LYS:HB2	2.02	0.42
2:D:77:SER:HA	2:D:89:GLY:HA2	2.02	0.42
2:D:821:ILE:HD11	2:D:828:ILE:CD1	2.49	0.42
2:D:939:GLN:HE21	2:D:950:ASN:HB2	1.84	0.42
2:F:269:ALA:HA	2:F:870:PRO:HA	2.00	0.42
2:H:256:LEU:HD13	2:H:606:GLY:HA3	2.01	0.42
2:D:244:SER:HB3	2:D:571:LEU:HB2	2.01	0.42
2:D:834:TYR:CZ	2:D:945:GLU:HG2	2.54	0.42
1:E:792:LYS:HE3	1:E:797:ASN:HD21	1.84	0.42
2:B:837:GLN:HB3	2:B:841:GLN:HB3	2.02	0.42
1:C:651:LEU:HD23	1:C:651:LEU:HA	1.90	0.42
1:C:812:ASP:OD2	1:C:815:LEU:HG	2.20	0.42
2:D:114:TYR:O	2:D:118:VAL:HG23	2.19	0.42
2:D:1281:TYR:HB2	2:D:1284:TYR:HD2	1.83	0.42
1:E:216:LEU:HB3	1:E:291:ILE:HB	2.01	0.42
2:F:475:LYS:HD2	2:F:479:THR:O	2.20	0.42
2:F:890:THR:HA	2:F:902:LYS:HE3	2.01	0.42
1:A:311:VAL:HB	1:A:323:TRP:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:475:LYS:HD2	2:B:479:THR:O	2.20	0.42
2:B:821:ILE:HD11	2:B:828:ILE:HD11	2.01	0.42
1:C:347:TRP:CH2	1:C:401:LYS:HG3	2.53	0.42
2:D:115:LEU:HD11	2:D:324:LEU:HD22	2.02	0.42
2:D:152:SER:HB2	2:D:172:LEU:HD22	2.02	0.42
2:D:668:ASN:HB2	2:D:669:TRP:CE3	2.54	0.42
2:D:1012:LEU:HD23	2:D:1012:LEU:HA	1.93	0.42
2:D:1150:LYS:HE2	2:D:1156:GLY:HA2	2.02	0.42
1:E:697:THR:HB	1:E:715:ASP:O	2.19	0.42
2:F:115:LEU:HD22	2:F:209:VAL:HG11	2.02	0.42
2:B:528:ASN:HD22	2:B:530:TRP:HE3	1.65	0.42
2:B:943:LYS:HB3	2:B:948:GLU:HB2	2.01	0.42
1:E:170:THR:HG22	1:E:173:GLU:H	1.85	0.42
1:E:436:LYS:HB2	1:E:441:ASP:HB3	2.01	0.42
2:F:170:PHE:CZ	2:F:344:TYR:HB3	2.55	0.42
2:F:756:LEU:HD12	2:F:760:THR:HG22	2.01	0.42
2:F:845:ILE:HA	2:F:846:PRO:HD3	1.93	0.42
2:H:299:PRO:HB2	2:H:609:LEU:HD12	2.02	0.42
1:A:136:ASN:H	1:A:136:ASN:ND2	2.11	0.41
1:A:253:PRO:HD2	1:A:263:GLY:HA3	2.02	0.41
1:A:359:GLN:HG2	1:A:405:VAL:HG12	2.01	0.41
1:C:347:TRP:CD1	1:C:353:LYS:HG3	2.55	0.41
2:F:771:ILE:H	2:F:771:ILE:HG13	1.69	0.41
1:G:67:ALA:HB2	1:G:81:LYS:HG2	2.01	0.41
2:H:923:ILE:HD12	2:H:983:ILE:HG22	2.00	0.41
2:H:1301:ARG:HH22	2:H:1319:GLU:CD	2.28	0.41
2:D:222:LYS:CE	2:D:321:TRP:HA	2.51	0.41
1:G:165:LYS:HD2	1:G:510:TYR:HB3	2.01	0.41
2:B:733:ASN:H	2:B:733:ASN:ND2	2.18	0.41
1:C:86:LYS:HB2	1:C:105:GLY:HA3	2.02	0.41
1:C:501:LEU:C	1:C:501:LEU:HD12	2.45	0.41
2:D:226:GLU:HB3	2:D:227:VAL:H	1.43	0.41
2:F:808:THR:HG21	2:F:817:ARG:NH2	2.35	0.41
2:F:1281:TYR:HB2	2:F:1284:TYR:HD2	1.86	0.41
2:H:201:TYR:CE1	2:H:345:ASP:HB3	2.56	0.41
2:H:933:PHE:HZ	2:H:939:GLN:HG2	1.85	0.41
1:A:639:MET:HB2	1:A:748:ASN:O	2.20	0.41
2:B:327:THR:HG21	2:B:367:VAL:HG21	2.02	0.41
2:F:475:LYS:HE3	2:F:1005:THR:HG21	2.03	0.41
1:G:261:SER:O	1:G:263:GLY:N	2.53	0.41
2:H:1031:PHE:CE2	2:H:1044:ILE:HD11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:710:ILE:HD12	2:B:740:TRP:HA	2.02	0.41
1:C:581:PRO:HG3	1:C:654:GLY:HA3	2.02	0.41
1:E:142:ASN:O	1:E:146:LYS:HB2	2.21	0.41
1:E:347:TRP:HH2	1:E:401:LYS:HG3	1.86	0.41
1:E:650:VAL:HG13	1:E:657:VAL:HG13	2.03	0.41
2:H:1281:TYR:HD2	2:H:1284:TYR:CE2	2.39	0.41
2:B:924:ASN:HB3	2:B:925:LYS:HG2	2.02	0.41
2:D:834:TYR:OH	2:D:945:GLU:HG2	2.21	0.41
1:E:706:GLU:OE1	1:E:706:GLU:N	2.54	0.41
2:F:528:ASN:OD1	2:F:530:TRP:O	2.39	0.41
1:G:411:SER:H	1:G:421:LYS:HE3	1.85	0.41
2:H:162:PRO:HG3	2:H:344:TYR:CE2	2.55	0.41
2:H:834:TYR:OH	2:H:945:GLU:HG2	2.20	0.41
2:B:391:ASN:ND2	2:B:418:ASN:HD22	2.18	0.41
2:B:422:GLY:HA2	2:B:439:SER:HB2	2.02	0.41
2:B:835:ARG:HB3	2:B:1122:ASN:HA	2.03	0.41
2:B:1165:ASN:HD22	2:B:1165:ASN:C	2.29	0.41
2:F:111:ASN:OD1	2:F:220:VAL:HG13	2.21	0.41
2:F:424:LYS:HD2	2:F:432:LYS:O	2.21	0.41
2:F:457:MET:HG3	2:F:466:ILE:HG13	2.02	0.41
2:H:151:PRO:HG3	2:H:180:TRP:CZ2	2.55	0.41
2:H:395:GLN:HE22	2:H:565:ARG:HD3	1.86	0.41
