



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:49 PM UTC

PDB ID : 3NBY / pdb_00003nby
Title : Crystal structure of the PKI NES-CRM1-RanGTP nuclear export complex
Authors : Guttler, T.; Madl, T.; Neumann, P.; Deichsel, D.; Corsini, L.; Monecke, T.;
Ficner, R.; Sattler, M.; Gorlich, D.
Deposited on : 2010-06-04
Resolution : 3.42 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

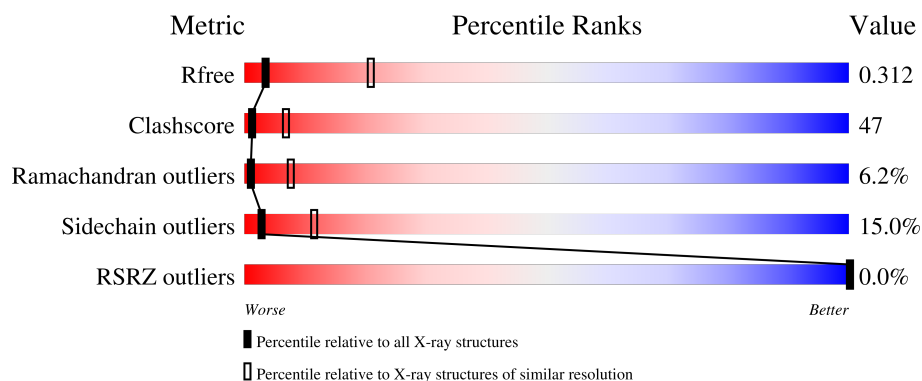
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.42 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	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)

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	B	361	21% 39% 14% • 25%
1	E	361	27% 35% 14% • 23%
2	C	176	30% 54% 11% • •
2	F	176	34% 48% 13% • •
3	A	1073	28% 53% 15% • •

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Mol	Chain	Length	Quality of chain
3	D	1073	29% 52% 16% ••

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24084 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 Snurportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	272	Total	C	N	O	S	0	0	0
			2193	1398	376	405	14			
1	E	277	Total	C	N	O	S	0	0	0
			2221	1416	380	410	15			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP O95149
B	0	SER	-	expression tag	UNP O95149
B	1	LEU	-	expression tag	UNP O95149
B	2	ASN	-	expression tag	UNP O95149
B	3	GLU	-	expression tag	UNP O95149
B	4	LEU	-	expression tag	UNP O95149
B	5	ALA	-	expression tag	UNP O95149
B	6	LEU	-	expression tag	UNP O95149
B	7	LYS	-	expression tag	UNP O95149
B	8	LEU	-	expression tag	UNP O95149
B	9	ALA	-	expression tag	UNP O95149
B	10	GLY	-	expression tag	UNP O95149
B	11	LEU	-	expression tag	UNP O95149
B	12	ASP	-	expression tag	UNP O95149
B	13	ILE	-	expression tag	UNP O95149
E	-1	GLY	-	expression tag	UNP O95149
E	0	SER	-	expression tag	UNP O95149
E	1	LEU	-	expression tag	UNP O95149
E	2	ASN	-	expression tag	UNP O95149
E	3	GLU	-	expression tag	UNP O95149
E	4	LEU	-	expression tag	UNP O95149
E	5	ALA	-	expression tag	UNP O95149
E	6	LEU	-	expression tag	UNP O95149
E	7	LYS	-	expression tag	UNP O95149
E	8	LEU	-	expression tag	UNP O95149

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Chain	Residue	Modelled	Actual	Comment	Reference
E	9	ALA	-	expression tag	UNP O95149
E	10	GLY	-	expression tag	UNP O95149
E	11	LEU	-	expression tag	UNP O95149
E	12	ASP	-	expression tag	UNP O95149
E	13	ILE	-	expression tag	UNP O95149

- Molecule 2 is a protein called GTP-binding nuclear protein Ran.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	171	Total	C	N	O	S	0	0	0
			1389	904	243	237	5			
2	F	171	Total	C	N	O	S	0	0	0
			1389	904	243	237	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	69	LEU	GLN	engineered mutation	UNP P62826
F	69	LEU	GLN	engineered mutation	UNP P62826

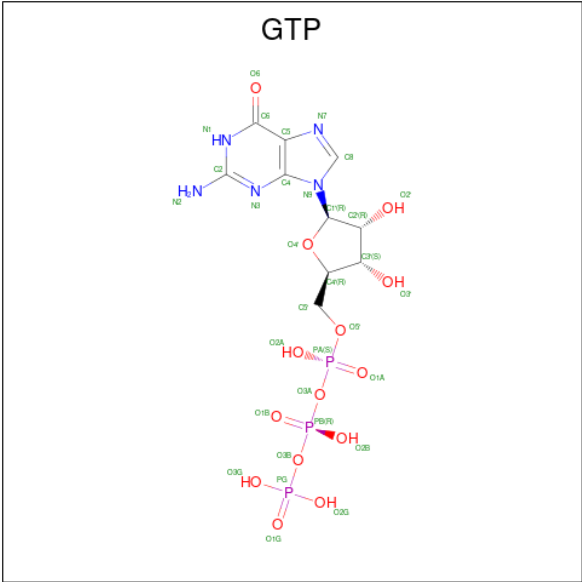
- Molecule 3 is a protein called Exportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	1041	Total	C	N	O	S	0	0	0
			8413	5397	1413	1549	54			
3	D	1041	Total	C	N	O	S	0	0	0
			8413	5397	1413	1549	54			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q6P5F9
A	0	SER	-	expression tag	UNP Q6P5F9
D	-1	GLY	-	expression tag	UNP Q6P5F9
D	0	SER	-	expression tag	UNP Q6P5F9

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	F	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

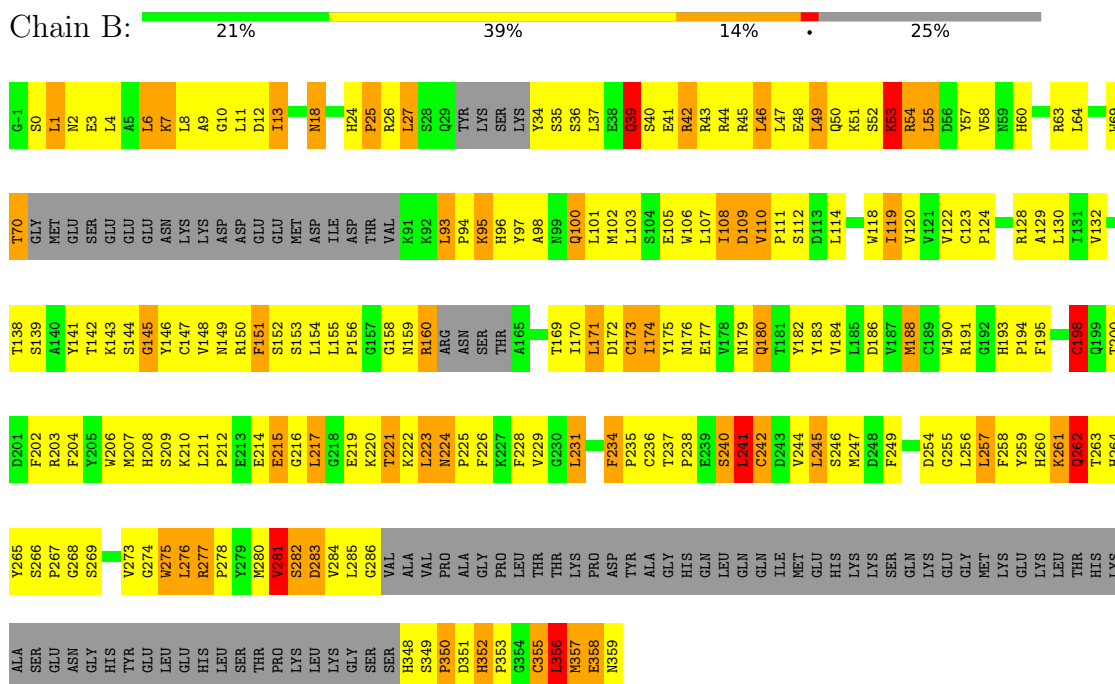
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		

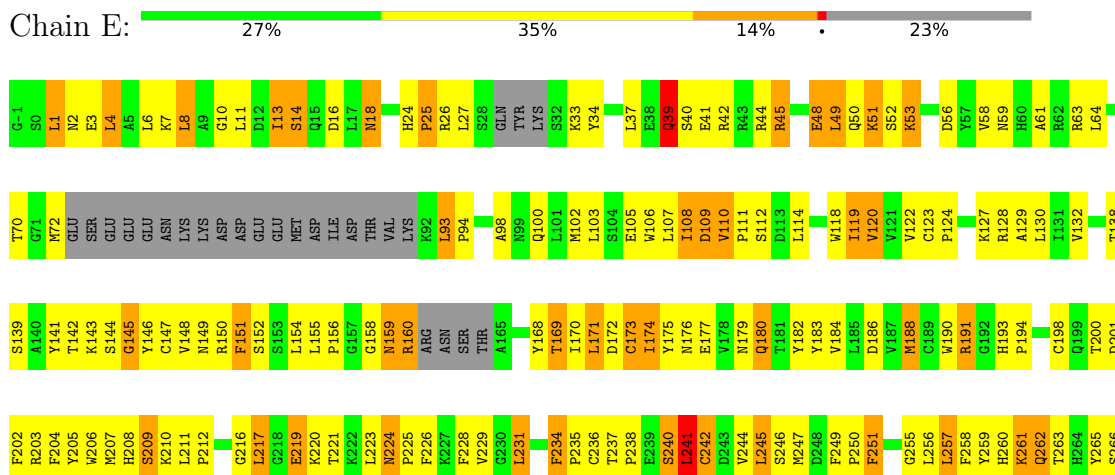
3 Residue-property plots

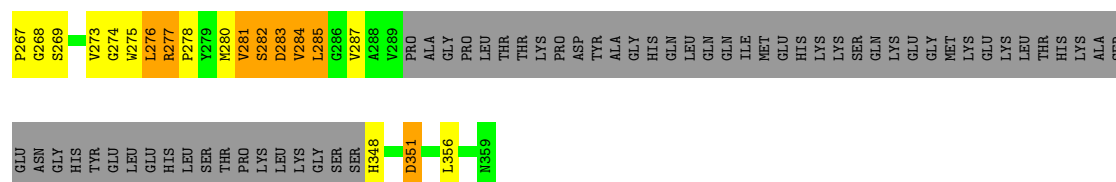
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Snurportin-1



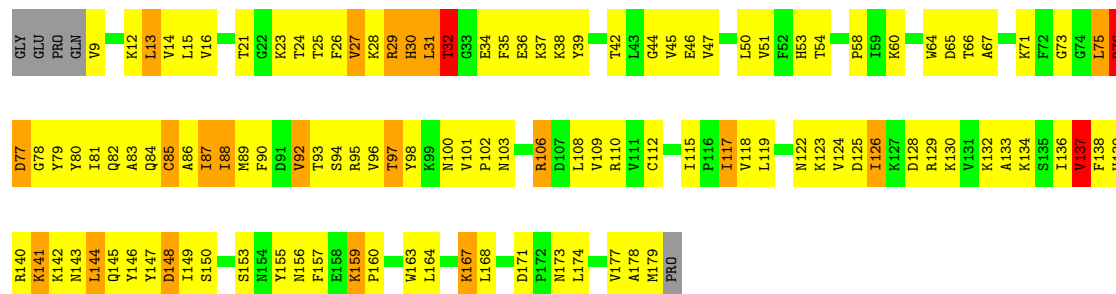
• Molecule 1: Snurportin-1





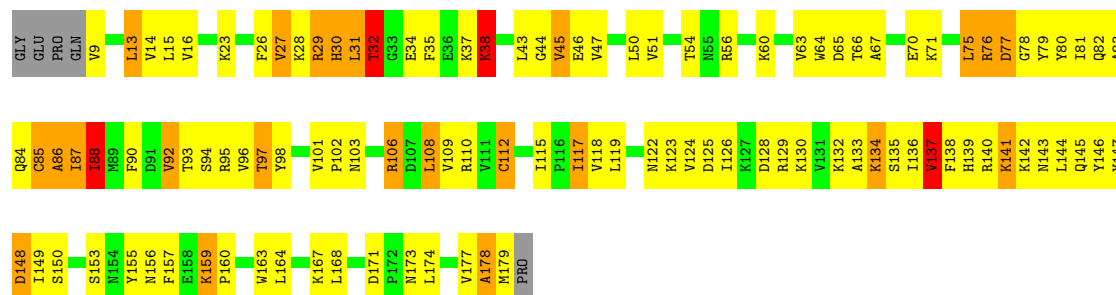
• Molecule 2: GTP-binding nuclear protein Ran

Chain C: 30% 54% 11% . .



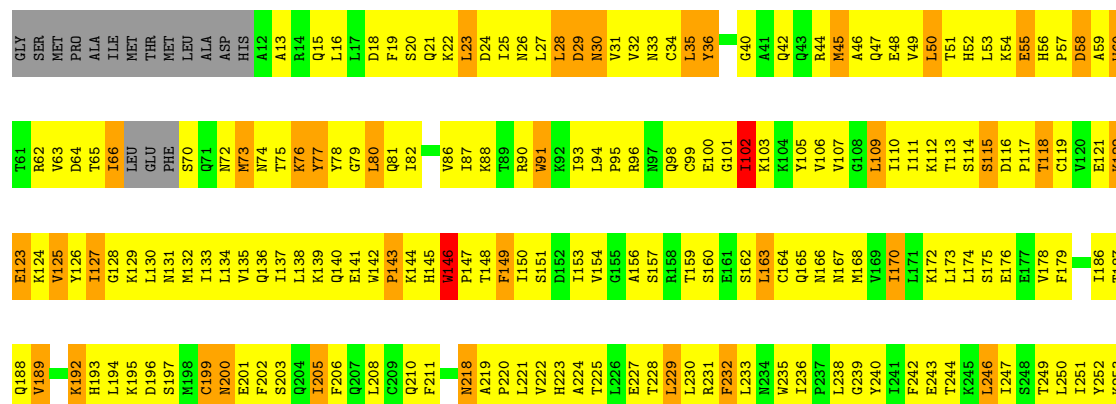
• Molecule 2: GTP-binding nuclear protein Ran

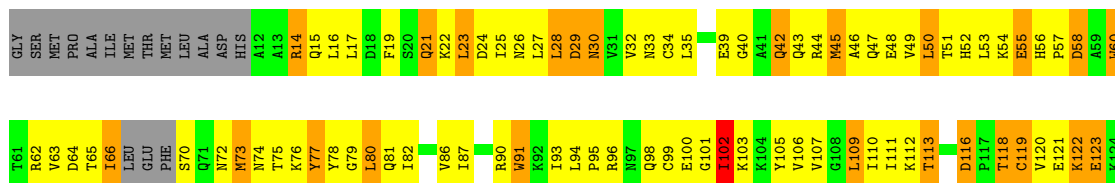
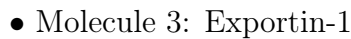
Chain F: 34% 48% 13% . .



• Molecule 3: Exportin-1

Chain A: 28% 53% 15% . .





D1007	T836	K872	T803	K741	V600	G533	H486	P392	S323	N256	A191	V126
D1008	A937	L873	H804	Q742	E606	K534	L467	L393	L324	V257	K192	Y127
P1009	G938	V874	A895	P743	V607	D535	D468	P258	F325	M259	H193	G128
A1010	L939	L875	T806	L744	M608	N536	Y469	S395	L326	F260	K129	L194
F1011	T940	D876	I807	I745	P609	K537	V470		C327	R261	D196	L130
M941	M941	S877	K810	I746	F610	A538	D471	H399	T328	R262	S197	M131
E1013	H942	S747	L878	S747	L611	I539	T472	F400	F329	V263	M198	M132
A943	A943	R748	L679	R748	D612	I540	E473	D401	L330	S264	C199	L133
S944	S944	T750	D681	T750	E613	A541	L474	L402	K331	L265	N200	L134
I945	I945	W751	P682	W751	E614		L475	P403	H333	K266	E201	V135
L946	L946	K752	F683	K752	E615	I544	M476	P404	H334	C267	F202	Q136
A947	A947	R684	E683	R684	L615			R405	G334	L268	S203	I137
T885	T885	T684	T684	T684	M616	I547	K479	R406	Q335	T268	Q204	L138
H886	H886	P685	P685	P685	N617	V548	L480	Q407	L336	T269	I205	K139
R887	R887	E686	E686	E686	L618		Q481	L408	L337	E270	F206	Q140
N888	N888	Q687	Q687	Q687	M619	Y551	N482	Y409	E338	I271	Q207	E141
V889	V889	W687	W687	W687	T620	P552	Q483		K339	A272	L208	W142
F892	F892	I691	I691	I691	E621	R553	V484	R417	R340	Q273	C209	F143
L894	L894	L692	L692	L692	T622	F554	N485		L341	V274	Q210	K144
A890	A890	K693	K693	K693	G623	L555	Q486	M420	N342	S275	F211	H145
D891	D891	T694	T694	T694	D624	R556	T487	V421	L343	Q277	Q217	P147
T892	T892	W696	W696	W696	L625	A557	W488	S422	R344	Q278	N218	T148
G893	G893	R697	R697	R697	Q626	H558	W489	R423		Y279	A219	F149
S895	S895	A698	A698	A698	P627	W559	S490	M424	L347	E280	P220	I150
S959	S959	K560	K560	K560	Q628	K560	W491		M348	E281	L221	S151
T960	T960	Q629	Q629	Q629	K562	F561		P427	A350	Q282	L222	D152
P961	P961	V630	V630	V630	L562	L562	T496	E428	L351	F283	W222	I153
L962	L962	H631	H631	H631	K563	T564	L497	V430	E362	E284	H223	V154
N963	N963	T632	T632	T632	F572	S505	C498	L431	I365	Q293	R231	E161
G965	G965	F633	F633	F633	W573		W499	V432	F366	L294	F232	L163
E954	E954	Y634	Y634	Y634	H574	H509	A500	V433	K367	K295	L233	G155
E955	E955	E635	E635	E635	E575	E510	I501	W440	I368	M297	W235	A156
I958	I958	I641	I641	I641	H575	E511	E502	R442	E371	L298	L238	M167
S959	S959	Q642	Q642	Q642	D576	D512	S503	E434	T290	M291	G239	M168
T960	T960	A643	A643	A643	H577	D513	E504	N435	T363	D292	Y240	Q165
P961	P961	T646	T646	T646	D578	E514	I504	Q437	E364	S160	L241	L170
L962	L962	D647	D647	D647	W579	K514	S505	E439	I366	Q293	F242	K172
S959	S959	Q647	Q647	Q647	H579	E515		W441	F366	L294	E243	S162
T960	T960	T648	T648	T648	D580	E516	E516	R443	I368	K296	L244	L163
P961	P961	Q650	Q650	Q650	Q581	F516	K514	T448	E372	M297	K245	S175
E954	E954	E651	E651	E651	D582	F517	E517	D449	W373	L300	L246	E176
A954	A954	E651	E651	E651	M583	V518	E518	S450	N374	K301	L247	E177
L958	L958	E651	E651	E651	D586	V520	E521	L451	H375	T302	T249	F179
S959	S959	E651	E651	E651	E651	E522	K522	N452	A377	I304	S248	W178
T960	T960	E651	E651	E651	E651	E522	K522	L453	A378	R305	L250	F179
P961	P961	E651	E651	E651	E651	E522	K522	Y454	E379	L306	L251	I186
L958	L958	E651	E651	E651	E651	E522	K522	M457	L380	A307	Y252	T187
S959	S959	E651	E651	E651	E651	E522	K522	R458	R382	Y308	K253	Q188
T960	T960	E651	E651	E651	E651	E522	K522	E459	E383	D313	F254	V189
P961	P961	E651	E651	E651	E651	E522	K522	T460	S384		L255	K190
L958	L958	E651	E651	E651	E651	E522	K522	L461	T388	Q316		
S959	S959	E651	E651	E651	E651	E522	K522	V462	S389	N317		
T960	T960	E651	E651	E651	E651	E522	K522	Y463	A390	F318		
P961	P961	E651	E651	E651	E651	E522	K522	L464				
L958	L958	E651	E651	E651	E651	E522	K522	T465	S391	L322		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.09Å 223.73Å 163.06Å 90.00° 100.63° 90.00°	Depositor
Resolution (Å)	38.63 – 3.42 38.63 – 3.42	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.63-3.42) 89.4 (38.63-3.42)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.95Å)	Xtriage
Refinement program	PHENIX 1.6.1_357	Depositor
R, R_{free}	0.258 , 0.315 0.257 , 0.312	Depositor DCC
R_{free} test set	5238 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.115 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	24084	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GTP

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	B	0.74	0/2250	1.17	20/3046 (0.7%)
1	E	0.74	0/2278	1.16	16/3084 (0.5%)
2	C	0.74	1/1423 (0.1%)	1.07	3/1921 (0.2%)
2	F	0.71	0/1423	1.10	10/1921 (0.5%)
3	A	0.74	5/8584 (0.1%)	1.12	45/11627 (0.4%)
3	D	0.74	2/8584 (0.0%)	1.13	46/11627 (0.4%)
All	All	0.74	8/24542 (0.0%)	1.13	140/33226 (0.4%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	491	TRP	NE1-CE2	6.63	1.44	1.37
3	A	466	HIS	CD2-NE2	6.09	1.44	1.37
3	D	491	TRP	NE1-CE2	5.96	1.44	1.37
3	A	664	VAL	CA-CB	5.64	1.60	1.54
3	D	521	ILE	CA-CB	5.56	1.61	1.54
3	A	466	HIS	CG-CD2	-5.33	1.29	1.35
2	C	126	ILE	CA-CB	-5.20	1.47	1.53
3	A	466	HIS	CE1-NE2	-5.06	1.27	1.32

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	391	SER	CA-C-N	12.13	135.00	119.84
3	D	391	SER	C-N-CA	12.13	135.00	119.84
3	D	116	ASP	CA-C-N	11.04	133.63	119.84
3	D	116	ASP	C-N-CA	11.04	133.63	119.84
1	B	224	ASN	CA-C-N	10.73	131.09	119.28
1	B	224	ASN	C-N-CA	10.73	131.09	119.28
3	D	488	GLU	N-CA-C	-10.40	99.90	112.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	488	GLU	N-CA-C	-10.11	100.25	112.59
1	E	224	ASN	CA-C-N	10.05	130.34	119.28
1	E	224	ASN	C-N-CA	10.05	130.34	119.28
1	E	93	LEU	CA-C-N	9.61	131.85	119.84
1	E	93	LEU	C-N-CA	9.61	131.85	119.84
3	A	608	MET	CA-C-N	9.53	131.75	119.84
3	A	608	MET	C-N-CA	9.53	131.75	119.84
3	D	742	GLN	CA-C-N	8.59	130.58	119.84
3	D	742	GLN	C-N-CA	8.59	130.58	119.84
3	A	742	GLN	CA-C-N	8.32	130.24	119.84
3	A	742	GLN	C-N-CA	8.32	130.24	119.84
3	D	608	MET	CA-C-N	8.17	128.65	119.83
3	D	608	MET	C-N-CA	8.17	128.65	119.83
3	D	635	GLU	N-CA-C	-7.91	102.66	111.28
3	D	757	LYS	N-CA-C	-7.36	104.11	113.23
3	D	206	PHE	N-CA-C	-7.26	103.31	111.07
1	E	42	ARG	NE-CZ-NH2	7.24	125.72	119.20
3	A	757	LYS	N-CA-C	-7.21	104.29	113.23
3	A	1008	ILE	CA-C-N	-7.10	111.17	119.05
3	A	1008	ILE	C-N-CA	-7.10	111.17	119.05
3	A	635	GLU	N-CA-C	-7.07	103.58	111.28
3	A	970	ASN	N-CA-C	7.06	118.77	111.14
3	D	621	ILE	CB-CA-C	-7.04	102.81	112.24
1	E	42	ARG	NE-CZ-NH1	-7.01	114.49	121.50
3	A	621	ILE	CB-CA-C	-7.00	102.87	112.24
3	A	36	TYR	N-CA-C	6.97	121.64	112.72
3	A	391	SER	CA-C-N	-6.94	111.16	119.84
3	A	391	SER	C-N-CA	-6.94	111.16	119.84
3	A	423	ARG	N-CA-C	-6.72	104.22	112.88
1	E	100	GLN	N-CA-C	-6.67	105.43	113.97
3	D	1008	ILE	CA-C-N	-6.65	111.67	119.05
3	D	1008	ILE	C-N-CA	-6.65	111.67	119.05
3	D	257	VAL	N-CA-C	6.59	114.65	107.60
3	A	257	VAL	N-CA-C	6.57	114.63	107.60
3	A	206	PHE	N-CA-C	-6.55	104.06	111.07
1	E	277	ARG	CA-C-N	6.51	127.97	119.84
1	E	277	ARG	C-N-CA	6.51	127.97	119.84
3	A	514	LYS	N-CA-C	-6.47	103.92	110.97
3	A	76	LYS	N-CA-C	-6.37	103.86	111.69
3	D	400	PHE	N-CA-C	-6.35	104.16	112.41
3	A	322	LEU	N-CA-C	-6.34	104.30	111.14
3	D	680	LYS	N-CA-C	-6.30	105.36	114.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	560	LYS	N-CA-C	-6.17	104.47	111.07
1	B	12	ASP	N-CA-C	6.15	119.15	108.76
3	D	120	VAL	N-CA-C	-6.14	105.30	112.98
3	D	922	ILE	N-CA-C	-6.13	106.94	111.90
3	D	423	ARG	N-CA-C	-6.13	104.30	112.94
3	D	441	VAL	N-CA-C	6.09	122.00	109.34
2	F	167	LYS	N-CA-C	6.06	117.69	111.14
1	B	173	CYS	N-CA-C	6.05	119.34	109.24
3	D	560	LYS	N-CA-C	-6.04	104.61	111.07
3	D	889	VAL	CB-CA-C	-6.01	103.92	112.22
3	A	922	ILE	N-CA-C	-6.00	107.04	111.90
3	A	470	VAL	N-CA-C	-5.95	103.65	111.09
2	F	159	LYS	CA-C-N	5.89	125.77	119.28
2	F	159	LYS	C-N-CA	5.89	125.77	119.28
3	D	559	TRP	N-CA-C	5.89	118.66	111.82
1	E	173	CYS	N-CA-C	5.84	118.72	109.50
3	D	470	VAL	N-CA-C	-5.83	103.81	111.09
3	D	626	GLN	CA-C-N	5.83	127.13	119.84
3	D	626	GLN	C-N-CA	5.83	127.13	119.84
3	A	889	VAL	CB-CA-C	-5.80	104.31	112.14
2	C	159	LYS	CA-C-N	5.80	125.66	119.28
2	C	159	LYS	C-N-CA	5.80	125.66	119.28
1	B	93	LEU	CA-C-N	5.75	127.03	119.84
1	B	93	LEU	C-N-CA	5.75	127.03	119.84
1	B	277	ARG	CA-C-N	5.73	127.00	119.84
1	B	277	ARG	C-N-CA	5.73	127.00	119.84
3	A	953	VAL	CB-CA-C	-5.72	104.65	111.97
3	A	751	VAL	CB-CA-C	-5.71	104.43	112.14
1	B	27	LEU	N-CA-C	5.69	119.32	112.38
1	B	100	GLN	N-CA-C	-5.66	106.73	113.97
2	F	86	ALA	N-CA-C	5.63	115.98	108.38
1	E	127	LYS	N-CA-C	5.61	117.67	108.52
3	D	826	VAL	N-CA-C	5.60	118.56	112.96
1	B	198	CYS	N-CA-C	5.60	118.94	109.76
1	E	120	VAL	N-CA-C	5.58	116.10	107.78
1	B	262	GLN	N-CA-C	5.58	118.87	112.57
2	C	167	LYS	N-CA-C	5.55	117.13	111.14
2	F	38	LYS	CA-C-N	-5.55	115.63	122.84
2	F	38	LYS	C-N-CA	-5.55	115.63	122.84
1	E	193	HIS	CA-C-N	5.53	125.85	119.93
1	E	193	HIS	C-N-CA	5.53	125.85	119.93
3	D	953	VAL	CB-CA-C	-5.51	104.91	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	559	TRP	N-CA-C	5.51	118.21	111.82
3	A	434	GLU	N-CA-C	5.49	117.67	108.73
3	D	491	TRP	CE2-CD2-CE3	-5.47	113.33	118.80
3	A	403	PRO	CA-C-N	5.47	126.67	119.84
3	A	403	PRO	C-N-CA	5.47	126.67	119.84
1	B	54	ARG	N-CA-C	-5.46	107.26	114.31
3	D	937	ALA	N-CA-C	-5.46	106.39	113.16
2	F	88	ILE	N-CA-C	-5.45	102.55	109.58
1	B	193	HIS	CA-C-N	5.45	126.65	119.84
1	B	193	HIS	C-N-CA	5.45	126.65	119.84
3	A	102	ILE	N-CA-C	-5.44	105.02	110.30
1	B	281	VAL	N-CA-C	5.43	115.88	110.23
3	D	292	MET	N-CA-C	-5.43	104.59	111.11
2	F	56	ARG	N-CA-C	5.40	116.15	108.54
1	B	221	THR	N-CA-C	5.38	115.13	108.19
3	A	680	LYS	N-CA-C	-5.38	106.65	114.12
2	F	178	ALA	N-CA-C	5.38	119.56	112.25
2	F	63	VAL	CB-CA-C	-5.37	106.11	111.80
3	D	751	VAL	CB-CA-C	-5.37	104.89	112.14
3	A	441	VAL	N-CA-C	5.35	116.41	108.65
3	A	550	GLN	N-CA-C	-5.33	106.78	113.28
3	D	284	GLU	N-CA-C	-5.32	105.38	111.07
1	E	251	PHE	N-CA-C	5.31	115.03	108.19
3	D	102	ILE	N-CA-C	-5.25	105.20	110.30
3	A	804	MET	N-CA-C	-5.24	105.64	111.36
3	D	322	LEU	N-CA-C	-5.24	105.48	111.14
3	D	826	VAL	CB-CA-C	-5.23	106.46	111.06
3	A	654	ILE	CB-CA-C	-5.22	103.65	112.16
3	D	904	VAL	N-CA-C	-5.21	105.63	110.53
1	B	42	ARG	CD-NE-CZ	5.21	131.69	124.40
3	D	403	PRO	CA-C-N	5.21	126.35	119.84
3	D	403	PRO	C-N-CA	5.21	126.35	119.84
3	A	292	MET	N-CA-C	-5.21	104.86	111.11
1	E	250	PRO	N-CA-C	-5.19	108.74	114.92
1	B	223	LEU	N-CA-C	-5.17	106.08	114.09
3	A	626	GLN	CA-C-N	5.14	126.26	119.84
3	A	626	GLN	C-N-CA	5.14	126.26	119.84
3	D	535	ASP	N-CA-C	-5.12	105.78	111.36
3	A	652	HIS	CA-C-N	5.12	127.14	120.28
3	A	652	HIS	C-N-CA	5.12	127.14	120.28
3	A	937	ALA	N-CA-C	-5.08	106.86	113.16
3	D	519	THR	CB-CA-C	-5.07	102.70	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	241	ILE	CB-CA-C	-5.05	105.58	111.94
3	A	904	VAL	N-CA-C	-5.04	105.79	110.53
3	D	557	ALA	N-CA-C	-5.04	107.13	113.28
3	A	485	ASN	N-CA-C	-5.03	104.75	111.24
3	A	826	VAL	N-CA-C	5.03	117.99	112.96
1	B	42	ARG	NE-CZ-NH2	-5.01	114.69	119.20
3	D	938	GLY	N-CA-C	-5.01	106.43	112.49

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	B	2193	0	2138	249	0
1	E	2221	0	2170	221	0
2	C	1389	0	1419	133	0
2	F	1389	0	1419	125	0
3	A	8413	0	8480	819	0
3	D	8413	0	8480	799	0
4	C	32	0	12	8	0
4	F	32	0	12	0	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
All	All	24084	0	24130	2256	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 47.

