



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:14 AM UTC

PDB ID : 5THP / pdb_00005thp
Title : Rhodocetin in complex with the integrin alpha2-A domain
Authors : McDougall, M.; Orriss, G.L.; Stetefeld, J.
Deposited on : 2016-09-30
Resolution : 3.01 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
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

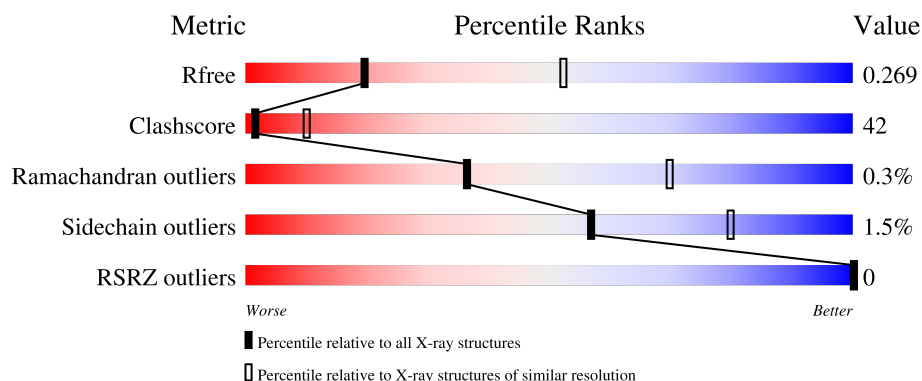
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

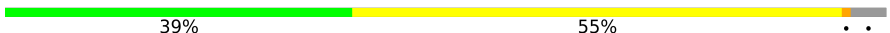
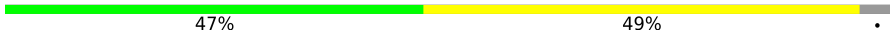
The reported resolution of this entry is 3.01 Å.

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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	135	
1	D	135	
1	G	135	
1	J	135	
1	M	135	

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Mol	Chain	Length	Quality of chain
1	P	135	
2	B	124	
2	E	124	
2	H	124	
2	K	124	
2	N	124	
2	Q	124	
3	C	217	
3	F	217	
3	I	217	
3	L	217	
3	O	217	
3	R	217	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CL	O	406	-	-	X	-
6	GOL	J	204	-	-	X	-
8	SO4	L	406	-	-	X	-
8	SO4	O	407	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 21018 atoms, of which 8 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 Snaclec rhodocetin subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			1006	638	171	188	9			
1	D	130	Total	C	N	O	S	0	0	0
			1022	642	176	196	8			
1	G	132	Total	C	N	O	S	0	0	0
			1064	671	185	199	9			
1	J	131	Total	C	N	O	S	0	0	0
			1046	658	180	199	9			
1	M	132	Total	C	N	O	S	0	0	0
			1041	655	178	199	9			
1	P	132	Total	C	N	O	S	0	0	0
			1058	666	182	201	9			

- Molecule 2 is a protein called Snaclec rhodocetin subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	119	Total	C	N	O	S	0	0	0
			987	641	167	170	9			
2	E	122	Total	C	N	O	S	0	0	0
			1006	650	169	178	9			
2	H	120	Total	C	N	O	S	0	0	0
			949	609	160	171	9			
2	K	108	Total	C	N	O	S	0	0	0
			885	572	149	157	7			
2	N	122	Total	C	N	O	S	0	0	0
			1029	667	174	179	9			
2	Q	122	Total	C	N	O	S	0	0	0
			1026	664	174	179	9			

- Molecule 3 is a protein called Integrin alpha-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	190	Total	C	N	O	S	0	0	0
			1435	905	244	282	4			
3	F	193	Total	C	N	O	S	0	0	0
			1443	908	246	284	5			
3	I	191	Total	C	N	O	S	0	0	0
			1396	882	232	277	5			
3	L	189	Total	C	N	O	S	0	0	0
			1392	878	236	273	5			
3	O	191	Total	C	N	O	S	0	0	0
			1430	907	235	283	5			
3	R	187	Total	C	N	O	S	0	0	0
			1407	892	236	274	5			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	150	MET	-	initiating methionine	UNP P17301
C	151	GLY	-	expression tag	UNP P17301
C	152	SER	-	expression tag	UNP P17301
C	153	SER	-	expression tag	UNP P17301
C	154	HIS	-	expression tag	UNP P17301
C	155	HIS	-	expression tag	UNP P17301
C	156	HIS	-	expression tag	UNP P17301
C	157	HIS	-	expression tag	UNP P17301
C	158	HIS	-	expression tag	UNP P17301
C	159	HIS	-	expression tag	UNP P17301
C	160	SER	-	expression tag	UNP P17301
C	161	SER	-	expression tag	UNP P17301
C	162	GLY	-	expression tag	UNP P17301
C	163	LEU	-	expression tag	UNP P17301
C	164	VAL	-	expression tag	UNP P17301
C	165	PRO	-	expression tag	UNP P17301
C	166	ARG	-	expression tag	UNP P17301
C	167	GLY	-	expression tag	UNP P17301
C	168	GLY	-	expression tag	UNP P17301
C	169	SER	-	expression tag	UNP P17301
F	150	MET	-	initiating methionine	UNP P17301
F	151	GLY	-	expression tag	UNP P17301
F	152	SER	-	expression tag	UNP P17301
F	153	SER	-	expression tag	UNP P17301
F	154	HIS	-	expression tag	UNP P17301
F	155	HIS	-	expression tag	UNP P17301
F	156	HIS	-	expression tag	UNP P17301
F	157	HIS	-	expression tag	UNP P17301

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Chain	Residue	Modelled	Actual	Comment	Reference
F	158	HIS	-	expression tag	UNP P17301
F	159	HIS	-	expression tag	UNP P17301
F	160	SER	-	expression tag	UNP P17301
F	161	SER	-	expression tag	UNP P17301
F	162	GLY	-	expression tag	UNP P17301
F	163	LEU	-	expression tag	UNP P17301
F	164	VAL	-	expression tag	UNP P17301
F	165	PRO	-	expression tag	UNP P17301
F	166	ARG	-	expression tag	UNP P17301
F	167	GLY	-	expression tag	UNP P17301
F	168	GLY	-	expression tag	UNP P17301
F	169	SER	-	expression tag	UNP P17301
I	150	MET	-	initiating methionine	UNP P17301
I	151	GLY	-	expression tag	UNP P17301
I	152	SER	-	expression tag	UNP P17301
I	153	SER	-	expression tag	UNP P17301
I	154	HIS	-	expression tag	UNP P17301
I	155	HIS	-	expression tag	UNP P17301
I	156	HIS	-	expression tag	UNP P17301
I	157	HIS	-	expression tag	UNP P17301
I	158	HIS	-	expression tag	UNP P17301
I	159	HIS	-	expression tag	UNP P17301
I	160	SER	-	expression tag	UNP P17301
I	161	SER	-	expression tag	UNP P17301
I	162	GLY	-	expression tag	UNP P17301
I	163	LEU	-	expression tag	UNP P17301
I	164	VAL	-	expression tag	UNP P17301
I	165	PRO	-	expression tag	UNP P17301
I	166	ARG	-	expression tag	UNP P17301
I	167	GLY	-	expression tag	UNP P17301
I	168	GLY	-	expression tag	UNP P17301
I	169	SER	-	expression tag	UNP P17301
L	150	MET	-	initiating methionine	UNP P17301
L	151	GLY	-	expression tag	UNP P17301
L	152	SER	-	expression tag	UNP P17301
L	153	SER	-	expression tag	UNP P17301
L	154	HIS	-	expression tag	UNP P17301
L	155	HIS	-	expression tag	UNP P17301
L	156	HIS	-	expression tag	UNP P17301
L	157	HIS	-	expression tag	UNP P17301
L	158	HIS	-	expression tag	UNP P17301
L	159	HIS	-	expression tag	UNP P17301

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Chain	Residue	Modelled	Actual	Comment	Reference
L	160	SER	-	expression tag	UNP P17301
L	161	SER	-	expression tag	UNP P17301
L	162	GLY	-	expression tag	UNP P17301
L	163	LEU	-	expression tag	UNP P17301
L	164	VAL	-	expression tag	UNP P17301
L	165	PRO	-	expression tag	UNP P17301
L	166	ARG	-	expression tag	UNP P17301
L	167	GLY	-	expression tag	UNP P17301
L	168	GLY	-	expression tag	UNP P17301
L	169	SER	-	expression tag	UNP P17301
O	150	MET	-	initiating methionine	UNP P17301
O	151	GLY	-	expression tag	UNP P17301
O	152	SER	-	expression tag	UNP P17301
O	153	SER	-	expression tag	UNP P17301
O	154	HIS	-	expression tag	UNP P17301
O	155	HIS	-	expression tag	UNP P17301
O	156	HIS	-	expression tag	UNP P17301
O	157	HIS	-	expression tag	UNP P17301
O	158	HIS	-	expression tag	UNP P17301
O	159	HIS	-	expression tag	UNP P17301
O	160	SER	-	expression tag	UNP P17301
O	161	SER	-	expression tag	UNP P17301
O	162	GLY	-	expression tag	UNP P17301
O	163	LEU	-	expression tag	UNP P17301
O	164	VAL	-	expression tag	UNP P17301
O	165	PRO	-	expression tag	UNP P17301
O	166	ARG	-	expression tag	UNP P17301
O	167	GLY	-	expression tag	UNP P17301
O	168	GLY	-	expression tag	UNP P17301
O	169	SER	-	expression tag	UNP P17301
R	150	MET	-	initiating methionine	UNP P17301
R	151	GLY	-	expression tag	UNP P17301
R	152	SER	-	expression tag	UNP P17301
R	153	SER	-	expression tag	UNP P17301
R	154	HIS	-	expression tag	UNP P17301
R	155	HIS	-	expression tag	UNP P17301
R	156	HIS	-	expression tag	UNP P17301
R	157	HIS	-	expression tag	UNP P17301
R	158	HIS	-	expression tag	UNP P17301
R	159	HIS	-	expression tag	UNP P17301
R	160	SER	-	expression tag	UNP P17301
R	161	SER	-	expression tag	UNP P17301

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Chain	Residue	Modelled	Actual	Comment	Reference
R	162	GLY	-	expression tag	UNP P17301
R	163	LEU	-	expression tag	UNP P17301
R	164	VAL	-	expression tag	UNP P17301
R	165	PRO	-	expression tag	UNP P17301
R	166	ARG	-	expression tag	UNP P17301
R	167	GLY	-	expression tag	UNP P17301
R	168	GLY	-	expression tag	UNP P17301
R	169	SER	-	expression tag	UNP P17301