2:H:835:ARG:CZ	2:H:849:GLN:OE1	2.68	0.41
2:H:1027:TRP:CE3	2:H:1046:LEU:HB3	2.56	0.41
1:E:204:GLY:HA3	1:E:424:ALA:O	2.20	0.41
2:F:371:PRO:HD2	2:F:374:TRP:CD2	2.55	0.41
1:G:661:PHE:HE1	1:G:668:LEU:HD23	1.80	0.41
1:A:220:TRP:O	1:A:287:PRO:HG2	2.20	0.41
2:B:276:ALA:HB2	2:B:655:PRO:HD3	2.01	0.41
2:B:945:GLU:H	2:B:945:GLU:HG3	1.38	0.41
2:B:1076:LYS:HE3	2:B:1171:GLN:HG3	2.02	0.41
2:D:851:LYS:HA	2:D:1123:LYS:NZ	2.36	0.41
2:D:923:ILE:HG22	2:D:1140:LEU:HG	2.03	0.41
1:E:808:LEU:HD11	2:F:702:LEU:HD12	2.03	0.41
2:F:524:PRO:HD2	2:F:557:MET:CE	2.45	0.41
2:F:536:ARG:NH1	2:F:686:ASN:HB3	2.36	0.41
2:F:664:TRP:HB2	2:F:898:THR:HA	2.03	0.41
1:G:28:PHE:HE2	1:G:42:PRO:HA	1.86	0.41
1:G:135:PRO:HA	1:G:337:PRO:HD2	2.02	0.41
1:G:433:LEU:HD23	1:G:534:LEU:HD11	2.03	0.41
1:G:461:ASP:HB3	2:H:811:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:987:ALA:HB1	2:H:1115:TYR:CG	2.55	0.41
2:B:457:MET:HA	2:B:465:PHE:O	2.20	0.41
2:B:847:PHE:CE1	2:B:850:VAL:HB	2.56	0.41
1:E:677:ALA:O	1:E:678:PRO:C	2.64	0.41
1:G:131:GLN:HG2	1:G:132:LEU:N	2.36	0.41
2:H:131:ARG:HG2	2:H:133:TYR:CZ	2.56	0.41
2:H:411:GLU:HB3	2:H:415:LYS:HD3	2.03	0.41
2:H:1221:MET:HB2	2:H:1225:LEU:HD11	2.03	0.41
2:B:345:ASP:HA	2:B:352:HIS:O	2.21	0.40
2:B:742:ARG:HG2	2:B:742:ARG:NH1	2.35	0.40
1:C:253:PRO:HG3	2:F:737:ASN:HD22	1.85	0.40
2:D:1260:ASP:OD1	2:D:1263:ARG:HB2	2.21	0.40
2:F:204:LEU:HD23	2:F:204:LEU:HA	1.98	0.40
2:H:180:TRP:O	2:H:184:LYS:HB2	2.21	0.40
2:H:834:TYR:CZ	2:H:945:GLU:HG2	2.55	0.40
2:H:945:GLU:H	2:H:945:GLU:HG3	1.36	0.40
1:A:405:VAL:HG22	1:A:501:LEU:HD11	2.03	0.40
2:B:199:ASN:O	2:B:344:TYR:HA	2.21	0.40
1:E:165:LYS:HB3	1:E:205:PHE:HB2	2.03	0.40
1:E:605:THR:HG22	1:E:606:THR:HG23	2.03	0.40
1:G:293:GLN:NE2	1:G:293:GLN:HA	2.35	0.40
2:H:594:PRO:HG2	2:H:1124:LEU:HD22	2.03	0.40
2:H:1248:THR:HB	2:H:1331:VAL:HG13	2.03	0.40
2:B:855:ASN:C	2:B:857:THR:N	2.78	0.40
2:B:1105:GLN:HB2	2:B:1107:TYR:CE2	2.56	0.40
1:C:97:ILE:HG22	1:C:134:VAL:HB	2.03	0.40
1:C:158:THR:CG2	1:C:163:LEU:HD13	2.52	0.40
2:D:994:SER:HB2	2:D:1137:MET:HE2	2.02	0.40
1:E:98:SER:HA	1:E:134:VAL:HG21	2.03	0.40
1:E:135:PRO:HB3	1:E:337:PRO:HG2	2.03	0.40
2:F:1038:ARG:HE	2:F:1038:ARG:HB2	1.63	0.40
2:F:1116:GLN:HB2	2:F:1120:THR:HA	2.03	0.40
1:G:749:GLN:HA	1:G:749:GLN:NE2	2.24	0.40
2:B:923:ILE:HD11	2:B:966:LEU:HD21	2.04	0.40
2:B:1234:VAL:CG1	2:B:1236:LEU:HG	2.51	0.40
1:C:782:LEU:HD22	1:C:788:ALA:HB2	2.03	0.40
1:E:143:GLN:HA	1:E:146:LYS:HE3	2.02	0.40
2:F:223:GLU:OE1	2:F:476:MET:HE3	2.20	0.40
2:F:467:PHE:CD1	2:F:542:VAL:HG21	2.56	0.40
2:F:756:LEU:HD12	2:F:760:THR:CG2	2.51	0.40
2:F:1030:THR:HB	2:F:1045:THR:OG1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:216:LEU:HD22	1:G:291:ILE:HD12	2.04	0.40
2:H:1265:PHE:C	2:H:1312:GLN:HE21	2.30	0.40
2:B:201:TYR:CE1	2:B:345:ASP:HB3	2.57	0.40
2:B:572:GLU:H	2:B:572:GLU:HG2	1.57	0.40
2:B:940:LYS:HB2	2:B:948:GLU:HB3	2.04	0.40
2:B:1003:ASN:ND2	2:B:1146:THR:HG21	2.37	0.40
2:D:276:ALA:HB2	2:D:655:PRO:HD3	2.03	0.40
1:E:111:VAL:HG11	1:E:309:ILE:HG21	2.03	0.40
2:H:742:ARG:HG2	2:H:742:ARG:NH1	2.34	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	773/802 (96%)	717 (93%)	50 (6%)	6 (1%)	16	27
1	C	771/802 (96%)	715 (93%)	48 (6%)	8 (1%)	12	20
1	E	777/802 (97%)	710 (91%)	60 (8%)	7 (1%)	14	24
1	G	778/802 (97%)	719 (92%)	50 (6%)	9 (1%)	10	17
2	B	1256/1334 (94%)	1162 (92%)	87 (7%)	7 (1%)	21	34
2	D	1253/1334 (94%)	1157 (92%)	84 (7%)	12 (1%)	12	20
2	F	1234/1334 (92%)	1139 (92%)	80 (6%)	15 (1%)	10	17
2	H	1231/1334 (92%)	1125 (91%)	91 (7%)	15 (1%)	10	17
All	All	8073/8544 (94%)	7444 (92%)	550 (7%)	79 (1%)	12	20