All (2256) 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)
3:A:328:THR:HA	3:A:331:LYS:HD3	1.27	1.14
3:D:328:THR:HA	3:D:331:LYS:HD3	1.33	1.09
3:D:961:PRO:HG2	3:D:973:PHE:HD2	1.16	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:GLU:O	1:B:7:LYS:HB2	1.53	1.07
3:D:996:LEU:HD13	3:D:1035:LEU:HD12	1.37	1.06
1:B:159:ASN:HB2	1:B:223:LEU:HD21	1.36	1.06
3:A:528:CYS:HB2	3:A:540:ILE:HG21	1.38	1.06
3:D:528:CYS:HB2	3:D:540:ILE:HG21	1.40	1.04
3:A:962:LEU:HB3	3:A:964:PRO:HD2	1.41	1.02
1:B:255:GLY:HA2	1:B:278:PRO:HD3	1.42	1.01
1:E:4:LEU:HA	1:E:7:LYS:CB	1.89	1.01
1:E:180:GLN:HE22	3:D:684:THR:HG22	1.25	1.01
3:D:892:THR:O	3:D:896:ILE:HG13	1.61	1.01
3:A:107:VAL:O	3:A:111:ILE:HG12	1.61	1.00
3:A:482:ASN:HA	3:A:486:GLY:HA3	1.43	1.00
1:E:4:LEU:HA	1:E:7:LYS:HB2	1.01	1.00
1:B:159:ASN:OD1	1:B:160:ARG:HD2	1.63	0.98
3:D:961:PRO:HG2	3:D:973:PHE:CD2	1.98	0.98
1:B:1:LEU:HD13	3:A:558:HIS:HD2	1.26	0.97
3:A:892:THR:O	3:A:896:ILE:HG13	1.63	0.97
3:D:482:ASN:HA	3:D:486:GLY:HA3	1.42	0.97
1:E:40:SER:HB2	1:E:109:ASP:HB2	1.45	0.96
1:E:4:LEU:CA	1:E:7:LYS:HB2	1.94	0.96
1:E:4:LEU:O	1:E:8:LEU:N	1.97	0.96
3:D:287:PHE:CE2	3:D:337:LEU:HD11	2.00	0.96
3:A:484:VAL:HG13	3:A:530:GLN:OE1	1.66	0.95
3:D:107:VAL:O	3:D:111:ILE:HG12	1.66	0.95
3:A:900:LEU:O	3:A:904:VAL:HG23	1.66	0.95
1:E:255:GLY:HA2	1:E:278:PRO:HD3	1.47	0.95
3:D:476:MET:HE3	3:D:501:ILE:HG12	1.44	0.95
2:C:148:ASP:HB3	2:C:155:TYR:HE2	1.31	0.94
2:C:32:THR:OG1	2:C:34:GLU:HG2	1.68	0.94
3:A:746:ARG:HG2	3:A:746:ARG:HH11	1.28	0.94
2:C:94:SER:O	2:C:97:THR:HG23	1.67	0.93
3:A:476:MET:HE3	3:A:501:ILE:HG12	1.50	0.93
1:B:40:SER:HB2	1:B:109:ASP:HB2	1.48	0.93
3:A:287:PHE:CE2	3:A:337:LEU:HD11	2.04	0.93
3:A:887:ARG:HD3	3:A:937:ALA:HB3	1.50	0.93
3:D:484:VAL:HG13	3:D:530:GLN:OE1	1.69	0.92
2:F:94:SER:O	2:F:97:THR:HG23	1.69	0.92
3:A:337:LEU:HD13	3:A:347:LEU:HD12	1.52	0.92
2:F:148:ASP:HB3	2:F:155:TYR:HE2	1.34	0.91
3:D:900:LEU:O	3:D:904:VAL:HG23	1.69	0.91
3:D:337:LEU:HD22	3:D:347:LEU:HB2	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:31:LEU:HD12	2:F:32:THR:HG22	1.50	0.91
2:F:77:ASP:HA	2:F:80:TYR:CD2	2.05	0.91
1:B:41:GLU:HG3	1:B:109:ASP:HB3	1.52	0.91
3:A:337:LEU:HD22	3:A:347:LEU:HB2	1.51	0.91
3:A:672:ALA:HB2	3:A:678:ILE:HD11	1.53	0.91
1:B:4:LEU:O	1:B:8:LEU:N	2.03	0.91
1:B:124:PRO:HD3	1:B:231:LEU:HD11	1.52	0.91
3:D:672:ALA:HB2	3:D:678:ILE:HD11	1.53	0.91
3:D:746:ARG:HG2	3:D:746:ARG:HH11	1.34	0.90
2:C:93:THR:HG21	2:C:126:ILE:HD12	1.54	0.90
3:A:434:GLU:HB2	3:A:439:GLU:O	1.72	0.89
2:C:44:GLY:HA3	3:A:45:MET:HE1	1.54	0.89
1:E:209:SER:C	1:E:210:LYS:HD2	1.97	0.89
3:A:1047:GLU:O	3:A:1051:LYS:HD3	1.72	0.88
1:B:4:LEU:HD11	3:A:518:VAL:HG13	1.56	0.88
1:E:41:GLU:HG3	1:E:109:ASP:HB3	1.54	0.88
1:B:64:LEU:HD23	1:B:170:ILE:HD13	1.57	0.88
3:D:887:ARG:HD3	3:D:937:ALA:HB3	1.54	0.87
1:E:8:LEU:HD23	3:D:564:THR:HG22	1.54	0.87
3:D:650:GLN:HE22	3:D:705:PRO:HG2	1.39	0.87
1:E:124:PRO:HD3	1:E:231:LEU:HD11	1.54	0.87
2:F:44:GLY:HA3	3:D:45:MET:HE1	1.57	0.86
3:A:650:GLN:HE22	3:A:705:PRO:HG2	1.41	0.86
1:B:55:LEU:HD12	1:B:55:LEU:H	1.38	0.86
3:A:899:THR:HG22	3:A:903:ASN:HD21	1.40	0.86
1:B:124:PRO:HD2	1:B:174:ILE:HD12	1.57	0.84
3:D:14:ARG:HH11	3:D:14:ARG:HG3	1.43	0.84
1:B:190:TRP:CD1	1:B:191:ARG:HG3	2.12	0.84
3:D:899:THR:HG22	3:D:903:ASN:HD21	1.43	0.84
3:D:633:PHE:O	3:D:636:ALA:HB3	1.78	0.83
1:B:160:ARG:NE	1:B:160:ARG:HA	1.93	0.83
1:B:13:ILE:HG21	3:A:575:GLU:CD	2.02	0.83
1:B:46:LEU:CD2	1:B:50:GLN:HE21	1.90	0.83
1:E:244:VAL:HG13	1:E:245:LEU:HD13	1.59	0.83
2:C:32:THR:HG1	2:C:34:GLU:HG2	1.44	0.83
1:B:160:ARG:HA	1:B:160:ARG:HE	1.42	0.83
2:C:77:ASP:HA	2:C:80:TYR:CD2	2.12	0.83
1:B:244:VAL:HG13	1:B:245:LEU:HD13	1.59	0.82
1:E:64:LEU:HD23	1:E:170:ILE:HD13	1.62	0.82
1:E:175:TYR:HB2	1:E:182:TYR:CE1	2.13	0.82
3:A:771:MET:HG2	3:A:775:ASN:HD22	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:225:THR:HA	3:D:228:THR:HG22	1.62	0.82
3:D:941:MET:O	3:D:945:ILE:HG13	1.79	0.82
1:B:63:ARG:HH12	1:B:70:THR:HB	1.43	0.82
3:A:736:GLY:O	3:A:739:VAL:HG23	1.80	0.82
1:E:51:LYS:NZ	1:E:263:THR:HA	1.94	0.82
2:F:93:THR:HG21	2:F:126:ILE:HD12	1.62	0.81
1:B:1:LEU:HD13	3:A:558:HIS:CD2	2.13	0.81
3:A:533:GLY:O	3:A:537:LYS:HG3	1.80	0.81
1:E:258:PHE:HD2	1:E:274:GLY:O	1.61	0.81
3:D:788:TYR:CE1	3:D:796:ARG:HB3	2.15	0.81
3:D:771:MET:HG2	3:D:775:ASN:HD22	1.44	0.81
3:A:33:ASN:HB3	3:A:44:ARG:HG3	1.63	0.81
1:B:209:SER:C	1:B:210:LYS:HD2	2.06	0.81
1:B:282:SER:HA	1:B:286:GLY:HA2	1.60	0.81
1:E:129:ALA:HA	1:E:141:TYR:O	1.81	0.81
1:B:110:VAL:HG11	1:B:285:LEU:HD13	1.62	0.81
1:B:172:ASP:HB2	1:B:188:MET:HE1	1.60	0.81
1:B:258:PHE:HD2	1:B:274:GLY:O	1.64	0.81
3:A:73:MET:HB2	3:A:122:LYS:HE3	1.61	0.80
3:A:823:PHE:HZ	3:A:852:LEU:HD13	1.46	0.80
3:A:633:PHE:O	3:A:636:ALA:HB3	1.82	0.80
1:E:175:TYR:HE2	1:E:177:GLU:HG2	1.45	0.80
1:B:129:ALA:HA	1:B:141:TYR:O	1.82	0.79
3:A:225:THR:HA	3:A:228:THR:HG22	1.64	0.79
3:A:575:GLU:HG2	3:A:580:VAL:HG11	1.63	0.79
1:E:190:TRP:CD1	1:E:191:ARG:HG3	2.17	0.79
3:A:926:ILE:O	3:A:930:VAL:HG23	1.82	0.79
1:B:37:LEU:HB2	1:B:39:GLN:NE2	1.97	0.79
3:A:899:THR:CG2	3:A:903:ASN:HD21	1.96	0.79
1:B:102:MET:HG3	1:B:266:SER:O	1.83	0.79
3:A:586:ASP:O	3:A:589:ILE:HG22	1.83	0.78
3:D:996:LEU:CD1	3:D:1035:LEU:HD12	2.12	0.78
3:A:569:LEU:HD21	3:A:587:THR:HG22	1.63	0.78
3:A:899:THR:HG22	3:A:903:ASN:ND2	1.99	0.78
2:C:28:LYS:O	2:C:32:THR:HG23	1.82	0.78
3:A:485:ASN:O	3:A:487:THR:N	2.16	0.78
3:A:834:ILE:HG22	3:A:845:ARG:HG2	1.65	0.78
3:D:225:THR:HA	3:D:228:THR:CG2	2.13	0.78
3:D:337:LEU:HD13	3:D:347:LEU:HD12	1.65	0.78
3:D:990:GLN:HB3	3:D:1028:GLU:HG2	1.64	0.78
3:A:219:ALA:HB3	3:A:220:PRO:HD3	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:219:ALA:HB3	3:D:220:PRO:HD3	1.66	0.78
3:D:569:LEU:HD21	3:D:587:THR:HG22	1.64	0.77
3:D:823:PHE:HZ	3:D:852:LEU:HD13	1.48	0.77
1:E:37:LEU:HB2	1:E:39:GLN:NE2	1.99	0.77
3:D:899:THR:HG22	3:D:903:ASN:ND2	2.00	0.77
1:E:160:ARG:CG	1:E:160:ARG:HH11	1.97	0.77
3:D:586:ASP:O	3:D:589:ILE:HG22	1.84	0.77
3:D:819:ILE:O	3:D:823:PHE:HB2	1.84	0.77
3:D:899:THR:CG2	3:D:903:ASN:HD21	1.98	0.77
3:D:926:ILE:O	3:D:930:VAL:HG23	1.84	0.77
3:A:60:TRP:CD1	3:A:60:TRP:H	1.99	0.77
1:B:144:SER:O	1:B:146:TYR:N	2.18	0.77
3:D:433:VAL:HG12	3:D:441:VAL:HG23	1.65	0.77
3:D:60:TRP:CD1	3:D:60:TRP:H	2.00	0.76
1:E:119:ILE:HD11	1:E:259:TYR:HB2	1.68	0.76
3:A:819:ILE:O	3:A:823:PHE:HB2	1.85	0.76
3:D:121:GLU:C	3:D:123:GLU:H	1.91	0.76
3:D:340:ARG:HB3	3:D:342:ASN:OD1	1.85	0.76
3:A:340:ARG:HB3	3:A:342:ASN:OD1	1.85	0.76
3:D:575:GLU:HG2	3:D:580:VAL:HG11	1.67	0.75
3:A:866:ILE:HB	3:A:867:PRO:HD2	1.68	0.75
3:D:632:THR:HA	3:D:697:ARG:HH22	1.51	0.75
3:D:706:PHE:CZ	3:D:709:GLN:HG2	2.21	0.75
1:B:119:ILE:HD11	1:B:259:TYR:HB2	1.68	0.75
3:D:123:GLU:O	3:D:127:ILE:HD13	1.85	0.75
3:A:337:LEU:CD2	3:A:347:LEU:HB2	2.17	0.75
3:A:274:VAL:HG12	3:A:275:SER:H	1.51	0.75
1:B:4:LEU:HA	1:B:7:LYS:HB2	1.68	0.75
1:B:175:TYR:HB2	1:B:182:TYR:CE1	2.21	0.74
3:A:518:VAL:O	3:A:522:LYS:HB2	1.86	0.74
1:E:56:ASP:OD1	1:E:59:ASN:HB2	1.85	0.74
2:C:122:ASN:O	2:C:123:LYS:HB2	1.87	0.74
2:F:177:VAL:HG22	2:F:178:ALA:H	1.52	0.74
3:D:238:LEU:HD22	3:D:242:PHE:HE2	1.52	0.74
1:B:55:LEU:HD13	1:B:57:TYR:CE2	2.22	0.74
1:B:175:TYR:HE2	1:B:177:GLU:HG2	1.51	0.74
1:E:102:MET:HG3	1:E:266:SER:O	1.87	0.74
3:A:225:THR:HA	3:A:228:THR:CG2	2.18	0.74
3:A:479:LYS:HE2	3:A:479:LYS:HA	1.69	0.74
3:D:555:LEU:HB3	3:D:562:LEU:HD13	1.68	0.74
3:A:941:MET:O	3:A:945:ILE:HG13	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:970:ASN:HD22	3:A:970:ASN:N	1.84	0.74
3:D:116:ASP:C	3:D:118:THR:H	1.96	0.74
3:D:479:LYS:HA	3:D:479:LYS:HE2	1.68	0.74
3:D:996:LEU:HD13	3:D:1035:LEU:CD1	2.17	0.73
3:A:238:LEU:HD22	3:A:242:PHE:HE2	1.52	0.73
3:A:681:ASP:HB3	3:A:684:THR:HG23	1.69	0.73
3:D:518:VAL:O	3:D:522:LYS:HB2	1.88	0.73
3:D:570:PHE:O	3:D:573:MET:HB2	1.87	0.73
1:B:119:ILE:HD13	1:B:259:TYR:O	1.87	0.73
2:F:110:ARG:NH2	3:D:176:GLU:OE1	2.20	0.73
2:F:126:ILE:HG22	2:F:128:ASP:H	1.54	0.73
1:B:51:LYS:HZ2	1:B:264:HIS:HB2	1.51	0.73
1:E:175:TYR:CE2	1:E:177:GLU:HG2	2.24	0.72
3:D:763:VAL:O	3:D:810:LYS:HG2	1.88	0.72
1:B:4:LEU:CD1	3:A:518:VAL:HG13	2.19	0.72
3:A:471:ASP:O	3:A:475:ILE:HG13	1.89	0.72
3:A:706:PHE:CZ	3:A:709:GLN:HG2	2.24	0.72
1:B:13:ILE:HD11	3:A:538:ALA:HA	1.71	0.72
2:F:90:PHE:HB2	2:F:97:THR:OG1	1.88	0.72
2:C:90:PHE:HB2	2:C:97:THR:OG1	1.89	0.72
3:D:608:MET:HE3	3:D:609:PRO:HD2	1.71	0.72
3:D:834:ILE:O	3:D:845:ARG:NH2	2.23	0.72
3:D:970:ASN:HD22	3:D:970:ASN:N	1.86	0.72
1:B:46:LEU:HD22	1:B:50:GLN:HE21	1.53	0.72
1:E:124:PRO:HD2	1:E:174:ILE:HD12	1.71	0.72
3:A:106:VAL:O	3:A:110:ILE:HG13	1.90	0.72
3:A:541:ALA:HA	3:A:544:ILE:HD12	1.71	0.72
3:D:23:LEU:HD11	3:D:26:ASN:HB2	1.72	0.72
3:D:274:VAL:HG12	3:D:275:SER:H	1.54	0.72
3:A:25:ILE:H	3:A:25:ILE:HD12	1.54	0.71
3:A:973:PHE:CD1	3:A:973:PHE:C	2.66	0.71
1:B:63:ARG:HH11	1:B:95:LYS:HZ2	1.36	0.71
2:C:14:VAL:HG21	2:C:80:TYR:CD1	2.25	0.71
3:D:105:TYR:O	3:D:109:LEU:HD12	1.91	0.71
3:D:698:ALA:O	3:D:702:VAL:HG23	1.90	0.71
1:B:24:HIS:HE1	1:B:108:ILE:HG23	1.56	0.71
3:A:327:CYS:O	3:A:331:LYS:HB3	1.90	0.71
3:A:788:TYR:CE1	3:A:796:ARG:HB3	2.26	0.71
3:D:224:ALA:O	3:D:228:THR:HG22	1.90	0.71
3:D:533:GLY:O	3:D:537:LYS:HG3	1.91	0.71
2:C:54:THR:HB	2:C:174:LEU:HD11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:293:GLN:O	3:D:297:MET:HG3	1.90	0.71
1:B:357:MET:HG3	3:A:719:ASN:ND2	2.05	0.71
3:A:575:GLU:CG	3:A:580:VAL:HG11	2.20	0.71
1:E:8:LEU:CD2	3:D:564:THR:HG22	2.20	0.71
1:E:172:ASP:HB2	1:E:188:MET:HE1	1.71	0.71
1:E:211:LEU:HB2	1:E:212:PRO:HD3	1.73	0.71
2:F:44:GLY:HA3	3:D:45:MET:CE	2.20	0.71
2:C:126:ILE:HG22	2:C:128:ASP:H	1.56	0.71
1:B:107:LEU:HB2	1:B:274:GLY:HA3	1.73	0.71
1:E:144:SER:O	1:E:146:TYR:N	2.24	0.71
1:B:13:ILE:HG21	3:A:575:GLU:OE1	1.90	0.70
1:B:241:LEU:O	1:B:244:VAL:HG12	1.91	0.70
2:F:54:THR:HB	2:F:174:LEU:HD11	1.72	0.70
3:D:106:VAL:O	3:D:110:ILE:HG13	1.91	0.70
3:D:497:LEU:O	3:D:501:ILE:HG13	1.91	0.70
3:D:681:ASP:HB3	3:D:684:THR:HG23	1.72	0.70
3:A:50:LEU:O	3:A:53:LEU:HG	1.92	0.70
1:E:119:ILE:HD13	1:E:259:TYR:O	1.91	0.70
3:A:698:ALA:O	3:A:702:VAL:HG23	1.91	0.70
3:A:141:GLU:HB2	3:A:145:HIS:HB2	1.73	0.70
2:F:14:VAL:HG21	2:F:80:TYR:CD1	2.27	0.70
3:A:632:THR:HA	3:A:697:ARG:HH22	1.57	0.69
3:A:770:GLN:O	3:A:774:GLU:HG3	1.92	0.69
2:C:93:THR:HG21	2:C:126:ILE:CD1	2.21	0.69
3:A:23:LEU:HD11	3:A:26:ASN:HB2	1.74	0.69
3:D:846:THR:HG23	3:D:888:ASN:HD22	1.58	0.69
1:E:241:LEU:O	1:E:244:VAL:HG12	1.91	0.69
2:F:122:ASN:O	2:F:123:LYS:HB2	1.92	0.69
3:D:179:PHE:CE1	3:D:195:LYS:HG3	2.26	0.69
3:D:1035:LEU:O	3:D:1036:GLU:C	2.35	0.69
3:A:763:VAL:O	3:A:810:LYS:HG2	1.92	0.69
3:A:804:MET:SD	3:A:807:ILE:HD11	2.33	0.69
3:A:497:LEU:O	3:A:501:ILE:HG13	1.91	0.69
1:E:282:SER:HB3	1:E:287:VAL:HA	1.74	0.69
1:B:151:PHE:N	1:B:151:PHE:HD1	1.91	0.69
3:A:823:PHE:CZ	3:A:852:LEU:HD13	2.27	0.69
3:D:50:LEU:O	3:D:53:LEU:HG	1.93	0.69
3:D:25:ILE:H	3:D:25:ILE:HD12	1.57	0.69
3:D:373:TRP:HA	3:D:373:TRP:CE3	2.28	0.69
1:B:24:HIS:O	1:B:26:ARG:N	2.26	0.68
3:A:224:ALA:O	3:A:228:THR:HG22	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:31:LEU:HB3	2:F:50:LEU:HD21	1.74	0.68
3:D:17:LEU:HD23	3:D:22:LYS:NZ	2.08	0.68
3:D:866:ILE:HB	3:D:867:PRO:HD2	1.73	0.68
3:A:45:MET:O	3:A:49:VAL:HG23	1.93	0.68
1:E:63:ARG:NH1	1:E:72:MET:HB2	2.07	0.68
1:E:160:ARG:HH11	1:E:160:ARG:HG2	1.55	0.68
2:F:103:ASN:O	2:F:106:ARG:HB3	1.94	0.68
3:A:658:MET:O	3:A:662:ASN:HB2	1.93	0.68
3:D:471:ASP:O	3:D:475:ILE:HG13	1.93	0.68
3:D:766:SER:H	3:D:810:LYS:NZ	1.91	0.68
3:A:109:LEU:O	3:A:113:THR:HG23	1.94	0.68
3:A:834:ILE:O	3:A:845:ARG:NH2	2.27	0.68
1:E:24:HIS:HE1	1:E:108:ILE:HG23	1.59	0.68
3:D:916:GLN:HE22	3:D:959:SER:HB2	1.58	0.68
3:D:14:ARG:HH11	3:D:14:ARG:CG	2.06	0.68
3:D:337:LEU:CD2	3:D:347:LEU:HB2	2.21	0.68
1:B:260:HIS:CE1	1:B:262:GLN:HG3	2.28	0.68
3:A:555:LEU:HB3	3:A:562:LEU:HD13	1.75	0.68
2:F:139:HIS:HB2	2:F:144:LEU:O	1.94	0.68
3:D:627:PRO:O	3:D:630:VAL:HG12	1.93	0.68
3:D:759:ILE:HD13	3:D:780:LEU:HD21	1.75	0.68
3:A:56:HIS:C	3:A:58:ASP:H	2.02	0.67
3:A:179:PHE:CE1	3:A:195:LYS:HG3	2.27	0.67
3:A:678:ILE:HD12	3:A:679:LEU:N	2.10	0.67
2:F:77:ASP:HB2	3:D:77:TYR:OH	1.94	0.67
1:E:107:LEU:HB2	1:E:274:GLY:HA3	1.76	0.67
1:B:175:TYR:CE2	1:B:177:GLU:HG2	2.30	0.67
3:D:834:ILE:HG22	3:D:845:ARG:HG2	1.76	0.67
1:E:24:HIS:ND1	1:E:25:PRO:HD2	2.09	0.67
3:D:631:HIS:CE1	3:D:693:LYS:HB2	2.29	0.67
3:D:823:PHE:CZ	3:D:852:LEU:HD13	2.29	0.67
3:A:164:CYS:SG	3:A:221:LEU:HD11	2.35	0.67
3:A:284:GLU:HG3	3:A:343:LEU:HD21	1.77	0.67
1:E:51:LYS:HZ1	1:E:263:THR:HA	1.58	0.67
3:A:179:PHE:HE1	3:A:195:LYS:HG3	1.59	0.67
1:E:217:LEU:HG	1:E:228:PHE:HB2	1.76	0.67
3:A:105:TYR:O	3:A:109:LEU:HD12	1.95	0.67
3:D:45:MET:O	3:D:49:VAL:HG23	1.94	0.67
3:D:770:GLN:O	3:D:774:GLU:HG3	1.95	0.67
1:B:106:TRP:CH2	1:B:280:MET:HE1	2.29	0.67
2:C:14:VAL:HG21	2:C:80:TYR:HD1	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:528:CYS:HB2	3:A:540:ILE:CG2	2.21	0.67
3:A:615:LEU:HD23	3:A:618:ILE:HD11	1.77	0.67
1:E:160:ARG:HG2	1:E:160:ARG:NH1	2.06	0.67
1:B:42:ARG:O	1:B:45:ARG:HB2	1.93	0.67
1:E:151:PHE:N	1:E:151:PHE:HD1	1.93	0.67
3:A:293:GLN:O	3:A:297:MET:HG3	1.94	0.66
3:A:704:HIS:CD2	3:A:767:ASN:H	2.13	0.66
3:D:593:GLN:HG3	3:D:639:TYR:CD2	2.29	0.66
2:C:75:LEU:HD12	2:C:75:LEU:N	2.10	0.66
3:A:570:PHE:O	3:A:573:MET:HB2	1.95	0.66
3:D:131:ASN:HD21	3:D:166:ASN:HD21	1.42	0.66
3:A:819:ILE:HD12	3:A:855:VAL:CG2	2.25	0.66
3:A:902:GLN:O	3:A:906:GLN:NE2	2.28	0.66
3:A:916:GLN:HE22	3:A:959:SER:HB2	1.60	0.66
3:A:1040:THR:HA	3:A:1043:ARG:HG2	1.76	0.66
3:D:179:PHE:HE1	3:D:195:LYS:HG3	1.59	0.66
3:D:678:ILE:HD12	3:D:679:LEU:N	2.11	0.66
1:B:211:LEU:HB2	1:B:212:PRO:HD3	1.78	0.66
3:A:150:ILE:HG23	3:A:151:SER:H	1.60	0.66
1:E:1:LEU:HD22	3:D:558:HIS:HD2	1.60	0.66
1:E:190:TRP:O	1:E:191:ARG:C	2.39	0.66
1:E:260:HIS:CE1	1:E:262:GLN:HG3	2.30	0.66
2:F:15:LEU:HD22	2:F:23:LYS:HB3	1.77	0.66
3:D:902:GLN:O	3:D:906:GLN:NE2	2.29	0.66
3:D:997:PHE:HD1	3:D:1014:HIS:CE1	2.14	0.66
1:B:154:LEU:HG	1:B:224:ASN:HB2	1.76	0.66
3:A:132:MET:O	3:A:132:MET:HE3	1.96	0.66
3:D:132:MET:O	3:D:132:MET:HE3	1.96	0.66
3:D:769:PRO:HG2	3:D:770:GLN:H	1.61	0.66
3:A:286:LEU:HD12	3:A:286:LEU:O	1.95	0.66
3:A:509:HIS:O	3:A:512:ASP:HB2	1.96	0.66
3:A:759:ILE:HD13	3:A:780:LEU:HD21	1.77	0.66
1:E:277:ARG:NH2	3:D:620:THR:HG21	2.11	0.66
2:F:14:VAL:HG21	2:F:80:TYR:HD1	1.60	0.66
3:D:819:ILE:HD12	3:D:855:VAL:CG2	2.25	0.66
3:A:78:TYR:O	3:A:81:GLN:HB2	1.96	0.65
3:D:168:MET:HE2	3:D:168:MET:HA	1.78	0.65
3:D:509:HIS:O	3:D:512:ASP:HB2	1.96	0.65
2:C:44:GLY:HA3	3:A:45:MET:CE	2.24	0.65
2:F:13:LEU:HD12	2:F:13:LEU:C	2.21	0.65
3:A:131:ASN:HD21	3:A:166:ASN:HD21	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:373:TRP:HA	3:D:373:TRP:HE3	1.61	0.65
2:C:139:HIS:HB2	2:C:144:LEU:O	1.97	0.65
3:A:762:TRP:HH2	3:A:772:VAL:HG22	1.61	0.65
1:E:147:CYS:SG	1:E:150:ARG:NH2	2.69	0.65
3:D:76:LYS:O	3:D:80:LEU:HD22	1.96	0.65
3:D:327:CYS:O	3:D:331:LYS:HB3	1.96	0.65
3:D:736:GLY:O	3:D:739:VAL:HG22	1.96	0.65
1:B:24:HIS:ND1	1:B:25:PRO:HD2	2.11	0.65
3:A:373:TRP:HA	3:A:373:TRP:CE3	2.32	0.65
1:E:24:HIS:O	1:E:26:ARG:N	2.27	0.65
3:D:905:ALA:HB3	3:D:906:GLN:NE2	2.11	0.65
3:A:900:LEU:HA	3:A:903:ASN:HD22	1.61	0.65
3:D:541:ALA:HA	3:D:544:ILE:HD12	1.79	0.65
1:B:175:TYR:CE2	1:B:177:GLU:HA	2.32	0.65
2:C:103:ASN:O	2:C:106:ARG:HB3	1.97	0.65
3:A:168:MET:HE2	3:A:168:MET:HA	1.78	0.65
1:E:1:LEU:O	1:E:4:LEU:HD12	1.97	0.65
3:D:266:LYS:O	3:D:270:GLU:HG2	1.96	0.65
3:D:658:MET:O	3:D:662:ASN:HB2	1.96	0.65
2:F:124:VAL:HG22	2:F:150:SER:HB2	1.77	0.65
3:D:150:ILE:HG23	3:D:151:SER:H	1.62	0.65
3:D:788:TYR:O	3:D:796:ARG:HG2	1.97	0.65
3:D:1008:ILE:C	3:D:1008:ILE:HD12	2.22	0.65
1:B:138:THR:HG22	1:B:151:PHE:CE1	2.32	0.65
2:C:148:ASP:HB3	2:C:155:TYR:CE2	2.23	0.65
3:A:1050:HIS:HB2	3:A:1054:MET:HE2	1.78	0.65
2:F:93:THR:HG21	2:F:126:ILE:CD1	2.26	0.65
1:B:63:ARG:NH1	1:B:95:LYS:NZ	2.45	0.64
3:A:30:ASN:HB3	3:A:47:GLN:NE2	2.12	0.64
3:A:766:SER:H	3:A:810:LYS:NZ	1.94	0.64
2:F:64:TRP:CE3	2:F:79:TYR:HB3	2.33	0.64
1:B:281:VAL:HG13	1:B:282:SER:H	1.63	0.64
3:A:218:ASN:C	3:A:218:ASN:OD1	2.40	0.64
1:E:175:TYR:CE2	1:E:177:GLU:HA	2.33	0.64
1:E:186:ASP:OD1	1:E:203:ARG:HD2	1.96	0.64
3:D:30:ASN:HB3	3:D:47:GLN:NE2	2.13	0.64
3:D:528:CYS:HB2	3:D:540:ILE:CG2	2.23	0.64
1:B:159:ASN:HB2	1:B:223:LEU:CD2	2.21	0.64
3:D:434:GLU:HG3	3:D:439:GLU:O	1.96	0.64
1:B:351:ASP:HB2	1:B:352:HIS:ND1	2.12	0.64
2:F:178:ALA:O	2:F:179:MET:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:GLU:O	1:B:7:LYS:CB	2.39	0.64
3:A:823:PHE:O	3:A:827:PHE:CB	2.45	0.64
3:A:1038:ARG:HA	3:A:1041:ALA:HB3	1.79	0.64
1:B:186:ASP:OD1	1:B:203:ARG:HD2	1.97	0.64
1:B:349:SER:HB3	1:B:350:PRO:HD2	1.80	0.64
3:A:56:HIS:N	3:A:57:PRO:HD3	2.13	0.64
1:E:255:GLY:C	1:E:256:LEU:HD23	2.23	0.64
2:F:92:VAL:HG13	2:F:122:ASN:O	1.98	0.64
3:D:336:LEU:HD12	3:D:336:LEU:O	1.96	0.64
3:D:804:MET:SD	3:D:807:ILE:HD11	2.38	0.64
1:B:4:LEU:HD11	3:A:518:VAL:HA	1.80	0.64
1:B:151:PHE:N	1:B:151:PHE:CD1	2.63	0.64
2:C:87:ILE:HA	2:C:118:VAL:O	1.97	0.64
3:A:336:LEU:HD12	3:A:336:LEU:O	1.96	0.64
3:D:56:HIS:C	3:D:58:ASP:H	2.06	0.64
3:D:150:ILE:HG21	3:D:201:GLU:CD	2.23	0.64
3:D:463:TYR:O	3:D:467:LEU:HG	1.98	0.64
3:A:299:PRO:HD2	3:A:302:THR:HG21	1.77	0.64
3:A:529:GLU:O	3:A:530:GLN:C	2.39	0.64
3:A:949:MET:O	3:A:953:VAL:HG23	1.97	0.64
2:F:101:VAL:HB	2:F:102:PRO:HD3	1.80	0.64
3:D:208:LEU:C	3:D:208:LEU:HD23	2.23	0.64
1:B:217:LEU:HG	1:B:228:PHE:HB2	1.79	0.64
2:C:13:LEU:C	2:C:13:LEU:HD12	2.22	0.64
3:A:860:PHE:N	3:A:861:PRO:HD2	2.13	0.64
3:D:485:ASN:O	3:D:487:THR:N	2.30	0.64
3:D:622:ILE:HG21	3:D:633:PHE:CD2	2.33	0.64
1:B:63:ARG:HH11	1:B:95:LYS:NZ	1.96	0.64
1:B:111:PRO:HD2	1:B:114:LEU:HD13	1.79	0.63
2:C:77:ASP:HB2	3:A:77:TYR:OH	1.97	0.63
2:C:115:ILE:O	2:C:115:ILE:HG13	1.98	0.63
3:A:290:THR:O	3:A:293:GLN:HB2	1.98	0.63
3:D:434:GLU:HA	3:D:439:GLU:O	1.98	0.63
3:D:766:SER:H	3:D:810:LYS:HZ3	1.46	0.63
3:D:798:PRO:HG3	3:D:844:HIS:CE1	2.32	0.63
3:A:82:ILE:O	3:A:86:VAL:HG23	1.98	0.63
3:D:78:TYR:O	3:D:81:GLN:HB2	1.99	0.63
3:D:575:GLU:CG	3:D:580:VAL:HG11	2.27	0.63
3:D:261:ARG:HD2	3:D:318:PHE:CG	2.33	0.63
3:D:650:GLN:NE2	3:D:705:PRO:HG2	2.12	0.63
3:D:960:THR:HG22	3:D:963:ASN:H	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:208:LEU:HD23	3:A:208:LEU:C	2.24	0.63
3:D:628:GLN:NE2	3:D:628:GLN:H	1.96	0.63
3:D:1008:ILE:HD12	3:D:1008:ILE:O	1.98	0.63
1:B:6:LEU:O	1:B:9:ALA:HB3	1.98	0.63
3:D:949:MET:O	3:D:953:VAL:HG23	1.98	0.63
1:B:120:VAL:HA	1:B:257:LEU:O	1.99	0.63
3:A:127:ILE:HG22	3:A:131:ASN:ND2	2.12	0.63
3:A:841:TYR:O	3:A:845:ARG:HG3	1.99	0.63
3:D:528:CYS:CB	3:D:540:ILE:HG21	2.24	0.63
3:D:1048:GLU:O	3:D:1052:LEU:HG	1.99	0.63
3:D:860:PHE:N	3:D:861:PRO:HD2	2.14	0.63
3:D:900:LEU:HA	3:D:903:ASN:HD22	1.64	0.63
3:A:762:TRP:CH2	3:A:772:VAL:HG22	2.34	0.62
3:A:1043:ARG:NH1	3:A:1043:ARG:HA	2.13	0.62
3:D:529:GLU:O	3:D:530:GLN:C	2.41	0.62
1:B:154:LEU:HD13	1:B:215:GLU:HG2	1.81	0.62
3:A:516:PHE:CE1	3:A:520:VAL:HG21	2.34	0.62
3:A:568:LYS:HE2	3:A:568:LYS:HA	1.79	0.62
3:A:997:PHE:HD1	3:A:1014:HIS:CE1	2.18	0.62
1:E:151:PHE:N	1:E:151:PHE:CD1	2.64	0.62
3:A:769:PRO:HG2	3:A:770:GLN:H	1.63	0.62
2:F:87:ILE:HA	2:F:118:VAL:O	1.99	0.62
3:D:299:PRO:HD2	3:D:302:THR:HG21	1.79	0.62
1:B:190:TRP:O	1:B:191:ARG:C	2.42	0.62
3:A:115:SER:HB3	3:A:162:SER:CB	2.28	0.62
3:A:627:PRO:O	3:A:630:VAL:HG12	1.99	0.62
1:E:154:LEU:HG	1:E:224:ASN:HB2	1.79	0.62
3:D:1003:SER:C	3:D:1005:ASN:H	2.06	0.62
2:C:92:VAL:HG13	2:C:122:ASN:O	2.00	0.62
1:E:106:TRP:CH2	1:E:280:MET:HE1	2.34	0.62
2:F:32:THR:OG1	2:F:34:GLU:HG2	2.00	0.62
3:D:56:HIS:N	3:D:57:PRO:HD3	2.15	0.62
3:D:860:PHE:HE1	3:D:900:LEU:HG	1.64	0.62
1:B:4:LEU:HD22	3:A:521:ILE:HD11	1.81	0.62
1:B:260:HIS:O	1:B:263:THR:HG22	2.00	0.62
1:B:277:ARG:NH2	3:A:620:THR:HG21	2.15	0.62
3:A:153:ILE:HA	3:A:156:ALA:HB3	1.81	0.62
3:A:804:MET:HB3	3:A:851:LEU:HD13	1.82	0.62
3:D:513:GLU:HA	3:D:516:PHE:HB3	1.80	0.62
3:D:637:VAL:O	3:D:641:ILE:HD12	1.99	0.62
3:A:150:ILE:HG21	3:A:201:GLU:CD	2.25	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:607:VAL:HG22	3:A:608:MET:SD	2.40	0.62
3:D:141:GLU:HB2	3:D:145:HIS:HB2	1.82	0.62
3:D:286:LEU:HD12	3:D:286:LEU:O	1.99	0.62
3:D:516:PHE:CE1	3:D:520:VAL:HG21	2.35	0.62
1:B:204:PHE:O	1:B:207:MET:HB2	2.00	0.62
2:C:64:TRP:CE3	2:C:79:TYR:HB3	2.35	0.62
3:A:337:LEU:HD22	3:A:347:LEU:CB	2.26	0.62
3:A:627:PRO:O	3:A:631:HIS:CD2	2.53	0.62
2:F:148:ASP:HB3	2:F:155:TYR:CE2	2.26	0.62
3:D:30:ASN:N	3:D:30:ASN:ND2	2.48	0.62
3:D:421:VAL:HG11	3:D:476:MET:HG2	1.81	0.62
3:A:123:GLU:C	3:A:125:VAL:H	2.06	0.62
3:A:266:LYS:O	3:A:270:GLU:HG2	1.98	0.62
3:A:513:GLU:HA	3:A:516:PHE:HB3	1.81	0.62
3:D:940:THR:OG1	3:D:1012:LYS:HE3	2.00	0.62
1:B:258:PHE:CD2	1:B:274:GLY:O	2.51	0.62
1:E:7:LYS:HB3	3:D:525:LEU:HD23	1.82	0.62
1:E:260:HIS:O	1:E:261:LYS:C	2.41	0.62
3:D:82:ILE:O	3:D:86:VAL:HG23	2.00	0.62
3:D:399:HIS:HB3	3:D:401:ASP:H	1.64	0.62
1:B:147:CYS:SG	1:B:150:ARG:NH2	2.72	0.61
3:A:30:ASN:N	3:A:30:ASN:ND2	2.48	0.61
3:A:74:ASN:O	3:A:77:TYR:HB3	2.00	0.61
3:A:193:HIS:O	3:A:197:SER:HB2	2.00	0.61
3:A:484:VAL:HG22	3:A:527:LEU:HB2	1.81	0.61
3:A:846:THR:HG23	3:A:888:ASN:HD22	1.65	0.61
1:E:111:PRO:HD2	1:E:114:LEU:HD13	1.82	0.61
1:E:180:GLN:NE2	3:D:684:THR:HG22	2.06	0.61
3:D:54:LYS:O	3:D:55:GLU:HB2	2.00	0.61
3:D:484:VAL:HG22	3:D:527:LEU:HB2	1.81	0.61
3:A:192:LYS:HA	3:A:192:LYS:HE3	1.82	0.61
1:E:98:ALA:HB2	1:E:145:GLY:N	2.15	0.61
1:E:260:HIS:O	1:E:263:THR:HG22	2.00	0.61
1:B:40:SER:O	1:B:44:ARG:HG3	2.00	0.61
1:B:110:VAL:HG11	1:B:285:LEU:CD1	2.30	0.61
1:E:258:PHE:CD2	1:E:274:GLY:O	2.49	0.61
3:D:615:LEU:HD23	3:D:618:ILE:HD11	1.83	0.61
1:B:63:ARG:NH1	1:B:70:THR:H	1.98	0.61
3:A:650:GLN:NE2	3:A:705:PRO:HG2	2.14	0.61
3:A:788:TYR:O	3:A:796:ARG:HG2	2.00	0.61
3:A:1008:ILE:C	3:A:1008:ILE:HD12	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:192:LYS:HA	3:D:192:LYS:HE3	1.83	0.61
3:D:996:LEU:HD22	3:D:1033:LEU:HD11	1.82	0.61
2:C:153:SER:O	3:A:433:VAL:HG21	2.00	0.61
3:A:388:THR:OG1	3:A:402:ILE:HD13	2.00	0.61
1:E:51:LYS:HZ3	1:E:263:THR:HA	1.65	0.61
1:B:46:LEU:HD23	1:B:50:GLN:HG3	1.82	0.61
1:B:98:ALA:HB2	1:B:145:GLY:N	2.16	0.61
1:B:225:PRO:HB2	1:B:226:PHE:CD2	2.36	0.61
3:D:847:ASN:O	3:D:848:PHE:C	2.42	0.61
3:D:153:ILE:HA	3:D:156:ALA:HB3	1.82	0.61
1:B:349:SER:HB3	1:B:350:PRO:CD	2.31	0.61
2:C:31:LEU:C	2:C:32:THR:HG22	2.25	0.61
3:A:70:SER:C	3:A:72:ASN:H	2.09	0.61
3:A:372:TYR:O	3:A:373:TRP:C	2.43	0.61
3:A:628:GLN:HA	3:A:631:HIS:HD2	1.66	0.61
3:A:628:GLN:NE2	3:A:628:GLN:H	1.99	0.61
3:A:877:SER:O	3:A:880:TRP:HB3	2.01	0.61
1:E:18:ASN:CG	1:E:108:ILE:HD11	2.26	0.61
3:A:116:ASP:C	3:A:118:THR:H	2.09	0.60
3:A:127:ILE:O	3:A:130:LEU:N	2.32	0.60
1:E:40:SER:O	1:E:44:ARG:HG3	2.01	0.60
2:F:115:ILE:HG13	2:F:115:ILE:O	2.01	0.60
3:D:846:THR:HG23	3:D:888:ASN:ND2	2.16	0.60
3:D:1044:GLN:HG3	3:D:1044:GLN:O	2.00	0.60
1:B:202:PHE:O	1:B:203:ARG:C	2.43	0.60
3:A:966:ASN:N	3:A:967:PRO:HD2	2.15	0.60
1:E:1:LEU:HG	1:E:2:ASN:N	2.10	0.60
3:D:337:LEU:HD23	3:D:343:LEU:HB3	1.83	0.60
1:B:130:LEU:HG	1:B:132:VAL:HG23	1.83	0.60
3:A:195:LYS:C	3:A:197:SER:H	2.07	0.60
3:A:373:TRP:HA	3:A:373:TRP:HE3	1.66	0.60
3:D:43:GLN:HA	3:D:46:ALA:HB3	1.83	0.60
3:D:945:ILE:O	3:D:949:MET:HG3	2.02	0.60
3:A:33:ASN:CB	3:A:44:ARG:HG3	2.31	0.60
3:A:77:TYR:O	3:A:78:TYR:C	2.44	0.60
3:A:99:CYS:HA	3:A:102:ILE:HD12	1.83	0.60
3:D:96:ARG:HH22	3:D:145:HIS:HB3	1.65	0.60
3:D:164:CYS:SG	3:D:221:LEU:HD11	2.42	0.60
3:D:704:HIS:HD2	3:D:766:SER:CB	2.13	0.60
1:B:1:LEU:CD1	3:A:558:HIS:HD2	2.08	0.60
3:A:116:ASP:HB2	3:A:119:CYS:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:178:VAL:HG11	3:A:194:LEU:HB3	1.84	0.60
3:A:344:ARG:O	3:A:348:MET:HG2	2.01	0.60
3:A:1014:HIS:O	3:A:1017:ASP:HB3	2.02	0.60
1:E:146:TYR:CD1	1:E:148:VAL:HG22	2.36	0.60
3:A:823:PHE:O	3:A:827:PHE:HB2	2.01	0.60
3:A:961:PRO:HD3	3:A:970:ASN:OD1	2.02	0.60
1:E:284:VAL:HG12	1:E:285:LEU:CD1	2.31	0.60
3:D:362:GLU:O	3:D:364:GLU:N	2.32	0.60
1:B:103:LEU:HD13	1:B:268:GLY:HA2	1.84	0.60
1:B:358:GLU:O	1:B:359:ASN:O	2.19	0.60
3:A:274:VAL:HG12	3:A:275:SER:N	2.17	0.60
3:D:568:LYS:HA	3:D:568:LYS:HE2	1.84	0.60
3:A:25:ILE:HD12	3:A:25:ILE:N	2.17	0.60
3:A:265:LEU:O	3:A:268:LEU:N	2.35	0.60
3:A:746:ARG:HG2	3:A:746:ARG:NH1	2.09	0.60
3:A:1008:ILE:HD12	3:A:1008:ILE:O	2.02	0.60
3:D:290:THR:O	3:D:293:GLN:HB2	2.02	0.60
3:D:859:CYS:C	3:D:861:PRO:HD2	2.27	0.60
3:D:919:PHE:CE1	3:D:949:MET:HE2	2.37	0.60
1:B:146:TYR:CD1	1:B:148:VAL:HG22	2.37	0.60
1:B:260:HIS:O	1:B:261:LYS:C	2.43	0.60
2:C:124:VAL:HG22	2:C:150:SER:HB2	1.83	0.60
1:E:240:SER:O	1:E:241:LEU:C	2.43	0.60
3:A:938:GLY:O	3:A:941:MET:N	2.35	0.59
1:E:138:THR:HG22	1:E:151:PHE:CE1	2.37	0.59
3:D:74:ASN:O	3:D:77:TYR:HB3	2.02	0.59
3:D:116:ASP:HB2	3:D:119:CYS:HB2	1.84	0.59
3:D:833:MET:HB3	3:D:841:TYR:CD1	2.37	0.59
3:A:1003:SER:C	3:A:1005:ASN:H	2.09	0.59
3:D:1000:GLY:HA2	3:D:1042:LEU:HD13	1.84	0.59
1:E:159:ASN:O	1:E:160:ARG:HG2	2.02	0.59
3:D:195:LYS:C	3:D:197:SER:H	2.08	0.59
3:D:484:VAL:HA	3:D:527:LEU:HD13	1.84	0.59
3:D:733:GLN:HB2	3:D:792:VAL:HG11	1.85	0.59
3:A:639:TYR:N	3:A:701:ALA:HB1	2.17	0.59
1:E:120:VAL:HA	1:E:257:LEU:O	2.03	0.59
3:A:285:THR:O	3:A:289:LEU:HB2	2.03	0.59
3:A:925:HIS:O	3:A:928:SER:HB3	2.02	0.59
1:E:4:LEU:HD22	3:D:521:ILE:HD11	1.84	0.59
1:E:280:MET:O	1:E:284:VAL:HG23	2.02	0.59
2:F:159:LYS:HB2	2:F:160:PRO:HD3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:515:ARG:HH11	3:D:515:ARG:HG3	1.68	0.59
3:A:1048:GLU:O	3:A:1052:LEU:HG	2.02	0.59
2:F:81:ILE:HD11	3:D:77:TYR:CD1	2.38	0.59
3:D:420:MET:HB2	3:D:461:LEU:HD13	1.83	0.59
3:D:678:ILE:HD12	3:D:679:LEU:HG	1.84	0.59
3:D:804:MET:HB3	3:D:851:LEU:HD13	1.84	0.59
3:A:632:THR:CA	3:A:697:ARG:HH22	2.16	0.59
3:D:337:LEU:HD22	3:D:347:LEU:CB	2.30	0.59
3:D:638:GLY:HA3	3:D:701:ALA:HB3	1.85	0.59
1:B:255:GLY:C	1:B:256:LEU:HD23	2.28	0.59
1:B:282:SER:HA	1:B:286:GLY:CA	2.30	0.59
3:A:766:SER:H	3:A:810:LYS:HZ3	1.47	0.59
3:A:833:MET:HB3	3:A:841:TYR:CD1	2.38	0.59
1:E:225:PRO:HB2	1:E:226:PHE:CD2	2.38	0.59
1:E:237:THR:O	1:E:238:PRO:C	2.45	0.59
3:D:704:HIS:CD2	3:D:767:ASN:H	2.21	0.59
3:A:631:HIS:CE1	3:A:693:LYS:HB2	2.37	0.59
3:D:95:PRO:HG2	3:D:98:GLN:HE21	1.68	0.59
1:B:4:LEU:HA	1:B:7:LYS:CB	2.32	0.59
1:E:11:LEU:HG	3:D:572:PHE:HZ	1.68	0.59
2:F:139:HIS:O	2:F:143:ASN:N	2.35	0.59
2:F:146:TYR:C	2:F:146:TYR:CD2	2.81	0.59
1:E:202:PHE:O	1:E:203:ARG:C	2.46	0.58
2:F:84:GLN:O	2:F:85:CYS:HB3	2.03	0.58
3:A:973:PHE:HD1	3:A:974:ILE:N	2.01	0.58
3:A:988:HIS:H	3:A:988:HIS:CD2	2.20	0.58
1:E:50:GLN:O	1:E:52:SER:N	2.31	0.58
3:D:621:ILE:HG22	3:D:622:ILE:HG23	1.85	0.58
3:D:762:TRP:CH2	3:D:772:VAL:HG22	2.38	0.58
1:B:206:TRP:O	1:B:210:LYS:HB2	2.03	0.58
2:F:75:LEU:HD12	2:F:75:LEU:N	2.18	0.58
3:D:823:PHE:O	3:D:827:PHE:CB	2.51	0.58
1:E:107:LEU:HD23	1:E:276:LEU:HD22	1.85	0.58
3:D:193:HIS:O	3:D:197:SER:HB2	2.03	0.58
3:D:961:PRO:HD3	3:D:970:ASN:OD1	2.03	0.58
1:B:58:VAL:HA	1:B:194:PRO:HG2	1.84	0.58
3:D:252:TYR:O	3:D:256:ASN:ND2	2.36	0.58
3:D:639:TYR:N	3:D:701:ALA:HB1	2.18	0.58
3:A:769:PRO:CG	3:A:770:GLN:H	2.16	0.58
3:D:803:THR:O	3:D:807:ILE:HG12	2.02	0.58
3:A:121:GLU:O	3:A:123:GLU:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1033:LEU:O	3:A:1034:PHE:C	2.47	0.58
1:E:130:LEU:HG	1:E:132:VAL:HG23	1.85	0.58
1:B:146:TYR:CE2	3:A:626:GLN:NE2	2.71	0.58
2:C:146:TYR:C	2:C:146:TYR:CD2	2.82	0.58
3:A:115:SER:HB3	3:A:162:SER:HB3	1.84	0.58
3:A:569:LEU:HD11	3:A:587:THR:HG21	1.85	0.58
2:C:137:VAL:HG12	2:C:140:ARG:NH1	2.19	0.58
3:A:202:PHE:O	3:A:205:ILE:HG23	2.04	0.58
3:A:859:CYS:C	3:A:861:PRO:HD2	2.29	0.58
3:D:528:CYS:HA	3:D:540:ILE:HD13	1.84	0.58
3:D:534:LYS:HE2	3:D:577:HIS:HB2	1.86	0.58
3:D:963:ASN:N	3:D:964:PRO:HD3	2.19	0.58
3:D:996:LEU:CD2	3:D:1033:LEU:HD11	2.33	0.58
3:A:93:ILE:CG2	3:A:1027:GLY:HA3	2.33	0.58
3:A:517:LEU:O	3:A:518:VAL:C	2.43	0.58
3:A:897:LEU:O	3:A:901:LEU:HG	2.03	0.58
2:C:39:TYR:HE1	4:C:217:GTP:O2B	1.86	0.57
3:A:256:ASN:OD1	3:A:257:VAL:HG23	2.04	0.57
1:E:356:LEU:O	3:D:719:ASN:ND2	2.37	0.57
2:F:88:ILE:HD11	2:F:117:ILE:CD1	2.34	0.57
3:D:16:LEU:C	3:D:17:LEU:HD12	2.29	0.57
3:D:344:ARG:O	3:D:348:MET:HG2	2.04	0.57
1:B:146:TYR:HD1	1:B:148:VAL:HG22	1.67	0.57
1:B:277:ARG:HB2	1:B:280:MET:HE3	1.85	0.57
3:A:252:TYR:O	3:A:256:ASN:ND2	2.37	0.57
3:A:515:ARG:HH11	3:A:515:ARG:HG3	1.69	0.57
2:F:138:PHE:HA	2:F:141:LYS:NZ	2.19	0.57
2:F:177:VAL:HG22	2:F:178:ALA:N	2.19	0.57
1:B:24:HIS:C	1:B:26:ARG:H	2.11	0.57
3:A:54:LYS:O	3:A:55:GLU:HB2	2.04	0.57
3:A:261:ARG:HD2	3:A:318:PHE:CG	2.39	0.57
3:D:121:GLU:C	3:D:123:GLU:N	2.61	0.57
3:D:769:PRO:CG	3:D:770:GLN:H	2.16	0.57
2:C:159:LYS:HB2	2:C:160:PRO:HD3	1.85	0.57
3:A:521:ILE:CG2	3:A:547:ILE:HG21	2.34	0.57
2:F:134:LYS:HE3	2:F:135:SER:OG	2.04	0.57
3:D:964:PRO:HG2	3:D:968:VAL:HB	1.86	0.57
1:B:258:PHE:O	1:B:273:VAL:HA	2.03	0.57
3:A:304:ILE:CG1	3:A:356:LEU:HB3	2.35	0.57
3:A:678:ILE:HD12	3:A:679:LEU:HG	1.86	0.57
3:A:746:ARG:HH11	3:A:746:ARG:CG	2.09	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:131:ASN:ND2	3:D:166:ASN:HD21	2.02	0.57
3:A:463:TYR:O	3:A:467:LEU:HG	2.04	0.57
3:A:1030:THR:HG23	3:A:1032:ASP:OD1	2.05	0.57
3:D:25:ILE:HD12	3:D:25:ILE:N	2.20	0.57
3:D:274:VAL:HG12	3:D:275:SER:N	2.20	0.57
3:D:768:ASP:CG	3:D:771:MET:HE3	2.30	0.57
3:D:877:SER:O	3:D:880:TRP:HB3	2.05	0.57
2:C:75:LEU:O	2:C:78:GLY:N	2.35	0.57
2:C:149:ILE:HG22	2:C:156:ASN:O	2.03	0.57
3:A:388:THR:O	3:A:389:SER:C	2.47	0.57
3:A:846:THR:HG23	3:A:888:ASN:ND2	2.19	0.57
1:E:103:LEU:HD13	1:E:268:GLY:HA2	1.87	0.57
1:E:206:TRP:O	1:E:210:LYS:HB2	2.05	0.57
3:D:77:TYR:O	3:D:78:TYR:C	2.48	0.57
3:D:389:SER:C	3:D:391:SER:H	2.10	0.57
3:D:943:ALA:HB2	3:D:1015:LEU:HD12	1.85	0.57
3:A:134:LEU:O	3:A:138:LEU:HG	2.05	0.57
3:A:637:VAL:O	3:A:641:ILE:HD12	2.05	0.57
2:F:88:ILE:HD11	2:F:117:ILE:HD11	1.87	0.57
3:D:265:LEU:O	3:D:268:LEU:N	2.38	0.57
3:D:823:PHE:O	3:D:827:PHE:HB2	2.04	0.57
3:D:871:PHE:CZ	3:D:875:LEU:HD11	2.40	0.57
1:B:49:LEU:HG	1:B:49:LEU:O	2.05	0.57
3:A:113:THR:HG21	3:A:126:TYR:HE2	1.69	0.57
3:A:276:VAL:O	3:A:277:SER:C	2.47	0.57
3:A:434:GLU:CB	3:A:439:GLU:O	2.51	0.57
3:A:574:HIS:HD2	3:A:624:ASP:HB2	1.69	0.57
3:A:875:LEU:O	3:A:878:ILE:N	2.37	0.57
3:A:974:ILE:O	3:A:975:GLN:C	2.47	0.57
3:D:304:ILE:CG1	3:D:356:LEU:HB3	2.35	0.57
3:A:56:HIS:C	3:A:58:ASP:N	2.61	0.57
3:D:202:PHE:O	3:D:205:ILE:HG23	2.05	0.57
1:B:98:ALA:HA	1:B:145:GLY:H	1.69	0.56
3:A:572:PHE:HD2	3:A:583:MET:HE1	1.70	0.56
3:A:866:ILE:HB	3:A:867:PRO:CD	2.35	0.56
1:E:10:GLY:HA3	1:E:34:TYR:CZ	2.40	0.56
1:E:244:VAL:CG1	1:E:245:LEU:HD13	2.33	0.56
3:A:484:VAL:HA	3:A:527:LEU:HD13	1.86	0.56
3:A:593:GLN:HG3	3:A:639:TYR:CD2	2.39	0.56
3:A:875:LEU:HD21	3:A:914:PHE:CE1	2.40	0.56
3:A:1000:GLY:HA2	3:A:1042:LEU:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:284:VAL:HG12	1:E:285:LEU:HD13	1.87	0.56
3:D:62:ARG:NH2	3:D:79:GLY:HA2	2.19	0.56
1:B:107:LEU:HD23	1:B:276:LEU:HD22	1.87	0.56
3:A:74:ASN:O	3:A:77:TYR:CB	2.54	0.56
3:A:76:LYS:O	3:A:80:LEU:HD22	2.05	0.56
3:A:210:GLN:O	3:A:211:PHE:C	2.49	0.56
3:A:420:MET:HB2	3:A:461:LEU:HD13	1.88	0.56
3:A:480:LEU:HB2	3:A:497:LEU:HD21	1.87	0.56
1:E:146:TYR:HD1	1:E:148:VAL:HG22	1.68	0.56
3:D:30:ASN:ND2	3:D:30:ASN:H	2.01	0.56
3:D:948:TYR:C	3:D:948:TYR:CD1	2.83	0.56
1:B:58:VAL:HG22	1:B:194:PRO:HG2	1.88	0.56
3:A:261:ARG:HD2	3:A:318:PHE:CD2	2.40	0.56
3:A:528:CYS:HA	3:A:540:ILE:HD13	1.87	0.56
3:A:905:ALA:HB3	3:A:906:GLN:NE2	2.20	0.56
3:A:1052:LEU:HD12	3:A:1053:GLN:HB2	1.86	0.56
1:E:277:ARG:HB2	1:E:280:MET:HE3	1.87	0.56
2:F:149:ILE:HG22	2:F:156:ASN:O	2.05	0.56
3:D:116:ASP:HB2	3:D:119:CYS:SG	2.46	0.56
3:D:678:ILE:C	3:D:680:LYS:H	2.12	0.56
3:D:762:TRP:HH2	3:D:772:VAL:HG22	1.68	0.56
3:D:938:GLY:O	3:D:941:MET:N	2.35	0.56
3:D:975:GLN:HG2	3:D:1002:PHE:CE1	2.40	0.56
2:C:138:PHE:HA	2:C:141:LYS:NZ	2.21	0.56
3:A:406:ARG:O	3:A:407:GLN:C	2.48	0.56
3:A:678:ILE:C	3:A:680:LYS:H	2.12	0.56
3:A:821:GLN:HA	3:D:597:ARG:HH21	1.71	0.56
1:E:6:LEU:C	1:E:6:LEU:HD23	2.30	0.56
2:C:66:THR:HG22	2:C:67:ALA:N	2.21	0.56
3:A:362:GLU:O	3:A:364:GLU:N	2.36	0.56
3:A:622:ILE:HG21	3:A:633:PHE:CD2	2.40	0.56
3:A:798:PRO:HG3	3:A:844:HIS:CE1	2.40	0.56
1:E:175:TYR:C	1:E:175:TYR:CD2	2.83	0.56
3:D:55:GLU:HG2	3:D:56:HIS:ND1	2.21	0.56
3:D:178:VAL:HG11	3:D:194:LEU:HB3	1.88	0.56
3:D:256:ASN:OD1	3:D:257:VAL:HG23	2.05	0.56
3:D:632:THR:HA	3:D:697:ARG:NH2	2.20	0.56
3:D:1004:LEU:HD21	3:D:1042:LEU:HD22	1.86	0.56
1:B:244:VAL:CG1	1:B:245:LEU:HD13	2.34	0.56
3:A:534:LYS:HE2	3:A:577:HIS:HB2	1.87	0.56
3:A:594:LYS:HE2	3:A:594:LYS:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:134:LEU:O	3:D:138:LEU:HG	2.06	0.56
3:A:62:ARG:NH2	3:A:79:GLY:HA2	2.20	0.56
3:A:123:GLU:C	3:A:125:VAL:N	2.63	0.56
3:A:962:LEU:HD13	3:A:968:VAL:HB	1.87	0.56
2:F:31:LEU:C	2:F:32:THR:HG22	2.31	0.56