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	B	1	Total Na 1 1	0	0
4	C	4	Total Na 4 4	0	0
4	D	3	Total Na 3 3	0	0
4	E	3	Total Na 3 3	0	0
4	F	2	Total Na 2 2	0	0
4	G	1	Total Na 1 1	0	0
4	H	1	Total Na 1 1	0	0
4	I	2	Total Na 2 2	0	0
4	J	2	Total Na 2 2	0	0
4	L	2	Total Na 2 2	0	0
4	M	1	Total Na 1 1	0	0
4	N	1	Total Na 1 1	0	0
4	O	3	Total Na 3 3	0	0
4	P	1	Total Na 1 1	0	0

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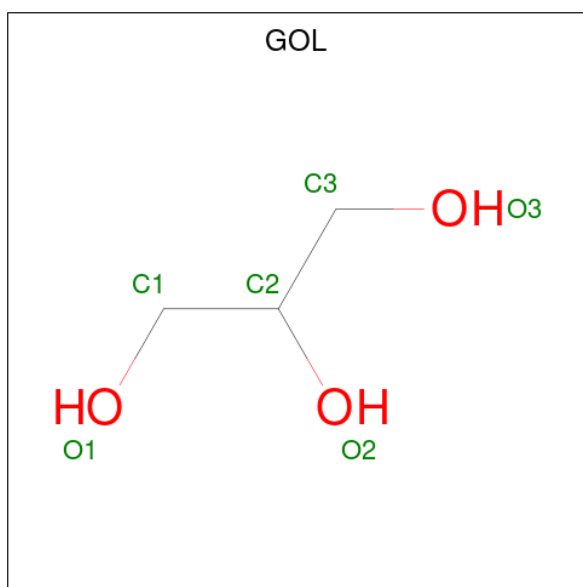
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Q	2	Total 2	Na 2	0	0
4	R	1	Total 1	Na 1	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Cl 1	0	0
5	C	4	Total 4	Cl 4	0	0
5	D	5	Total 5	Cl 5	0	0
5	E	3	Total 3	Cl 3	0	0
5	F	1	Total 1	Cl 1	0	0
5	G	2	Total 2	Cl 2	0	0
5	H	2	Total 2	Cl 2	0	0
5	I	3	Total 3	Cl 3	0	0
5	J	1	Total 1	Cl 1	0	0
5	L	2	Total 2	Cl 2	0	0
5	M	2	Total 2	Cl 2	0	0
5	N	3	Total 3	Cl 3	0	0
5	O	1	Total 1	Cl 1	0	0
5	P	2	Total 2	Cl 2	0	0
5	Q	2	Total 2	Cl 2	0	0
5	R	1	Total 1	Cl 1	0	0

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	0	0	
			6	3	3			
6	C	1	Total	C	O	0	0	
			6	3	3			
6	G	1	Total	C	O	0	0	
			6	3	3			
6	G	1	Total	C	H	O	0	0
			14	3	8	3		
6	H	1	Total	C	O	0	0	
			6	3	3			
6	J	1	Total	C	O	0	0	
			6	3	3			
6	J	1	Total	C	O	0	0	
			6	3	3			
6	P	1	Total	C	O	0	0	
			6	3	3			

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

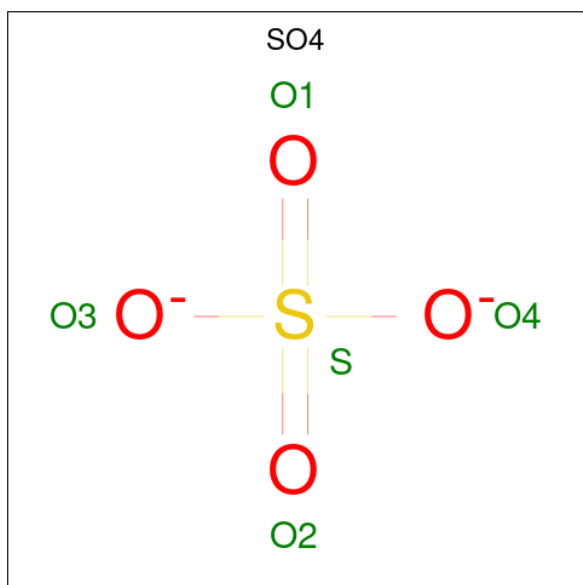
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Mg	0	0
			1	1		
7	F	1	Total	Mg	0	0
			1	1		
7	I	1	Total	Mg	0	0
			1	1		
7	L	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	O	1	Total	Mg	0	0
			1	1		
7	R	1	Total	Mg	0	0
			1	1		

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	O	S	0	0
			5	4	1		
8	D	1	Total	O	S	0	0
			5	4	1		
8	E	1	Total	O	S	0	0
			5	4	1		
8	F	1	Total	O	S	0	0
			5	4	1		
8	F	1	Total	O	S	0	0
			5	4	1		
8	I	1	Total	O	S	0	0
			5	4	1		
8	L	1	Total	O	S	0	0
			5	4	1		
8	O	1	Total	O	S	0	0
			5	4	1		
8	O	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	R	1	Total	O	S	0	0
			5	4	1		

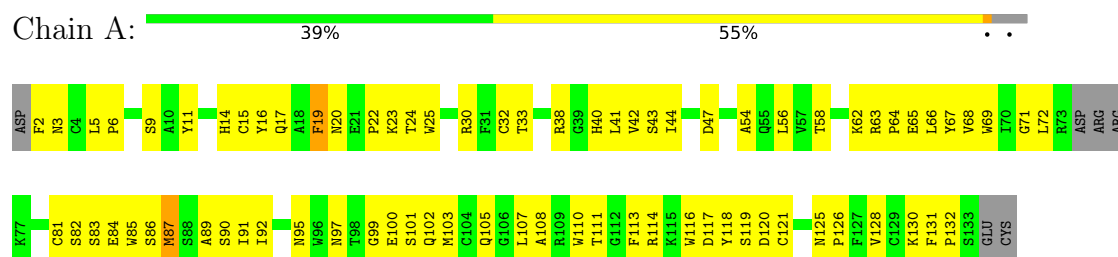
- Molecule 9 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	16	Total	O		0	0
			16	16			
9	B	7	Total	O		0	0
			7	7			
9	C	15	Total	O		0	0
			15	15			
9	D	19	Total	O		0	0
			19	19			
9	E	9	Total	O		0	0
			9	9			
9	F	11	Total	O		0	0
			11	11			
9	G	16	Total	O		0	0
			16	16			
9	H	7	Total	O		0	0
			7	7			
9	I	16	Total	O		0	0
			16	16			
9	J	10	Total	O		0	0
			10	10			
9	K	8	Total	O		0	0
			8	8			
9	L	17	Total	O		0	0
			17	17			
9	M	6	Total	O		0	0
			6	6			
9	N	7	Total	O		0	0
			7	7			
9	O	20	Total	O		0	0
			20	20			
9	P	6	Total	O		0	0
			6	6			
9	Q	14	Total	O		0	0
			14	14			
9	R	14	Total	O		0	0
			14	14			

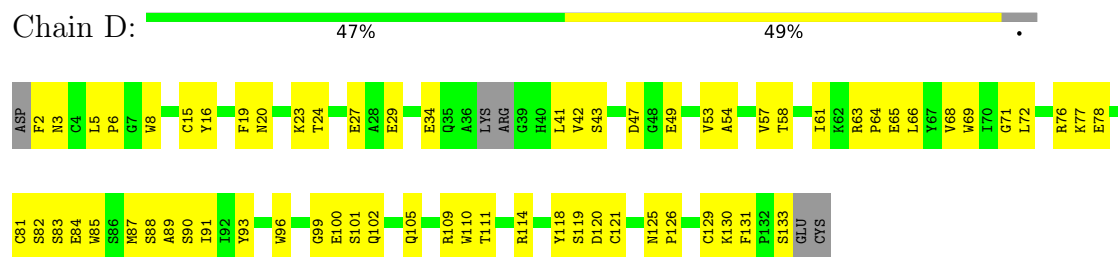
3 Residue-property plots

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.

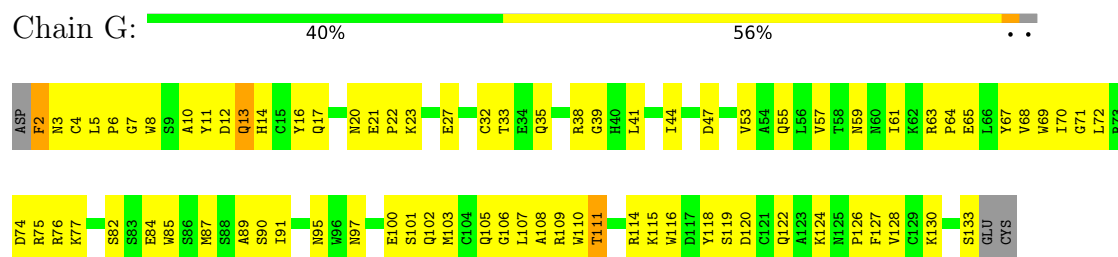
- Molecule 1: Snaclec rhodocetin subunit gamma



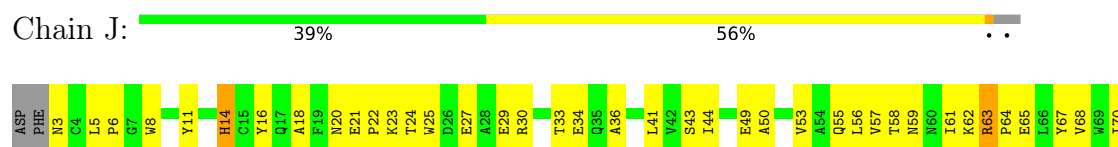
- Molecule 1: Snaclec rhodocetin subunit gamma



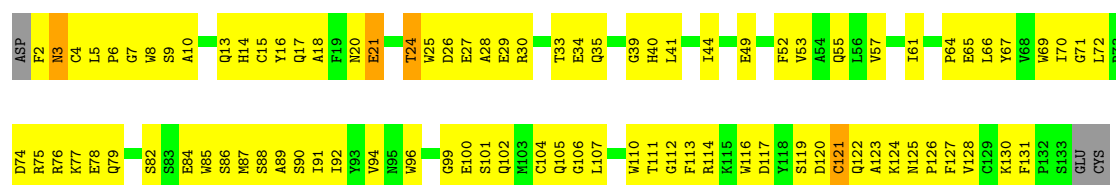
- Molecule 1: Snaclec rhodocetin subunit gamma