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	366	THR

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Mol	Chain	Res	Type
1	A	367	SER
1	C	368	THR
2	D	618	GLY
2	D	1157	THR
2	D	1158	ALA
2	F	150	ASN
2	F	847	PHE
2	F	857	THR
2	F	1157	THR
2	F	1158	ALA
1	G	262	SER
1	G	368	THR
1	G	783	SER
1	G	784	GLU
2	H	618	GLY
2	H	1157	THR
2	H	1262	ASN
1	A	368	THR
1	A	512	ASP
2	B	618	GLY
2	B	854	ASN
1	C	795	ASP
2	D	987	ALA
1	E	795	ASP
2	F	618	GLY
2	F	988	ASP
2	F	1259	ILE
1	G	782	LEU
1	G	795	ASP
2	H	1188	GLU
2	H	1259	ILE
2	H	1347	ASN
2	B	847	PHE
2	B	1188	GLU
1	C	182	ASN
1	C	284	ASP
2	D	1188	GLU
1	E	284	ASP
1	E	367	SER
2	F	684	ASN
2	F	1258	GLN
2	F	1263	ARG

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Mol	Chain	Res	Type
2	F	1326	GLN
1	G	232	GLY
2	H	1326	GLN
1	A	365	THR
2	D	226	GLU
2	D	1263	ARG
1	E	232	GLY
1	E	453	ILE
2	H	684	ASN
2	H	1258	GLN
2	B	586	ARG
1	C	367	SER
1	C	446	ASP
1	C	453	ILE
2	D	1187	LYS
1	E	368	THR
1	G	453	ILE
1	G	563	GLY
2	H	874	SER
2	B	855	ASN
1	C	563	GLY
2	D	264	MET
2	D	684	ASN
1	E	167	LYS
2	F	852	PRO
2	F	874	SER
2	H	97	ASN
2	H	1187	LYS
1	A	453	ILE
2	B	143	ILE
2	D	771	ILE
2	H	846	PRO
2	F	143	ILE
2	H	836	VAL
2	H	1345	PRO
2	D	143	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	685/701 (98%)	611 (89%)	74 (11%)	6	9
1	C	683/701 (97%)	607 (89%)	76 (11%)	6	9
1	E	684/701 (98%)	605 (88%)	79 (12%)	5	8
1	G	685/701 (98%)	615 (90%)	70 (10%)	7	10
2	B	1112/1171 (95%)	949 (85%)	163 (15%)	3	4
2	D	1109/1171 (95%)	954 (86%)	155 (14%)	3	5
2	F	1097/1171 (94%)	937 (85%)	160 (15%)	3	4
2	H	1093/1171 (93%)	943 (86%)	150 (14%)	3	5
All	All	7148/7488 (96%)	6221 (87%)	927 (13%)	4	6

All (927) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LYS
1	A	48	THR
1	A	56	SER
1	A	57	LEU
1	A	65	GLN
1	A	66	ILE
1	A	79	LEU
1	A	84	ASP
1	A	90	GLU
1	A	104	GLN
1	A	107	LYS
1	A	125	THR
1	A	131	GLN
1	A	136	ASN
1	A	149	ILE
1	A	150	LEU
1	A	154	LEU
1	A	155	THR
1	A	159	LEU
1	A	163	LEU
1	A	171	GLN
1	A	176	LEU
1	A	189	ASN
1	A	190	GLN

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Mol	Chain	Res	Type
1	A	208	THR
1	A	209	THR
1	A	229	THR
1	A	243	THR
1	A	247	GLU
1	A	254	SER
1	A	264	THR
1	A	275	LEU
1	A	294	LEU
1	A	305	THR
1	A	317	LEU
1	A	319	SER
1	A	334	SER
1	A	350	ASP
1	A	351	LYS
1	A	366	THR
1	A	386	SER
1	A	391	VAL
1	A	393	ASP
1	A	395	ILE
1	A	401	LYS
1	A	419	SER
1	A	421	LYS
1	A	444	THR
1	A	453	ILE
1	A	494	SER
1	A	500	SER
1	A	508	ASN
1	A	532	GLU
1	A	537	ARG
1	A	568	VAL
1	A	571	SER
1	A	574	GLN
1	A	576	ARG
1	A	605	THR
1	A	638	VAL
1	A	657	VAL
1	A	665	ASN
1	A	670	SER
1	A	676	ILE
1	A	687	THR
1	A	706	GLU