3:D:632:THR:CA	3:D:697:ARG:HH22	2.17	0.56
3:D:983:LYS:HE2	3:D:991:ASP:HA	1.87	0.56
2:C:45:VAL:HG22	2:C:46:GLU:N	2.21	0.56
3:A:30:ASN:ND2	3:A:30:ASN:H	2.02	0.56
3:A:117:PRO:O	3:A:118:THR:OG1	2.22	0.56
3:A:973:PHE:C	3:A:973:PHE:HD1	2.10	0.56
1:B:240:SER:O	1:B:241:LEU:C	2.47	0.56
2:C:81:ILE:HD11	3:A:77:TYR:CD1	2.42	0.56
3:A:95:PRO:HG2	3:A:98:GLN:HE21	1.71	0.56
1:B:63:ARG:CZ	1:B:70:THR:H	2.19	0.55
1:E:45:ARG:NH1	1:E:49:LEU:CD2	2.69	0.55
1:E:110:VAL:HB	1:E:285:LEU:HD11	1.88	0.55
3:D:227:GLU:HG2	3:D:263:VAL:CG1	2.36	0.55
3:D:261:ARG:HD2	3:D:318:PHE:CD2	2.41	0.55
3:D:847:ASN:O	3:D:849:PHE:N	2.39	0.55
3:A:46:ALA:O	3:A:50:LEU:HD12	2.06	0.55
3:A:919:PHE:CE1	3:A:949:MET:HE2	2.42	0.55
3:D:704:HIS:HD2	3:D:766:SER:CA	2.19	0.55
3:A:290:THR:HG21	3:A:325:PHE:CE2	2.41	0.55
3:A:637:VAL:HG12	3:A:641:ILE:HD12	1.88	0.55
1:E:58:VAL:HG22	1:E:194:PRO:HG2	1.88	0.55
1:B:175:TYR:C	1:B:175:TYR:CD2	2.84	0.55
3:A:142:TRP:CZ3	3:A:197:SER:HB3	2.42	0.55
3:A:421:VAL:HG11	3:A:476:MET:HG2	1.87	0.55
3:A:704:HIS:HD2	3:A:766:SER:CA	2.20	0.55
1:E:4:LEU:HD23	3:D:522:LYS:HG3	1.87	0.55
3:D:925:HIS:O	3:D:928:SER:HB3	2.06	0.55
1:B:107:LEU:HB3	1:B:276:LEU:HD13	1.89	0.55
1:B:152:SER:O	1:B:225:PRO:CD	2.54	0.55
2:C:155:TYR:HE1	3:A:429:GLU:OE2	1.90	0.55
3:A:672:ALA:HB1	3:A:679:LEU:HD11	1.89	0.55
3:A:736:GLY:C	3:A:738:MET:N	2.64	0.55
3:A:914:PHE:CE1	3:A:918:TYR:HD1	2.24	0.55
3:D:99:CYS:HA	3:D:102:ILE:HD12	1.87	0.55
3:A:56:HIS:O	3:A:58:ASP:N	2.40	0.55
3:A:95:PRO:HG2	3:A:98:GLN:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:517:LEU:O	3:D:518:VAL:C	2.46	0.55
3:D:972:MET:O	3:D:976:ASP:HB2	2.07	0.55
1:B:98:ALA:CA	1:B:145:GLY:H	2.19	0.55
1:B:106:TRP:HH2	1:B:280:MET:HE1	1.70	0.55
1:B:351:ASP:O	3:A:715:LEU:HD12	2.06	0.55
3:A:30:ASN:HB3	3:A:47:GLN:HE21	1.69	0.55
3:A:790:ARG:NH1	3:D:647:GLN:HB2	2.21	0.55
3:D:594:LYS:HE2	3:D:594:LYS:HA	1.88	0.55
3:D:747:SER:O	3:D:750:THR:HB	2.07	0.55
3:A:128:GLY:O	3:A:132:MET:HB2	2.07	0.55
3:A:962:LEU:CD1	3:A:968:VAL:HB	2.36	0.55
1:E:114:LEU:HD12	1:E:118:TRP:CG	2.41	0.55
1:E:204:PHE:O	1:E:207:MET:HB2	2.07	0.55
3:D:66:ILE:HG22	3:D:76:LYS:HD2	1.86	0.55
3:D:123:GLU:C	3:D:125:VAL:H	2.13	0.55
3:D:247:ILE:O	3:D:251:ILE:HG13	2.05	0.55
3:D:432:VAL:HG23	3:D:432:VAL:O	2.06	0.55
3:D:515:ARG:HH11	3:D:515:ARG:CG	2.19	0.55
3:D:552:PRO:O	3:D:556:ARG:HG3	2.07	0.55
1:B:210:LYS:HD2	1:B:210:LYS:N	2.18	0.55
2:C:84:GLN:O	2:C:85:CYS:HB3	2.07	0.55
2:C:122:ASN:HA	2:C:149:ILE:O	2.07	0.55
2:C:139:HIS:O	2:C:143:ASN:N	2.40	0.55
3:A:406:ARG:C	3:A:408:LEU:N	2.62	0.55
3:A:638:GLY:HA3	3:A:701:ALA:HB3	1.89	0.55
2:F:28:LYS:O	2:F:32:THR:HG23	2.07	0.55
3:D:179:PHE:CE2	3:D:235:TRP:CE2	2.95	0.55
3:D:225:THR:CA	3:D:228:THR:HG22	2.34	0.55
3:D:383:GLU:OE1	3:D:405:ARG:HB2	2.07	0.55
3:D:559:TRP:HH2	3:D:610:PHE:HB2	1.72	0.55
3:D:737:GLU:OE1	3:D:794:ALA:HB1	2.07	0.55
3:A:55:GLU:HG2	3:A:56:HIS:ND1	2.22	0.55
3:A:616:ASN:OD1	3:A:656:LYS:HE3	2.06	0.55
2:F:66:THR:HG22	2:F:67:ALA:N	2.22	0.55
3:D:616:ASN:OD1	3:D:656:LYS:HE3	2.06	0.55
3:D:870:GLN:O	3:D:873:LEU:N	2.39	0.55
1:B:352:HIS:ND1	1:B:352:HIS:N	2.49	0.54
1:E:13:ILE:HD11	3:D:572:PHE:CZ	2.42	0.54
3:D:866:ILE:HB	3:D:867:PRO:CD	2.37	0.54
3:D:962:LEU:O	3:D:963:ASN:HB3	2.07	0.54
2:C:101:VAL:HB	2:C:102:PRO:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:280:GLU:HG3	3:A:336:LEU:CD1	2.37	0.54
3:A:515:ARG:HH11	3:A:515:ARG:CG	2.19	0.54
3:A:639:TYR:CE1	3:A:701:ALA:HA	2.42	0.54
3:A:816:THR:HG23	3:A:859:CYS:SG	2.47	0.54
1:E:152:SER:O	1:E:225:PRO:CD	2.54	0.54
3:D:280:GLU:HG3	3:D:336:LEU:CD1	2.37	0.54
3:D:521:ILE:CG2	3:D:547:ILE:HG21	2.36	0.54
1:B:351:ASP:OD2	3:A:712:ARG:HA	2.08	0.54
3:A:26:ASN:O	3:A:29:ASP:HB2	2.07	0.54
3:A:132:MET:HE3	3:A:135:VAL:HB	1.89	0.54
3:A:276:VAL:CG2	3:A:280:GLU:HA	2.37	0.54
3:A:286:LEU:HD12	3:A:286:LEU:C	2.32	0.54
2:F:98:TYR:HA	2:F:101:VAL:HG23	1.88	0.54
3:D:26:ASN:O	3:D:29:ASP:HB2	2.07	0.54
3:D:95:PRO:HG2	3:D:98:GLN:HB3	1.90	0.54
3:A:378:ALA:O	3:A:382:ARG:HG3	2.07	0.54
3:A:383:GLU:OE1	3:A:405:ARG:HB2	2.07	0.54
3:A:676:VAL:O	3:A:676:VAL:HG12	2.07	0.54
3:A:948:TYR:CD1	3:A:948:TYR:C	2.85	0.54
1:E:175:TYR:HB2	1:E:182:TYR:CD1	2.42	0.54
2:F:81:ILE:HG22	2:F:82:GLN:HG3	1.89	0.54
3:D:417:ARG:NE	3:D:464:LEU:O	2.34	0.54
3:D:626:GLN:HB2	3:D:627:PRO:HD2	1.89	0.54
3:D:716:ASP:O	3:D:717:MET:C	2.51	0.54
3:A:940:THR:OG1	3:A:1012:LYS:HE3	2.08	0.54
3:D:271:ILE:O	3:D:274:VAL:HG23	2.07	0.54
3:D:306:LEU:O	3:D:308:TYR:N	2.40	0.54
3:D:988:HIS:H	3:D:988:HIS:CD2	2.24	0.54
1:B:4:LEU:HD22	3:A:521:ILE:CD1	2.38	0.54
2:C:31:LEU:C	2:C:32:THR:CG2	2.80	0.54
2:C:110:ARG:NH2	3:A:176:GLU:OE1	2.40	0.54
3:A:983:LYS:HE2	3:A:991:ASP:HA	1.89	0.54
1:E:14:SER:HB2	1:E:16:ASP:OD2	2.07	0.54
1:E:159:ASN:HB2	1:E:223:LEU:HD11	1.90	0.54
2:F:159:LYS:N	2:F:160:PRO:CD	2.71	0.54
1:B:18:ASN:CG	1:B:108:ILE:HD11	2.33	0.54
3:A:239:GLY:O	3:A:244:THR:HG23	2.08	0.54
3:A:704:HIS:HD2	3:A:766:SER:CB	2.21	0.54
1:E:4:LEU:O	1:E:7:LYS:N	2.40	0.54
1:E:209:SER:O	1:E:210:LYS:HD2	2.06	0.54
3:D:227:GLU:HG2	3:D:263:VAL:HG11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:287:PHE:CD2	3:D:337:LEU:HD11	2.42	0.54
3:A:337:LEU:HD23	3:A:343:LEU:HB3	1.89	0.54
3:A:514:LYS:O	3:A:515:ARG:C	2.49	0.54
3:A:847:ASN:O	3:A:850:LEU:N	2.41	0.54
3:D:378:ALA:O	3:D:382:ARG:HG3	2.07	0.54
3:D:433:VAL:HG13	3:D:434:GLU:N	2.22	0.54
3:A:178:VAL:CG1	3:A:194:LEU:HB3	2.37	0.54
3:A:1036:GLU:O	3:A:1037:GLU:C	2.51	0.54
1:E:142:THR:HG23	1:E:148:VAL:HG21	1.88	0.54
2:F:29:ARG:HB3	2:F:157:PHE:HZ	1.73	0.54
3:D:962:LEU:C	3:D:964:PRO:HD3	2.33	0.54
2:C:15:LEU:HD22	2:C:23:LYS:HB3	1.89	0.54
3:A:20:SER:HB2	3:A:22:LYS:HD3	1.90	0.54
3:A:127:ILE:HG22	3:A:131:ASN:HD21	1.72	0.54
3:A:304:ILE:HG13	3:A:356:LEU:HB3	1.90	0.54
3:A:405:ARG:O	3:A:408:LEU:HB2	2.08	0.54
3:A:632:THR:HA	3:A:697:ARG:NH2	2.22	0.54
3:A:131:ASN:ND2	3:A:166:ASN:HD21	2.05	0.53
1:E:348:HIS:CD2	3:D:708:ILE:O	2.61	0.53
3:D:30:ASN:HB3	3:D:47:GLN:HE21	1.71	0.53
3:D:668:ILE:HG22	3:D:668:ILE:O	2.08	0.53
3:A:819:ILE:N	3:A:820:PRO:HD2	2.22	0.53
2:F:156:ASN:HB3	2:F:159:LYS:HG3	1.88	0.53
3:D:133:ILE:O	3:D:136:GLN:HB2	2.08	0.53
2:C:75:LEU:N	2:C:75:LEU:CD1	2.72	0.53
3:A:569:LEU:HD21	3:A:587:THR:CG2	2.34	0.53
3:A:819:ILE:HD12	3:A:855:VAL:HG21	1.89	0.53
3:A:964:PRO:HD2	3:A:968:VAL:HG21	1.91	0.53
3:A:218:ASN:OD1	3:A:218:ASN:O	2.27	0.53
3:A:247:ILE:O	3:A:251:ILE:HG13	2.07	0.53
3:A:293:GLN:O	3:A:296:GLN:HB3	2.08	0.53
3:A:871:PHE:CZ	3:A:875:LEU:HD11	2.44	0.53
1:E:173:CYS:SG	1:E:184:VAL:HG22	2.49	0.53
3:D:304:ILE:HG13	3:D:356:LEU:HB3	1.91	0.53
3:D:574:HIS:HD2	3:D:624:ASP:HB2	1.73	0.53
3:D:746:ARG:HH11	3:D:746:ARG:CG	2.12	0.53
3:D:905:ALA:HB3	3:D:906:GLN:HE22	1.72	0.53
3:D:1047:GLU:O	3:D:1051:LYS:HE2	2.08	0.53
3:A:179:PHE:CE2	3:A:235:TRP:CE2	2.96	0.53
3:A:953:VAL:HG11	3:A:974:ILE:HD13	1.89	0.53
3:D:272:ALA:HB1	3:D:329:PHE:HD1	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:238:LEU:HD22	3:A:242:PHE:CE2	2.40	0.53
2:F:85:CYS:HB2	2:F:164:LEU:HD22	1.91	0.53
3:D:819:ILE:HD12	3:D:855:VAL:HG21	1.91	0.53
3:D:914:PHE:CE1	3:D:918:TYR:HD1	2.26	0.53
3:D:1014:HIS:O	3:D:1017:ASP:HB3	2.08	0.53
1:B:3:GLU:HB3	3:A:522:LYS:NZ	2.24	0.53
1:B:220:LYS:C	1:B:221:THR:HG23	2.33	0.53
2:C:81:ILE:HG22	2:C:82:GLN:HG3	1.91	0.53
3:A:35:LEU:O	3:A:36:TYR:HD1	1.91	0.53
1:E:1:LEU:HD13	3:D:558:HIS:CD2	2.43	0.53
2:F:155:TYR:HE1	3:D:429:GLU:OE2	1.92	0.53
3:D:15:GLN:C	3:D:16:LEU:HD12	2.34	0.53
3:D:334:GLY:C	3:D:336:LEU:H	2.16	0.53
3:D:628:GLN:HA	3:D:631:HIS:HD2	1.74	0.53
3:A:615:LEU:CD2	3:A:618:ILE:HD11	2.38	0.53
3:A:417:ARG:NE	3:A:464:LEU:O	2.36	0.53
3:A:1004:LEU:HD21	3:A:1042:LEU:HD22	1.90	0.53
3:D:238:LEU:HD22	3:D:242:PHE:CE2	2.40	0.53
2:C:36:GLU:OE2	2:C:38:LYS:HE2	2.08	0.53
3:A:334:GLY:C	3:A:336:LEU:H	2.16	0.53
3:A:733:GLN:HB2	3:A:792:VAL:HG11	1.92	0.53
3:A:943:ALA:HB2	3:A:1015:LEU:HD12	1.89	0.53
1:E:4:LEU:HD11	3:D:518:VAL:HG13	1.89	0.53
1:E:258:PHE:O	1:E:273:VAL:HA	2.08	0.53
2:F:137:VAL:HG12	2:F:140:ARG:NH1	2.24	0.53
3:D:132:MET:HE3	3:D:135:VAL:HB	1.91	0.53
3:D:749:ARG:O	3:D:753:ARG:HG3	2.09	0.53
1:B:106:TRP:HZ3	1:B:276:LEU:HA	1.74	0.52
2:C:123:LYS:C	2:C:125:ASP:H	2.15	0.52
3:A:66:ILE:HG22	3:A:76:LYS:HD2	1.90	0.52
1:E:146:TYR:CD1	1:E:146:TYR:C	2.88	0.52
3:D:46:ALA:O	3:D:50:LEU:HD12	2.09	0.52
3:D:476:MET:CE	3:D:501:ILE:HG12	2.28	0.52
3:D:517:LEU:HD11	3:D:551:TYR:CG	2.44	0.52
3:D:819:ILE:N	3:D:820:PRO:HD2	2.23	0.52
3:D:997:PHE:CD1	3:D:1014:HIS:NE2	2.77	0.52
3:D:1034:PHE:O	3:D:1035:LEU:O	2.27	0.52
2:C:92:VAL:CG2	2:C:129:ARG:HG3	2.39	0.52
3:A:20:SER:O	3:A:22:LYS:N	2.42	0.52
3:A:259:MET:C	3:A:261:ARG:H	2.16	0.52
3:A:821:GLN:HA	3:D:597:ARG:NH2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:15:LEU:CD2	2:F:23:LYS:HG2	2.39	0.52
1:B:46:LEU:HD22	1:B:50:GLN:NE2	2.23	0.52
1:B:183:TYR:HA	1:B:229:VAL:O	2.10	0.52
2:C:35:PHE:HE2	2:C:37:LYS:HG2	1.74	0.52
3:A:249:THR:O	3:A:253:LYS:HB3	2.10	0.52
3:A:271:ILE:C	3:A:273:GLY:H	2.17	0.52
3:A:860:PHE:HE1	3:A:900:LEU:HG	1.74	0.52
1:B:4:LEU:O	1:B:7:LYS:N	2.42	0.52
1:B:119:ILE:CD1	1:B:259:TYR:HB2	2.37	0.52
3:A:334:GLY:C	3:A:336:LEU:N	2.66	0.52
3:A:860:PHE:N	3:A:861:PRO:CD	2.71	0.52
1:E:98:ALA:HA	1:E:145:GLY:H	1.73	0.52
1:B:142:THR:C	1:B:144:SER:N	2.67	0.52
3:A:870:GLN:O	3:A:873:LEU:N	2.42	0.52
3:A:953:VAL:CG1	3:A:974:ILE:HD13	2.39	0.52
1:E:237:THR:O	1:E:240:SER:N	2.42	0.52
3:D:103:LYS:HE3	3:D:146:TRP:CD1	2.44	0.52
3:D:128:GLY:O	3:D:132:MET:HB2	2.10	0.52
3:D:168:MET:SD	3:D:225:THR:HG23	2.49	0.52
3:D:293:GLN:O	3:D:296:GLN:HB3	2.10	0.52
3:D:324:LEU:CD2	3:D:368:ILE:HD13	2.40	0.52
1:B:169:THR:HG22	1:B:171:LEU:HD21	1.91	0.52
3:A:736:GLY:C	3:A:738:MET:H	2.16	0.52
3:D:615:LEU:HA	3:D:618:ILE:HG13	1.89	0.52
1:E:98:ALA:CA	1:E:145:GLY:H	2.22	0.52
2:F:75:LEU:O	2:F:78:GLY:N	2.40	0.52
3:D:50:LEU:C	3:D:52:HIS:H	2.18	0.52
3:D:816:THR:HG23	3:D:859:CYS:SG	2.49	0.52
3:D:1003:SER:C	3:D:1005:ASN:N	2.67	0.52
3:A:271:ILE:O	3:A:274:VAL:HG23	2.09	0.52
3:A:572:PHE:CD2	3:A:583:MET:HE1	2.44	0.52
3:A:1052:LEU:HD12	3:A:1053:GLN:N	2.25	0.52
3:D:28:LEU:O	3:D:32:VAL:HG23	2.09	0.52
3:D:286:LEU:HD12	3:D:286:LEU:C	2.35	0.52
3:D:1049:LYS:C	3:D:1051:LYS:H	2.18	0.52
1:B:48:GLU:C	1:B:50:GLN:H	2.16	0.52
2:C:119:LEU:HD23	2:C:146:TYR:HD1	1.74	0.52
3:A:658:MET:HE2	3:A:695:ASN:ND2	2.25	0.52
1:E:146:TYR:CE2	3:D:626:GLN:NE2	2.78	0.52
2:F:123:LYS:C	2:F:125:ASP:H	2.17	0.52
3:D:56:HIS:C	3:D:58:ASP:N	2.67	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:56:HIS:O	3:D:58:ASP:N	2.43	0.52
3:D:434:GLU:O	3:D:435:ASN:O	2.28	0.52
3:D:572:PHE:HD2	3:D:583:MET:HE1	1.75	0.52
3:A:51:THR:O	3:A:51:THR:HG22	2.09	0.52
3:A:268:LEU:O	3:A:269:THR:C	2.53	0.52
3:D:95:PRO:HG2	3:D:98:GLN:CB	2.40	0.52
3:D:116:ASP:C	3:D:118:THR:N	2.67	0.52
3:D:134:LEU:O	3:D:134:LEU:HD12	2.10	0.52
3:D:882:PHE:HA	3:D:890:ALA:HA	1.91	0.52
3:D:1004:LEU:HD21	3:D:1042:LEU:CD2	2.39	0.52
3:A:30:ASN:HB2	3:A:48:GLU:OE2	2.10	0.51
3:A:95:PRO:HG2	3:A:98:GLN:CB	2.40	0.51
3:A:133:ILE:O	3:A:136:GLN:HB2	2.10	0.51
3:A:621:ILE:HG22	3:A:622:ILE:HG23	1.92	0.51
3:A:695:ASN:HD21	3:A:709:GLN:HE21	1.58	0.51
3:A:798:PRO:HG2	3:A:843:GLU:OE1	2.09	0.51
3:D:29:ASP:O	3:D:33:ASN:ND2	2.43	0.51
3:D:74:ASN:O	3:D:77:TYR:CB	2.58	0.51
3:D:163:LEU:O	3:D:163:LEU:HD23	2.10	0.51
3:D:417:ARG:O	3:D:421:VAL:HG23	2.10	0.51
1:B:146:TYR:CD1	1:B:146:TYR:C	2.89	0.51
1:B:237:THR:O	1:B:240:SER:N	2.43	0.51
3:A:833:MET:HB3	3:A:841:TYR:HD1	1.75	0.51
3:A:882:PHE:HA	3:A:890:ALA:HA	1.91	0.51
1:E:107:LEU:HB3	1:E:276:LEU:HD13	1.92	0.51
3:D:17:LEU:HD23	3:D:22:LYS:HZ2	1.75	0.51
3:D:860:PHE:N	3:D:861:PRO:CD	2.72	0.51
1:B:234:PHE:N	1:B:234:PHE:CD1	2.78	0.51
1:B:357:MET:CG	3:A:719:ASN:HD21	2.23	0.51
2:C:155:TYR:O	2:C:156:ASN:C	2.54	0.51
3:A:647:GLN:O	3:A:651:GLU:HG3	2.10	0.51
1:E:58:VAL:HA	1:E:194:PRO:HG2	1.91	0.51
3:D:424:MET:HA	3:D:457:MET:CE	2.41	0.51
3:D:600:VAL:HG11	3:D:640:MET:O	2.11	0.51
3:D:658:MET:HE2	3:D:695:ASN:ND2	2.24	0.51
2:C:42:THR:OG1	4:C:217:GTP:O1G	2.25	0.51
2:C:92:VAL:HG23	2:C:129:ARG:HG3	1.92	0.51
1:E:52:SER:O	1:E:53:LYS:C	2.54	0.51
1:E:63:ARG:HH22	1:E:70:THR:HG23	1.76	0.51
3:D:102:ILE:O	3:D:103:LYS:C	2.54	0.51
3:D:430:VAL:O	3:D:430:VAL:CG1	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:LEU:HD11	3:A:518:VAL:CG1	2.35	0.51
1:B:142:THR:C	1:B:144:SER:H	2.18	0.51
1:B:142:THR:HG23	1:B:148:VAL:HG21	1.91	0.51
1:B:280:MET:O	1:B:284:VAL:HG23	2.10	0.51
2:C:13:LEU:HB2	2:C:85:CYS:SG	2.51	0.51
3:A:306:LEU:O	3:A:308:TYR:N	2.43	0.51
3:A:509:HIS:HB2	3:A:512:ASP:OD2	2.11	0.51
3:A:521:ILE:HG22	3:A:547:ILE:HG21	1.92	0.51
2:F:155:TYR:O	2:F:156:ASN:C	2.54	0.51
3:D:660:LEU:O	3:D:661:PRO:C	2.51	0.51
3:D:804:MET:HA	3:D:807:ILE:HG12	1.93	0.51
1:B:215:GLU:HG2	1:B:216:GLY:H	1.75	0.51
2:C:117:ILE:HG23	2:C:144:LEU:HD22	1.91	0.51
3:A:74:ASN:O	3:A:77:TYR:N	2.44	0.51
3:A:223:HIS:NE2	3:A:263:VAL:HG21	2.25	0.51
3:A:406:ARG:HA	3:A:409:TYR:HD2	1.74	0.51
3:D:347:LEU:O	3:D:351:LEU:HB2	2.09	0.51
2:C:47:VAL:O	2:C:47:VAL:HG23	2.09	0.51
3:A:875:LEU:O	3:A:876:ASP:C	2.53	0.51
2:F:98:TYR:HE1	2:F:136:ILE:HG23	1.75	0.51
1:B:357:MET:HG3	3:A:719:ASN:HD21	1.75	0.51
3:A:157:SER:HB3	3:A:164:CYS:HB2	1.92	0.51
3:A:432:VAL:O	3:A:433:VAL:HB	2.10	0.51
3:D:238:LEU:CD2	3:D:242:PHE:HE2	2.23	0.51
1:B:41:GLU:HG3	1:B:109:ASP:CB	2.35	0.51
1:B:357:MET:CG	3:A:719:ASN:ND2	2.74	0.51
3:A:912:GLN:OE1	3:A:958:ILE:HG12	2.11	0.51
3:A:914:PHE:CD1	3:A:918:TYR:HD1	2.28	0.51
3:A:970:ASN:N	3:A:970:ASN:ND2	2.56	0.51
3:A:1006:GLN:HB2	3:A:1049:LYS:HG2	1.91	0.51
1:E:119:ILE:CD1	1:E:259:TYR:HB2	2.39	0.51
3:D:51:THR:O	3:D:51:THR:HG22	2.11	0.51
3:D:317:ASN:O	3:D:318:PHE:C	2.52	0.51
3:D:406:ARG:C	3:D:408:LEU:N	2.65	0.51
3:D:672:ALA:HB1	3:D:679:LEU:HD11	1.93	0.51
3:D:871:PHE:CE2	3:D:875:LEU:HD11	2.46	0.51
3:D:875:LEU:HD21	3:D:914:PHE:CE1	2.46	0.51
3:D:906:GLN:NE2	3:D:906:GLN:N	2.58	0.51
1:B:51:LYS:NZ	1:B:264:HIS:HB2	2.23	0.51
3:A:142:TRP:HH2	3:A:197:SER:C	2.19	0.51
3:A:938:GLY:O	3:A:939:LEU:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1038:ARG:HA	3:A:1041:ALA:CB	2.40	0.51
3:D:123:GLU:C	3:D:125:VAL:N	2.68	0.51
3:D:134:LEU:HD23	3:D:170:ILE:HD12	1.94	0.51
3:A:257:VAL:O	3:A:257:VAL:HG12	2.11	0.50
3:A:299:PRO:HD2	3:A:302:THR:CG2	2.41	0.50
1:E:281:VAL:HG13	1:E:282:SER:H	1.76	0.50
3:D:30:ASN:N	3:D:30:ASN:HD22	2.07	0.50
3:D:44:ARG:O	3:D:47:GLN:HG2	2.11	0.50
3:D:95:PRO:CG	3:D:98:GLN:HE21	2.24	0.50
3:D:491:TRP:CH2	3:D:535:ASP:HB3	2.46	0.50
3:D:912:GLN:OE1	3:D:958:ILE:HG12	2.11	0.50
1:B:180:GLN:OE1	3:A:684:THR:HG22	2.10	0.50
3:A:44:ARG:O	3:A:47:GLN:HG2	2.11	0.50
3:A:95:PRO:CG	3:A:98:GLN:HE21	2.24	0.50
3:A:103:LYS:HE3	3:A:146:TRP:CD1	2.46	0.50
3:A:225:THR:CA	3:A:228:THR:HG22	2.39	0.50
1:E:122:VAL:HG22	1:E:256:LEU:HD22	1.93	0.50
3:D:150:ILE:O	3:D:154:VAL:HG23	2.11	0.50
3:D:259:MET:C	3:D:261:ARG:H	2.17	0.50
3:D:436:ASP:O	3:D:436:ASP:OD2	2.28	0.50
1:B:98:ALA:HB1	1:B:144:SER:HA	1.93	0.50
1:B:234:PHE:HB3	1:B:235:PRO:HD2	1.94	0.50
3:A:803:THR:O	3:A:807:ILE:HG12	2.11	0.50
2:F:122:ASN:HA	2:F:149:ILE:O	2.12	0.50
3:D:139:LYS:HD2	3:D:186:ILE:HD11	1.93	0.50
3:D:841:TYR:O	3:D:845:ARG:HG3	2.12	0.50
3:A:378:ALA:HB1	3:A:382:ARG:NH1	2.26	0.50
3:A:823:PHE:O	3:A:827:PHE:HB3	2.11	0.50
2:F:132:LYS:O	2:F:135:SER:N	2.38	0.50
3:D:249:THR:O	3:D:253:LYS:HB3	2.11	0.50
3:D:569:LEU:HD11	3:D:587:THR:HG21	1.94	0.50
1:B:138:THR:HG22	1:B:151:PHE:CZ	2.45	0.50
1:B:152:SER:O	1:B:225:PRO:HD3	2.12	0.50
2:C:117:ILE:CG1	2:C:118:VAL:N	2.74	0.50
3:A:28:LEU:O	3:A:32:VAL:HG23	2.11	0.50
3:A:101:GLY:O	3:A:105:TYR:HB2	2.10	0.50
3:A:280:GLU:HG3	3:A:336:LEU:HD13	1.92	0.50
3:A:1043:ARG:HA	3:A:1043:ARG:CZ	2.41	0.50
1:E:106:TRP:HH2	1:E:280:MET:HE1	1.75	0.50
3:D:142:TRP:CZ3	3:D:197:SER:HB3	2.46	0.50
3:D:178:VAL:CG1	3:D:194:LEU:HB3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:ASP:HB2	1:B:352:HIS:CE1	2.46	0.50
3:A:1003:SER:C	3:A:1005:ASN:N	2.69	0.50
2:F:31:LEU:HB3	2:F:50:LEU:CD2	2.39	0.50
2:F:38:LYS:HD2	3:D:840:GLU:HA	1.92	0.50
3:D:290:THR:HG21	3:D:325:PHE:CE2	2.46	0.50
3:D:539:ILE:HG22	3:D:540:ILE:N	2.27	0.50
3:D:569:LEU:HD21	3:D:587:THR:CG2	2.38	0.50
3:D:675:ASN:C	3:D:677:ASP:H	2.20	0.50
3:D:709:GLN:O	3:D:712:ARG:HB3	2.11	0.50
3:D:870:GLN:O	3:D:873:LEU:HB3	2.11	0.50
3:A:168:MET:SD	3:A:225:THR:HG23	2.51	0.50
3:A:552:PRO:O	3:A:556:ARG:HG3	2.11	0.50
3:A:1046:GLN:HE22	3:A:1049:LYS:NZ	2.10	0.50
1:E:1:LEU:CD2	3:D:558:HIS:HD2	2.24	0.50
3:D:123:GLU:OE1	3:D:123:GLU:HA	2.11	0.50
3:D:130:LEU:O	3:D:131:ASN:C	2.54	0.50
3:D:271:ILE:C	3:D:273:GLY:H	2.19	0.50
3:D:334:GLY:C	3:D:336:LEU:N	2.68	0.50
3:D:1038:ARG:O	3:D:1041:ALA:HB3	2.12	0.50
1:B:39:GLN:O	1:B:39:GLN:HG2	2.11	0.50
1:B:357:MET:CB	3:A:719:ASN:HD21	2.24	0.50
2:C:31:LEU:O	2:C:32:THR:HG22	2.12	0.50
3:A:424:MET:HA	3:A:457:MET:CE	2.41	0.50
3:A:749:ARG:O	3:A:753:ARG:HG3	2.12	0.50
1:E:41:GLU:HG3	1:E:109:ASP:CB	2.36	0.50
1:E:176:ASN:OD1	1:E:179:ASN:HB2	2.12	0.50
2:F:47:VAL:HG12	2:F:64:TRP:CG	2.47	0.50
2:F:171:ASP:C	2:F:171:ASP:OD1	2.55	0.50
1:B:122:VAL:HG22	1:B:256:LEU:HD22	1.94	0.50
3:A:615:LEU:HA	3:A:618:ILE:HG13	1.92	0.50
1:E:234:PHE:HB3	1:E:235:PRO:HD2	1.94	0.50
3:D:393:LEU:HD23	3:D:394:LEU:H	1.77	0.50
3:D:879:ILE:HD12	3:D:879:ILE:N	2.27	0.50
3:D:962:LEU:O	3:D:963:ASN:CB	2.59	0.50
3:D:1004:LEU:HD12	3:D:1014:HIS:HB2	1.93	0.50
3:A:15:GLN:HG2	3:A:16:LEU:O	2.12	0.49
3:A:276:VAL:HG23	3:A:283:PHE:CD2	2.46	0.49
3:A:847:ASN:O	3:A:848:PHE:C	2.55	0.49
3:A:924:GLN:NE2	3:A:977:TYR:OH	2.45	0.49
1:E:234:PHE:N	1:E:234:PHE:CD1	2.79	0.49
3:D:300:LEU:HB3	3:D:352:HIS:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:406:ARG:O	3:D:407:GLN:C	2.54	0.49
3:D:676:VAL:O	3:D:676:VAL:HG12	2.11	0.49
3:D:736:GLY:C	3:D:738:MET:N	2.69	0.49
3:D:974:ILE:N	3:D:974:ILE:HD12	2.27	0.49
1:B:106:TRP:CZ3	1:B:276:LEU:HA	2.46	0.49
1:B:119:ILE:HD11	1:B:259:TYR:CB	2.40	0.49
3:A:50:LEU:C	3:A:52:HIS:H	2.21	0.49
3:A:72:ASN:O	3:A:75:THR:N	2.44	0.49
3:A:129:LYS:O	3:A:133:ILE:HG13	2.12	0.49
3:A:195:LYS:C	3:A:197:SER:N	2.69	0.49
2:F:45:VAL:HG22	2:F:46:GLU:N	2.27	0.49
2:F:117:ILE:CG1	2:F:118:VAL:N	2.75	0.49
3:D:142:TRP:N	3:D:143:PRO:HD2	2.27	0.49
3:D:276:VAL:O	3:D:276:VAL:HG13	2.10	0.49
3:D:637:VAL:HG12	3:D:641:ILE:HD12	1.93	0.49
3:D:963:ASN:N	3:D:964:PRO:CD	2.75	0.49
1:B:149:ASN:HD22	1:B:150:ARG:H	1.60	0.49
3:A:56:HIS:N	3:A:57:PRO:CD	2.75	0.49
3:A:96:ARG:HH22	3:A:145:HIS:HB3	1.76	0.49
3:A:423:ARG:O	3:A:424:MET:C	2.53	0.49
3:A:526:GLY:O	3:A:530:GLN:HG3	2.12	0.49
3:A:528:CYS:CB	3:A:540:ILE:HG21	2.26	0.49
3:A:559:TRP:HH2	3:A:610:PHE:HB2	1.77	0.49
3:A:697:ARG:NH2	3:A:697:ARG:HG3	2.26	0.49
3:A:945:ILE:O	3:A:949:MET:HG3	2.12	0.49
3:D:63:VAL:O	3:D:76:LYS:HE3	2.13	0.49
3:D:843:GLU:O	3:D:844:HIS:C	2.54	0.49
1:E:25:PRO:HG2	1:E:108:ILE:HD13	1.95	0.49
3:D:28:LEU:O	3:D:28:LEU:HD23	2.11	0.49
3:D:195:LYS:C	3:D:197:SER:N	2.70	0.49
3:D:865:ALA:O	3:D:866:ILE:HG23	2.11	0.49
2:C:31:LEU:O	2:C:31:LEU:HG	2.10	0.49
2:C:75:LEU:HD11	3:A:49:VAL:HG22	1.95	0.49
3:A:163:LEU:O	3:A:163:LEU:HD23	2.13	0.49
3:A:362:GLU:C	3:A:364:GLU:H	2.19	0.49
3:A:654:ILE:O	3:A:654:ILE:HG22	2.10	0.49
3:A:739:VAL:O	3:A:742:GLN:HG2	2.12	0.49
3:D:526:GLY:O	3:D:530:GLN:HG3	2.13	0.49
1:B:237:THR:O	1:B:238:PRO:C	2.55	0.49
3:A:29:ASP:O	3:A:33:ASN:ND2	2.45	0.49
3:A:313:ASP:HA	3:A:316:GLN:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:329:PHE:CE1	3:A:333:HIS:HD2	2.30	0.49
3:A:547:ILE:HG22	3:A:548:VAL:N	2.26	0.49
3:A:997:PHE:CD1	3:A:1014:HIS:NE2	2.80	0.49
1:E:106:TRP:CZ3	1:E:276:LEU:HA	2.48	0.49
3:D:572:PHE:CD2	3:D:583:MET:HE1	2.47	0.49
3:D:966:ASN:HB3	3:D:967:PRO:HD3	1.94	0.49
1:B:69:TRP:HB3	1:B:95:LYS:HE3	1.94	0.49
1:B:155:LEU:HG	1:B:217:LEU:HD11	1.95	0.49
3:A:709:GLN:O	3:A:712:ARG:HB3	2.12	0.49
3:D:19:PHE:CD1	3:D:19:PHE:C	2.89	0.49
3:D:365:ILE:HG22	3:D:366:PHE:N	2.28	0.49
3:D:1035:LEU:O	3:D:1037:GLU:N	2.46	0.49
3:A:552:PRO:HA	3:A:555:LEU:HD12	1.95	0.49
3:A:1004:LEU:HD21	3:A:1042:LEU:CD2	2.42	0.49
1:E:142:THR:C	1:E:144:SER:H	2.19	0.49
3:D:157:SER:HB3	3:D:164:CYS:HB2	1.94	0.49
3:D:509:HIS:O	3:D:510:GLU:C	2.56	0.49
3:D:639:TYR:CE1	3:D:701:ALA:HA	2.48	0.49
3:D:974:ILE:O	3:D:975:GLN:C	2.54	0.49
1:B:160:ARG:NE	1:B:160:ARG:CA	2.68	0.49
3:A:30:ASN:N	3:A:30:ASN:HD22	2.09	0.49
3:A:116:ASP:C	3:A:118:THR:N	2.71	0.49
3:A:153:ILE:HA	3:A:156:ALA:CB	2.43	0.49
3:A:255:LEU:HD12	3:A:268:LEU:CD1	2.42	0.49
3:A:450:SER:O	3:A:453:LEU:N	2.46	0.49
3:A:650:GLN:O	3:A:654:ILE:HG13	2.12	0.49
2:F:70:GLU:OE2	3:D:1023:LYS:NZ	2.43	0.49
3:D:676:VAL:HG13	3:D:679:LEU:HD12	1.94	0.49
3:A:146:TRP:CE3	3:A:149:PHE:HB2	2.47	0.49
3:A:276:VAL:O	3:A:278:GLN:N	2.46	0.49
3:A:458:ARG:HG3	3:A:503:SER:HB2	1.94	0.49
3:A:804:MET:HA	3:A:807:ILE:HG12	1.95	0.49
3:A:1008:ILE:HG13	3:A:1009:PRO:HD3	1.94	0.49
3:D:297:MET:O	3:D:299:PRO:HD3	2.13	0.49
3:D:423:ARG:C	3:D:457:MET:HE1	2.38	0.49
3:D:875:LEU:O	3:D:878:ILE:N	2.45	0.49
3:A:127:ILE:CG2	3:A:131:ASN:HD21	2.26	0.48
3:A:279:TYR:O	3:A:283:PHE:CD2	2.66	0.48
1:E:11:LEU:HG	3:D:572:PHE:CZ	2.48	0.48
1:E:142:THR:C	1:E:144:SER:N	2.70	0.48
1:E:210:LYS:HD2	1:E:210:LYS:N	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:299:PRO:HD2	3:D:302:THR:CG2	2.43	0.48
1:B:236:CYS:HA	1:B:241:LEU:HD21	1.94	0.48
2:C:47:VAL:HG12	2:C:64:TRP:CG	2.48	0.48
2:C:138:PHE:O	2:C:139:HIS:C	2.56	0.48
2:C:156:ASN:HB3	2:C:159:LYS:HG3	1.93	0.48
3:A:962:LEU:HB3	3:A:964:PRO:CD	2.30	0.48
1:E:1:LEU:HG	1:E:2:ASN:HD22	1.78	0.48
1:E:106:TRP:HZ3	1:E:276:LEU:HA	1.79	0.48
2:F:178:ALA:O	2:F:179:MET:CB	2.61	0.48
3:D:279:TYR:O	3:D:283:PHE:CD2	2.65	0.48
3:D:400:PHE:O	3:D:400:PHE:CD1	2.66	0.48
3:D:406:ARG:NH2	3:D:467:LEU:O	2.46	0.48
3:D:833:MET:HB3	3:D:841:TYR:HD1	1.75	0.48
3:D:897:LEU:O	3:D:901:LEU:HG	2.13	0.48
3:D:900:LEU:HD23	3:D:900:LEU:C	2.37	0.48
2:C:171:ASP:C	2:C:171:ASP:OD1	2.56	0.48
3:A:672:ALA:HA	3:A:675:ASN:O	2.12	0.48
1:E:39:GLN:O	1:E:39:GLN:HG2	2.12	0.48
2:F:77:ASP:HA	2:F:80:TYR:CE2	2.45	0.48
3:D:218:ASN:O	3:D:222:VAL:HG23	2.13	0.48
3:D:284:GLU:CG	3:D:336:LEU:HD11	2.42	0.48
3:D:420:MET:O	3:D:424:MET:HB2	2.14	0.48
3:A:672:ALA:CB	3:A:678:ILE:HD11	2.37	0.48
3:A:786:ILE:HD13	3:D:645:THR:HG21	1.94	0.48
3:A:1036:GLU:O	3:A:1039:GLU:N	2.46	0.48
1:E:351:ASP:OD2	1:E:351:ASP:N	2.40	0.48
3:D:405:ARG:O	3:D:408:LEU:HB2	2.13	0.48
3:D:840:GLU:O	3:D:845:ARG:NH1	2.46	0.48
3:D:879:ILE:HG12	3:D:925:HIS:CD2	2.48	0.48
3:D:1021:GLN:HE22	3:D:1033:LEU:HD13	1.79	0.48
3:D:1035:LEU:O	3:D:1038:ARG:N	2.46	0.48
2:C:13:LEU:HD12	2:C:14:VAL:O	2.12	0.48
2:C:75:LEU:CD1	3:A:49:VAL:HG22	2.44	0.48
2:C:79:TYR:OH	3:A:45:MET:HE3	2.13	0.48
2:C:132:LYS:O	2:C:133:ALA:C	2.54	0.48
2:C:159:LYS:N	2:C:160:PRO:CD	2.77	0.48
4:C:217:GTP:O3B	4:C:217:GTP:O1A	2.32	0.48
3:A:134:LEU:HD23	3:A:170:ILE:HD12	1.96	0.48
3:A:430:VAL:O	3:A:430:VAL:CG1	2.61	0.48
3:A:552:PRO:O	3:A:553:ARG:C	2.55	0.48
3:A:879:ILE:HG12	3:A:925:HIS:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:988:HIS:CD2	3:A:988:HIS:N	2.81	0.48
1:E:130:LEU:HD11	1:E:170:ILE:CG2	2.43	0.48
2:F:117:ILE:HG23	2:F:144:LEU:HD22	1.94	0.48
3:D:1003:SER:O	3:D:1005:ASN:N	2.47	0.48
1:B:214:GLU:O	1:B:215:GLU:C	2.57	0.48
3:A:232:PHE:O	3:A:236:ILE:HG23	2.14	0.48
3:A:324:LEU:CD2	3:A:368:ILE:HD13	2.44	0.48
3:A:476:MET:CE	3:A:501:ILE:HG12	2.35	0.48
3:A:768:ASP:CG	3:A:771:MET:HE3	2.39	0.48
3:D:272:ALA:HB1	3:D:329:PHE:CD1	2.49	0.48
1:B:1:LEU:HD23	1:B:1:LEU:H	1.79	0.48
2:C:81:ILE:HD11	3:A:77:TYR:CG	2.49	0.48
3:A:188:GLN:NE2	3:A:1013:GLU:HG3	2.28	0.48
3:D:138:LEU:C	3:D:140:GLN:H	2.19	0.48
3:D:188:GLN:NE2	3:D:1013:GLU:HG3	2.29	0.48
3:A:551:TYR:O	3:A:554:PHE:HB3	2.14	0.48
3:A:769:PRO:CG	3:A:770:GLN:N	2.77	0.48
3:A:894:LEU:HA	3:A:894:LEU:HD23	1.48	0.48
3:D:122:LYS:O	3:D:123:GLU:O	2.32	0.48
3:D:424:MET:HE3	3:D:454:TYR:CE1	2.48	0.48
3:D:611:ILE:O	3:D:614:ILE:HB	2.14	0.48
3:D:802:SER:O	3:D:806:ILE:HG13	2.13	0.48
3:D:1022:ILE:CG1	3:D:1023:LYS:N	2.76	0.48
2:C:29:ARG:HB3	2:C:157:PHE:HZ	1.79	0.48
3:A:383:GLU:OE2	3:A:405:ARG:HG3	2.14	0.48
3:A:600:VAL:HG11	3:A:640:MET:O	2.14	0.48
3:A:962:LEU:O	3:A:963:ASN:HB2	2.14	0.48
3:D:280:GLU:HG3	3:D:336:LEU:HD13	1.94	0.48
3:D:924:GLN:NE2	3:D:977:TYR:OH	2.47	0.48
1:B:1:LEU:HD22	3:A:514:LYS:NZ	2.28	0.48
1:B:60:HIS:CE1	1:B:100:GLN:HE22	2.32	0.48
2:C:24:THR:OG1	4:C:217:GTP:O1G	2.32	0.48
3:A:139:LYS:HD2	3:A:186:ILE:HD11	1.96	0.48
3:A:329:PHE:CE1	3:A:333:HIS:CD2	3.02	0.48
3:A:376:LEU:HG	3:A:380:LEU:HD12	1.95	0.48
3:A:424:MET:HE3	3:A:454:TYR:CE1	2.49	0.48
3:A:517:LEU:HD11	3:A:551:TYR:CG	2.49	0.48
3:D:448:THR:O	3:D:449:ASP:C	2.57	0.48
3:D:504:ILE:O	3:D:504:ILE:HD12	2.14	0.48
1:B:58:VAL:HA	1:B:194:PRO:CG	2.44	0.47
3:A:150:ILE:O	3:A:154:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:687:GLN:O	3:A:691:ILE:HB	2.14	0.47
3:A:831:LEU:HD13	3:A:848:PHE:CZ	2.49	0.47
3:D:127:ILE:HG22	3:D:128:GLY:N	2.29	0.47
3:D:157:SER:HB3	3:D:164:CYS:CB	2.44	0.47
3:D:329:PHE:CE1	3:D:333:HIS:HD2	2.30	0.47
3:A:56:HIS:HB3	3:A:82:ILE:CG2	2.44	0.47
3:A:246:LEU:O	3:A:249:THR:N	2.46	0.47
3:A:317:ASN:O	3:A:318:PHE:C	2.55	0.47
3:A:865:ALA:O	3:A:866:ILE:HG23	2.13	0.47
2:F:138:PHE:O	2:F:141:LYS:HD2	2.14	0.47
3:D:56:HIS:N	3:D:57:PRO:CD	2.77	0.47
3:D:62:ARG:HH12	3:D:82:ILE:HD13	1.79	0.47
3:D:102:ILE:O	3:D:105:TYR:N	2.47	0.47
3:D:578:ASP:OD2	3:D:578:ASP:N	2.47	0.47
1:B:55:LEU:H	1:B:55:LEU:CD1	2.09	0.47
1:B:98:ALA:CB	1:B:144:SER:HA	2.44	0.47
3:A:138:LEU:C	3:A:140:GLN:H	2.20	0.47
3:D:138:LEU:C	3:D:140:GLN:N	2.72	0.47
3:D:491:TRP:CD2	3:D:539:ILE:HD12	2.49	0.47
3:D:547:ILE:HG22	3:D:548:VAL:N	2.28	0.47
1:B:18:ASN:ND2	1:B:36:SER:OG	2.47	0.47
1:B:247:MET:HB2	1:B:249:PHE:CE1	2.49	0.47
2:C:145:GLN:HE21	2:C:163:TRP:CD1	2.32	0.47
3:A:55:GLU:HB3	3:A:57:PRO:HD3	1.97	0.47
3:A:239:GLY:HA2	3:A:243:GLU:OE2	2.13	0.47
3:A:509:HIS:O	3:A:510:GLU:C	2.58	0.47
3:A:871:PHE:CE2	3:A:875:LEU:HD11	2.49	0.47
3:A:964:PRO:O	3:A:968:VAL:HG22	2.13	0.47
1:E:240:SER:C	1:E:242:CYS:N	2.73	0.47
1:E:284:VAL:CG1	1:E:285:LEU:HD13	2.44	0.47
3:D:80:LEU:HB3	3:D:133:ILE:HD11	1.95	0.47
3:D:129:LYS:O	3:D:133:ILE:HG13	2.14	0.47
3:D:372:TYR:O	3:D:373:TRP:C	2.57	0.47
3:D:615:LEU:CD2	3:D:618:ILE:HD11	2.43	0.47
3:D:875:LEU:O	3:D:876:ASP:C	2.57	0.47
1:B:235:PRO:O	1:B:240:SER:OG	2.31	0.47
2:C:88:ILE:HD11	2:C:117:ILE:HD11	1.97	0.47
2:C:88:ILE:HD11	2:C:117:ILE:CD1	2.44	0.47
3:A:491:TRP:CH2	3:A:535:ASP:HB3	2.49	0.47
3:A:975:GLN:HG3	3:A:998:VAL:CG1	2.44	0.47
3:A:1004:LEU:HD12	3:A:1014:HIS:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:30:ASN:HB2	3:D:48:GLU:OE2	2.15	0.47
3:D:179:PHE:CE2	3:D:235:TRP:CD2	3.02	0.47
3:D:306:LEU:C	3:D:308:TYR:N	2.72	0.47
3:D:362:GLU:C	3:D:364:GLU:H	2.22	0.47
3:D:376:LEU:HG	3:D:380:LEU:HD12	1.96	0.47
3:D:697:ARG:O	3:D:698:ALA:C	2.57	0.47
3:D:887:ARG:CD	3:D:937:ALA:HB3	2.37	0.47
1:B:24:HIS:C	1:B:26:ARG:N	2.72	0.47
1:B:155:LEU:HD11	1:B:228:PHE:CZ	2.49	0.47
3:A:875:LEU:HD21	3:A:914:PHE:HE1	1.80	0.47
3:A:898:PHE:HD2	3:A:945:ILE:HG12	1.80	0.47
1:E:119:ILE:HD11	1:E:259:TYR:CB	2.43	0.47
1:E:200:THR:OG1	1:E:263:THR:HG23	2.14	0.47
2:F:16:VAL:HG23	2:F:88:ILE:HA	1.95	0.47
3:D:153:ILE:HA	3:D:156:ALA:CB	2.45	0.47
3:D:282:GLN:OE1	3:D:282:GLN:N	2.47	0.47
3:D:313:ASP:HA	3:D:316:GLN:HG3	1.96	0.47
3:D:484:VAL:CG1	3:D:530:GLN:OE1	2.54	0.47
3:D:860:PHE:CE1	3:D:900:LEU:HG	2.47	0.47
1:B:13:ILE:CG2	3:A:575:GLU:OE1	2.59	0.47
1:B:52:SER:O	1:B:53:LYS:C	2.57	0.47
2:C:98:TYR:HE1	2:C:136:ILE:HG23	1.79	0.47
3:A:100:GLU:O	3:A:103:LYS:HB3	2.15	0.47
3:A:122:LYS:O	3:A:123:GLU:O	2.32	0.47
3:A:146:TRP:N	3:A:147:PRO:CD	2.77	0.47
3:A:656:LYS:O	3:A:656:LYS:HG2	2.13	0.47
3:A:668:ILE:HG22	3:A:668:ILE:O	2.14	0.47
3:A:675:ASN:C	3:A:677:ASP:H	2.23	0.47
1:E:122:VAL:HG11	1:E:249:PHE:CE2	2.49	0.47
1:E:183:TYR:HA	1:E:229:VAL:O	2.14	0.47
1:E:244:VAL:HG13	1:E:245:LEU:CD1	2.39	0.47
2:F:124:VAL:HG21	2:F:155:TYR:CD2	2.50	0.47
2:F:140:ARG:NH2	3:D:371:GLU:OE1	2.39	0.47
3:D:344:ARG:NE	3:D:408:LEU:HD21	2.30	0.47
3:D:406:ARG:HA	3:D:409:TYR:HD2	1.78	0.47
3:D:915:TYR:HA	3:D:919:PHE:HB2	1.96	0.47
3:D:938:GLY:O	3:D:939:LEU:C	2.57	0.47
3:D:1047:GLU:HA	3:D:1050:HIS:NE2	2.29	0.47
1:B:1:LEU:HG	1:B:2:ASN:N	2.30	0.47
3:A:63:VAL:O	3:A:76:LYS:HE3	2.15	0.47
3:A:579:GLY:C	3:A:581:GLN:N	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:731:ALA:HB1	3:A:739:VAL:HG11	1.95	0.47
3:A:843:GLU:O	3:A:844:HIS:C	2.57	0.47
1:E:13:ILE:HD11	3:D:572:PHE:CE2	2.49	0.47
1:E:25:PRO:HG2	1:E:108:ILE:CD1	2.45	0.47
3:D:23:LEU:HD11	3:D:26:ASN:CB	2.44	0.47
3:D:239:GLY:O	3:D:244:THR:HG23	2.15	0.47
3:D:255:LEU:HD23	3:D:255:LEU:O	2.14	0.47
3:D:704:HIS:HD2	3:D:766:SER:HA	1.80	0.47
3:D:769:PRO:CG	3:D:770:GLN:N	2.78	0.47
3:D:847:ASN:O	3:D:850:LEU:N	2.47	0.47
1:B:63:ARG:NH1	1:B:95:LYS:HZ2	2.05	0.47
3:A:378:ALA:HB1	3:A:382:ARG:HH12	1.79	0.47
3:A:578:ASP:OD2	3:A:578:ASP:N	2.48	0.47
2:F:23:LYS:O	2:F:27:VAL:HG13	2.15	0.47
3:D:100:GLU:OE2	3:D:103:LYS:HD3	2.14	0.47
3:D:127:ILE:O	3:D:130:LEU:N	2.48	0.47
3:D:142:TRP:HH2	3:D:197:SER:C	2.23	0.47
3:D:146:TRP:CE3	3:D:149:PHE:HB2	2.49	0.47
3:D:257:VAL:O	3:D:257:VAL:HG12	2.15	0.47
3:D:458:ARG:O	3:D:462:VAL:HG23	2.15	0.47
2:C:26:PHE:CZ	2:C:30:HIS:CE1	3.03	0.47
2:C:138:PHE:O	2:C:141:LYS:HD2	2.15	0.47
3:A:102:ILE:O	3:A:103:LYS:C	2.58	0.47
3:A:716:ASP:O	3:A:717:MET:C	2.58	0.47
3:A:970:ASN:O	3:A:971:GLN:C	2.58	0.47
3:A:973:PHE:CD1	3:A:974:ILE:N	2.81	0.47
2:F:132:LYS:O	2:F:133:ALA:C	2.56	0.47
3:D:718:LEU:HA	3:D:718:LEU:HD23	1.56	0.47
1:B:47:LEU:HA	1:B:47:LEU:HD23	1.62	0.46
1:B:114:LEU:HD12	1:B:118:TRP:CG	2.50	0.46
1:B:352:HIS:HA	1:B:353:PRO:HD3	1.79	0.46
3:A:125:VAL:O	3:A:126:TYR:C	2.58	0.46
3:A:747:SER:O	3:A:750:THR:HB	2.15	0.46
3:D:258:PRO:O	3:D:261:ARG:HB3	2.15	0.46
3:D:378:ALA:HB1	3:D:382:ARG:NH1	2.30	0.46
1:B:63:ARG:NH1	1:B:95:LYS:HZ1	2.10	0.46
3:A:351:LEU:HA	3:A:351:LEU:HD23	1.55	0.46
3:A:704:HIS:CD2	3:A:767:ASN:N	2.83	0.46
3:A:730:ALA:O	3:A:731:ALA:C	2.57	0.46
3:A:840:GLU:O	3:A:845:ARG:NH1	2.47	0.46
3:A:918:TYR:O	3:A:922:ILE:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:12:LYS:O	2:C:12:LYS:HG2	2.15	0.46
2:C:98:TYR:HA	2:C:101:VAL:HG23	1.96	0.46
3:A:28:LEU:O	3:A:28:LEU:HD23	2.15	0.46
3:A:66:ILE:HD13	3:A:66:ILE:H	1.80	0.46
3:A:93:ILE:HG23	3:A:1027:GLY:HA3	1.96	0.46
3:A:219:ALA:CB	3:A:220:PRO:HD3	2.43	0.46
3:A:240:TYR:O	3:A:244:THR:HG21	2.15	0.46
3:A:287:PHE:CD2	3:A:337:LEU:HD11	2.50	0.46
3:A:935:HIS:ND1	3:A:935:HIS:N	2.63	0.46
3:A:952:LEU:O	3:A:952:LEU:HD23	2.15	0.46
2:F:28:LYS:O	2:F:29:ARG:C	2.58	0.46
2:F:81:ILE:HD11	3:D:77:TYR:CG	2.51	0.46
3:D:101:GLY:O	3:D:105:TYR:HB2	2.14	0.46
3:D:125:VAL:O	3:D:126:TYR:C	2.58	0.46
3:D:514:LYS:O	3:D:515:ARG:C	2.58	0.46
3:D:521:ILE:HG22	3:D:547:ILE:HG21	1.97	0.46
3:D:627:PRO:O	3:D:631:HIS:CD2	2.69	0.46
3:D:752:LYS:O	3:D:755:THR:HB	2.15	0.46
3:D:970:ASN:O	3:D:971:GLN:C	2.58	0.46
1:B:25:PRO:HG2	1:B:108:ILE:CD1	2.45	0.46
2:C:45:VAL:HG22	2:C:46:GLU:H	1.79	0.46
2:C:50:LEU:O	2:C:60:LYS:HA	2.16	0.46
3:A:240:TYR:O	3:A:244:THR:CG2	2.63	0.46
3:A:272:ALA:HB1	3:A:329:PHE:HD1	1.80	0.46
3:A:465:THR:O	3:A:469:TYR:HB3	2.16	0.46
3:A:906:GLN:NE2	3:A:906:GLN:N	2.63	0.46
1:E:4:LEU:C	1:E:7:LYS:H	2.23	0.46
1:E:240:SER:O	1:E:242:CYS:N	2.49	0.46
2:F:64:TRP:HE3	2:F:79:TYR:HB3	1.78	0.46
2:F:75:LEU:N	2:F:75:LEU:CD1	2.79	0.46
2:F:83:ALA:O	2:F:115:ILE:HG21	2.15	0.46
3:D:119:CYS:C	3:D:121:GLU:H	2.23	0.46
3:D:660:LEU:HD12	3:D:660:LEU:N	2.30	0.46
1:B:105:GLU:O	1:B:106:TRP:C	2.59	0.46
2:C:83:ALA:O	2:C:115:ILE:HG21	2.16	0.46
2:C:124:VAL:HG21	2:C:155:TYR:CD2	2.51	0.46
3:A:90:ARG:O	3:A:91:TRP:C	2.59	0.46
3:A:189:VAL:HG11	3:A:1038:ARG:HG3	1.97	0.46
3:A:269:THR:HG22	3:A:270:GLU:N	2.29	0.46
3:A:445:MET:HE2	3:A:445:MET:HB3	1.74	0.46
3:D:246:LEU:O	3:D:249:THR:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:244:THR:C	3:A:246:LEU:H	2.24	0.46
3:A:297:MET:O	3:A:299:PRO:HD3	2.16	0.46
3:A:306:LEU:C	3:A:308:TYR:N	2.73	0.46
3:A:724:LEU:HD12	3:A:751:VAL:HB	1.97	0.46
3:A:813:GLY:HA2	3:A:816:THR:OG1	2.16	0.46
3:A:964:PRO:HB2	3:A:968:VAL:CG1	2.46	0.46
3:A:1029:ASP:O	3:A:1030:THR:C	2.58	0.46
3:D:90:ARG:O	3:D:91:TRP:C	2.59	0.46
3:D:347:LEU:HD23	3:D:347:LEU:C	2.41	0.46
3:D:894:LEU:HA	3:D:894:LEU:HD23	1.48	0.46
2:C:15:LEU:CD2	2:C:23:LYS:HG2	2.45	0.46
2:C:156:ASN:ND2	2:C:159:LYS:HE3	2.31	0.46
3:A:25:ILE:H	3:A:25:ILE:CD1	2.25	0.46
3:A:87:ILE:HG23	3:A:91:TRP:CE3	2.50	0.46
3:A:229:LEU:O	3:A:233:LEU:HG	2.15	0.46
3:A:255:LEU:C	3:A:257:VAL:H	2.23	0.46
3:A:718:LEU:HA	3:A:718:LEU:HD23	1.48	0.46
3:A:819:ILE:N	3:A:820:PRO:CD	2.79	0.46
3:A:914:PHE:CE1	3:A:918:TYR:CD1	3.04	0.46
3:D:87:ILE:HG23	3:D:91:TRP:CE3	2.51	0.46
3:D:467:LEU:O	3:D:468:ASP:HB2	2.16	0.46
3:D:816:THR:HG23	3:D:859:CYS:CB	2.46	0.46
3:D:1008:ILE:C	3:D:1008:ILE:CD1	2.86	0.46
2:C:153:SER:HB2	3:A:431:LEU:HD21	1.98	0.46
3:A:144:LYS:C	3:A:145:HIS:CD2	2.94	0.46