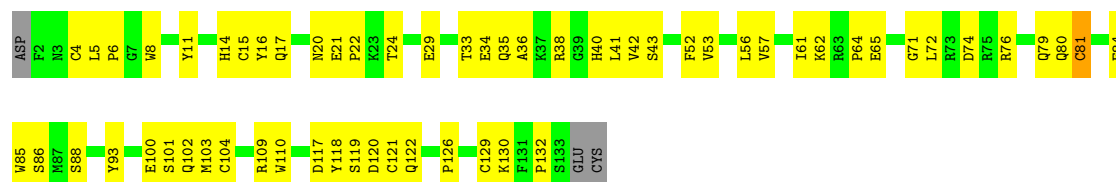
- Molecule 1: Snaclec rhodocetin subunit gamma



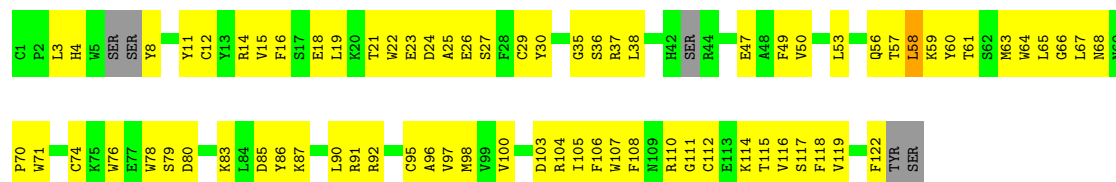
- Molecule 1: Snaclec rhodocetin subunit gamma



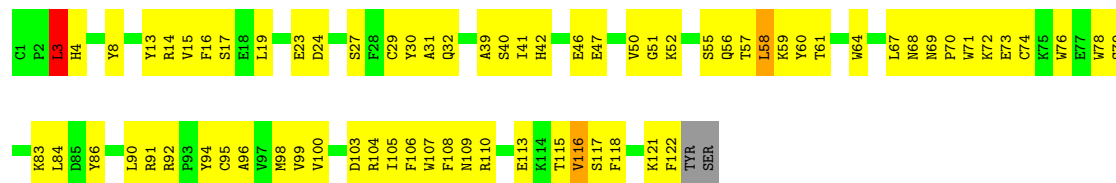
- Molecule 1: Snaclec rhodocetin subunit gamma



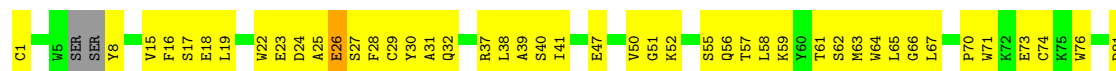
- Molecule 2: Snaclec rhodocetin subunit delta



- Molecule 2: Snaclec rhodocetin subunit delta

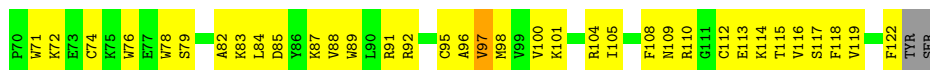
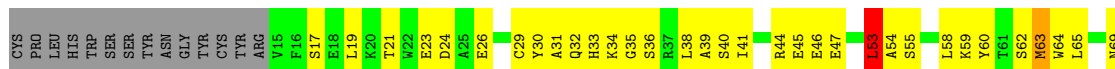


- Molecule 2: Snaclec rhodocetin subunit delta

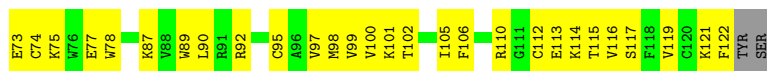
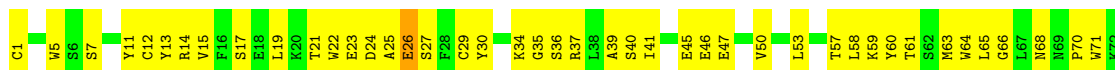




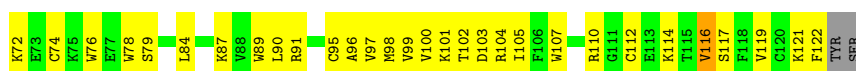
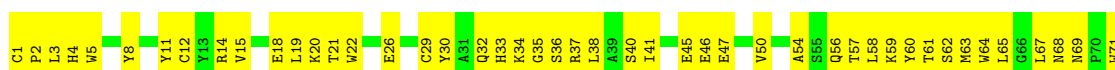
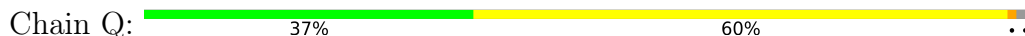
• Molecule 2: Snaclec rhodocetin subunit delta



• Molecule 2: Snaclec rhodocetin subunit delta



• Molecule 2: Snaclec rhodocetin subunit delta

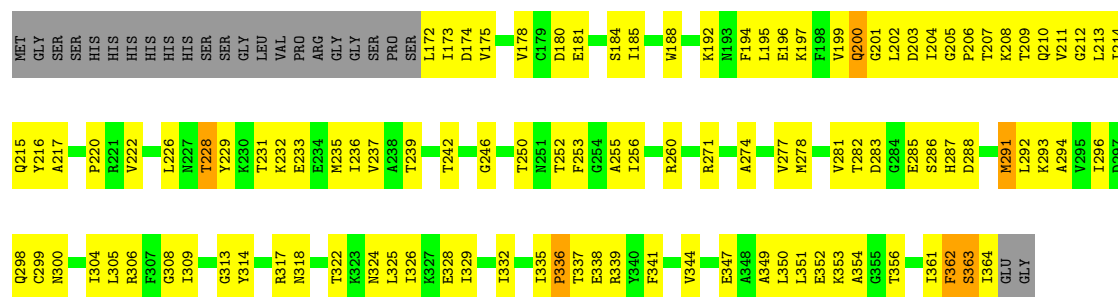


• Molecule 3: Integrin alpha-2



• Molecule 3: Integrin alpha-2

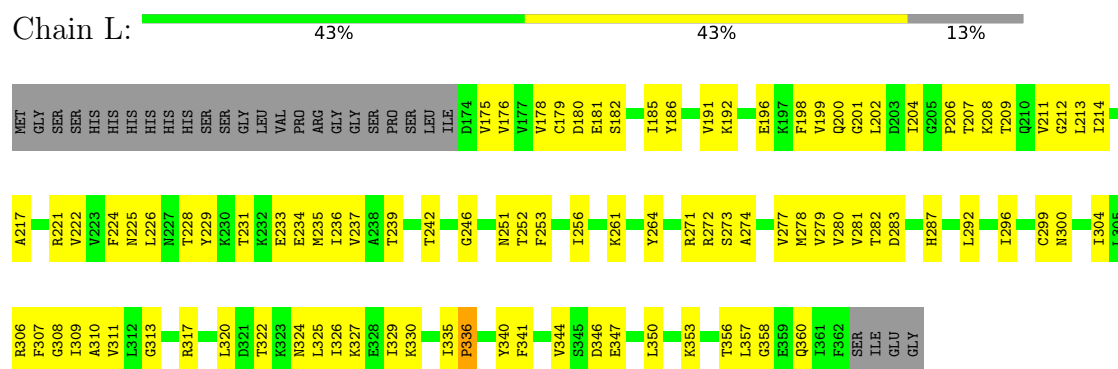




• Molecule 3: Integrin alpha-2



• Molecule 3: Integrin alpha-2



• Molecule 3: Integrin alpha-2



• Molecule 3: Integrin alpha-2

Chain R: 41% 45% 14%

MET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	PRO	ARG	GLY	GLY	SER	PRO	S171	L172	L173	ASP	V175	V176	V177	V178	C179	D180	E181	I185	Y186	E196	V199	Q200	G201	L202	D203	I1E	GLY	P206	T207	K208	T209	Q210	V211	G212	L213	I214	Q215	Y216	A217	R221	V222
V223	F224	N225	L226	N227	T228	Y229	E233	E234	N235	I236	V237	A238	T239	T242	S243	T244	Y245	G246	GLY	ASP	L249	T250	N251	T252	F253	I256	A259	A263	Y264	R271	R272	S273	A274	T275	R276	V277	N278	V279	V280	V281	T282	D283	S286	H287	L292	I304	L305	R306	I309					
A310	V311	L312	N318	A319	L320	D321	T322	L325	I326	K327	E328	I329	I335	P336	T337	E338	R339	Y340	F341	Y344	S345	D346	E347	A348	A349	E352	K353	A354	G355	T356	L357	G358	E359	Q360	I361	F362	SER	I1E	GLU	GLY														

4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	130.76Å 130.76Å 251.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.87 – 3.01 19.87 – 3.01	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.87-3.01) 99.6 (19.87-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.98Å)	Xtriage
Refinement program	PHENIX (1.10.1-2155_2155: ???)	Depositor
R, R_{free}	0.221 , 0.270 0.221 , 0.269	Depositor DCC
R_{free} test set	4301 reflections (2.97%)	wwPDB-VP
Wilson B-factor (Å ²)	71.1	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 60.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.467 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21018	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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: CL, MG, SO4, GOL, NA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.11	0/1036	0.32	0/1409
1	D	0.09	0/1053	0.38	0/1435
1	G	0.09	0/1096	0.33	0/1488
1	J	0.09	0/1077	0.32	0/1464
1	M	0.10	0/1072	0.40	0/1460
1	P	0.08	0/1090	0.31	0/1481
2	B	0.09	0/1018	0.41	2/1377 (0.1%)
2	E	0.10	0/1040	0.38	1/1410 (0.1%)
2	H	0.10	0/978	0.40	0/1330
2	K	0.11	0/913	0.43	0/1235
2	N	0.09	0/1064	0.33	0/1439
2	Q	0.09	0/1061	0.38	0/1435
3	C	0.11	0/1456	0.31	1/1976 (0.1%)
3	F	0.10	0/1465	0.35	1/1991 (0.1%)
3	I	0.14	0/1419	0.41	0/1937
3	L	0.09	0/1414	0.36	0/1927
3	O	0.11	0/1452	0.31	0/1976
3	R	0.09	0/1426	0.30	0/1936
All	All	0.10	0/21130	0.36	5/28706 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	M	0	1
2	E	0	1
2	K	0	2
3	F	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	I	0	1
All	All	0	8