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Mol	Chain	Res	Type
1	A	732	ASN
1	A	745	ILE
1	A	770	GLN
1	A	782	LEU
1	A	796	GLN
1	A	803	LYS
1	A	806	ASN
1	A	811	ILE
2	B	63	GLU
2	B	83	GLU
2	B	88	PHE
2	B	91	VAL
2	B	94	GLN
2	B	99	ASN
2	B	105	LYS
2	B	109	ASP
2	B	113	LYS
2	B	125	GLN
2	B	127	ASN
2	B	130	ILE
2	B	142	ASP
2	B	150	ASN
2	B	153	THR
2	B	154	VAL
2	B	182	GLU
2	B	187	VAL
2	B	200	LEU
2	B	203	VAL
2	B	204	LEU
2	B	219	GLN
2	B	226	GLU
2	B	233	SER
2	B	238	GLN
2	B	242	LYS
2	B	256	LEU
2	B	264	MET
2	B	265	SER
2	B	270	THR
2	B	272	THR
2	B	277	LEU
2	B	280	GLU
2	B	291	LEU

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Mol	Chain	Res	Type
2	B	301	LYS
2	B	318	THR
2	B	322	LYS
2	B	324	LEU
2	B	328	ASP
2	B	333	GLU
2	B	334	LYS
2	B	350	GLU
2	B	358	VAL
2	B	384	ILE
2	B	393	LEU
2	B	396	THR
2	B	403	ARG
2	B	411	GLU
2	B	420	SER
2	B	431	LYS
2	B	432	LYS
2	B	437	LYS
2	B	448	GLU
2	B	453	ASN
2	B	458	VAL
2	B	479	THR
2	B	523	LEU
2	B	528	ASN
2	B	529	ARG
2	B	562	THR
2	B	565	ARG
2	B	567	LYS
2	B	570	GLN
2	B	572	GLU
2	B	582	GLN
2	B	587	GLU
2	B	610	GLN
2	B	620	HIS
2	B	632	VAL
2	B	642	SER
2	B	649	LYS
2	B	673	LEU
2	B	679	SER
2	B	681	ASN
2	B	701	ASP
2	B	707	SER

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Mol	Chain	Res	Type
2	B	708	ASP
2	B	709	LYS
2	B	710	ILE
2	B	720	GLU
2	B	725	ARG
2	B	728	GLN
2	B	732	LEU
2	B	733	ASN
2	B	742	ARG
2	B	746	VAL
2	B	751	THR
2	B	756	LEU
2	B	768	LEU
2	B	771	ILE
2	B	790	SER
2	B	795	THR
2	B	803	VAL
2	B	806	MET
2	B	835	ARG
2	B	841	GLN
2	B	843	ASN
2	B	849	GLN
2	B	850	VAL
2	B	857	THR
2	B	869	THR
2	B	871	SER
2	B	906	GLN
2	B	921	VAL
2	B	922	LEU
2	B	935	LYS
2	B	939	GLN
2	B	945	GLU
2	B	947	ASN
2	B	956	GLU
2	B	965	LEU
2	B	974	THR
2	B	979	THR
2	B	986	LYS
2	B	1002	LEU
2	B	1005	THR
2	B	1012	LEU
2	B	1015	ILE

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Mol	Chain	Res	Type
2	B	1017	ASP
2	B	1029	ILE
2	B	1036	ARG
2	B	1039	THR
2	B	1044	ILE
2	B	1045	THR
2	B	1047	SER
2	B	1052	GLN
2	B	1059	GLN
2	B	1061	TRP
2	B	1089	ASN
2	B	1123	LYS
2	B	1136	ASN
2	B	1143	LEU
2	B	1157	THR
2	B	1164	ASN
2	B	1165	ASN
2	B	1170	SER
2	B	1171	GLN
2	B	1172	THR
2	B	1184	GLU
2	B	1187	LYS
2	B	1191	SER
2	B	1224	LYS
2	B	1230	SER
2	B	1234	VAL
2	B	1240	GLN
2	B	1246	SER
2	B	1249	GLU
2	B	1251	ILE
2	B	1258	GLN
2	B	1259	ILE
2	B	1262	ASN
2	B	1270	THR
2	B	1271	GLU
2	B	1288	LEU
2	B	1305	ILE
2	B	1308	SER
2	B	1310	GLU
2	B	1314	LEU
2	B	1318	LEU
2	B	1325	THR

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Mol	Chain	Res	Type
2	B	1335	SER
2	B	1341	THR
2	B	1342	VAL
1	C	48	THR
1	C	57	LEU
1	C	65	GLN
1	C	66	ILE
1	C	69	GLN
1	C	73	ASN
1	C	79	LEU
1	C	85	VAL
1	C	92	SER
1	C	95	ASN
1	C	101	SER
1	C	107	LYS
1	C	117	SER
1	C	123	LYS
1	C	136	ASN
1	C	149	ILE
1	C	150	LEU
1	C	154	LEU
1	C	155	THR
1	C	163	LEU
1	C	165	LYS
1	C	170	THR
1	C	183	GLN
1	C	208	THR
1	C	224	GLU
1	C	243	THR
1	C	247	GLU
1	C	254	SER
1	C	264	THR
1	C	275	LEU
1	C	291	ILE
1	C	294	LEU
1	C	305	THR
1	C	351	LYS
1	C	363	LYS
1	C	366	THR
1	C	391	VAL
1	C	393	ASP
1	C	395	ILE