3:A:167:ASN:HA	3:A:170:ILE:HG13	1.98	0.46
3:A:676:VAL:HG13	3:A:679:LEU:HD12	1.97	0.46
1:E:13:ILE:HG22	3:D:537:LYS:CB	2.45	0.46
3:D:56:HIS:HB3	3:D:82:ILE:CG2	2.45	0.46
3:D:144:LYS:HB2	3:D:145:HIS:CD2	2.50	0.46
3:D:552:PRO:O	3:D:553:ARG:C	2.58	0.46
3:D:841:TYR:O	3:D:842:PRO:C	2.56	0.46
3:D:879:ILE:HD12	3:D:879:ILE:H	1.81	0.46
2:C:73:GLY:HA3	2:C:76:ARG:NH2	2.31	0.46
3:A:142:TRP:N	3:A:143:PRO:HD2	2.31	0.46
3:A:402:ILE:H	3:A:402:ILE:HG12	1.48	0.46
3:A:804:MET:HE2	3:A:822:ILE:HD13	1.97	0.46
3:A:1007:ASP:OD1	3:A:1010:ALA:HB2	2.16	0.46
1:E:238:PRO:HA	1:E:241:LEU:HD12	1.96	0.46
3:D:268:LEU:HD23	3:D:268:LEU:HA	1.79	0.46
3:D:378:ALA:HA	3:D:463:TYR:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:887:ARG:O	3:D:891:ASP:HB2	2.16	0.46
3:D:973:PHE:O	3:D:973:PHE:HD1	1.99	0.46
3:A:109:LEU:O	3:A:112:LYS:HG3	2.16	0.46
3:A:138:LEU:C	3:A:140:GLN:N	2.74	0.46
3:A:258:PRO:O	3:A:261:ARG:HB3	2.16	0.46
1:E:247:MET:HB2	1:E:249:PHE:CE1	2.51	0.46
2:F:146:TYR:CD2	2:F:147:TYR:N	2.84	0.46
3:D:39:GLU:CD	3:D:39:GLU:C	2.83	0.46
3:D:223:HIS:HD2	3:D:223:HIS:O	1.99	0.46
1:B:93:LEU:HA	1:B:94:PRO:HD3	1.74	0.45
1:B:280:MET:O	1:B:283:ASP:HB2	2.14	0.45
2:C:42:THR:OG1	4:C:217:GTP:PG	2.74	0.45
2:C:45:VAL:CG2	2:C:46:GLU:H	2.29	0.45
3:A:282:GLN:OE1	3:A:282:GLN:N	2.48	0.45
3:A:704:HIS:HD2	3:A:766:SER:HA	1.80	0.45
2:F:45:VAL:CG2	2:F:46:GLU:N	2.78	0.45
2:F:86:ALA:C	2:F:87:ILE:HG13	2.41	0.45
3:D:480:LEU:HB2	3:D:497:LEU:HD21	1.98	0.45
3:D:801:LEU:HD11	3:D:830:THR:HG21	1.97	0.45
3:D:847:ASN:C	3:D:849:PHE:N	2.75	0.45
3:D:950:PHE:O	3:D:953:VAL:HB	2.16	0.45
1:B:60:HIS:HE1	1:B:100:GLN:HE22	1.63	0.45
1:B:107:LEU:HB2	1:B:274:GLY:CA	2.44	0.45
3:A:107:VAL:O	3:A:111:ILE:CG1	2.50	0.45
3:A:150:ILE:HG23	3:A:151:SER:N	2.28	0.45
3:A:467:LEU:O	3:A:468:ASP:HB2	2.16	0.45
1:E:277:ARG:HH22	3:D:620:THR:HG21	1.80	0.45
2:F:139:HIS:N	2:F:139:HIS:ND1	2.64	0.45
3:D:55:GLU:HB3	3:D:57:PRO:HD3	1.98	0.45
3:D:195:LYS:O	3:D:197:SER:N	2.49	0.45
3:D:675:ASN:ND2	3:D:677:ASP:HB2	2.31	0.45
3:D:906:GLN:N	3:D:906:GLN:CD	2.72	0.45
3:D:964:PRO:HG2	3:D:968:VAL:CB	2.46	0.45
1:B:154:LEU:HD13	1:B:215:GLU:CG	2.46	0.45
3:A:102:ILE:O	3:A:105:TYR:N	2.49	0.45
3:A:164:CYS:O	3:A:165:GLN:C	2.59	0.45
3:A:583:MET:SD	3:A:583:MET:C	3.00	0.45
2:F:71:LYS:HE2	3:D:932:ASP:OD1	2.17	0.45
3:D:329:PHE:CE1	3:D:333:HIS:CD2	3.05	0.45
3:D:378:ALA:HB1	3:D:382:ARG:HH12	1.80	0.45
3:D:839:GLU:O	3:D:840:GLU:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1008:ILE:HG13	3:D:1009:PRO:HD3	1.97	0.45
3:D:1022:ILE:HG13	3:D:1023:LYS:N	2.31	0.45
1:B:48:GLU:C	1:B:50:GLN:N	2.73	0.45
3:A:344:ARG:NE	3:A:408:LEU:HD21	2.32	0.45
3:A:930:VAL:HG11	3:A:1015:LEU:HD22	1.97	0.45
3:A:1003:SER:O	3:A:1005:ASN:N	2.50	0.45
1:E:348:HIS:NE2	3:D:708:ILE:O	2.49	0.45
2:F:145:GLN:HE21	2:F:163:TRP:CD1	2.35	0.45
2:F:153:SER:HB2	3:D:431:LEU:HD21	1.99	0.45
3:D:113:THR:HG22	3:D:119:CYS:SG	2.57	0.45
3:D:647:GLN:O	3:D:651:GLU:HG3	2.16	0.45
3:D:715:LEU:O	3:D:718:LEU:HB2	2.17	0.45
3:D:746:ARG:HG2	3:D:746:ARG:NH1	2.15	0.45
3:D:785:LEU:HD11	3:D:804:MET:HG2	1.97	0.45
3:D:819:ILE:N	3:D:820:PRO:CD	2.80	0.45
3:D:973:PHE:CD1	3:D:973:PHE:C	2.92	0.45
1:B:240:SER:C	1:B:242:CYS:N	2.75	0.45
1:B:241:LEU:C	1:B:244:VAL:HG12	2.42	0.45
3:A:103:LYS:O	3:A:107:VAL:HG23	2.15	0.45
3:A:130:LEU:O	3:A:131:ASN:C	2.59	0.45
3:A:946:LEU:HA	3:A:946:LEU:HD12	1.61	0.45
3:A:966:ASN:N	3:A:967:PRO:CD	2.80	0.45
1:E:152:SER:O	1:E:225:PRO:HD2	2.16	0.45
1:E:235:PRO:O	1:E:240:SER:OG	2.32	0.45
2:F:84:GLN:O	2:F:168:LEU:HD21	2.17	0.45
3:D:172:LYS:O	3:D:175:SER:HB3	2.16	0.45
3:D:268:LEU:O	3:D:269:THR:C	2.59	0.45
1:B:245:LEU:HA	1:B:245:LEU:HD12	1.55	0.45
1:B:281:VAL:HG13	1:B:282:SER:N	2.30	0.45
2:C:13:LEU:HD12	2:C:14:VAL:C	2.42	0.45
3:A:122:LYS:HD2	3:A:122:LYS:HA	1.59	0.45
3:A:378:ALA:HA	3:A:463:TYR:CE2	2.52	0.45
3:A:406:ARG:NH2	3:A:467:LEU:O	2.50	0.45
3:A:458:ARG:O	3:A:462:VAL:HG23	2.16	0.45
3:A:632:THR:N	3:A:697:ARG:HH22	2.15	0.45
3:A:691:ILE:CG2	3:A:692:LEU:N	2.79	0.45
3:A:847:ASN:O	3:A:849:PHE:N	2.50	0.45
2:F:31:LEU:O	2:F:32:THR:HG22	2.15	0.45
2:F:106:ARG:O	2:F:110:ARG:HG3	2.15	0.45
3:D:164:CYS:O	3:D:165:GLN:C	2.59	0.45
1:B:54:ARG:H	1:B:55:LEU:HD12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:118:THR:HG22	3:A:121:GLU:HG3	1.99	0.45
3:A:563:LYS:HE2	3:A:606:GLU:OE2	2.16	0.45
3:A:837:ASP:O	3:A:845:ARG:NH2	2.49	0.45
1:E:1:LEU:O	1:E:4:LEU:CD1	2.64	0.45
3:D:634:TYR:O	3:D:657:TYR:OH	2.30	0.45
3:D:837:ASP:O	3:D:845:ARG:NH2	2.49	0.45
1:B:107:LEU:O	1:B:276:LEU:HD11	2.17	0.45
3:A:372:TYR:O	3:A:375:HIS:N	2.50	0.45
3:A:729:SER:O	3:A:730:ALA:C	2.59	0.45
3:A:950:PHE:O	3:A:953:VAL:HB	2.16	0.45
3:D:509:HIS:HB2	3:D:512:ASP:OD2	2.17	0.45
3:D:736:GLY:O	3:D:737:GLU:C	2.60	0.45
3:D:918:TYR:O	3:D:922:ILE:HG13	2.17	0.45
3:D:988:HIS:CD2	3:D:988:HIS:N	2.84	0.45
1:B:284:VAL:O	1:B:284:VAL:HG12	2.17	0.45
3:A:60:TRP:CD1	3:A:60:TRP:N	2.76	0.45
3:A:250:LEU:HA	3:A:250:LEU:HD23	1.71	0.45
3:A:300:LEU:HB3	3:A:352:HIS:CE1	2.52	0.45
3:A:396:GLY:O	3:A:397:SER:O	2.34	0.45
3:A:448:THR:O	3:A:449:ASP:C	2.60	0.45
3:A:628:GLN:O	3:A:631:HIS:HB2	2.17	0.45
1:E:37:LEU:HB2	1:E:39:GLN:CD	2.42	0.45
3:D:269:THR:HG22	3:D:270:GLU:N	2.30	0.45
3:D:304:ILE:HG12	3:D:356:LEU:HB3	1.99	0.45
3:D:351:LEU:HA	3:D:351:LEU:HD23	1.47	0.45
3:D:551:TYR:O	3:D:554:PHE:HB3	2.17	0.45
3:D:914:PHE:CD1	3:D:918:TYR:HD1	2.34	0.45
1:B:69:TRP:CE3	1:B:95:LYS:HD3	2.52	0.45
1:B:111:PRO:CD	1:B:114:LEU:HD13	2.45	0.45
3:A:27:LEU:HA	3:A:30:ASN:OD1	2.16	0.45
3:A:223:HIS:HD2	3:A:223:HIS:O	2.00	0.45
3:A:268:LEU:HD23	3:A:268:LEU:HA	1.80	0.45
3:A:303:ASN:C	3:A:303:ASN:OD1	2.59	0.45
3:A:729:SER:OG	3:A:792:VAL:HG13	2.17	0.45
3:A:1032:ASP:OD1	3:A:1032:ASP:N	2.49	0.45
1:E:200:THR:O	1:E:201:ASP:C	2.60	0.45
2:F:138:PHE:O	2:F:139:HIS:C	2.60	0.45
3:D:66:ILE:HD13	3:D:66:ILE:H	1.82	0.45
3:D:116:ASP:HB2	3:D:119:CYS:CB	2.45	0.45
3:D:186:ILE:HG22	3:D:187:THR:O	2.17	0.45
3:D:930:VAL:HG11	3:D:1015:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:952:LEU:O	3:D:952:LEU:HD23	2.17	0.45
3:A:18:ASP:CG	3:A:19:PHE:N	2.75	0.44
3:A:697:ARG:O	3:A:698:ALA:C	2.59	0.44
1:E:152:SER:O	1:E:225:PRO:HD3	2.16	0.44
2:F:26:PHE:CZ	2:F:30:HIS:CE1	3.05	0.44
2:F:108:LEU:CD1	2:F:112:CYS:SG	3.05	0.44
3:D:60:TRP:CD1	3:D:60:TRP:N	2.76	0.44
3:D:658:MET:HE2	3:D:695:ASN:HD21	1.82	0.44
3:D:898:PHE:HD2	3:D:945:ILE:HG12	1.83	0.44
3:D:1014:HIS:O	3:D:1015:LEU:C	2.59	0.44
1:B:41:GLU:CG	1:B:109:ASP:HB3	2.36	0.44
1:B:357:MET:HE1	3:A:676:VAL:HG11	1.99	0.44
2:C:45:VAL:CG2	2:C:46:GLU:N	2.80	0.44
3:A:72:ASN:O	3:A:73:MET:C	2.60	0.44
3:A:304:ILE:HG12	3:A:356:LEU:HB3	1.99	0.44
3:A:332:GLU:HG3	3:A:332:GLU:O	2.17	0.44
3:A:423:ARG:C	3:A:457:MET:HE1	2.42	0.44
3:A:515:ARG:CG	3:A:515:ARG:NH1	2.79	0.44
3:A:643:ALA:O	3:A:644:GLN:C	2.59	0.44
3:A:643:ALA:O	3:A:645:THR:HG23	2.17	0.44
3:A:660:LEU:O	3:A:661:PRO:C	2.57	0.44
3:A:824:ASP:O	3:A:825:ALA:C	2.60	0.44
3:A:834:ILE:HG21	3:A:845:ARG:HA	1.99	0.44
3:A:1007:ASP:O	3:A:1010:ALA:HB3	2.18	0.44
2:F:45:VAL:CG2	2:F:46:GLU:H	2.30	0.44
2:F:94:SER:HB3	2:F:97:THR:CG2	2.47	0.44
3:D:190:LYS:O	3:D:194:LEU:HD13	2.16	0.44
3:D:337:LEU:CD2	3:D:343:LEU:HB3	2.46	0.44
3:D:503:SER:O	3:D:505:SER:N	2.49	0.44
3:D:608:MET:HE3	3:D:609:PRO:CD	2.43	0.44
3:D:721:TYR:CE2	3:D:784:VAL:HG22	2.52	0.44
2:C:85:CYS:HB2	2:C:164:LEU:HD22	1.99	0.44
2:C:132:LYS:C	2:C:134:LYS:N	2.74	0.44
2:C:139:HIS:O	2:C:140:ARG:C	2.58	0.44
3:A:102:ILE:H	3:A:102:ILE:HG13	1.55	0.44
3:A:340:ARG:C	3:A:342:ASN:H	2.25	0.44
3:A:855:VAL:O	3:A:859:CYS:HB2	2.17	0.44
1:E:260:HIS:O	1:E:262:GLN:N	2.50	0.44
3:D:76:LYS:O	3:D:77:TYR:C	2.60	0.44
3:D:129:LYS:O	3:D:132:MET:HB3	2.16	0.44
3:D:680:LYS:HB3	3:D:680:LYS:HE2	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:ASP:HB2	1:B:188:MET:CE	2.39	0.44
1:B:211:LEU:N	1:B:212:PRO:CD	2.80	0.44
3:A:149:PHE:O	3:A:150:ILE:C	2.58	0.44
3:A:417:ARG:O	3:A:418:LEU:C	2.60	0.44
3:A:539:ILE:HG22	3:A:540:ILE:N	2.33	0.44
3:A:736:GLY:O	3:A:738:MET:N	2.51	0.44
3:A:871:PHE:O	3:A:872:LYS:C	2.57	0.44
3:A:915:TYR:HA	3:A:919:PHE:HB2	1.98	0.44
1:E:4:LEU:HD22	3:D:521:ILE:CD1	2.46	0.44
3:D:50:LEU:C	3:D:52:HIS:N	2.75	0.44
3:D:72:ASN:O	3:D:75:THR:N	2.50	0.44
3:D:78:TYR:CE2	3:D:82:ILE:HD11	2.52	0.44
3:D:103:LYS:O	3:D:107:VAL:HG23	2.16	0.44
3:D:223:HIS:NE2	3:D:263:VAL:HG21	2.32	0.44
3:D:255:LEU:HD12	3:D:268:LEU:CD1	2.47	0.44
3:D:592:ALA:O	3:D:596:ARG:HB3	2.17	0.44
3:D:656:LYS:O	3:D:656:LYS:HG2	2.16	0.44
2:C:122:ASN:O	2:C:123:LYS:CB	2.60	0.44
3:A:157:SER:HB3	3:A:164:CYS:CB	2.47	0.44
3:A:329:PHE:CD1	3:A:333:HIS:HD2	2.35	0.44
2:F:13:LEU:HD12	2:F:14:VAL:C	2.43	0.44
3:D:106:VAL:O	3:D:107:VAL:C	2.60	0.44
3:D:291:MET:O	3:D:292:MET:C	2.60	0.44
3:D:831:LEU:HD12	3:D:834:ILE:HD11	1.99	0.44
3:D:879:ILE:HA	3:D:882:PHE:CE2	2.52	0.44
2:C:88:ILE:HD13	2:C:88:ILE:N	2.33	0.44
3:A:179:PHE:CE2	3:A:235:TRP:CD2	3.05	0.44
3:A:654:ILE:O	3:A:654:ILE:CG2	2.64	0.44
3:A:735:ASN:HB2	3:A:739:VAL:CG2	2.48	0.44
3:A:870:GLN:O	3:A:873:LEU:HB3	2.18	0.44
1:E:281:VAL:C	1:E:283:ASP:H	2.26	0.44
2:F:31:LEU:C	2:F:32:THR:CG2	2.90	0.44
2:F:50:LEU:O	2:F:60:LYS:HA	2.17	0.44
3:D:55:GLU:CG	3:D:56:HIS:H	2.31	0.44
3:D:199:CYS:O	3:D:200:ASN:C	2.61	0.44
3:D:389:SER:C	3:D:391:SER:N	2.75	0.44
3:D:678:ILE:C	3:D:680:LYS:N	2.75	0.44
3:D:887:ARG:HD2	3:D:887:ARG:HA	1.76	0.44
3:D:912:GLN:H	3:D:912:GLN:HG2	1.57	0.44
3:A:98:GLN:O	3:A:102:ILE:HG13	2.18	0.44
3:A:279:TYR:O	3:A:283:PHE:HD2	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:426:LYS:HG3	3:A:499:TRP:CH2	2.53	0.44
3:A:485:ASN:C	3:A:487:THR:H	2.25	0.44
3:A:659:LEU:HD23	3:A:659:LEU:HA	1.77	0.44
3:A:704:HIS:C	3:A:706:PHE:H	2.25	0.44
3:A:800:VAL:O	3:A:801:LEU:C	2.61	0.44
3:A:963:ASN:N	3:A:964:PRO:CD	2.80	0.44
1:E:1:LEU:HD22	3:D:558:HIS:CD2	2.45	0.44
2:F:92:VAL:CG2	2:F:129:ARG:HG3	2.47	0.44
3:D:210:GLN:O	3:D:211:PHE:C	2.58	0.44
3:D:465:THR:O	3:D:469:TYR:HB3	2.18	0.44
3:D:515:ARG:CG	3:D:515:ARG:NH1	2.79	0.44
3:D:672:ALA:CB	3:D:678:ILE:HD11	2.38	0.44
1:B:39:GLN:O	1:B:40:SER:C	2.61	0.44
1:B:200:THR:OG1	1:B:263:THR:HG23	2.17	0.44
2:C:139:HIS:N	2:C:139:HIS:ND1	2.66	0.44
3:A:786:ILE:O	3:A:789:GLN:HB3	2.17	0.44
3:A:801:LEU:HD11	3:A:830:THR:HG21	1.99	0.44
3:A:894:LEU:HB3	3:A:941:MET:HE2	2.00	0.44
1:E:211:LEU:N	1:E:212:PRO:CD	2.81	0.44
3:D:172:LYS:O	3:D:176:GLU:HG3	2.18	0.44
3:D:824:ASP:O	3:D:825:ALA:C	2.61	0.44
3:A:32:VAL:O	3:A:36:TYR:HB2	2.17	0.44
3:A:88:LYS:HE2	3:A:136:GLN:NE2	2.33	0.44
3:A:721:TYR:CE2	3:A:784:VAL:HG22	2.53	0.44
3:A:879:ILE:HD12	3:A:879:ILE:N	2.33	0.44
1:E:114:LEU:HD12	1:E:118:TRP:CD1	2.53	0.44
3:D:137:ILE:O	3:D:140:GLN:HB2	2.18	0.44
3:D:291:MET:HE3	3:D:291:MET:HB3	1.70	0.44
3:D:643:ALA:O	3:D:645:THR:HG23	2.18	0.44
3:D:804:MET:HE2	3:D:822:ILE:HD13	2.00	0.44
3:D:920:CYS:HB3	3:D:977:TYR:HE2	1.81	0.44
1:B:1:LEU:HD22	3:A:514:LYS:HE3	2.00	0.43
1:B:188:MET:HE3	1:B:265:TYR:CE1	2.53	0.43
3:A:622:ILE:HD13	3:A:630:VAL:HG23	2.00	0.43
3:A:735:ASN:HB2	3:A:739:VAL:HG22	1.99	0.43
3:A:748:MET:O	3:A:749:ARG:C	2.61	0.43
1:E:56:ASP:CG	1:E:59:ASN:HB2	2.43	0.43
1:E:103:LEU:HD21	1:E:143:LYS:HD3	2.00	0.43
1:E:149:ASN:HD22	1:E:150:ARG:H	1.66	0.43
3:D:672:ALA:HA	3:D:675:ASN:O	2.17	0.43
1:B:102:MET:HE3	1:B:273:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:504:ILE:HD12	3:A:504:ILE:O	2.19	0.43
3:A:516:PHE:O	3:A:519:THR:HB	2.18	0.43
3:A:678:ILE:C	3:A:680:LYS:N	2.75	0.43
3:A:962:LEU:HA	3:A:973:PHE:HE2	1.84	0.43
1:E:236:CYS:HA	1:E:241:LEU:HD21	2.00	0.43
3:D:150:ILE:CG2	3:D:201:GLU:CD	2.89	0.43
3:D:255:LEU:C	3:D:257:VAL:H	2.26	0.43
3:D:424:MET:HE3	3:D:454:TYR:CD1	2.53	0.43
1:B:63:ARG:NH1	1:B:70:THR:N	2.66	0.43
2:C:23:LYS:HE3	4:C:217:GTP:O1B	2.18	0.43
3:A:44:ARG:HD3	3:A:44:ARG:HA	1.81	0.43
3:A:379:GLU:OE2	3:A:382:ARG:NH2	2.37	0.43
3:A:592:ALA:O	3:A:596:ARG:HB3	2.18	0.43
3:A:768:ASP:OD1	3:A:768:ASP:C	2.61	0.43
1:E:13:ILE:HG22	3:D:537:LYS:HB3	2.00	0.43
1:E:124:PRO:HB3	1:E:251:PHE:CD2	2.53	0.43
1:E:146:TYR:CE1	1:E:147:CYS:O	2.72	0.43
1:E:202:PHE:O	1:E:205:TYR:N	2.51	0.43
2:F:29:ARG:HB3	2:F:157:PHE:CZ	2.53	0.43
3:D:303:ASN:OD1	3:D:303:ASN:C	2.60	0.43
3:D:450:SER:O	3:D:453:LEU:N	2.51	0.43
3:D:760:SER:O	3:D:761:GLY:C	2.60	0.43
3:A:58:ASP:O	3:A:59:ALA:C	2.61	0.43
3:A:134:LEU:O	3:A:134:LEU:HD12	2.18	0.43
3:A:229:LEU:O	3:A:229:LEU:HD22	2.17	0.43
3:A:267:CYS:O	3:A:268:LEU:C	2.61	0.43
3:A:822:ILE:O	3:A:824:ASP:N	2.51	0.43
3:D:17:LEU:HD23	3:D:22:LYS:HZ1	1.80	0.43
3:D:25:ILE:H	3:D:25:ILE:CD1	2.27	0.43
3:D:559:TRP:CH2	3:D:610:PHE:HB2	2.53	0.43
1:B:175:TYR:HB2	1:B:182:TYR:CD1	2.53	0.43
1:B:278:PRO:O	1:B:281:VAL:HG12	2.18	0.43
2:C:53:HIS:HB2	2:C:179:MET:O	2.18	0.43
2:C:171:ASP:OD1	2:C:174:LEU:N	2.52	0.43
3:A:22:LYS:HD2	3:A:22:LYS:HA	1.64	0.43
3:A:62:ARG:HH12	3:A:82:ILE:HD13	1.84	0.43
3:A:503:SER:O	3:A:505:SER:N	2.50	0.43
3:A:816:THR:HG23	3:A:859:CYS:CB	2.48	0.43
3:A:1007:ASP:OD2	3:A:1009:PRO:HD2	2.18	0.43
2:F:119:LEU:HD23	2:F:146:TYR:HD1	1.84	0.43
3:D:217:GLN:H	3:D:217:GLN:HG3	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:384:SER:CB	3:D:403:PRO:HG2	2.48	0.43
3:D:516:PHE:O	3:D:519:THR:HB	2.19	0.43
3:D:946:LEU:HA	3:D:946:LEU:HD12	1.57	0.43
1:B:98:ALA:CB	1:B:145:GLY:H	2.32	0.43
2:C:123:LYS:C	2:C:125:ASP:N	2.77	0.43
3:A:141:GLU:O	3:A:142:TRP:C	2.61	0.43
3:A:142:TRP:HZ3	3:A:197:SER:HB3	1.83	0.43
3:A:516:PHE:CE1	3:A:520:VAL:CG2	3.00	0.43
3:A:887:ARG:CD	3:A:937:ALA:HB3	2.35	0.43
3:A:954:GLU:O	3:A:955:GLU:HG3	2.19	0.43
1:E:158:GLY:O	1:E:159:ASN:HB3	2.18	0.43
3:D:141:GLU:O	3:D:142:TRP:C	2.61	0.43
3:D:150:ILE:HG23	3:D:151:SER:N	2.30	0.43
3:D:247:ILE:H	3:D:247:ILE:HG13	1.63	0.43
3:D:516:PHE:CE1	3:D:520:VAL:CG2	3.01	0.43
3:D:635:GLU:OE1	3:D:697:ARG:HD2	2.19	0.43
3:D:739:VAL:C	3:D:741:LYS:H	2.25	0.43
3:D:778:PRO:O	3:D:781:LEU:HB2	2.19	0.43
3:D:800:VAL:O	3:D:801:LEU:C	2.61	0.43
3:D:970:ASN:N	3:D:970:ASN:ND2	2.58	0.43
3:D:1029:ASP:O	3:D:1030:THR:C	2.60	0.43
3:A:203:SER:C	3:A:205:ILE:H	2.27	0.43
3:A:424:MET:HE3	3:A:454:TYR:CD1	2.53	0.43
3:A:879:ILE:HA	3:A:882:PHE:CE2	2.53	0.43
3:A:904:VAL:CG1	3:A:911:ALA:HA	2.49	0.43
3:A:926:ILE:HG21	3:A:946:LEU:HD13	2.01	0.43
1:E:138:THR:HG22	1:E:151:PHE:CZ	2.53	0.43
2:F:134:LYS:HG3	2:F:135:SER:N	2.34	0.43
3:D:168:MET:CE	3:D:171:LEU:HD12	2.49	0.43
3:D:997:PHE:CD1	3:D:1014:HIS:CE1	3.01	0.43
2:C:23:LYS:O	2:C:27:VAL:HG13	2.19	0.43
3:A:287:PHE:HB2	3:A:329:PHE:CE2	2.54	0.43
3:A:822:ILE:C	3:A:824:ASP:N	2.77	0.43
3:A:899:THR:HG23	3:A:903:ASN:HD21	1.81	0.43
1:E:241:LEU:C	1:E:244:VAL:HG12	2.44	0.43
3:D:30:ASN:CB	3:D:47:GLN:NE2	2.79	0.43
3:D:777:VAL:O	3:D:780:LEU:HB2	2.18	0.43
3:D:823:PHE:O	3:D:827:PHE:HB3	2.18	0.43
3:D:831:LEU:HD13	3:D:848:PHE:CZ	2.54	0.43
3:D:935:HIS:N	3:D:935:HIS:ND1	2.67	0.43
1:B:34:TYR:HB3	1:B:35:SER:H	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:LEU:HD13	1:B:57:TYR:HE2	1.76	0.43
1:B:103:LEU:CD1	1:B:268:GLY:HA2	2.49	0.43
1:B:173:CYS:SG	1:B:184:VAL:HG22	2.59	0.43
1:B:238:PRO:HA	1:B:241:LEU:HD12	1.99	0.43
1:B:350:PRO:HB2	1:B:351:ASP:H	1.61	0.43
3:A:30:ASN:CB	3:A:47:GLN:NE2	2.80	0.43
3:A:186:ILE:HG22	3:A:187:THR:O	2.19	0.43
3:A:778:PRO:N	3:A:779:PRO:CD	2.82	0.43
3:A:802:SER:O	3:A:806:ILE:HG13	2.18	0.43
3:A:839:GLU:O	3:A:840:GLU:C	2.61	0.43
3:A:962:LEU:HD13	3:A:968:VAL:CB	2.48	0.43
1:E:39:GLN:O	1:E:40:SER:C	2.61	0.43
1:E:278:PRO:O	1:E:281:VAL:HG12	2.18	0.43
2:F:47:VAL:HG11	2:F:64:TRP:CE2	2.54	0.43
3:D:55:GLU:HG2	3:D:56:HIS:H	1.84	0.43
3:D:100:GLU:O	3:D:103:LYS:HB3	2.19	0.43
3:D:612:ASP:O	3:D:613:GLU:C	2.61	0.43
3:D:625:LEU:HB3	3:D:629:GLN:HB2	2.01	0.43
3:D:748:MET:O	3:D:749:ARG:C	2.62	0.43
1:B:195:PHE:HA	1:B:198:CYS:SG	2.59	0.43
1:B:240:SER:O	1:B:242:CYS:N	2.52	0.43
3:A:137:ILE:O	3:A:140:GLN:HB2	2.19	0.43
3:A:144:LYS:C	3:A:145:HIS:HD2	2.27	0.43
3:A:238:LEU:CD2	3:A:242:PHE:HE2	2.27	0.43
3:A:420:MET:O	3:A:424:MET:HB2	2.19	0.43
3:A:823:PHE:HD1	3:A:823:PHE:HA	1.72	0.43
3:A:1008:ILE:C	3:A:1008:ILE:CD1	2.89	0.43
3:D:704:HIS:C	3:D:706:PHE:H	2.26	0.43
1:B:7:LYS:HD2	3:A:522:LYS:CG	2.49	0.42
2:C:64:TRP:HE3	2:C:79:TYR:HB3	1.82	0.42
3:A:443:GLU:OE1	3:A:443:GLU:HA	2.19	0.42
3:A:906:GLN:N	3:A:906:GLN:CD	2.75	0.42
3:A:964:PRO:HB2	3:A:968:VAL:HG11	2.00	0.42
1:E:155:LEU:HG	1:E:217:LEU:HD11	2.01	0.42
2:F:156:ASN:HB3	2:F:159:LYS:CG	2.48	0.42
3:D:1007:ASP:OD1	3:D:1010:ALA:HB2	2.19	0.42
1:B:69:TRP:CD2	1:B:95:LYS:O	2.73	0.42
3:A:27:LEU:HD23	3:A:75:THR:HG23	2.01	0.42
3:A:66:ILE:HG22	3:A:76:LYS:NZ	2.33	0.42
3:A:323:SER:O	3:A:327:CYS:HB3	2.19	0.42
3:A:365:ILE:HG22	3:A:366:PHE:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:637:VAL:HG12	3:A:641:ILE:CD1	2.49	0.42
1:E:1:LEU:HD21	1:E:2:ASN:ND2	2.35	0.42
3:D:203:SER:C	3:D:205:ILE:H	2.27	0.42
3:D:244:THR:C	3:D:246:LEU:H	2.27	0.42
3:D:338:GLU:C	3:D:340:ARG:H	2.27	0.42
3:D:443:GLU:OE1	3:D:443:GLU:HA	2.19	0.42
3:D:525:LEU:HD12	3:D:525:LEU:HA	1.82	0.42
3:D:563:LYS:HE2	3:D:606:GLU:OE2	2.18	0.42
3:D:575:GLU:O	3:D:581:GLN:HG3	2.19	0.42
2:C:26:PHE:CE1	2:C:30:HIS:CE1	3.07	0.42
3:A:195:LYS:O	3:A:197:SER:N	2.53	0.42
3:A:259:MET:C	3:A:261:ARG:N	2.72	0.42
3:A:391:SER:C	3:A:392:PRO:O	2.61	0.42
3:A:611:ILE:O	3:A:612:ASP:C	2.62	0.42
3:A:715:LEU:O	3:A:718:LEU:HB2	2.19	0.42
3:A:887:ARG:O	3:A:891:ASP:HB2	2.19	0.42
3:D:218:ASN:OD1	3:D:218:ASN:C	2.63	0.42
3:D:222:VAL:HG11	3:D:254:PHE:HE1	1.84	0.42
3:D:559:TRP:CD1	3:D:559:TRP:C	2.92	0.42
3:D:822:ILE:C	3:D:824:ASP:N	2.76	0.42
2:C:35:PHE:CE2	2:C:37:LYS:HG2	2.54	0.42
2:C:73:GLY:HA3	2:C:76:ARG:CZ	2.50	0.42
3:A:110:ILE:O	3:A:111:ILE:C	2.61	0.42
3:A:565:VAL:O	3:A:565:VAL:CG1	2.63	0.42
3:A:612:ASP:O	3:A:613:GLU:C	2.62	0.42
1:E:122:VAL:HG11	1:E:249:PHE:CZ	2.54	0.42
2:F:15:LEU:HD22	2:F:23:LYS:CB	2.49	0.42
3:D:27:LEU:HA	3:D:30:ASN:OD1	2.18	0.42
3:D:110:ILE:O	3:D:111:ILE:C	2.62	0.42
3:D:223:HIS:CD2	3:D:223:HIS:C	2.96	0.42
3:D:228:THR:O	3:D:232:PHE:CD2	2.72	0.42
3:D:265:LEU:HD11	3:D:325:PHE:HB2	2.02	0.42
3:D:470:VAL:O	3:D:474:ILE:HG13	2.18	0.42
3:D:720:VAL:O	3:D:721:TYR:C	2.61	0.42
3:D:914:PHE:CE1	3:D:918:TYR:CD1	3.07	0.42
1:B:63:ARG:NH1	1:B:70:THR:HB	2.24	0.42
2:C:21:THR:HG21	2:C:89:MET:HB3	2.01	0.42
2:C:84:GLN:O	2:C:168:LEU:HD21	2.19	0.42
3:A:27:LEU:C	3:A:29:ASP:H	2.26	0.42
3:A:35:LEU:C	3:A:36:TYR:HD1	2.27	0.42
3:A:55:GLU:CG	3:A:56:HIS:H	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:80:LEU:HD21	3:A:126:TYR:CE1	2.54	0.42
3:A:559:TRP:CD1	3:A:559:TRP:C	2.93	0.42
3:A:941:MET:O	3:A:942:HIS:C	2.62	0.42
1:E:107:LEU:O	1:E:276:LEU:HD11	2.20	0.42
1:E:245:LEU:HA	1:E:245:LEU:HD12	1.57	0.42
2:F:75:LEU:HD11	3:D:49:VAL:HG22	2.02	0.42
3:D:279:TYR:O	3:D:283:PHE:HD2	2.02	0.42
3:D:298:LEU:O	3:D:353:TYR:OH	2.28	0.42
3:D:422:SER:O	3:D:496:THR:HG21	2.20	0.42
3:D:611:ILE:HG23	3:D:612:ASP:N	2.32	0.42
3:D:704:HIS:CD2	3:D:766:SER:HA	2.55	0.42
3:D:724:LEU:HD12	3:D:751:VAL:HB	2.00	0.42
3:D:871:PHE:O	3:D:872:LYS:C	2.59	0.42
3:D:962:LEU:HD23	3:D:968:VAL:HG11	2.00	0.42
3:D:1007:ASP:O	3:D:1010:ALA:HB3	2.20	0.42
1:B:9:ALA:C	1:B:11:LEU:H	2.27	0.42
1:B:220:LYS:C	1:B:221:THR:CG2	2.92	0.42
2:C:177:VAL:HG22	2:C:178:ALA:N	2.35	0.42
3:A:80:LEU:HB3	3:A:133:ILE:HD11	2.00	0.42
3:A:127:ILE:O	3:A:130:LEU:HB2	2.20	0.42
3:A:199:CYS:O	3:A:200:ASN:C	2.62	0.42
3:A:222:VAL:HG11	3:A:254:PHE:HE1	1.85	0.42
3:A:272:ALA:HB1	3:A:329:PHE:CD1	2.55	0.42
3:A:433:VAL:O	3:A:433:VAL:CG1	2.66	0.42
3:A:785:LEU:HD11	3:A:804:MET:HG2	2.01	0.42
3:A:841:TYR:O	3:A:842:PRO:C	2.62	0.42
3:A:862:ALA:O	3:A:865:ALA:N	2.52	0.42
3:A:920:CYS:HB3	3:A:977:TYR:HE2	1.84	0.42
3:A:939:LEU:HD21	3:A:1016:ARG:HH11	1.83	0.42
2:F:47:VAL:O	2:F:47:VAL:HG23	2.18	0.42
3:D:430:VAL:O	3:D:430:VAL:HG13	2.20	0.42
3:D:500:ALA:O	3:D:503:SER:OG	2.32	0.42
3:D:637:VAL:HG12	3:D:641:ILE:CD1	2.50	0.42
3:D:1029:ASP:HB3	3:D:1030:THR:H	1.63	0.42
1:B:96:HIS:HB3	1:B:97:TYR:H	1.65	0.42
2:C:117:ILE:HG12	2:C:118:VAL:N	2.34	0.42
3:A:50:LEU:C	3:A:52:HIS:N	2.77	0.42
3:A:78:TYR:CE2	3:A:82:ILE:HD11	2.54	0.42
3:A:406:ARG:O	3:A:408:LEU:N	2.52	0.42
3:A:470:VAL:O	3:A:474:ILE:HG13	2.19	0.42
3:A:485:ASN:C	3:A:487:THR:N	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1038:ARG:HH21	3:A:1042:LEU:CD2	2.33	0.42
1:E:3:GLU:O	1:E:7:LYS:HB2	2.20	0.42
1:E:155:LEU:HD11	1:E:228:PHE:CZ	2.55	0.42
3:D:127:ILE:N	3:D:127:ILE:HD12	2.35	0.42
3:D:133:ILE:O	3:D:136:GLN:N	2.52	0.42
3:D:401:ASP:O	3:D:403:PRO:HD3	2.20	0.42
3:D:911:ALA:O	3:D:912:GLN:C	2.62	0.42
1:B:153:SER:N	1:B:158:GLY:O	2.44	0.42
2:C:38:LYS:HA	3:A:842:PRO:CG	2.50	0.42
2:C:155:TYR:CD1	3:A:445:MET:SD	3.12	0.42
3:A:94:LEU:HB2	3:A:99:CYS:SG	2.60	0.42
3:D:14:ARG:C	3:D:14:ARG:HD2	2.44	0.42
3:D:16:LEU:HB3	3:D:17:LEU:H	1.62	0.42
3:D:146:TRP:N	3:D:147:PRO:CD	2.82	0.42
3:D:472:THR:O	3:D:473:GLU:C	2.63	0.42
3:D:687:GLN:O	3:D:691:ILE:HB	2.20	0.42
1:B:241:LEU:HA	1:B:244:VAL:HG12	2.02	0.42
2:C:42:THR:H	4:C:217:GTP:PG	2.43	0.42
3:A:149:PHE:CZ	3:A:153:ILE:HD13	2.54	0.42
3:A:173:LEU:O	3:A:174:LEU:C	2.63	0.42
3:A:422:SER:O	3:A:496:THR:HG21	2.20	0.42
3:A:704:HIS:CD2	3:A:766:SER:HA	2.55	0.42
3:A:850:LEU:O	3:A:853:GLN:HB3	2.20	0.42
3:A:887:ARG:HD2	3:A:887:ARG:HA	1.79	0.42
1:E:18:ASN:ND2	1:E:108:ILE:HD11	2.35	0.42
1:E:58:VAL:HA	1:E:194:PRO:CG	2.50	0.42
1:E:93:LEU:HA	1:E:94:PRO:HD3	1.61	0.42
2:F:123:LYS:C	2:F:125:ASP:N	2.78	0.42
2:F:146:TYR:CG	2:F:147:TYR:N	2.87	0.42
3:D:98:GLN:O	3:D:102:ILE:HG13	2.19	0.42
3:D:681:ASP:HA	3:D:682:PRO:HD3	1.95	0.42
3:D:722:LYS:HD3	3:D:783:ALA:HA	2.02	0.42
3:D:953:VAL:O	3:D:955:GLU:N	2.53	0.42
3:D:990:GLN:C	3:D:992:ALA:N	2.76	0.42
1:B:43:ARG:O	1:B:44:ARG:C	2.62	0.42
1:B:60:HIS:CD2	1:B:93:LEU:HB3	2.55	0.42
1:B:101:LEU:N	1:B:101:LEU:HD23	2.34	0.42
2:C:100:ASN:O	2:C:101:VAL:C	2.63	0.42
3:A:409:TYR:O	3:A:410:LEU:C	2.63	0.42
3:A:503:SER:C	3:A:505:SER:H	2.28	0.42
3:A:531:LYS:HD3	3:A:531:LYS:HA	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:704:HIS:C	3:A:706:PHE:N	2.78	0.42
3:A:760:SER:O	3:A:761:GLY:C	2.62	0.42
3:A:777:VAL:O	3:A:780:LEU:HB2	2.20	0.42
3:A:939:LEU:HD12	3:A:939:LEU:HA	1.80	0.42
3:A:1032:ASP:O	3:A:1034:PHE:CE1	2.73	0.42
1:E:41:GLU:CG	1:E:109:ASP:HB3	2.38	0.42
1:E:48:GLU:H	1:E:48:GLU:HG2	1.55	0.42
1:E:122:VAL:O	1:E:122:VAL:HG12	2.19	0.42
2:F:13:LEU:HD12	2:F:14:VAL:O	2.18	0.42
3:D:40:GLY:C	3:D:42:GLN:N	2.78	0.42
3:D:208:LEU:C	3:D:208:LEU:CD2	2.92	0.42
3:D:617:ASN:O	3:D:618:ILE:C	2.62	0.42
3:D:695:ASN:HD22	3:D:695:ASN:HA	1.54	0.42
3:D:704:HIS:C	3:D:706:PHE:N	2.78	0.42
3:D:926:ILE:HG21	3:D:946:LEU:HD13	2.02	0.42
1:B:1:LEU:HD22	3:A:514:LYS:CE	2.50	0.41
1:B:8:LEU:HG	1:B:8:LEU:O	2.20	0.41
3:A:91:TRP:CZ3	3:A:102:ILE:HD13	2.55	0.41
3:A:298:LEU:O	3:A:353:TYR:OH	2.28	0.41
3:A:334:GLY:O	3:A:337:LEU:N	2.50	0.41
3:A:667:SER:C	3:A:669:ILE:N	2.77	0.41
1:E:10:GLY:HA3	1:E:34:TYR:CE1	2.55	0.41
1:E:111:PRO:CD	1:E:114:LEU:HD13	2.48	0.41
1:E:220:LYS:C	1:E:221:THR:HG23	2.45	0.41
3:D:729:SER:OG	3:D:792:VAL:HG13	2.20	0.41
3:D:732:ILE:HA	3:D:739:VAL:HG21	2.02	0.41
3:D:842:PRO:O	3:D:843:GLU:C	2.63	0.41
2:C:86:ALA:C	2:C:87:ILE:HG13	2.45	0.41
3:A:165:GLN:HA	3:A:221:LEU:HD13	2.01	0.41
3:A:208:LEU:C	3:A:208:LEU:CD2	2.92	0.41
3:A:255:LEU:HD12	3:A:268:LEU:HD12	2.02	0.41
3:A:262:ASN:OD1	3:A:318:PHE:HA	2.20	0.41
3:A:534:LYS:CE	3:A:577:HIS:HB2	2.48	0.41
3:A:575:GLU:O	3:A:581:GLN:HG3	2.20	0.41
3:A:608:MET:HA	3:A:609:PRO:HD3	1.62	0.41
3:A:695:ASN:HD22	3:A:695:ASN:HA	1.57	0.41
3:A:862:ALA:O	3:A:863:PHE:C	2.63	0.41
1:E:175:TYR:CD2	1:E:175:TYR:O	2.73	0.41
3:D:287:PHE:HB2	3:D:329:PHE:CE2	2.55	0.41
3:D:423:ARG:HG3	3:D:423:ARG:HH11	1.86	0.41
3:D:953:VAL:C	3:D:955:GLU:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:PRO:CG	1:B:114:LEU:HD13	2.51	0.41
1:B:260:HIS:O	1:B:262:GLN:N	2.53	0.41
2:C:167:LYS:HA	2:C:167:LYS:HD2	1.92	0.41
3:A:246:LEU:O	3:A:247:ILE:C	2.63	0.41
3:A:607:VAL:HG22	3:A:608:MET:HG2	2.02	0.41
3:A:1038:ARG:HH21	3:A:1042:LEU:HD21	1.83	0.41
2:F:98:TYR:CE1	2:F:136:ILE:HG23	2.54	0.41
3:D:80:LEU:HD21	3:D:126:TYR:CE1	2.55	0.41
3:D:329:PHE:CD1	3:D:333:HIS:HD2	2.37	0.41
3:D:330:LEU:HB2	3:D:372:TYR:CE1	2.55	0.41
3:D:771:MET:HE3	3:D:771:MET:HB3	1.62	0.41
3:D:952:LEU:HD23	3:D:952:LEU:C	2.45	0.41
3:D:964:PRO:HG2	3:D:968:VAL:CG1	2.50	0.41
3:D:974:ILE:C	3:D:976:ASP:N	2.79	0.41
3:A:133:ILE:O	3:A:136:GLN:N	2.53	0.41
3:A:291:MET:HE3	3:A:291:MET:HB3	1.74	0.41
3:A:962:LEU:HB2	3:A:973:PHE:HD2	1.85	0.41
1:E:244:VAL:HA	1:E:247:MET:HG3	2.02	0.41
2:F:132:LYS:O	2:F:134:LYS:N	2.53	0.41
3:D:24:ASP:C	3:D:26:ASN:N	2.78	0.41
3:D:91:TRP:CZ3	3:D:102:ILE:HD13	2.55	0.41
3:D:388:THR:HG21	3:D:402:ILE:HD13	2.02	0.41
3:D:813:GLY:HA2	3:D:816:THR:OG1	2.21	0.41
3:D:939:LEU:HD21	3:D:1016:ARG:HH11	1.84	0.41
3:D:954:GLU:O	3:D:955:GLU:HG3	2.20	0.41
1:B:103:LEU:HD21	1:B:143:LYS:HD3	2.03	0.41
1:B:176:ASN:OD1	1:B:179:ASN:N	2.54	0.41
1:B:244:VAL:HG13	1:B:245:LEU:CD1	2.40	0.41
1:B:244:VAL:HA	1:B:247:MET:HG3	2.03	0.41
2:C:77:ASP:HA	2:C:80:TYR:CE2	2.52	0.41
3:A:227:GLU:O	3:A:230:LEU:HB3	2.20	0.41
3:A:551:TYR:N	3:A:552:PRO:CD	2.83	0.41
3:A:742:GLN:HB2	3:A:743:PRO:HD2	2.03	0.41
3:A:753:ARG:C	3:A:755:THR:H	2.29	0.41
3:A:864:LEU:HD23	3:A:864:LEU:HA	1.81	0.41
3:A:990:GLN:C	3:A:992:ALA:N	2.77	0.41
1:E:119:ILE:HD13	1:E:119:ILE:H	1.85	0.41
2:F:141:LYS:HD2	2:F:141:LYS:H	1.86	0.41
3:D:72:ASN:O	3:D:73:MET:C	2.63	0.41
3:D:427:PRO:HD3	3:D:499:TRP:CD2	2.55	0.41
3:D:667:SER:O	3:D:671:GLN:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:695:ASN:HD21	3:D:709:GLN:HE21	1.67	0.41
3:D:729:SER:O	3:D:730:ALA:C	2.63	0.41
3:D:736:GLY:C	3:D:738:MET:H	2.27	0.41
2:C:13:LEU:HD12	2:C:13:LEU:O	2.20	0.41
2:C:141:LYS:HD2	2:C:141:LYS:H	1.85	0.41
3:A:24:ASP:C	3:A:26:ASN:N	2.78	0.41
3:A:374:ASN:HD22	3:A:374:ASN:C	2.28	0.41
3:A:430:VAL:O	3:A:430:VAL:HG13	2.20	0.41
3:A:626:GLN:HB2	3:A:627:PRO:HD2	2.02	0.41
3:A:721:TYR:CD2	3:A:784:VAL:HG22	2.56	0.41
1:E:98:ALA:CB	1:E:145:GLY:H	2.34	0.41
1:E:226:PHE:HZ	3:D:683:GLU:OE1	2.03	0.41
1:E:348:HIS:N	3:D:707:VAL:HG13	2.36	0.41
2:F:35:PHE:CE2	2:F:37:LYS:HG2	2.55	0.41
2:F:66:THR:HG22	2:F:67:ALA:H	1.84	0.41
3:D:622:ILE:HD13	3:D:630:VAL:HG23	2.03	0.41
2:C:71:LYS:HE2	3:A:932:ASP:OD1	2.20	0.41
3:A:594:LYS:HE2	3:A:594:LYS:CA	2.49	0.41
3:A:792:VAL:O	3:A:793:PRO:C	2.63	0.41
3:A:1015:LEU:HA	3:A:1015:LEU:HD23	1.82	0.41
3:A:1040:THR:HA	3:A:1043:ARG:CG	2.49	0.41
1:E:245:LEU:HD21	1:E:281:VAL:HG11	2.03	0.41
3:D:340:ARG:C	3:D:342:ASN:H	2.29	0.41
3:D:631:HIS:CE1	3:D:693:LYS:CB	3.02	0.41
3:D:744:LEU:HD12	3:D:744:LEU:O	2.21	0.41
3:D:911:ALA:O	3:D:914:PHE:HB3	2.21	0.41
1:B:130:LEU:HD11	1:B:170:ILE:CG2	2.51	0.41
3:A:172:LYS:O	3:A:175:SER:HB3	2.20	0.41
3:A:372:TYR:O	3:A:374:ASN:N	2.53	0.41
3:A:780:LEU:O	3:A:781:LEU:C	2.64	0.41
3:A:949:MET:O	3:A:952:LEU:HB3	2.20	0.41
1:E:8:LEU:C	1:E:10:GLY:N	2.79	0.41
1:E:262:GLN:HE21	1:E:262:GLN:HB2	1.66	0.41
3:D:93:ILE:CG2	3:D:1027:GLY:HA3	2.51	0.41
3:D:178:VAL:O	3:D:178:VAL:HG12	2.20	0.41
3:D:697:ARG:NH2	3:D:697:ARG:HG3	2.35	0.41
3:D:823:PHE:HD1	3:D:823:PHE:HA	1.72	0.41
3:D:997:PHE:HD1	3:D:1014:HIS:NE2	2.18	0.41
2:C:25:THR:O	2:C:26:PHE:C	2.64	0.41
2:C:66:THR:HG22	2:C:67:ALA:H	1.84	0.41
2:C:106:ARG:O	2:C:110:ARG:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:146:TYR:CD2	2:C:147:TYR:N	2.89	0.41
3:A:23:LEU:HD11	3:A:26:ASN:CB	2.46	0.41
3:A:72:ASN:O	3:A:74:ASN:N	2.54	0.41
3:A:168:MET:HG3	3:A:225:THR:OG1	2.21	0.41
3:A:223:HIS:CD2	3:A:223:HIS:C	2.97	0.41
3:A:340:ARG:C	3:A:342:ASN:N	2.77	0.41
3:A:421:VAL:HG22	3:A:461:LEU:HD21	2.03	0.41
3:A:508:MET:O	3:A:509:HIS:C	2.63	0.41
3:A:667:SER:O	3:A:671:GLN:HG3	2.21	0.41
3:A:975:GLN:HG3	3:A:998:VAL:HG12	2.03	0.41
3:A:1014:HIS:O	3:A:1015:LEU:C	2.63	0.41
1:E:61:ALA:HB1	1:E:168:TYR:HE1	1.86	0.41
1:E:105:GLU:O	1:E:106:TRP:C	2.64	0.41
1:E:154:LEU:HD23	1:E:154:LEU:HA	1.82	0.41
1:E:241:LEU:O	1:E:242:CYS:C	2.64	0.41
2:F:171:ASP:OD1	2:F:174:LEU:N	2.54	0.41
3:D:27:LEU:CD2	3:D:75:THR:HG23	2.51	0.41
3:D:161:GLU:O	3:D:164:CYS:HB3	2.20	0.41
3:D:198:MET:O	3:D:202:PHE:HB2	2.21	0.41
3:D:240:TYR:O	3:D:244:THR:CG2	2.69	0.41
3:D:391:SER:HA	3:D:392:PRO:HD3	1.73	0.41
3:D:516:PHE:O	3:D:520:VAL:HG23	2.21	0.41
3:D:531:LYS:HA	3:D:531:LYS:HD3	1.84	0.41
3:D:552:PRO:HA	3:D:555:LEU:HD12	2.03	0.41
3:D:850:LEU:O	3:D:853:GLN:HB3	2.21	0.41
3:D:853:GLN:O	3:D:857:SER:OG	2.36	0.41
3:D:983:LYS:HE2	3:D:991:ASP:OD1	2.21	0.41
3:D:1007:ASP:OD2	3:D:1009:PRO:HD2	2.21	0.41
1:B:25:PRO:HG2	1:B:108:ILE:HD13	2.03	0.41
1:B:355:CYS:O	1:B:356:LEU:CB	2.69	0.41
2:C:9:VAL:HG22	2:C:58:PRO:O	2.21	0.41
3:A:40:GLY:C	3:A:42:GLN:N	2.79	0.41
3:A:247:ILE:H	3:A:247:ILE:HG13	1.59	0.41
3:A:347:LEU:C	3:A:347:LEU:HD23	2.46	0.41
3:A:660:LEU:HB2	3:A:661:PRO:HD3	2.03	0.41
3:A:746:ARG:NH1	3:A:746:ARG:CG	2.76	0.41
3:A:911:ALA:O	3:A:914:PHE:HB3	2.21	0.41
3:A:952:LEU:HD23	3:A:952:LEU:C	2.46	0.41
1:E:2:ASN:N	1:E:2:ASN:HD22	2.19	0.41
1:E:63:ARG:NH1	1:E:72:MET:CB	2.81	0.41
1:E:122:VAL:HG21	1:E:249:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:35:PHE:HE2	2:F:37:LYS:HG2	1.86	0.41
3:D:14:ARG:CG	3:D:14:ARG:NH1	2.75	0.41
3:D:27:LEU:C	3:D:29:ASP:H	2.28	0.41
3:D:55:GLU:HG2	3:D:56:HIS:N	2.36	0.41
3:D:165:GLN:HA	3:D:221:LEU:HD13	2.03	0.41
3:D:229:LEU:O	3:D:233:LEU:HG	2.21	0.41
3:D:247:ILE:HG21	3:D:286:LEU:HB2	2.03	0.41
3:D:394:LEU:C	3:D:394:LEU:HD23	2.46	0.41
3:D:615:LEU:HA	3:D:618:ILE:CG1	2.51	0.41
1:B:208:HIS:CD2	1:B:208:HIS:N	2.90	0.40
3:A:271:ILE:C	3:A:273:GLY:N	2.78	0.40
3:A:347:LEU:O	3:A:351:LEU:HB2	2.20	0.40
3:A:970:ASN:O	3:A:973:PHE:HB3	2.21	0.40
1:E:13:ILE:HD12	1:E:13:ILE:HG21	1.85	0.40
1:E:63:ARG:NH1	1:E:70:THR:H	2.19	0.40
1:E:169:THR:HG22	1:E:171:LEU:HD21	2.02	0.40
1:E:208:HIS:CD2	1:E:208:HIS:N	2.90	0.40
1:E:216:GLY:O	1:E:219:GLU:N	2.54	0.40
1:E:255:GLY:O	1:E:256:LEU:HD23	2.20	0.40
2:F:156:ASN:ND2	2:F:159:LYS:HE3	2.36	0.40
3:D:149:PHE:CZ	3:D:153:ILE:HD13	2.56	0.40
3:D:287:PHE:HZ	3:D:350:ALA:CB	2.34	0.40
3:D:588:PHE:CE2	3:D:636:ALA:HB1	2.56	0.40
3:D:948:TYR:CE1	3:D:952:LEU:HD12	2.56	0.40
3:D:990:GLN:C	3:D:992:ALA:H	2.29	0.40
1:B:105:GLU:O	1:B:274:GLY:HA2	2.20	0.40
3:A:219:ALA:HB3	3:A:220:PRO:CD	2.41	0.40
3:A:326:LEU:HD23	3:A:326:LEU:HA	1.89	0.40
3:A:997:PHE:CD1	3:A:1014:HIS:CE1	3.05	0.40
1:E:102:MET:SD	1:E:265:TYR:HA	2.61	0.40
2:F:75:LEU:CD1	3:D:49:VAL:HG22	2.51	0.40
2:F:132:LYS:C	2:F:134:LYS:N	2.77	0.40
3:D:127:ILE:O	3:D:130:LEU:HB2	2.21	0.40
3:D:260:PHE:O	3:D:261:ARG:C	2.64	0.40
3:D:594:LYS:HE2	3:D:594:LYS:CA	2.50	0.40
3:D:672:ALA:O	3:D:676:VAL:HG22	2.22	0.40
3:D:786:ILE:O	3:D:789:GLN:HB3	2.21	0.40
3:D:855:VAL:O	3:D:859:CYS:HB2	2.21	0.40
3:D:938:GLY:O	3:D:940:THR:N	2.54	0.40
3:D:953:VAL:C	3:D:955:GLU:H	2.29	0.40
1:B:7:LYS:HD2	3:A:522:LYS:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:LEU:HB2	1:B:39:GLN:CD	2.44	0.40
1:B:257:LEU:CD1	1:B:275:TRP:HB2	2.52	0.40
2:C:37:LYS:HA	4:C:217:GTP:O2'	2.21	0.40
3:A:287:PHE:HZ	3:A:350:ALA:CB	2.35	0.40
1:E:216:GLY:O	1:E:217:LEU:C	2.65	0.40
2:F:164:LEU:HA	2:F:164:LEU:HD23	1.91	0.40
3:D:227:GLU:HG2	3:D:263:VAL:HG13	2.03	0.40
3:D:402:ILE:H	3:D:402:ILE:HG12	1.56	0.40
2:C:38:LYS:HA	3:A:842:PRO:HG3	2.04	0.40
3:A:55:GLU:HG2	3:A:56:HIS:H	1.86	0.40
3:A:672:ALA:O	3:A:676:VAL:HG22	2.22	0.40
3:A:973:PHE:O	3:A:976:ASP:CB	2.69	0.40
2:F:135:SER:O	2:F:137:VAL:HG22	2.21	0.40
3:D:94:LEU:HB2	3:D:99:CYS:SG	2.62	0.40
3:D:219:ALA:HB3	3:D:220:PRO:CD	2.41	0.40
3:D:251:ILE:HG22	3:D:293:GLN:HG3	2.04	0.40
3:D:259:MET:C	3:D:261:ARG:N	2.74	0.40
3:D:328:THR:HG23	3:D:331:LYS:NZ	2.35	0.40
3:D:704:HIS:CD2	3:D:766:SER:CB	3.00	0.40
3:D:988:HIS:O	3:D:989:LEU:C	2.64	0.40
1:B:24:HIS:HA	1:B:25:PRO:HD3	1.97	0.40
1:B:254:ASP:O	1:B:277:ARG:NE	2.49	0.40
1:B:260:HIS:CE1	1:B:262:GLN:CG	3.00	0.40
2:C:16:VAL:HG23	2:C:88:ILE:HA	2.03	0.40
3:A:232:PHE:HD2	3:A:232:PHE:HA	1.71	0.40
3:A:255:LEU:O	3:A:255:LEU:HD23	2.21	0.40
3:A:437:GLN:HB2	3:A:439:GLU:HG3	2.02	0.40
3:A:617:ASN:O	3:A:618:ILE:C	2.64	0.40
3:A:997:PHE:HD1	3:A:1014:HIS:NE2	2.19	0.40
1:E:107:LEU:HB2	1:E:274:GLY:CA	2.47	0.40
2:F:92:VAL:HG23	2:F:129:ARG:HG3	2.03	0.40
3:D:15:GLN:O	3:D:16:LEU:HD12	2.21	0.40
3:D:27:LEU:HD23	3:D:75:THR:HG23	2.04	0.40
3:D:102:ILE:HG13	3:D:102:ILE:H	1.60	0.40
3:D:383:GLU:OE2	3:D:405:ARG:HG3	2.21	0.40
3:D:407:GLN:HE21	3:D:407:GLN:HB3	1.66	0.40
3:D:745:ILE:HD13	3:D:745:ILE:HA	1.83	0.40
3:D:1008:ILE:O	3:D:1012:LYS:HB2	2.21	0.40
3:D:1043:ARG:HA	3:D:1043:ARG:HD2	1.72	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	262/361 (73%)	206 (79%)	38 (14%)	18 (7%)	1	6
1	E	267/361 (74%)	211 (79%)	39 (15%)	17 (6%)	1	7
2	C	169/176 (96%)	139 (82%)	23 (14%)	7 (4%)	2	14
2	F	169/176 (96%)	138 (82%)	24 (14%)	7 (4%)	2	14
3	A	1037/1073 (97%)	760 (73%)	206 (20%)	71 (7%)	1	6
3	D	1037/1073 (97%)	755 (73%)	220 (21%)	62 (6%)	1	8
All	All	2941/3220 (91%)	2209 (75%)	550 (19%)	182 (6%)	1	8