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	LEU	CB-CA-C	-6.12	109.50	116.54
3	F	200	GLN	N-CA-C	5.40	119.56	112.92
2	B	58	LEU	CA-C-N	5.28	131.21	121.70
2	B	58	LEU	C-N-CA	5.28	131.21	121.70
3	C	200	GLN	N-CA-C	5.10	119.19	112.92

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	PHE	Peptide
2	E	58	LEU	Peptide
3	F	206	PRO	Peptide
3	F	207	THR	Peptide
3	I	202	LEU	Peptide
2	K	53	LEU	Peptide
2	K	55	SER	Peptide
1	M	3	ASN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1006	0	890	96	0
1	D	1022	0	879	73	0
1	G	1064	0	962	100	0
1	J	1046	0	938	100	0
1	M	1041	0	920	115	0
1	P	1058	0	944	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	987	0	922	83	0
2	E	1006	0	929	92	0
2	H	949	0	847	73	0
2	K	885	0	823	87	0
2	N	1029	0	976	83	0
2	Q	1026	0	967	96	0
3	C	1435	0	1384	123	0
3	F	1443	0	1387	120	0
3	I	1396	0	1294	121	0
3	L	1392	0	1323	113	0
3	O	1430	0	1367	136	0
3	R	1407	0	1358	103	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	4	0	0	0	0
4	D	3	0	0	0	0
4	E	3	0	0	0	0
4	F	2	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	2	0	0	0	0
4	J	2	0	0	0	0
4	L	2	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	3	0	0	0	0
4	P	1	0	0	0	0
4	Q	2	0	0	0	0
4	R	1	0	0	0	0
5	A	1	0	0	0	0
5	C	4	0	0	2	0
5	D	5	0	0	0	0
5	E	3	0	0	1	0
5	F	1	0	0	1	0
5	G	2	0	0	0	0
5	H	2	0	0	1	0
5	I	3	0	0	2	0
5	J	1	0	0	0	0
5	L	2	0	0	0	0
5	M	2	0	0	2	0
5	N	3	0	0	0	0
5	O	1	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	2	0	0	0	0
5	Q	2	0	0	0	0
5	R	1	0	0	0	0
6	A	6	0	8	0	0
6	C	6	0	8	0	0
6	G	12	8	16	0	0
6	H	6	0	8	1	0
6	J	12	0	16	11	0
6	P	6	0	8	0	0
7	C	1	0	0	0	0
7	F	1	0	0	0	0
7	I	1	0	0	0	0
7	L	1	0	0	0	0
7	O	1	0	0	0	0
7	R	1	0	0	0	0
8	C	5	0	0	0	0
8	D	5	0	0	1	0
8	E	5	0	0	1	0
8	F	10	0	0	1	0
8	I	5	0	0	0	0
8	L	5	0	0	2	0
8	O	10	0	0	5	0
8	R	5	0	0	0	0
9	A	16	0	0	10	0
9	B	7	0	0	5	0
9	C	15	0	0	8	0
9	D	19	0	0	6	0
9	E	9	0	0	6	0
9	F	11	0	0	10	0
9	G	16	0	0	10	0
9	H	7	0	0	5	0
9	I	16	0	0	6	0
9	J	10	0	0	5	0
9	K	8	0	0	11	0
9	L	17	0	0	6	0
9	M	6	0	0	3	0
9	N	7	0	0	5	0
9	O	20	0	0	16	0
9	P	6	0	0	2	0
9	Q	14	0	0	10	0
9	R	14	0	0	7	0
All	All	21010	8	19174	1683	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 42.