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Mol	Chain	Res	Type
1	C	421	LYS
1	C	444	THR
1	C	446	ASP
1	C	483	LYS
1	C	496	VAL
1	C	502	ILE
1	C	508	ASN
1	C	533	ARG
1	C	537	ARG
1	C	540	GLN
1	C	568	VAL
1	C	571	SER
1	C	574	GLN
1	C	576	ARG
1	C	580	VAL
1	C	629	LEU
1	C	638	VAL
1	C	639	MET
1	C	657	VAL
1	C	670	SER
1	C	674	ASN
1	C	676	ILE
1	C	679	ILE
1	C	716	SER
1	C	719	LYS
1	C	732	ASN
1	C	733	MET
1	C	745	ILE
1	C	765	VAL
1	C	782	LEU
1	C	784	GLU
1	C	785	GLU
1	C	793	ASP
1	C	796	GLN
1	C	806	ASN
1	C	813	THR
1	C	815	LEU
2	D	83	GLU
2	D	88	PHE
2	D	91	VAL
2	D	99	ASN
2	D	111	ASN

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Mol	Chain	Res	Type
2	D	112	LEU
2	D	113	LYS
2	D	120	LYS
2	D	127	ASN
2	D	130	ILE
2	D	138	ARG
2	D	142	ASP
2	D	154	VAL
2	D	163	ILE
2	D	182	GLU
2	D	187	VAL
2	D	200	LEU
2	D	203	VAL
2	D	204	LEU
2	D	219	GLN
2	D	222	LYS
2	D	226	GLU
2	D	238	GLN
2	D	242	LYS
2	D	249	SER
2	D	256	LEU
2	D	270	THR
2	D	272	THR
2	D	277	LEU
2	D	291	LEU
2	D	301	LYS
2	D	316	GLU
2	D	318	THR
2	D	324	LEU
2	D	328	ASP
2	D	333	GLU
2	D	334	LYS
2	D	350	GLU
2	D	358	VAL
2	D	384	ILE
2	D	393	LEU
2	D	396	THR
2	D	420	SER
2	D	432	LYS
2	D	437	LYS
2	D	438	ASN
2	D	448	GLU

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Mol	Chain	Res	Type
2	D	453	ASN
2	D	458	VAL
2	D	479	THR
2	D	523	LEU
2	D	529	ARG
2	D	547	ASN
2	D	562	THR
2	D	565	ARG
2	D	567	LYS
2	D	570	GLN
2	D	572	GLU
2	D	587	GLU
2	D	610	GLN
2	D	632	VAL
2	D	642	SER
2	D	649	LYS
2	D	650	LEU
2	D	662	TYR
2	D	673	LEU
2	D	681	ASN
2	D	701	ASP
2	D	707	SER
2	D	709	LYS
2	D	710	ILE
2	D	720	GLU
2	D	725	ARG
2	D	728	GLN
2	D	732	LEU
2	D	733	ASN
2	D	735	ASN
2	D	737	ASN
2	D	742	ARG
2	D	746	VAL
2	D	756	LEU
2	D	768	LEU
2	D	771	ILE
2	D	773	ASN
2	D	795	THR
2	D	797	SER
2	D	803	VAL
2	D	835	ARG
2	D	841	GLN

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Mol	Chain	Res	Type
2	D	843	ASN
2	D	850	VAL
2	D	857	THR
2	D	874	SER
2	D	906	GLN
2	D	921	VAL
2	D	922	LEU
2	D	935	LYS
2	D	939	GLN
2	D	945	GLU
2	D	947	ASN
2	D	956	GLU
2	D	965	LEU
2	D	974	THR
2	D	979	THR
2	D	988	ASP
2	D	1002	LEU
2	D	1012	LEU
2	D	1017	ASP
2	D	1029	ILE
2	D	1036	ARG
2	D	1039	THR
2	D	1044	ILE
2	D	1045	THR
2	D	1047	SER
2	D	1052	GLN
2	D	1059	GLN
2	D	1061	TRP
2	D	1089	ASN
2	D	1108	GLN
2	D	1117	THR
2	D	1120	THR
2	D	1123	LYS
2	D	1136	ASN
2	D	1143	LEU
2	D	1146	THR
2	D	1164	ASN
2	D	1169	VAL
2	D	1171	GLN
2	D	1172	THR
2	D	1178	THR
2	D	1184	GLU

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Mol	Chain	Res	Type
2	D	1187	LYS
2	D	1190	THR
2	D	1191	SER
2	D	1219	THR
2	D	1224	LYS
2	D	1230	SER
2	D	1234	VAL
2	D	1240	GLN
2	D	1244	SER
2	D	1260	ASP
2	D	1262	ASN
2	D	1270	THR
2	D	1271	GLU
2	D	1288	LEU
2	D	1301	ARG
2	D	1305	ILE
2	D	1310	GLU
2	D	1314	LEU
2	D	1318	LEU
2	D	1324	GLN
2	D	1327	GLN
2	D	1341	THR
2	D	1342	VAL
2	D	1348	GLN
1	E	27	THR
1	E	31	LYS
1	E	38	THR
1	E	48	THR
1	E	57	LEU
1	E	65	GLN
1	E	66	ILE
1	E	69	GLN
1	E	79	LEU
1	E	88	LYS
1	E	95	ASN
1	E	101	SER
1	E	102	THR
1	E	103	SER
1	E	107	LYS
1	E	136	ASN
1	E	149	ILE
1	E	150	LEU

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Mol	Chain	Res	Type
1	E	154	LEU
1	E	155	THR
1	E	163	LEU
1	E	165	LYS
1	E	170	THR
1	E	186	SER
1	E	187	GLN
1	E	217	SER
1	E	226	ILE
1	E	243	THR
1	E	251	ASP
1	E	254	SER
1	E	264	THR
1	E	275	LEU
1	E	284	ASP
1	E	294	LEU
1	E	305	THR
1	E	330	GLN
1	E	331	GLU
1	E	349	GLU
1	E	351	LYS
1	E	363	LYS
1	E	366	THR
1	E	376	LYS
1	E	391	VAL
1	E	393	ASP
1	E	395	ILE
1	E	409	SER
1	E	419	SER
1	E	421	LYS
1	E	466	VAL
1	E	472	ASN
1	E	490	LYS
1	E	496	VAL
1	E	537	ARG
1	E	540	GLN
1	E	543	VAL
1	E	574	GLN
1	E	576	ARG
1	E	580	VAL
1	E	595	LYS
1	E	604	VAL