All (182) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	39	GLN
1	B	145	GLY
1	B	180	GLN
1	B	217	LEU
2	C	76	ARG
3	A	55	GLU
3	A	114	SER
3	A	123	GLU
3	A	127	ILE
3	A	200	ASN
3	A	326	LEU
3	A	397	SER
3	A	433	VAL
3	A	450	SER
3	A	468	ASP
3	A	486	GLY
3	A	939	LEU
3	A	963	ASN
3	A	1028	GLU
1	E	39	GLN

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Mol	Chain	Res	Type
1	E	145	GLY
1	E	180	GLN
1	E	217	LEU
2	F	76	ARG
3	D	42	GLN
3	D	55	GLU
3	D	123	GLU
3	D	127	ILE
3	D	200	ASN
3	D	326	LEU
3	D	363	THR
3	D	392	PRO
3	D	435	ASN
3	D	450	SER
3	D	468	ASP
3	D	627	PRO
3	D	848	PHE
3	D	939	LEU
3	D	963	ASN
3	D	1029	ASP
3	D	1035	LEU
3	D	1036	GLU
1	B	53	LYS
2	C	32	THR
2	C	87	ILE
3	A	115	SER
3	A	118	THR
3	A	125	VAL
3	A	269	THR
3	A	277	SER
3	A	297	MET
3	A	307	ALA
3	A	388	THR
3	A	435	ASN
3	A	504	ILE
3	A	627	PRO
3	A	674	LYS
3	A	730	ALA
3	A	743	PRO
3	A	769	PRO
3	A	823	PHE
3	A	843	GLU