All (1683) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:PHE:HA	1:A:20:ASN:HB3	1.23	1.14
2:B:56:GLN:HG3	2:B:57:THR:HG23	1.35	1.08
1:A:87:MET:HB3	2:B:37:ARG:HD2	1.29	1.07
2:K:92:ARG:NH1	2:K:113:GLU:OE2	1.88	1.06
1:M:87:MET:HE2	1:M:89:ALA:HB3	1.39	1.05
3:I:199:VAL:O	3:I:201:GLY:N	1.90	1.03
3:C:343:ASN:HA	3:C:344:VAL:HB	1.39	1.02
3:I:196:GLU:O	3:I:199:VAL:HG12	1.58	1.02
2:Q:58:LEU:HA	2:Q:59:LYS:HB3	1.44	1.00
3:R:208:LYS:HG2	3:R:209:THR:HG23	1.41	1.00
1:A:64:PRO:HB2	1:A:66:LEU:HD11	1.47	0.96
3:F:184:SER:OG	3:F:283:ASP:OD2	1.83	0.96
1:D:102:GLN:HA	1:D:120:ASP:HA	1.47	0.95
3:O:203:ASP:HB2	3:O:204:ILE:HA	1.46	0.95
1:M:102:GLN:HA	1:M:120:ASP:HA	1.47	0.95
1:G:70:ILE:HD11	1:G:105:GLN:HG3	1.48	0.94
3:I:335:ILE:HG22	5:I:404:CL:CL	2.04	0.94
1:P:64:PRO:HA	1:P:65:GLU:HB2	1.50	0.94
2:H:16:PHE:CB	2:H:17:SER:HA	1.96	0.93
3:O:261:LYS:NZ	8:O:407:SO4:O4	2.01	0.93
1:A:19:PHE:HA	1:A:20:ASN:CB	1.98	0.93
3:C:178:VAL:HG12	3:C:214:ILE:HD11	1.52	0.92
3:C:273:SER:HB3	3:C:274:ALA:HB2	1.51	0.92
3:O:178:VAL:HG12	3:O:214:ILE:HD11	1.51	0.91
1:M:25:TRP:HB3	1:M:121:CYS:HB3	1.52	0.91
1:G:101:SER:HA	1:G:102:GLN:HB3	1.50	0.90
2:K:44:ARG:H	2:K:44:ARG:HD3	1.37	0.90
1:M:101:SER:HA	1:M:102:GLN:HB3	1.52	0.90
3:F:304:ILE:O	3:F:306:ARG:NH1	2.05	0.90
3:I:199:VAL:HG11	3:I:236:ILE:HG22	1.54	0.90
1:G:114:ARG:NH1	9:G:301:HOH:O	1.97	0.90
3:O:272:ARG:HB3	3:O:273:SER:O	1.72	0.89
1:P:101:SER:HA	1:P:102:GLN:HB3	1.54	0.89
3:R:175:VAL:HG12	3:R:277:VAL:HB	1.53	0.89
1:P:76:ARG:NH1	1:P:81:CYS:HB3	1.88	0.89
1:D:76:ARG:HD3	1:D:78:GLU:HB2	1.54	0.88
1:G:114:ARG:N	9:G:303:HOH:O	2.06	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:34:GLU:HG3	1:M:35:GLN:HG3	1.54	0.88
1:J:101:SER:HA	1:J:102:GLN:HB3	1.53	0.88
2:Q:3:LEU:HG	2:Q:4:HIS:H	1.39	0.88
2:H:59:LYS:NZ	5:H:203:CL:CL	2.44	0.87
1:D:87:MET:SD	2:E:42:HIS:NE2	2.47	0.87
3:L:261:LYS:NZ	9:L:501:HOH:O	2.03	0.86
1:A:101:SER:HA	1:A:102:GLN:HB3	1.55	0.86
3:I:173:ILE:HG13	3:I:209:THR:HG22	1.57	0.86
2:K:59:LYS:H	2:K:59:LYS:HD3	1.40	0.86
3:F:175:VAL:HG23	3:F:211:VAL:HG23	1.57	0.85
3:O:184:SER:OG	3:O:283:ASP:OD2	1.92	0.85
1:D:114:ARG:NH1	9:D:301:HOH:O	2.10	0.85
2:Q:58:LEU:HD23	2:Q:61:THR:HA	1.58	0.84
2:H:29:CYS:SG	9:H:304:HOH:O	2.35	0.84
1:J:44:ILE:HD13	6:J:204:GOL:HO2	1.42	0.84
1:G:65:GLU:HG3	1:G:126:PRO:HD3	1.57	0.83
1:A:47:ASP:OD2	1:G:115:LYS:NZ	2.12	0.83
2:K:65:LEU:N	9:K:203:HOH:O	2.11	0.82
1:M:102:GLN:HB2	1:M:120:ASP:HB2	1.60	0.82
2:B:30:TYR:HA	2:B:36:SER:HB3	1.62	0.82
1:D:87:MET:SD	2:E:40:SER:OG	2.36	0.82
1:D:102:GLN:OE1	2:E:91:ARG:NH1	2.12	0.82
2:B:83:LYS:H	2:B:83:LYS:HD3	1.45	0.82
2:Q:69:ASN:OD1	9:Q:301:HOH:O	1.98	0.82
3:C:232:LYS:NZ	9:C:502:HOH:O	2.12	0.81
1:J:64:PRO:HA	1:J:65:GLU:HB2	1.62	0.81
2:K:64:TRP:H	2:K:118:PHE:HA	1.43	0.81
3:L:272:ARG:H	3:L:273:SER:HA	1.45	0.81
3:C:272:ARG:HB3	3:C:273:SER:O	1.80	0.81
1:D:85:TRP:N	1:D:89:ALA:O	2.13	0.81
3:F:200:GLN:N	3:F:201:GLY:HA3	1.94	0.81
3:O:317:ARG:NH2	3:O:347:GLU:OE1	2.15	0.80
5:F:405:CL:CL	9:F:510:HOH:O	2.35	0.80
1:M:123:ALA:HB1	1:M:124:LYS:HB3	1.64	0.80
2:Q:58:LEU:HA	2:Q:59:LYS:CB	2.10	0.80
2:B:35:GLY:HA3	2:B:36:SER:HB2	1.63	0.80
3:C:184:SER:OG	3:C:283:ASP:OD2	1.99	0.79
3:C:175:VAL:HG23	3:C:211:VAL:HG23	1.64	0.79
1:G:70:ILE:HG13	1:G:72:LEU:H	1.46	0.79
3:O:361:ILE:HG13	9:O:505:HOH:O	1.81	0.79
2:E:68:ASN:ND2	8:E:207:SO4:O4	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:344:VAL:HG11	3:C:350:LEU:HD23	1.63	0.79
3:C:286:SER:OG	3:C:328:GLU:OE2	2.01	0.79
1:J:5:LEU:HD12	1:J:6:PRO:HD2	1.65	0.79
2:B:58:LEU:HB3	2:B:59:LYS:C	2.07	0.79
2:H:81:ASP:OD1	6:H:204:GOL:O1	2.00	0.79
2:N:12:CYS:H	2:N:122:PHE:HB2	1.47	0.79
3:F:199:VAL:C	3:F:201:GLY:HA3	2.08	0.79
2:N:100:VAL:HG13	2:N:105:ILE:HG12	1.64	0.79
2:Q:100:VAL:HG22	2:Q:102:THR:H	1.48	0.78
1:A:102:GLN:N	1:A:120:ASP:HA	1.97	0.78
2:K:21:THR:OG1	2:K:112:CYS:O	2.00	0.78
3:L:178:VAL:HG12	3:L:214:ILE:HD11	1.65	0.78
1:P:17:GLN:O	9:P:301:HOH:O	2.00	0.78
2:H:58:LEU:HA	2:H:59:LYS:HG2	1.65	0.78
3:O:273:SER:HB3	3:O:274:ALA:HB2	1.65	0.78
1:G:102:GLN:N	1:G:120:ASP:HA	2.00	0.77
1:A:68:VAL:O	9:A:301:HOH:O	2.03	0.77
3:I:199:VAL:HG13	3:I:200:GLN:H	1.50	0.77
3:L:344:VAL:HG21	3:L:350:LEU:HD23	1.67	0.77
2:K:29:CYS:HB2	2:K:32:GLN:HB2	1.65	0.77
2:Q:29:CYS:HA	2:Q:30:TYR:C	2.08	0.77
3:I:244:GLN:NE2	5:I:406:CL:CL	2.53	0.77
3:L:310:ALA:HB2	3:L:329:ILE:HG12	1.65	0.77
2:H:17:SER:OG	2:H:18:GLU:OE1	2.03	0.77
1:J:3:ASN:N	9:J:302:HOH:O	2.17	0.77
1:G:47:ASP:OD2	9:G:302:HOH:O	2.01	0.76
2:K:114:LYS:HD3	2:K:115:THR:H	1.50	0.76
1:P:102:GLN:N	1:P:120:ASP:HA	2.01	0.76
3:L:299:CYS:SG	9:L:511:HOH:O	2.42	0.76
2:Q:33:HIS:CE1	2:Q:122:PHE:HA	2.20	0.76
3:C:272:ARG:HB3	3:C:273:SER:C	2.10	0.76
2:K:17:SER:HA	2:K:58:LEU:HD11	1.67	0.76
3:O:185:ILE:HD11	3:O:283:ASP:HB2	1.67	0.76
3:O:203:ASP:CB	3:O:204:ILE:HA	2.16	0.76
3:C:199:VAL:C	3:C:201:GLY:HA3	2.11	0.76
1:J:44:ILE:HD13	6:J:204:GOL:O2	1.84	0.76
3:O:261:LYS:NZ	8:O:407:SO4:S	2.59	0.76
2:K:64:TRP:HB2	2:K:118:PHE:HB3	1.68	0.75
1:M:87:MET:O	1:M:88:SER:OG	2.05	0.75
3:O:214:ILE:HG22	3:O:222:VAL:HA	1.67	0.75
2:B:58:LEU:HD13	2:B:61:THR:HA	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:272:ARG:CB	3:I:273:SER:HB3	2.16	0.75
3:F:178:VAL:HG13	3:F:214:ILE:HD11	1.68	0.75
2:Q:56:GLN:HG2	2:Q:57:THR:H	1.52	0.75
2:N:17:SER:HB3	2:N:58:LEU:HB3	1.66	0.75
3:I:278:MET:HG3	3:I:306:ARG:CB	2.17	0.75
1:J:101:SER:OG	1:J:103:MET:HG2	1.86	0.75
1:M:104:CYS:HB2	1:M:119:SER:O	1.86	0.75
3:O:200:GLN:N	3:O:201:GLY:HA3	2.02	0.75
1:M:2:PHE:HB2	1:M:3:ASN:HA	1.67	0.75
1:M:101:SER:CA	1:M:102:GLN:HB3	2.17	0.75
1:J:33:THR:O	6:J:205:GOL:O1	2.03	0.74
3:C:313:GLY:O	3:C:317:ARG:HG3	1.87	0.74
3:L:214:ILE:HG22	3:L:222:VAL:HA	1.70	0.74
2:K:85:ASP:O	9:K:201:HOH:O	2.03	0.74
3:L:211:VAL:O	3:L:226:LEU:HA	1.87	0.74
3:L:304:ILE:O	3:L:306:ARG:NH1	2.21	0.74
2:N:35:GLY:N	2:N:36:SER:OG	2.21	0.74
1:M:24:THR:O	1:M:28:ALA:N	2.15	0.74
3:O:334:SER:OG	9:O:501:HOH:O	2.05	0.74
1:A:87:MET:CB	2:B:37:ARG:HD2	2.13	0.74
3:R:352:GLU:O	9:R:501:HOH:O	2.05	0.74
1:J:102:GLN:HA	1:J:119:SER:O	1.88	0.74
3:R:200:GLN:HA	3:R:201:GLY:C	2.11	0.74
1:A:102:GLN:OE1	2:B:91:ARG:NH2	2.21	0.73
1:M:102:GLN:HG3	1:M:120:ASP:N	2.03	0.73
1:G:2:PHE:N	1:G:133:SER:O	2.21	0.73
3:O:272:ARG:HB3	3:O:273:SER:C	2.13	0.73