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Mol	Chain	Res	Type
1	E	605	THR
1	E	638	VAL
1	E	640	SER
1	E	657	VAL
1	E	679	ILE
1	E	680	SER
1	E	705	GLN
1	E	706	GLU
1	E	717	SER
1	E	732	ASN
1	E	733	MET
1	E	745	ILE
1	E	770	GLN
1	E	772	THR
1	E	782	LEU
1	E	796	GLN
1	E	806	ASN
1	E	813	THR
1	E	815	LEU
2	F	63	GLU
2	F	83	GLU
2	F	88	PHE
2	F	91	VAL
2	F	99	ASN
2	F	100	ILE
2	F	105	LYS
2	F	113	LYS
2	F	130	ILE
2	F	131	ARG
2	F	147	LYS
2	F	148	MET
2	F	149	GLU
2	F	154	VAL
2	F	163	ILE
2	F	173	THR
2	F	182	GLU
2	F	187	VAL
2	F	200	LEU
2	F	203	VAL
2	F	204	LEU
2	F	219	GLN
2	F	225	LEU

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Mol	Chain	Res	Type
2	F	238	GLN
2	F	242	LYS
2	F	256	LEU
2	F	259	THR
2	F	270	THR
2	F	272	THR
2	F	273	ARG
2	F	277	LEU
2	F	291	LEU
2	F	301	LYS
2	F	312	GLU
2	F	315	LYS
2	F	316	GLU
2	F	322	LYS
2	F	324	LEU
2	F	328	ASP
2	F	333	GLU
2	F	334	LYS
2	F	350	GLU
2	F	358	VAL
2	F	384	ILE
2	F	393	LEU
2	F	396	THR
2	F	411	GLU
2	F	420	SER
2	F	432	LYS
2	F	437	LYS
2	F	448	GLU
2	F	453	ASN
2	F	457	MET
2	F	458	VAL
2	F	479	THR
2	F	501	THR
2	F	523	LEU
2	F	555	LEU
2	F	562	THR
2	F	565	ARG
2	F	567	LYS
2	F	570	GLN
2	F	572	GLU
2	F	587	GLU
2	F	610	GLN

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Mol	Chain	Res	Type
2	F	616	LYS
2	F	620	HIS
2	F	632	VAL
2	F	642	SER
2	F	649	LYS
2	F	650	LEU
2	F	662	TYR
2	F	673	LEU
2	F	679	SER
2	F	681	ASN
2	F	685	GLU
2	F	707	SER
2	F	709	LYS
2	F	710	ILE
2	F	725	ARG
2	F	728	GLN
2	F	732	LEU
2	F	733	ASN
2	F	737	ASN
2	F	742	ARG
2	F	746	VAL
2	F	756	LEU
2	F	763	GLN
2	F	768	LEU
2	F	771	ILE
2	F	773	ASN
2	F	803	VAL
2	F	806	MET
2	F	809	GLN
2	F	835	ARG
2	F	845	ILE
2	F	849	GLN
2	F	850	VAL
2	F	853	SER
2	F	855	ASN
2	F	856	SER
2	F	921	VAL
2	F	922	LEU
2	F	930	ASN
2	F	931	ASP
2	F	935	LYS
2	F	945	GLU

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Mol	Chain	Res	Type
2	F	947	ASN
2	F	956	GLU
2	F	965	LEU
2	F	974	THR
2	F	978	SER
2	F	979	THR
2	F	988	ASP
2	F	1002	LEU
2	F	1012	LEU
2	F	1029	ILE
2	F	1032	THR
2	F	1036	ARG
2	F	1044	ILE
2	F	1045	THR
2	F	1050	GLN
2	F	1052	GLN
2	F	1059	GLN
2	F	1061	TRP
2	F	1069	LEU
2	F	1071	SER
2	F	1074	THR
2	F	1089	ASN
2	F	1108	GLN
2	F	1117	THR
2	F	1120	THR
2	F	1123	LYS
2	F	1136	ASN
2	F	1171	GLN
2	F	1172	THR
2	F	1173	ILE
2	F	1184	GLU
2	F	1187	LYS
2	F	1190	THR
2	F	1191	SER
2	F	1224	LYS
2	F	1230	SER
2	F	1234	VAL
2	F	1240	GLN
2	F	1246	SER
2	F	1260	ASP
2	F	1262	ASN
2	F	1270	THR

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Mol	Chain	Res	Type
2	F	1271	GLU
2	F	1288	LEU
2	F	1293	SER
2	F	1305	ILE
2	F	1310	GLU
2	F	1314	LEU
2	F	1318	LEU
2	F	1337	THR
2	F	1341	THR
2	F	1342	VAL
2	F	1348	GLN
1	G	56	SER
1	G	57	LEU
1	G	65	GLN
1	G	66	ILE
1	G	69	GLN
1	G	79	LEU
1	G	90	GLU
1	G	98	SER
1	G	101	SER
1	G	102	THR
1	G	107	LYS
1	G	118	THR
1	G	149	ILE
1	G	150	LEU
1	G	155	THR
1	G	159	LEU
1	G	163	LEU
1	G	165	LYS
1	G	170	THR
1	G	186	SER
1	G	224	GLU
1	G	243	THR
1	G	254	SER
1	G	275	LEU
1	G	284	ASP
1	G	291	ILE
1	G	294	LEU
1	G	305	THR
1	G	326	GLU
1	G	331	GLU
1	G	332	ASN