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Mol	Chain	Res	Type
3	A	848	PHE
3	A	1027	GLY
3	A	1037	GLU
1	E	25	PRO
1	E	51	LYS
1	E	159	ASN
3	D	269	THR
3	D	297	MET
3	D	307	ALA
3	D	486	GLY
3	D	504	ILE
3	D	712	ARG
3	D	737	GLU
3	D	769	PRO
3	D	965	GLY
1	B	10	GLY
1	B	25	PRO
1	B	156	PRO
1	B	261	LYS
1	B	350	PRO
2	C	65	ASP
2	C	106	ARG
3	A	13	ALA
3	A	64	ASP
3	A	122	LYS
3	A	143	PRO
3	A	149	PHE
3	A	362	GLU
3	A	363	THR
3	A	530	GLN
3	A	712	ARG
3	A	737	GLU
3	A	781	LEU
3	A	954	GLU
1	E	53	LYS
1	E	156	PRO
2	F	32	THR
2	F	106	ARG
3	D	64	ASP
3	D	125	VAL
3	D	143	PRO
3	D	530	GLN

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Mol	Chain	Res	Type
3	D	730	ALA
3	D	743	PRO
3	D	823	PHE
3	D	843	GLU
3	D	954	GLU
1	B	49	LEU
1	B	240	SER
3	A	124	LYS
3	A	246	LEU
3	A	268	LEU
3	A	392	PRO
3	A	679	LEU
3	A	961	PRO
1	E	191	ARG
1	E	240	SER
1	E	242	CYS
1	E	261	LYS
2	F	87	ILE
3	D	21	GLN
3	D	65	THR
3	D	77	TYR
3	D	122	LYS
3	D	149	PHE
3	D	196	ASP
3	D	217	GLN
3	D	246	LEU
3	D	268	LEU
3	D	362	GLU
3	D	679	LEU
3	D	781	LEU
3	D	820	PRO
1	B	241	LEU
1	B	242	CYS
1	B	356	LEU
1	B	358	GLU
2	C	85	CYS
3	A	21	GLN
3	A	65	THR
3	A	77	TYR
3	A	91	TRP
3	A	341	LEU
3	A	510	GLU