2:E:73:GLU:OE1	2:E:73:GLU:N	2.21	0.73
1:A:19:PHE:CA	1:A:20:ASN:HB3	2.11	0.73
3:I:251:ASN:OD1	3:I:287:HIS:HB3	1.88	0.73
3:O:199:VAL:C	3:O:201:GLY:HA3	2.12	0.73
3:R:353:LYS:O	3:R:356:THR:HG22	1.88	0.73
2:H:50:VAL:HG12	2:H:63:MET:HE1	1.70	0.73
3:C:362:PHE:O	9:C:501:HOH:O	2.07	0.73
3:O:222:VAL:N	5:O:406:CL:CL	2.55	0.73
1:P:79:GLN:HG3	1:P:80:GLN:H	1.53	0.73
1:A:89:ALA:N	9:A:302:HOH:O	2.21	0.73
3:L:182:SER:OG	9:L:502:HOH:O	2.06	0.73
1:G:102:GLN:CA	1:G:120:ASP:HA	2.19	0.73
3:R:251:ASN:OD1	3:R:287:HIS:HB3	1.89	0.73
1:D:101:SER:HA	1:D:102:GLN:HB3	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:84:GLU:HB2	1:P:88:SER:HA	1.70	0.72
3:O:260:ARG:NH2	8:O:407:SO4:O1	2.21	0.72
1:A:67:TYR:O	1:A:126:PRO:HD2	1.87	0.72
2:B:15:VAL:HG22	2:B:119:VAL:HG12	1.69	0.72
3:F:325:LEU:O	9:F:501:HOH:O	2.07	0.72
2:H:1:CYS:SG	2:H:8:TYR:N	2.62	0.72
1:M:25:TRP:CB	1:M:121:CYS:HB3	2.19	0.72
1:P:102:GLN:H	1:P:120:ASP:HA	1.54	0.72
2:Q:41:ILE:CG2	2:Q:47:GLU:HB2	2.20	0.72
2:B:8:TYR:N	9:B:302:HOH:O	2.21	0.72
1:J:64:PRO:HD3	1:J:109:ARG:NH1	2.05	0.72
3:L:179:CYS:HA	3:L:281:VAL:HG22	1.72	0.72
3:C:197:LYS:HD2	3:C:200:GLN:HE21	1.54	0.72
1:A:114:ARG:NH1	9:A:303:HOH:O	2.22	0.72
3:F:172:LEU:N	9:F:504:HOH:O	2.22	0.72
3:F:215:GLN:OE1	9:F:502:HOH:O	2.08	0.72
2:B:21:THR:OG1	9:B:301:HOH:O	2.07	0.71
3:I:178:VAL:HG13	3:I:214:ILE:HD11	1.71	0.71
3:F:199:VAL:HG21	3:F:235:MET:HE3	1.70	0.71
3:F:205:GLY:O	3:F:208:LYS:HB2	1.90	0.71
3:O:226:LEU:O	9:O:502:HOH:O	2.08	0.71
2:N:59:LYS:HG3	2:N:60:TYR:H	1.55	0.71
3:C:353:LYS:O	3:C:356:THR:HG22	1.91	0.71
1:M:87:MET:HE2	1:M:89:ALA:CB	2.18	0.71
3:C:312:LEU:HD23	3:C:322:THR:HG21	1.72	0.71
1:G:115:LYS:HG3	2:H:88:VAL:CG1	2.21	0.71
3:F:185:ILE:HD11	3:F:283:ASP:HB3	1.72	0.71
1:M:13:GLN:O	1:M:14:HIS:ND1	2.23	0.71
3:O:286:SER:OG	3:O:328:GLU:OE2	2.08	0.71
3:F:352:GLU:OE1	3:F:353:LYS:NZ	2.24	0.71
1:D:101:SER:CA	1:D:102:GLN:HB3	2.21	0.70
2:K:97:VAL:HA	9:K:203:HOH:O	1.89	0.70
3:L:175:VAL:HG23	3:L:211:VAL:HG23	1.72	0.70
1:P:102:GLN:OE1	2:Q:91:ARG:NH1	2.19	0.70
2:N:100:VAL:N	9:N:301:HOH:O	2.18	0.70
2:B:65:LEU:HD13	2:B:98:MET:HE3	1.73	0.70
1:M:5:LEU:HD23	1:M:6:PRO:O	1.92	0.70
2:Q:33:HIS:HE1	2:Q:122:PHE:HA	1.55	0.70
2:H:19:LEU:HD22	2:H:117:SER:OG	1.92	0.70
3:O:355:GLY:O	3:O:359:GLU:HG2	1.91	0.70
3:I:334:SER:HB2	3:I:340:TYR:CE2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:79:SER:O	9:K:202:HOH:O	2.10	0.70
1:D:24:THR:HG23	1:D:27:GLU:H	1.54	0.70
2:K:29:CYS:HA	2:K:30:TYR:C	2.17	0.70
3:L:281:VAL:HG12	3:L:309:ILE:HB	1.72	0.70
2:Q:41:ILE:HG21	2:Q:47:GLU:HB2	1.74	0.70
1:D:57:VAL:O	1:D:61:ILE:N	2.24	0.70
2:Q:59:LYS:O	9:Q:302:HOH:O	2.09	0.70
3:C:273:SER:HB3	3:C:274:ALA:CB	2.22	0.69
1:G:57:VAL:HG13	1:G:61:ILE:HD12	1.74	0.69
3:C:272:ARG:H	3:C:273:SER:HA	1.57	0.69
1:G:5:LEU:HD12	1:G:6:PRO:HD2	1.74	0.69
1:D:64:PRO:HG3	1:D:109:ARG:HH22	1.56	0.69
1:G:63:ARG:HG3	1:G:65:GLU:HG2	1.75	0.69
3:O:199:VAL:HG21	3:O:235:MET:HE3	1.73	0.69
1:G:105:GLN:O	9:G:304:HOH:O	2.11	0.69
1:M:49:GLU:OE2	1:M:130:LYS:NZ	2.26	0.69
2:Q:38:LEU:HG	9:Q:306:HOH:O	1.92	0.69
3:R:233:GLU:O	3:R:236:ILE:HG13	1.92	0.69
1:A:102:GLN:H	1:A:120:ASP:HA	1.55	0.69
1:D:64:PRO:HA	1:D:65:GLU:HB2	1.74	0.69
2:H:52:LYS:O	2:H:56:GLN:HG3	1.91	0.69
3:O:357:LEU:O	9:O:503:HOH:O	2.10	0.69
3:F:204:ILE:HG12	3:F:235:MET:HE1	1.75	0.69
3:I:253:PHE:N	9:I:502:HOH:O	2.25	0.69
3:L:175:VAL:HG12	3:L:277:VAL:HB	1.73	0.69
3:F:178:VAL:HG22	3:F:214:ILE:HD11	1.73	0.69
3:O:197:LYS:HD3	3:O:200:GLN:HE21	1.57	0.69
3:F:214:ILE:HG22	3:F:222:VAL:HA	1.75	0.68
3:I:271:ARG:O	9:I:501:HOH:O	2.11	0.68
2:K:78:TRP:CD1	2:K:82:ALA:HB3	2.28	0.68
3:O:274:ALA:O	3:O:275:THR:HG22	1.93	0.68
2:Q:71:TRP:HA	2:Q:74:CYS:SG	2.33	0.68
1:A:19:PHE:O	1:A:126:PRO:HB3	1.92	0.68
3:F:313:GLY:O	3:F:317:ARG:HG3	1.92	0.68
3:I:281:VAL:HG22	3:I:309:ILE:HD12	1.75	0.68
3:L:308:GLY:O	3:L:341:PHE:HA	1.93	0.68
1:A:82:SER:OG	2:B:70:PRO:HA	1.93	0.68
3:L:202:LEU:HD12	3:L:202:LEU:O	1.93	0.68
2:Q:41:ILE:O	9:Q:303:HOH:O	2.10	0.68
1:J:14:HIS:HD2	1:J:130:LYS:HE3	1.57	0.68
1:J:64:PRO:HA	1:J:65:GLU:CB	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:218:ASN:N	9:O:508:HOH:O	2.26	0.68
3:F:203:ASP:HA	3:F:232:LYS:HE2	1.75	0.68
3:I:199:VAL:HG11	3:I:236:ILE:CG2	2.24	0.68
1:J:70:ILE:HG13	1:J:72:LEU:H	1.59	0.68
3:L:324:ASN:O	3:L:327:LYS:HG2	1.94	0.68
1:G:8:TRP:O	9:G:305:HOH:O	2.11	0.68
1:D:16:TYR:HE1	1:D:42:VAL:HG23	1.58	0.68
3:I:173:ILE:N	9:I:506:HOH:O	2.26	0.67
1:M:17:GLN:O	1:M:128:VAL:HG13	1.93	0.67
2:Q:101:LYS:O	2:Q:102:THR:OG1	2.12	0.67
1:A:69:TRP:CD1	1:A:125:ASN:HB2	2.30	0.67
1:D:29:GLU:OE2	1:D:41:LEU:HG	1.94	0.67
2:H:41:ILE:HG21	2:H:47:GLU:HB2	1.75	0.67
2:Q:114:LYS:NZ	9:Q:305:HOH:O	2.26	0.67
3:C:181:GLU:CD	3:C:245:TYR:HB3	2.20	0.67
1:J:50:ALA:HA	6:J:204:GOL:O2	1.94	0.67
1:J:41:LEU:HB3	1:J:70:ILE:O	1.94	0.67
3:I:175:VAL:HA	3:I:277:VAL:O	1.95	0.67
1:P:110:TRP:HE1	2:Q:90:LEU:HD23	1.59	0.67
1:M:35:GLN:N	1:M:35:GLN:OE1	2.27	0.67
3:F:328:GLU:HB3	9:F:501:HOH:O	1.94	0.67
3:F:329:ILE:HD13	9:F:501:HOH:O	1.93	0.67
2:Q:21:THR:OG1	2:Q:112:CYS:O	2.11	0.67
1:A:101:SER:OG	1:A:103:MET:HG2	1.93	0.67
1:G:65:GLU:HG3	1:G:126:PRO:CD	2.25	0.67
1:D:71:GLY:O	2:E:79:SER:N	2.26	0.66
1:G:89:ALA:O	1:G:90:SER:OG	2.11	0.66
3:I:272:ARG:H	3:I:273:SER:C	2.02	0.66
1:J:85:TRP:NE1	1:J:91:ILE:HD13	2.10	0.66
1:G:41:LEU:HB3	1:G:70:ILE:O	1.95	0.66
1:G:55:GLN:O	1:G:59:ASN:ND2	2.21	0.66
2:K:96:ALA:O	9:K:203:HOH:O	2.12	0.66
3:O:251:ASN:OD1	3:O:287:HIS:HB3	1.96	0.66
3:O:352:GLU:O	9:O:504:HOH:O	2.13	0.66
2:N:12:CYS:N	2:N:122:PHE:HB2	2.11	0.66
2:E:19:LEU:HD22	2:E:116:VAL:HA	1.78	0.66
1:G:63:ARG:CG	1:G:65:GLU:HG2	2.25	0.66
1:J:87:MET:HE1	2:K:38:LEU:O	1.96	0.66
3:I:173:ILE:HG22	3:I:275:THR:HG21	1.78	0.65
1:A:65:GLU:O	1:A:66:LEU:HD12	1.96	0.65
2:K:114:LYS:HD3	2:K:115:THR:N	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:360:GLN:OE1	9:O:505:HOH:O	2.14	0.65
1:P:102:GLN:HA	1:P:119:SER:O	1.96	0.65
2:Q:38:LEU:N	9:Q:306:HOH:O	2.28	0.65
2:Q:101:LYS:HE3	2:Q:104:ARG:NH2	2.11	0.65
3:L:175:VAL:HA	3:L:277:VAL:O	1.96	0.65
1:M:112:GLY:O	1:M:114:ARG:NH1	2.29	0.65
1:D:102:GLN:CA	1:D:120:ASP:HA	2.26	0.65
3:O:265:SER:O	3:O:270:GLY:N	2.28	0.65
1:A:66:LEU:HD13	1:A:126:PRO:HD2	1.77	0.65
1:A:101:SER:CA	1:A:102:GLN:HB3	2.25	0.65