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Mol	Chain	Res	Type
1	G	351	LYS
1	G	363	LYS
1	G	366	THR
1	G	376	LYS
1	G	391	VAL
1	G	395	ILE
1	G	396	ILE
1	G	419	SER
1	G	421	LYS
1	G	453	ILE
1	G	496	VAL
1	G	500	SER
1	G	531	GLN
1	G	532	GLU
1	G	537	ARG
1	G	540	GLN
1	G	543	VAL
1	G	568	VAL
1	G	574	GLN
1	G	576	ARG
1	G	580	VAL
1	G	605	THR
1	G	629	LEU
1	G	638	VAL
1	G	652	THR
1	G	657	VAL
1	G	665	ASN
1	G	671	THR
1	G	676	ILE
1	G	679	ILE
1	G	713	ILE
1	G	732	ASN
1	G	745	ILE
1	G	749	GLN
1	G	765	VAL
1	G	770	GLN
1	G	782	LEU
1	G	796	GLN
1	G	806	ASN
2	H	63	GLU
2	H	83	GLU
2	H	88	PHE

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Mol	Chain	Res	Type
2	H	91	VAL
2	H	95	ASN
2	H	96	ASP
2	H	105	LYS
2	H	113	LYS
2	H	114	TYR
2	H	130	ILE
2	H	131	ARG
2	H	149	GLU
2	H	154	VAL
2	H	163	ILE
2	H	182	GLU
2	H	187	VAL
2	H	200	LEU
2	H	203	VAL
2	H	204	LEU
2	H	219	GLN
2	H	225	LEU
2	H	238	GLN
2	H	242	LYS
2	H	256	LEU
2	H	258	GLU
2	H	259	THR
2	H	270	THR
2	H	272	THR
2	H	277	LEU
2	H	291	LEU
2	H	301	LYS
2	H	316	GLU
2	H	324	LEU
2	H	328	ASP
2	H	333	GLU
2	H	334	LYS
2	H	350	GLU
2	H	358	VAL
2	H	384	ILE
2	H	391	ASN
2	H	393	LEU
2	H	396	THR
2	H	411	GLU
2	H	420	SER
2	H	432	LYS

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Mol	Chain	Res	Type
2	H	436	LYS
2	H	438	ASN
2	H	448	GLU
2	H	453	ASN
2	H	458	VAL
2	H	479	THR
2	H	523	LEU
2	H	551	LEU
2	H	560	THR
2	H	562	THR
2	H	565	ARG
2	H	567	LYS
2	H	570	GLN
2	H	572	GLU
2	H	587	GLU
2	H	610	GLN
2	H	620	HIS
2	H	632	VAL
2	H	633	ASN
2	H	649	LYS
2	H	650	LEU
2	H	659	SER
2	H	662	TYR
2	H	668	ASN
2	H	673	LEU
2	H	679	SER
2	H	681	ASN
2	H	701	ASP
2	H	707	SER
2	H	709	LYS
2	H	710	ILE
2	H	720	GLU
2	H	725	ARG
2	H	728	GLN
2	H	732	LEU
2	H	737	ASN
2	H	742	ARG
2	H	746	VAL
2	H	768	LEU
2	H	771	ILE
2	H	803	VAL
2	H	806	MET

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Mol	Chain	Res	Type
2	H	835	ARG
2	H	841	GLN
2	H	843	ASN
2	H	845	ILE
2	H	849	GLN
2	H	850	VAL
2	H	857	THR
2	H	906	GLN
2	H	921	VAL
2	H	922	LEU
2	H	939	GLN
2	H	945	GLU
2	H	947	ASN
2	H	956	GLU
2	H	965	LEU
2	H	986	LYS
2	H	988	ASP
2	H	992	SER
2	H	994	SER
2	H	1002	LEU
2	H	1012	LEU
2	H	1017	ASP
2	H	1024	LEU
2	H	1032	THR
2	H	1036	ARG
2	H	1044	ILE
2	H	1045	THR
2	H	1050	GLN
2	H	1052	GLN
2	H	1059	GLN
2	H	1061	TRP
2	H	1069	LEU
2	H	1074	THR
2	H	1117	THR
2	H	1120	THR
2	H	1123	LYS
2	H	1136	ASN
2	H	1143	LEU
2	H	1169	VAL
2	H	1171	GLN
2	H	1172	THR
2	H	1174	ASN

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Mol	Chain	Res	Type
2	H	1184	GLU
2	H	1187	LYS
2	H	1191	SER
2	H	1224	LYS
2	H	1230	SER
2	H	1234	VAL
2	H	1240	GLN
2	H	1267	LEU
2	H	1270	THR
2	H	1288	LEU
2	H	1293	SER
2	H	1301	ARG
2	H	1305	ILE
2	H	1310	GLU
2	H	1314	LEU
2	H	1318	LEU
2	H	1319	GLU
2	H	1328	PHE
2	H	1341	THR
2	H	1342	VAL
2	H	1348	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (258) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	171	GLN
1	A	183	GLN
1	A	191	HIS
1	A	194	ASN
1	A	211	ASN
1	A	270	ASN
1	A	293	GLN
1	A	450	ASN
1	A	454	ASN
1	A	460	GLN
1	A	530	ASN
1	A	531	GLN
1	A	574	GLN
1	A	599	ASN
1	A	645	ASN
1	A	662	ASN

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Mol	Chain	Res	Type
1	A	665	ASN
1	A	722	HIS
1	A	796	GLN
1	A	797	ASN
2	B	95	ASN
2	B	99	ASN
2	B	125	GLN
2	B	127	ASN
2	B	144	ASN
2	B	181	ASN
2	B	217	ASN
2	B	235	ASN
2	B	302	HIS
2	B	360	HIS
2	B	382	HIS
2	B	391	ASN
2	B	528	ASN
2	B	547	ASN
2	B	570	GLN
2	B	582	GLN
2	B	620	HIS
2	B	665	GLN
2	B	668	ASN
2	B	733	ASN
2	B	773	ASN
2	B	841	GLN
2	B	849	GLN
2	B	895	ASN
2	B	924	ASN
2	B	939	GLN
2	B	947	ASN
2	B	1011	ASN
2	B	1050	GLN
2	B	1119	ASN
2	B	1122	ASN
2	B	1136	ASN
2	B	1165	ASN
2	B	1171	GLN
2	B	1258	GLN
2	B	1327	GLN
2	B	1333	ASN
1	C	36	ASN