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Mol	Chain	Res	Type
3	A	807	ILE
3	A	820	PRO
3	A	899	THR
3	A	971	GLN
3	A	1005	ASN
1	E	18	ASN
2	F	85	CYS
3	D	91	TRP
3	D	341	LEU
3	D	510	GLU
3	D	899	THR
3	D	1037	GLU
1	B	18	ASN
1	B	267	PRO
3	A	482	ASN
1	E	241	LEU
1	E	267	PRO
2	F	65	ASP
3	D	235	TRP
3	D	335	GLN
3	A	258	PRO
3	A	484	VAL
3	A	540	ILE
3	D	807	ILE
3	D	961	PRO
3	D	1027	GLY
1	E	284	VAL
3	D	258	PRO
3	D	540	ILE
3	D	451	ILE
3	A	146	TRP
2	F	137	VAL
2	C	137	VAL
3	A	31	VAL
3	A	451	ILE
3	A	676	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	244/323 (76%)	197 (81%)	47 (19%)	1	6
1	E	247/323 (76%)	204 (83%)	43 (17%)	2	8
2	C	150/154 (97%)	124 (83%)	26 (17%)	2	8
2	F	150/154 (97%)	120 (80%)	30 (20%)	1	5
3	A	945/973 (97%)	820 (87%)	125 (13%)	4	15
3	D	945/973 (97%)	815 (86%)	130 (14%)	3	14
All	All	2681/2900 (92%)	2280 (85%)	401 (15%)	3	11