1:M:2:PHE:HD1	1:M:3:ASN:HB3	1.62	0.65
2:B:103:ASP:OD1	2:B:104:ARG:HG2	1.96	0.65
2:K:30:TYR:HB3	2:K:31:ALA:HA	1.79	0.65
3:I:224:PHE:HB2	3:I:228:THR:HG21	1.78	0.65
3:L:179:CYS:HA	3:L:281:VAL:CG2	2.27	0.65
3:L:336:PRO:O	9:L:503:HOH:O	2.14	0.65
8:L:406:SO4:O4	9:L:502:HOH:O	2.13	0.65
3:C:279:VAL:HG22	3:C:307:PHE:HB2	1.78	0.65
3:C:184:SER:OG	9:C:503:HOH:O	2.14	0.65
3:F:175:VAL:HG12	3:F:277:VAL:HB	1.78	0.65
3:C:173:ILE:O	3:C:209:THR:HA	1.97	0.64
3:I:281:VAL:HG22	3:I:309:ILE:HB	1.79	0.64
1:M:84:GLU:HB2	1:M:88:SER:HA	1.79	0.64
3:O:175:VAL:HG23	3:O:211:VAL:HG23	1.78	0.64
3:C:312:LEU:HD23	3:C:322:THR:CG2	2.26	0.64
3:O:324:ASN:N	9:O:509:HOH:O	2.29	0.64
1:A:85:TRP:HB2	1:A:89:ALA:HB3	1.80	0.64
1:G:102:GLN:HA	1:G:119:SER:O	1.97	0.64
2:H:64:TRP:N	2:H:117:SER:O	2.25	0.64
2:Q:11:TYR:CD2	2:Q:122:PHE:HB3	2.32	0.64
1:A:42:VAL:HG12	9:A:306:HOH:O	1.97	0.64
1:M:17:GLN:OE1	1:M:18:ALA:N	2.30	0.64
1:M:16:TYR:CD2	1:M:130:LYS:HD2	2.33	0.64
3:I:199:VAL:C	3:I:201:GLY:H	1.98	0.64
1:J:101:SER:CA	1:J:102:GLN:HB3	2.25	0.64
2:B:30:TYR:CA	2:B:36:SER:HB3	2.28	0.64
3:O:204:ILE:HG12	3:O:235:MET:CE	2.28	0.64
3:O:264:TYR:OH	3:O:277:VAL:O	2.15	0.64
3:I:178:VAL:HG12	3:I:216:TYR:CE1	2.33	0.63
1:J:120:ASP:HB3	1:J:123:ALA:HB2	1.79	0.63
3:L:330:LYS:HE2	3:L:341:PHE:CZ	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:92:ARG:NH1	2:N:113:GLU:OE2	2.30	0.63
2:N:98:MET:HE3	2:N:105:ILE:HG21	1.80	0.63
1:P:100:GLU:O	1:P:102:GLN:HB3	1.97	0.63
3:R:173:ILE:HG13	3:R:209:THR:HG22	1.81	0.63
3:C:197:LYS:HA	3:C:200:GLN:NE2	2.12	0.63
1:J:67:TYR:HB2	1:J:125:ASN:ND2	2.13	0.63
3:O:199:VAL:CG2	3:O:235:MET:HE3	2.28	0.63
1:A:72:LEU:HD11	2:B:76:TRP:HB3	1.81	0.63
1:G:101:SER:CA	1:G:102:GLN:HB3	2.25	0.63
3:L:199:VAL:HG21	3:L:235:MET:HE3	1.79	0.63
1:D:24:THR:OG1	1:D:121:CYS:O	2.17	0.63
1:D:68:VAL:HA	1:D:126:PRO:O	1.99	0.63
3:I:173:ILE:HG22	3:I:275:THR:CG2	2.29	0.63
1:J:113:PHE:O	6:J:204:GOL:O3	2.10	0.63
2:Q:1:CYS:N	9:Q:307:HOH:O	2.32	0.63
1:A:87:MET:HB3	2:B:37:ARG:CD	2.19	0.63
2:B:58:LEU:CD1	2:B:61:THR:HA	2.29	0.63
2:N:23:GLU:O	2:N:27:SER:HB2	1.98	0.63
1:P:101:SER:CA	1:P:102:GLN:HB3	2.26	0.63
3:F:253:PHE:HB3	3:F:291:MET:HG2	1.80	0.63
3:I:296:ILE:O	3:I:300:ASN:N	2.31	0.63
3:O:196:GLU:O	3:O:200:GLN:HG2	1.99	0.63
3:O:335:ILE:HG13	3:O:336:PRO:HA	1.81	0.63
1:A:11:TYR:HB3	1:A:16:TYR:CE2	2.34	0.63
1:D:76:ARG:HG2	1:D:78:GLU:H	1.64	0.63
2:E:58:LEU:HA	2:E:59:LYS:CB	2.29	0.63
1:G:101:SER:OG	1:G:103:MET:HG2	1.98	0.63
1:J:64:PRO:HD3	1:J:109:ARG:HH12	1.63	0.63
1:J:89:ALA:O	9:J:301:HOH:O	2.16	0.63
2:N:19:LEU:HB3	2:N:115:THR:OG1	1.98	0.63
2:Q:58:LEU:HD23	2:Q:61:THR:CA	2.29	0.63
3:C:326:ILE:HG23	3:C:341:PHE:CZ	2.34	0.63
1:M:90:SER:OG	1:M:92:ILE:HG23	1.99	0.63
3:R:199:VAL:O	3:R:202:LEU:HB2	1.99	0.63
1:G:102:GLN:H	1:G:120:ASP:HA	1.62	0.63
1:J:118:TYR:CE2	2:K:91:ARG:HG2	2.33	0.63
2:K:26:GLU:N	2:K:26:GLU:OE1	2.31	0.63
3:O:211:VAL:O	3:O:226:LEU:HA	1.99	0.63
3:F:196:GLU:O	3:F:200:GLN:HG2	1.99	0.62
2:K:19:LEU:HD12	2:K:19:LEU:O	1.99	0.62
3:L:231:THR:HG22	3:L:234:GLU:OE1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:64:PRO:O	1:G:109:ARG:NH1	2.32	0.62
1:M:114:ARG:NH2	3:R:207:THR:O	2.31	0.62
1:D:102:GLN:HA	1:D:120:ASP:CA	2.26	0.62
2:H:61:THR:HB	2:H:100:VAL:HG22	1.81	0.62
2:K:64:TRP:HB2	2:K:118:PHE:CB	2.28	0.62
1:P:102:GLN:CA	1:P:120:ASP:HA	2.29	0.62
1:A:84:GLU:HG2	1:A:85:TRP:H	1.63	0.62
3:R:173:ILE:HD11	3:R:209:THR:HB	1.80	0.62
2:E:41:ILE:HG21	2:E:47:GLU:HB2	1.80	0.62
2:K:82:ALA:C	2:K:83:LYS:HD2	2.23	0.62
3:O:204:ILE:HG12	3:O:235:MET:HE1	1.81	0.62
1:A:5:LEU:HD12	1:A:6:PRO:HD2	1.80	0.62
3:C:312:LEU:N	3:C:345:SER:O	2.33	0.62
1:P:29:GLU:O	1:P:33:THR:HG23	2.00	0.62
1:P:34:GLU:HB2	1:P:35:GLN:HG3	1.82	0.62
3:R:259:ALA:O	3:R:263:ALA:HB3	2.00	0.62
1:G:7:GLY:O	1:G:17:GLN:NE2	2.33	0.62
1:J:20:ASN:OD1	1:J:61:ILE:HA	2.00	0.62
3:L:281:VAL:HG12	3:L:309:ILE:HD12	1.80	0.62
3:O:252:THR:O	3:O:256:ILE:HG13	2.00	0.62
1:P:61:ILE:O	1:P:62:LYS:HD2	2.00	0.62
3:R:215:GLN:NE2	3:R:242:THR:OG1	2.32	0.62
3:C:178:VAL:HG12	3:C:214:ILE:CD1	2.29	0.62
3:C:224:PHE:HB2	3:C:228:THR:HG21	1.81	0.62
3:O:192:LYS:O	3:O:196:GLU:HG3	1.99	0.62
3:O:353:LYS:O	3:O:356:THR:HG22	1.99	0.62
1:G:102:GLN:HA	1:G:120:ASP:HA	1.81	0.62
1:J:110:TRP:HB3	3:L:246:GLY:O	2.00	0.62
3:R:252:THR:O	3:R:256:ILE:HG13	1.99	0.62
1:G:20:ASN:OD1	1:G:61:ILE:HA	2.01	0.61
1:J:85:TRP:N	1:J:89:ALA:O	2.25	0.61
3:L:178:VAL:CG2	3:L:280:VAL:HG22	2.30	0.61
3:L:330:LYS:HE2	3:L:341:PHE:HZ	1.64	0.61
3:O:178:VAL:CG2	3:O:280:VAL:HG12	2.30	0.61
1:P:118:TYR:CD2	2:Q:91:ARG:HD2	2.35	0.61
1:M:86:SER:N	2:N:66:GLY:O	2.33	0.61
3:F:181:GLU:O	3:F:246:GLY:HA2	1.98	0.61
2:K:88:VAL:O	2:K:89:TRP:HB3	2.00	0.61
3:O:194:PHE:CD1	3:O:354:ALA:HB2	2.36	0.61
1:A:102:GLN:HA	1:A:119:SER:O	2.00	0.61
3:C:197:LYS:CD	3:C:200:GLN:HE21	2.12	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:41:ILE:HG12	2:H:65:LEU:HD11	1.82	0.61
2:K:64:TRP:N	2:K:118:PHE:HA	2.15	0.61
1:M:82:SER:OG	2:N:70:PRO:HA	1.99	0.61
3:O:272:ARG:H	3:O:273:SER:HA	1.63	0.61
3:R:271:ARG:HA	3:R:272:ARG:CB	2.29	0.61
1:A:102:GLN:CA	1:A:120:ASP:HA	2.30	0.61
3:F:172:LEU:HA	3:F:208:LYS:O	2.00	0.61
3:I:303:ASN:HA	3:I:304:ILE:HB	1.83	0.61
1:J:30:ARG:O	1:J:34:GLU:HG3	2.00	0.61
1:M:53:VAL:O	1:M:57:VAL:HG23	2.00	0.61
1:M:76:ARG:HG2	9:M:301:HOH:O	2.00	0.61
1:P:34:GLU:N	1:P:34:GLU:OE1	2.33	0.61
3:O:199:VAL:O	3:O:202:LEU:N	2.33	0.61
3:I:214:ILE:HG22	3:I:222:VAL:HA	1.83	0.61
3:L:322:THR:O	3:L:326:ILE:HD13	2.01	0.61
3:F:204:ILE:HG12	3:F:235:MET:CE	2.30	0.61
2:K:32:GLN:N	2:K:32:GLN:OE1	2.34	0.61
2:Q:98:MET:SD	2:Q:105:ILE:HD11	2.41	0.61
1:G:85:TRP:CG	2:H:40:SER:HG	2.19	0.60
3:L:185:ILE:HD11	3:L:283:ASP:HB2	1.82	0.60
3:R:211:VAL:C	3:R:226:LEU:HD23	2.26	0.60
2:B:15:VAL:HG22	2:B:119:VAL:CG1	2.30	0.60
2:B:23:GLU:HG2	9:B:301:HOH:O	2.01	0.60
1:D:102:GLN:HG3	1:D:119:SER:CA	2.32	0.60
2:E:58:LEU:HD22	2:E:60:TYR:O	2.01	0.60
1:M:74:ASP:O	9:M:301:HOH:O	2.16	0.60
3:C:343:ASN:HA	3:C:344:VAL:CB	2.16	0.60
2:E:83:LYS:H	2:E:83:LYS:HD3	1.66	0.60
2:H:26:GLU:OE2	2:H:26:GLU:N	2.34	0.60
1:M:34:GLU:HG3	1:M:35:GLN:HA	1.84	0.60
3:O:175:VAL:HA	3:O:277:VAL:O	2.02	0.60
1:A:24:THR:CB	1:A:25:TRP:HA	2.32	0.60
2:H:16:PHE:CB	2:H:17:SER:CA	2.75	0.60
3:I:173:ILE:HD12	3:I:173:ILE:O	2.01	0.60