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Mol	Chain	Res	Type
1	C	69	GLN
1	C	104	GLN
1	C	136	ASN
1	C	171	GLN
1	C	182	ASN
1	C	183	GLN
1	C	189	ASN
1	C	190	GLN
1	C	194	ASN
1	C	211	ASN
1	C	285	GLN
1	C	335	ASN
1	C	352	GLN
1	C	354	GLN
1	C	445	ASN
1	C	454	ASN
1	C	530	ASN
1	C	531	GLN
1	C	569	ASN
1	C	574	GLN
1	C	599	ASN
1	C	665	ASN
1	C	770	GLN
1	C	796	GLN
1	C	797	ASN
1	C	804	ASN
1	C	814	GLN
2	D	59	GLN
2	D	72	ASN
2	D	111	ASN
2	D	127	ASN
2	D	136	ASN
2	D	144	ASN
2	D	218	ASN
2	D	235	ASN
2	D	360	HIS
2	D	382	HIS
2	D	438	ASN
2	D	494	ASN
2	D	528	ASN
2	D	547	ASN
2	D	548	GLN

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Mol	Chain	Res	Type
2	D	570	GLN
2	D	620	HIS
2	D	631	ASN
2	D	634	ASN
2	D	665	GLN
2	D	684	ASN
2	D	728	GLN
2	D	733	ASN
2	D	773	ASN
2	D	815	ASN
2	D	823	ASN
2	D	924	ASN
2	D	939	GLN
2	D	947	ASN
2	D	975	ASN
2	D	977	ASN
2	D	1011	ASN
2	D	1050	GLN
2	D	1052	GLN
2	D	1164	ASN
2	D	1171	GLN
2	D	1297	GLN
2	D	1324	GLN
2	D	1327	GLN
2	D	1333	ASN
1	E	65	GLN
1	E	73	ASN
1	E	96	ASN
1	E	136	ASN
1	E	143	GLN
1	E	189	ASN
1	E	191	HIS
1	E	194	ASN
1	E	200	ASN
1	E	293	GLN
1	E	308	HIS
1	E	330	GLN
1	E	369	ASN
1	E	371	HIS
1	E	380	GLN
1	E	394	GLN
1	E	454	ASN

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Mol	Chain	Res	Type
1	E	472	ASN
1	E	503	ASN
1	E	530	ASN
1	E	574	GLN
1	E	665	ASN
1	E	748	ASN
1	E	751	GLN
1	E	770	GLN
1	E	797	ASN
2	F	71	ASN
2	F	95	ASN
2	F	126	GLN
2	F	127	ASN
2	F	144	ASN
2	F	150	ASN
2	F	155	GLN
2	F	181	ASN
2	F	218	ASN
2	F	235	ASN
2	F	302	HIS
2	F	351	ASN
2	F	352	HIS
2	F	388	ASN
2	F	391	ASN
2	F	418	ASN
2	F	547	ASN
2	F	570	GLN
2	F	620	HIS
2	F	634	ASN
2	F	733	ASN
2	F	763	GLN
2	F	773	ASN
2	F	841	GLN
2	F	843	ASN
2	F	862	ASN
2	F	947	ASN
2	F	958	ASN
2	F	1011	ASN
2	F	1052	GLN
2	F	1122	ASN
2	F	1181	ASN
2	F	1207	ASN

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Mol	Chain	Res	Type
2	F	1235	ASN
2	F	1311	ASN
2	F	1333	ASN
2	F	1347	ASN
2	F	1348	GLN
1	G	59	GLN
1	G	65	GLN
1	G	72	HIS
1	G	73	ASN
1	G	96	ASN
1	G	131	GLN
1	G	171	GLN
1	G	180	GLN
1	G	183	GLN
1	G	285	GLN
1	G	293	GLN
1	G	308	HIS
1	G	344	ASN
1	G	352	GLN
1	G	359	GLN
1	G	380	GLN
1	G	445	ASN
1	G	454	ASN
1	G	508	ASN
1	G	574	GLN
1	G	662	ASN
1	G	665	ASN
1	G	674	ASN
1	G	732	ASN
1	G	749	GLN
1	G	751	GLN
1	G	797	ASN
1	G	804	ASN
1	G	814	GLN
2	H	59	GLN
2	H	71	ASN
2	H	95	ASN
2	H	97	ASN
2	H	127	ASN
2	H	144	ASN
2	H	217	ASN
2	H	218	ASN

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Mol	Chain	Res	Type
2	H	235	ASN
2	H	391	ASN
2	H	395	GLN
2	H	418	ASN
2	H	570	GLN
2	H	620	HIS
2	H	631	ASN
2	H	634	ASN
2	H	721	ASN
2	H	728	GLN
2	H	773	ASN
2	H	812	ASN
2	H	815	ASN
2	H	823	ASN
2	H	837	GLN
2	H	854	ASN
2	H	932	GLN
2	H	939	GLN
2	H	947	ASN
2	H	958	ASN
2	H	967	HIS
2	H	975	ASN
2	H	1003	ASN
2	H	1011	ASN
2	H	1052	GLN
2	H	1136	ASN
2	H	1207	ASN
2	H	1311	ASN
2	H	1312	GLN
2	H	1333	ASN
2	H	1348	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	781/802 (97%)	-1.81	0 100 100	8, 29, 71, 112	0
1	C	779/802 (97%)	-1.82	0 100 100	9, 28, 73, 99	0
1	E	783/802 (97%)	-1.82	0 100 100	7, 29, 68, 109	0
1	G	784/802 (97%)	-1.80	0 100 100	8, 32, 69, 104	0
2	B	1268/1334 (95%)	-1.80	0 100 100	7, 29, 76, 130	0
2	D	1265/1334 (94%)	-1.83	0 100 100	6, 27, 73, 118	0
2	F	1250/1334 (93%)	-1.63	0 100 100	9, 44, 103, 136	0
2	H	1247/1334 (93%)	-1.53	0 100 100	14, 55, 115, 149	0
All	All	8157/8544 (95%)	-1.74	0 100 100	6, 34, 91, 149	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.