All (401) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	0	SER
1	B	1	LEU
1	B	6	LEU
1	B	7	LYS
1	B	13	ILE
1	B	27	LEU
1	B	39	GLN
1	B	46	LEU
1	B	53	LYS
1	B	55	LEU
1	B	70	THR
1	B	95	LYS
1	B	108	ILE
1	B	109	ASP
1	B	110	VAL
1	B	112	SER
1	B	119	ILE
1	B	123	CYS
1	B	128	ARG
1	B	139	SER
1	B	151	PHE
1	B	160	ARG
1	B	171	LEU
1	B	174	ILE
1	B	188	MET
1	B	198	CYS
1	B	215	GLU

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Mol	Chain	Res	Type
1	B	219	GLU
1	B	222	LYS
1	B	231	LEU
1	B	234	PHE
1	B	241	LEU
1	B	245	LEU
1	B	246	SER
1	B	257	LEU
1	B	262	GLN
1	B	269	SER
1	B	275	TRP
1	B	276	LEU
1	B	281	VAL
1	B	282	SER
1	B	283	ASP
1	B	348	HIS
1	B	352	HIS
1	B	355	CYS
1	B	356	LEU
1	B	357	MET
2	C	13	LEU
2	C	27	VAL
2	C	29	ARG
2	C	30	HIS
2	C	31	LEU
2	C	32	THR
2	C	51	VAL
2	C	75	LEU
2	C	76	ARG
2	C	77	ASP
2	C	88	ILE
2	C	92	VAL
2	C	95	ARG
2	C	96	VAL
2	C	97	THR
2	C	108	LEU
2	C	109	VAL
2	C	112	CYS
2	C	117	ILE
2	C	130	LYS
2	C	137	VAL
2	C	141	LYS

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Mol	Chain	Res	Type
2	C	142	LYS
2	C	144	LEU
2	C	148	ASP
2	C	173	ASN
3	A	23	LEU
3	A	28	LEU
3	A	29	ASP
3	A	30	ASN
3	A	34	CYS
3	A	35	LEU
3	A	45	MET
3	A	50	LEU
3	A	58	ASP
3	A	60	TRP
3	A	66	ILE
3	A	73	MET
3	A	80	LEU
3	A	102	ILE
3	A	109	LEU
3	A	146	TRP
3	A	148	THR
3	A	159	THR
3	A	160	SER
3	A	163	LEU
3	A	170	ILE
3	A	189	VAL
3	A	192	LYS
3	A	196	ASP
3	A	199	CYS
3	A	205	ILE
3	A	218	ASN
3	A	229	LEU
3	A	231	ARG
3	A	232	PHE
3	A	263	VAL
3	A	265	LEU
3	A	266	LYS
3	A	277	SER
3	A	285	THR
3	A	286	LEU
3	A	294	LEU
3	A	313	ASP

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Mol	Chain	Res	Type
3	A	323	SER
3	A	327	CYS
3	A	331	LYS
3	A	335	GLN
3	A	336	LEU
3	A	337	LEU
3	A	353	TYR
3	A	365	ILE
3	A	374	ASN
3	A	379	GLU
3	A	388	THR
3	A	391	SER
3	A	393	LEU
3	A	398	GLN
3	A	402	ILE
3	A	406	ARG
3	A	422	SER
3	A	430	VAL
3	A	433	VAL
3	A	440	VAL
3	A	443	GLU
3	A	452	ASN
3	A	460	THR
3	A	464	LEU
3	A	465	THR
3	A	487	THR
3	A	490	SER
3	A	515	ARG
3	A	525	LEU
3	A	539	ILE
3	A	547	ILE
3	A	565	VAL
3	A	569	LEU
3	A	578	ASP
3	A	606	GLU
3	A	607	VAL
3	A	613	GLU
3	A	617	ASN
3	A	622	ILE
3	A	641	ILE
3	A	649	VAL
3	A	659	LEU

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Mol	Chain	Res	Type
3	A	662	ASN
3	A	680	LYS
3	A	684	THR
3	A	685	VAL
3	A	691	ILE
3	A	695	ASN
3	A	708	ILE
3	A	720	VAL
3	A	739	VAL
3	A	743	PRO
3	A	746	ARG
3	A	749	ARG
3	A	771	MET
3	A	781	LEU
3	A	785	LEU
3	A	804	MET
3	A	816	THR
3	A	823	PHE
3	A	852	LEU
3	A	855	VAL
3	A	872	LYS
3	A	885	THR
3	A	892	THR
3	A	895	GLN
3	A	907	GLU
3	A	916	GLN
3	A	920	CYS
3	A	926	ILE
3	A	928	SER
3	A	935	HIS
3	A	940	THR
3	A	946	LEU
3	A	948	TYR
3	A	962	LEU
3	A	969	ASN
3	A	970	ASN
3	A	973	PHE
3	A	976	ASP
3	A	988	HIS
3	A	1008	ILE
3	A	1013	GLU
3	A	1020	VAL

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Mol	Chain	Res	Type
3	A	1032	ASP
3	A	1033	LEU
3	A	1035	LEU
1	E	1	LEU
1	E	4	LEU
1	E	8	LEU
1	E	13	ILE
1	E	14	SER
1	E	27	LEU
1	E	33	LYS
1	E	39	GLN
1	E	45	ARG
1	E	48	GLU
1	E	49	LEU
1	E	108	ILE
1	E	109	ASP
1	E	110	VAL
1	E	112	SER
1	E	119	ILE
1	E	123	CYS
1	E	128	ARG
1	E	139	SER
1	E	151	PHE
1	E	160	ARG
1	E	169	THR
1	E	171	LEU
1	E	174	ILE
1	E	188	MET
1	E	198	CYS
1	E	209	SER
1	E	219	GLU
1	E	231	LEU
1	E	234	PHE
1	E	241	LEU
1	E	245	LEU
1	E	246	SER
1	E	257	LEU
1	E	262	GLN
1	E	269	SER
1	E	275	TRP
1	E	276	LEU
1	E	281	VAL

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Mol	Chain	Res	Type
1	E	282	SER
1	E	283	ASP
1	E	285	LEU
1	E	351	ASP
2	F	9	VAL
2	F	13	LEU
2	F	27	VAL
2	F	29	ARG
2	F	30	HIS
2	F	31	LEU
2	F	32	THR
2	F	38	LYS
2	F	43	LEU
2	F	45	VAL
2	F	51	VAL
2	F	75	LEU
2	F	76	ARG
2	F	77	ASP
2	F	88	ILE
2	F	92	VAL
2	F	95	ARG
2	F	96	VAL
2	F	97	THR
2	F	108	LEU
2	F	109	VAL
2	F	112	CYS
2	F	117	ILE
2	F	130	LYS
2	F	134	LYS
2	F	137	VAL
2	F	141	LYS
2	F	142	LYS
2	F	148	ASP
2	F	173	ASN
3	D	14	ARG
3	D	21	GLN
3	D	23	LEU
3	D	28	LEU
3	D	29	ASP
3	D	30	ASN
3	D	34	CYS
3	D	35	LEU

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Mol	Chain	Res	Type
3	D	45	MET
3	D	50	LEU
3	D	58	ASP
3	D	60	TRP
3	D	66	ILE
3	D	70	SER
3	D	73	MET
3	D	80	LEU
3	D	102	ILE
3	D	109	LEU
3	D	112	LYS
3	D	113	THR
3	D	118	THR
3	D	119	CYS
3	D	146	TRP
3	D	148	THR
3	D	157	SER
3	D	159	THR
3	D	160	SER
3	D	163	LEU
3	D	170	ILE
3	D	189	VAL
3	D	192	LYS
3	D	199	CYS
3	D	205	ILE
3	D	210	GLN
3	D	217	GLN
3	D	229	LEU
3	D	231	ARG
3	D	263	VAL
3	D	265	LEU
3	D	266	LYS
3	D	277	SER
3	D	286	LEU
3	D	294	LEU
3	D	313	ASP
3	D	323	SER
3	D	327	CYS
3	D	331	LYS
3	D	335	GLN
3	D	336	LEU
3	D	337	LEU

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Mol	Chain	Res	Type
3	D	351	LEU
3	D	353	TYR
3	D	365	ILE
3	D	374	ASN
3	D	379	GLU
3	D	389	SER
3	D	393	LEU
3	D	395	SER
3	D	401	ASP
3	D	402	ILE
3	D	406	ARG
3	D	422	SER
3	D	430	VAL
3	D	433	VAL
3	D	437	GLN
3	D	443	GLU
3	D	452	ASN
3	D	460	THR
3	D	465	THR
3	D	485	ASN
3	D	487	THR
3	D	490	SER
3	D	515	ARG
3	D	517	LEU
3	D	525	LEU
3	D	539	ILE
3	D	547	ILE
3	D	565	VAL
3	D	569	LEU
3	D	578	ASP
3	D	606	GLU
3	D	607	VAL
3	D	613	GLU
3	D	617	ASN
3	D	622	ILE
3	D	641	ILE
3	D	649	VAL
3	D	659	LEU
3	D	662	ASN
3	D	680	LYS
3	D	684	THR
3	D	685	VAL

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Mol	Chain	Res	Type
3	D	691	ILE
3	D	695	ASN
3	D	708	ILE
3	D	720	VAL
3	D	739	VAL
3	D	743	PRO
3	D	746	ARG
3	D	747	SER
3	D	749	ARG
3	D	771	MET
3	D	781	LEU
3	D	785	LEU
3	D	804	MET
3	D	816	THR
3	D	823	PHE
3	D	852	LEU
3	D	855	VAL
3	D	857	SER
3	D	872	LYS
3	D	885	THR
3	D	892	THR
3	D	907	GLU
3	D	916	GLN
3	D	920	CYS
3	D	926	ILE
3	D	928	SER
3	D	935	HIS
3	D	940	THR
3	D	946	LEU
3	D	948	TYR
3	D	970	ASN
3	D	976	ASP
3	D	988	HIS
3	D	1008	ILE
3	D	1013	GLU
3	D	1020	VAL
3	D	1030	THR
3	D	1053	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	18	ASN
1	B	50	GLN
1	B	60	HIS
1	B	149	ASN
1	B	180	GLN
1	B	199	GLN
1	B	208	HIS
1	B	262	GLN
2	C	82	GLN
2	C	103	ASN
2	C	156	ASN
3	A	30	ASN
3	A	47	GLN
3	A	98	GLN
3	A	131	ASN
3	A	193	HIS
3	A	204	GLN
3	A	321	ASN
3	A	333	HIS
3	A	374	ASN
3	A	399	HIS
3	A	407	GLN
3	A	437	GLN
3	A	466	HIS
3	A	483	GLN
3	A	536	ASN
3	A	574	HIS
3	A	593	GLN
3	A	617	ASN
3	A	626	GLN
3	A	628	GLN
3	A	631	HIS
3	A	650	GLN
3	A	675	ASN
3	A	695	ASN
3	A	704	HIS
3	A	727	ASN
3	A	742	GLN
3	A	767	ASN
3	A	775	ASN
3	A	858	HIS
3	A	888	ASN
3	A	903	ASN

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Mol	Chain	Res	Type
3	A	906	GLN
3	A	916	GLN
3	A	924	GLN
3	A	951	ASN
3	A	963	ASN
3	A	969	ASN
3	A	970	ASN
3	A	971	GLN
3	A	975	GLN
3	A	988	HIS
3	A	990	GLN
3	A	993	GLN
3	A	1005	ASN
3	A	1006	GLN
3	A	1046	GLN
1	E	2	ASN
1	E	18	ASN
1	E	60	HIS
1	E	149	ASN
1	E	199	GLN
1	E	208	HIS
1	E	262	GLN
1	E	348	HIS
2	F	82	GLN
2	F	103	ASN
2	F	156	ASN
3	D	26	ASN
3	D	30	ASN
3	D	43	GLN
3	D	47	GLN
3	D	71	GLN
3	D	98	GLN
3	D	131	ASN
3	D	145	HIS
3	D	193	HIS
3	D	204	GLN
3	D	210	GLN
3	D	223	HIS
3	D	321	ASN
3	D	333	HIS
3	D	352	HIS
3	D	374	ASN

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Mol	Chain	Res	Type
3	D	407	GLN
3	D	437	GLN
3	D	466	HIS
3	D	483	GLN
3	D	536	ASN
3	D	574	HIS
3	D	593	GLN
3	D	617	ASN
3	D	626	GLN
3	D	628	GLN
3	D	631	HIS
3	D	675	ASN
3	D	695	ASN
3	D	704	HIS
3	D	742	GLN
3	D	767	ASN
3	D	775	ASN
3	D	789	GLN
3	D	853	GLN
3	D	858	HIS
3	D	888	ASN
3	D	903	ASN
3	D	906	GLN
3	D	916	GLN
3	D	924	GLN
3	D	951	ASN
3	D	970	ASN
3	D	993	GLN
3	D	1005	ASN
3	D	1021	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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	GTP	C	217	5	33,34,34	0.93	1 (3%)	50,54,54	2.01	12 (24%)
4	GTP	F	217	5	33,34,34	0.95	2 (6%)	50,54,54	1.64	10 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	C	217	5	-	9/22/38/38	0/3/3/3
4	GTP	F	217	5	-	2/22/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	217	GTP	PB-O3B	2.38	1.62	1.59
4	C	217	GTP	C2-N3	2.30	1.38	1.33
4	F	217	GTP	C2-N3	2.00	1.38	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	217	GTP	C5-C4-N3	-6.27	118.42	128.39
4	C	217	GTP	C2-N3-C4	5.42	121.64	112.30
4	F	217	GTP	C2-N3-C4	4.09	119.34	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	217	GTP	C5-C4-N3	-3.93	122.14	128.39
4	C	217	GTP	C4-C5-N7	-3.69	104.83	110.67
4	C	217	GTP	C8-N7-C5	3.57	110.63	104.26
4	F	217	GTP	N9-C8-N7	-3.46	106.98	113.40
4	C	217	GTP	C2'-C1'-N9	3.24	122.27	113.25
4	C	217	GTP	N9-C4-N3	2.96	131.87	125.95
4	C	217	GTP	C2-N1-C6	-2.91	119.84	125.11
4	F	217	GTP	C8-N7-C5	2.89	109.41	104.26
4	C	217	GTP	O2'-C2'-C3'	-2.84	102.73	111.82
4	C	217	GTP	O4'-C1'-N9	-2.83	101.95	108.36
4	F	217	GTP	C2-N1-C6	-2.65	120.30	125.11
4	C	217	GTP	N9-C8-N7	-2.48	108.80	113.40
4	F	217	GTP	O2G-PG-O3B	2.45	112.85	104.64
4	F	217	GTP	C5-C6-N1	2.29	119.09	113.25
4	F	217	GTP	N9-C4-N3	2.25	130.46	125.95
4	C	217	GTP	C5-C4-N9	2.25	109.68	105.66
4	F	217	GTP	C4-C5-N7	-2.20	107.18	110.67
4	F	217	GTP	O2B-PB-O3B	2.04	112.78	107.27
4	C	217	GTP	O3'-C3'-C4'	-2.03	105.25	111.08

There are no chirality outliers.

All (11) torsion outliers are listed below:

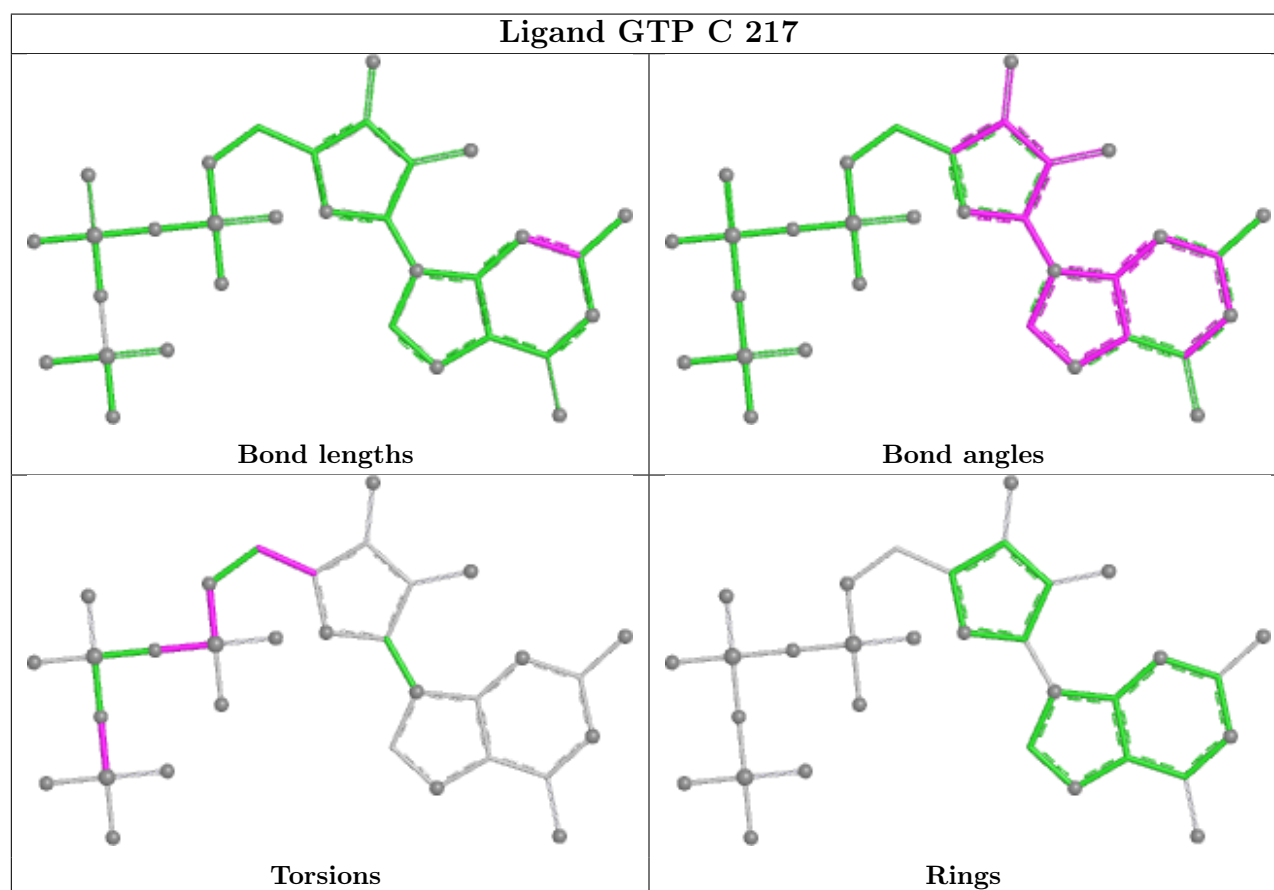
Mol	Chain	Res	Type	Atoms
4	C	217	GTP	PB-O3B-PG-O3G
4	C	217	GTP	C5'-O5'-PA-O3A
4	C	217	GTP	C5'-O5'-PA-O1A
4	C	217	GTP	C5'-O5'-PA-O2A
4	C	217	GTP	O4'-C4'-C5'-O5'
4	C	217	GTP	C3'-C4'-C5'-O5'
4	F	217	GTP	O4'-C4'-C5'-O5'
4	C	217	GTP	PB-O3B-PG-O1G
4	C	217	GTP	PB-O3A-PA-O1A
4	C	217	GTP	PB-O3A-PA-O2A
4	F	217	GTP	PG-O3B-PB-O2B

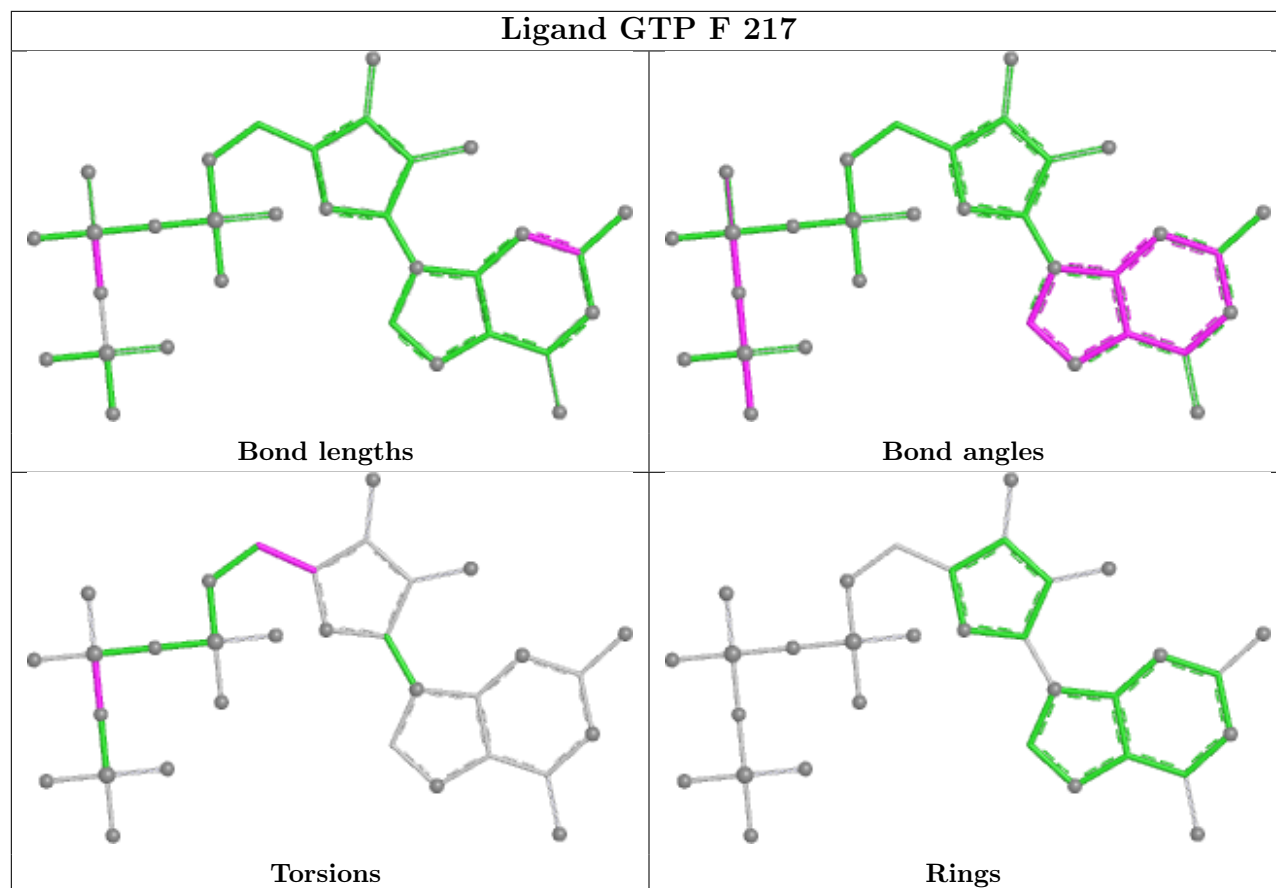
There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	217	GTP	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	B	272/361 (75%)	-1.35	0 100 100	7, 29, 72, 91	4 (1%)
1	E	277/361 (76%)	-1.36	0 100 100	7, 29, 80, 111	7 (2%)
2	C	171/176 (97%)	-1.43	0 100 100	10, 28, 58, 84	1 (0%)
2	F	171/176 (97%)	-1.45	0 100 100	10, 27, 56, 80	0
3	A	1041/1073 (97%)	-1.35	1 (0%) 92 92	4, 35, 90, 141	6 (0%)
3	D	1041/1073 (97%)	-1.37	0 100 100	5, 35, 89, 147	13 (1%)
All	All	2973/3220 (92%)	-1.37	1 (0%) 100 100	4, 32, 85, 147	31 (1%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	967	PRO	2.5

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](#)

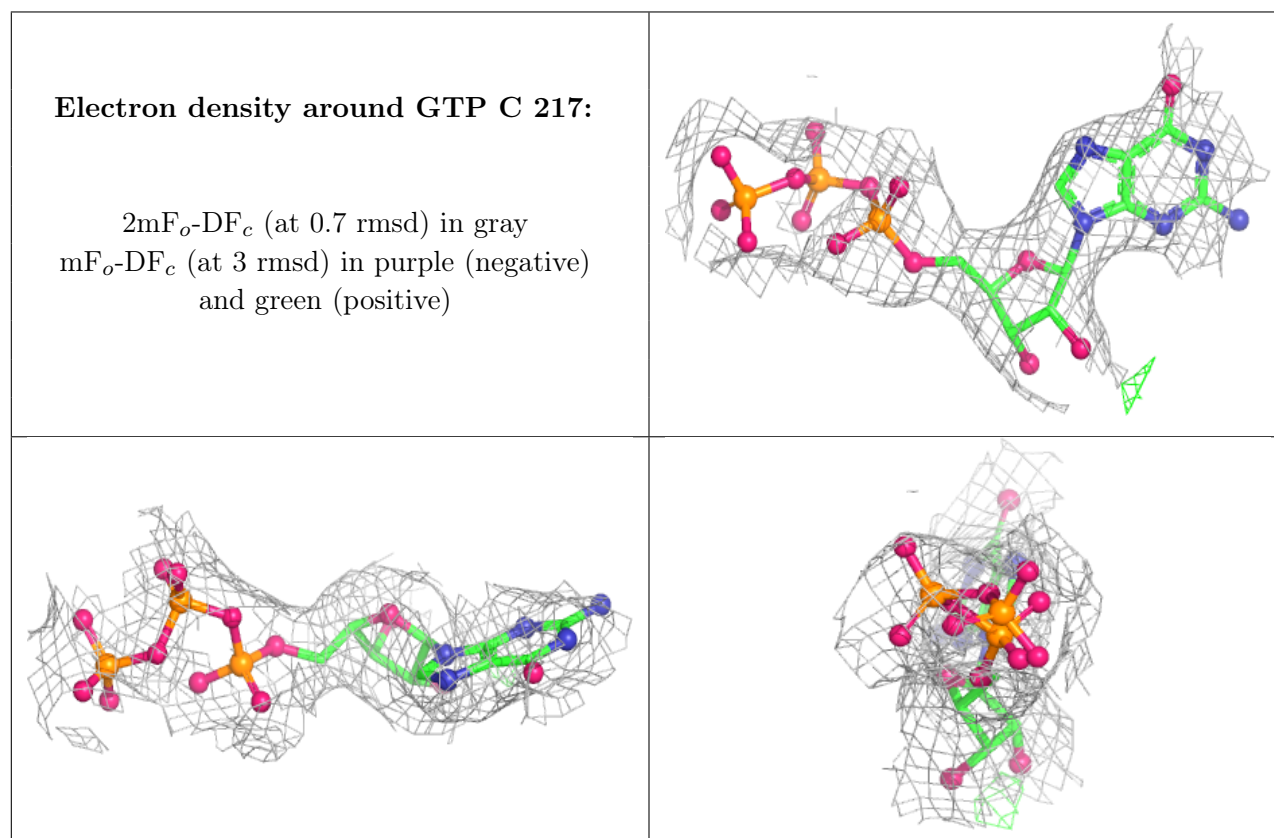
There are no oligosaccharides in this entry.

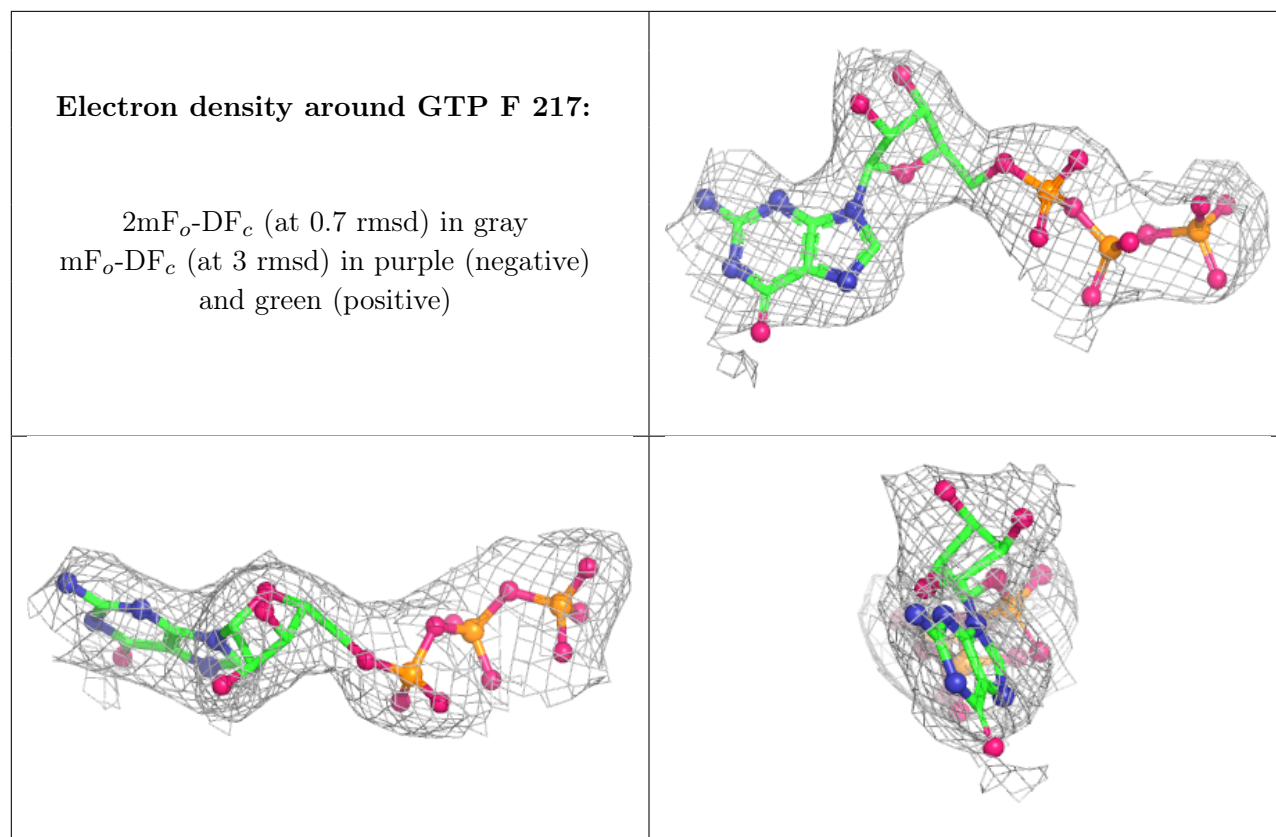
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GTP	C	217	32/32	1.00	0.02	10,21,47,63	0
4	GTP	F	217	32/32	1.00	0.02	7,18,30,35	0
5	MG	C	218	1/1	1.00	0.04	0,0,0,0	0
5	MG	F	218	1/1	1.00	0.02	6,6,6,6	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.