1:D:82:SER:OG	2:E:70:PRO:HA	2.02	0.60
2:E:100:VAL:HG13	2:E:105:ILE:HG12	1.83	0.60
3:F:174:ASP:OD1	3:F:271:ARG:NH1	2.35	0.60
1:G:85:TRP:NE1	1:G:90:SER:O	2.35	0.60
1:J:91:ILE:HG12	9:J:301:HOH:O	2.00	0.60
3:R:178:VAL:CG2	3:R:280:VAL:HG12	2.31	0.60
2:B:14:ARG:NH1	2:B:15:VAL:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:55:GLN:O	1:J:59:ASN:ND2	2.18	0.60
3:O:275:THR:HG23	3:O:275:THR:O	2.01	0.60
5:O:406:CL:CL	3:R:227:ASN:ND2	2.72	0.60
3:I:325:LEU:HD23	3:I:329:ILE:HD13	1.83	0.60
3:R:207:THR:CG2	3:R:208:LYS:HB2	2.32	0.60
1:G:23:LYS:HB3	1:G:27:GLU:HG2	1.83	0.60
1:J:14:HIS:CD2	1:J:130:LYS:HE3	2.36	0.60
2:K:97:VAL:HG11	2:K:108:PHE:CZ	2.37	0.60
2:Q:56:GLN:HG2	2:Q:57:THR:N	2.15	0.60
3:R:214:ILE:HG23	3:R:221:ARG:O	2.02	0.60
1:A:95:ASN:ND2	2:B:105:ILE:O	2.34	0.60
3:C:355:GLY:O	3:C:359:GLU:HG2	2.01	0.60
3:F:173:ILE:HD12	3:F:173:ILE:O	2.02	0.60
3:I:252:THR:O	3:I:256:ILE:HG13	2.02	0.60
1:M:4:CYS:HB2	1:M:10:ALA:HB2	1.84	0.60
3:C:175:VAL:HA	3:C:277:VAL:O	2.02	0.59
2:E:58:LEU:HB3	2:E:59:LYS:HB3	1.83	0.59
3:F:199:VAL:CG2	3:F:235:MET:HE3	2.32	0.59
1:J:85:TRP:CD1	2:K:40:SER:HG	2.20	0.59
3:O:185:ILE:CD1	3:O:283:ASP:HB2	2.32	0.59
1:P:74:ASP:HB3	1:P:103:MET:CE	2.32	0.59
2:Q:101:LYS:HB3	9:Q:304:HOH:O	2.02	0.59
2:B:85:ASP:OD1	2:B:86:TYR:N	2.32	0.59
1:D:100:GLU:C	1:D:102:GLN:HB3	2.27	0.59
3:O:175:VAL:HG12	3:O:277:VAL:HB	1.84	0.59
2:Q:98:MET:HE2	2:Q:107:TRP:HE1	1.66	0.59
3:L:186:TYR:N	3:L:347:GLU:OE1	2.24	0.59
1:M:2:PHE:CB	1:M:3:ASN:HA	2.30	0.59
1:M:8:TRP:CZ3	1:M:130:LYS:HA	2.37	0.59
3:R:215:GLN:OE1	3:R:221:ARG:NH2	2.35	0.59
2:E:69:ASN:OD1	2:E:72:LYS:N	2.36	0.59
3:L:224:PHE:HB2	3:L:228:THR:HG21	1.83	0.59
1:M:87:MET:HE1	2:N:40:SER:CB	2.32	0.59
3:R:329:ILE:HG22	3:R:341:PHE:HD1	1.67	0.59
3:F:363:SER:OG	3:F:364:ILE:HA	2.03	0.59
2:H:24:ASP:O	2:H:28:PHE:HB2	2.03	0.59
1:M:65:GLU:CB	1:M:126:PRO:HD3	2.33	0.59
3:O:337:THR:O	3:O:340:TYR:N	2.36	0.59
1:P:35:GLN:OE1	1:P:35:GLN:N	2.36	0.59
1:J:16:TYR:CE2	1:J:130:LYS:HD2	2.38	0.59
2:Q:41:ILE:HG13	2:Q:98:MET:HE1	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:212:GLY:N	3:C:226:LEU:HD23	2.18	0.59
3:C:252:THR:O	3:C:256:ILE:HG13	2.03	0.59
2:H:98:MET:HE2	2:H:107:TRP:HE1	1.67	0.59
2:K:109:ASN:ND2	9:K:205:HOH:O	2.23	0.59
3:C:219:ASN:O	9:C:505:HOH:O	2.16	0.58
3:F:253:PHE:CB	3:F:291:MET:HG2	2.33	0.58
1:A:64:PRO:HB2	1:A:66:LEU:CD1	2.27	0.58
3:C:310:ALA:O	3:C:343:ASN:HB2	2.04	0.58
3:F:178:VAL:HG13	3:F:214:ILE:CD1	2.33	0.58
2:K:44:ARG:HD3	2:K:44:ARG:N	2.15	0.58
1:D:81:CYS:HB3	2:E:73:GLU:O	2.03	0.58
1:D:83:SER:O	1:D:90:SER:HA	2.03	0.58
2:E:92:ARG:NH1	2:E:113:GLU:OE2	2.32	0.58
1:G:23:LYS:N	1:G:124:LYS:HB3	2.18	0.58
2:H:50:VAL:HG12	2:H:63:MET:CE	2.32	0.58
3:R:179:CYS:HA	3:R:281:VAL:CG1	2.32	0.58
3:O:243:SER:HB2	3:R:234:GLU:OE2	2.04	0.58
3:F:185:ILE:CD1	3:F:283:ASP:HB3	2.32	0.58
3:F:317:ARG:NH2	3:F:347:GLU:OE1	2.37	0.58
2:N:1:CYS:N	9:N:302:HOH:O	2.36	0.58
1:P:61:ILE:C	1:P:62:LYS:HD2	2.28	0.58
3:R:310:ALA:HB1	3:R:325:LEU:CD2	2.33	0.58
3:C:343:ASN:CA	3:C:344:VAL:HB	2.26	0.58
3:F:328:GLU:O	3:F:332:ILE:HG13	2.03	0.58
3:F:364:ILE:O	9:F:503:HOH:O	2.17	0.58
2:H:73:GLU:OE1	2:H:73:GLU:N	2.36	0.58
1:M:91:ILE:HG22	1:M:91:ILE:O	2.03	0.58
1:A:87:MET:HG3	9:A:302:HOH:O	2.04	0.58
2:B:21:THR:HG23	2:B:24:ASP:H	1.67	0.58
2:H:22:TRP:HH2	2:H:67:LEU:H	1.51	0.58
3:C:215:GLN:HG3	3:C:223:VAL:HG21	1.84	0.58
1:G:35:GLN:OE1	1:G:35:GLN:N	2.26	0.58
1:J:44:ILE:HG21	6:J:204:GOL:O2	2.02	0.58
3:L:272:ARG:H	3:L:273:SER:CA	2.16	0.58
1:A:64:PRO:O	1:A:66:LEU:HG	2.03	0.58
1:G:70:ILE:HG12	9:G:304:HOH:O	2.03	0.58
1:J:18:ALA:HB2	1:J:56:LEU:HD22	1.86	0.58
1:J:43:SER:HA	2:K:78:TRP:CZ3	2.38	0.58
1:J:102:GLN:N	1:J:120:ASP:HA	2.19	0.58
3:L:178:VAL:HG12	3:L:214:ILE:CD1	2.32	0.58
1:M:102:GLN:HG3	1:M:119:SER:C	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:173:ILE:HG13	3:R:209:THR:CG2	2.33	0.58
2:B:58:LEU:HD13	2:B:61:THR:CA	2.33	0.57
3:I:178:VAL:HG12	3:I:216:TYR:CD1	2.39	0.57
3:R:199:VAL:CG2	3:R:235:MET:HE3	2.33	0.57
1:D:5:LEU:HD23	1:D:6:PRO:N	2.20	0.57
3:F:349:ALA:O	3:F:352:GLU:HG3	2.04	0.57
3:L:252:THR:O	3:L:256:ILE:HG13	2.03	0.57
1:G:23:LYS:HE3	1:G:27:GLU:HG2	1.85	0.57
3:I:173:ILE:CG1	3:I:209:THR:HG22	2.33	0.57
2:N:110:ARG:NH1	8:O:402:SO4:O3	2.37	0.57
3:R:176:VAL:HG12	3:R:264:TYR:OH	2.05	0.57
1:A:22:PRO:HB3	1:A:126:PRO:HA	1.85	0.57
3:F:325:LEU:HD12	9:F:501:HOH:O	2.03	0.57
1:M:34:GLU:HG3	1:M:35:GLN:CG	2.32	0.57
2:B:110:ARG:NH1	2:B:114:LYS:HB3	2.20	0.57
3:F:344:VAL:HG21	3:F:350:LEU:HD23	1.87	0.57
1:M:72:LEU:HB2	2:N:78:TRP:CZ3	2.40	0.57
1:P:5:LEU:HD12	1:P:6:PRO:HD2	1.85	0.57
1:A:22:PRO:O	1:A:23:LYS:NZ	2.38	0.57
1:A:90:SER:HB2	1:A:92:ILE:HD11	1.86	0.57
2:E:103:ASP:OD1	2:E:104:ARG:N	2.33	0.57
2:Q:15:VAL:HA	2:Q:119:VAL:HG12	1.87	0.57
1:A:110:TRP:HZ2	2:B:90:LEU:HD11	1.69	0.57
1:M:102:GLN:HG2	1:M:102:GLN:O	2.04	0.57
1:M:105:GLN:HA	1:M:117:ASP:O	2.05	0.57
3:O:233:GLU:O	3:O:236:ILE:HG13	2.05	0.57
3:I:199:VAL:HG13	3:I:200:GLN:N	2.18	0.56
3:I:206:PRO:HA	3:I:210:GLN:HG3	1.86	0.56
3:I:296:ILE:HA	3:I:299:CYS:SG	2.45	0.56
3:L:204:ILE:HA	3:L:209:THR:O	2.05	0.56
2:Q:58:LEU:CD2	2:Q:61:THR:HA	2.31	0.56
3:R:310:ALA:HB1	3:R:325:LEU:HD21	1.87	0.56
3:R:335:ILE:HA	3:R:336:PRO:C	2.29	0.56
1:D:34:GLU:OE2	1:D:34:GLU:N	2.36	0.56
3:F:173:ILE:HD12	3:F:209:THR:HB	1.86	0.56
1:J:70:ILE:HD11	1:J:105:GLN:CB	2.35	0.56
2:K:29:CYS:CB	2:K:32:GLN:HB2	2.32	0.56
1:M:3:ASN:OD1	1:M:5:LEU:HA	2.05	0.56
2:N:21:THR:HG23	2:N:24:ASP:H	1.70	0.56
2:N:92:ARG:HE	3:O:249:LEU:HD21	1.70	0.56
1:G:87:MET:HE2	2:H:37:ARG:CB	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:301:HIS:C	3:I:303:ASN:H	2.14	0.56
2:N:35:GLY:N	2:N:36:SER:CB	2.69	0.56
3:O:260:ARG:NH2	3:O:298:GLN:OE1	2.37	0.56
2:Q:58:LEU:HD23	2:Q:60:TYR:O	2.06	0.56
3:F:228:THR:HG23	3:F:229:TYR:H	1.70	0.56
3:F:239:THR:O	3:F:242:THR:HG22	2.06	0.56
1:G:44:ILE:HB	1:G:116:TRP:HZ2	1.70	0.56
2:N:14:ARG:NH1	2:N:15:VAL:O	2.38	0.56
2:N:87:LYS:HB3	2:N:89:TRP:CH2	2.40	0.56
1:A:22:PRO:HB3	1:A:126:PRO:CA	2.36	0.56
3:F:236:ILE:HD12	3:F:237:VAL:N	2.21	0.56
1:M:84:GLU:C	1:M:91:ILE:HD11	2.31	0.56
2:B:50:VAL:HG22	2:B:63:MET:HE1	1.86	0.56
3:F:194:PHE:CD1	3:F:354:ALA:HB2	2.41	0.56
1:J:85:TRP:CG	2:K:40:SER:HG	2.24	0.56
2:K:21:THR:HG23	2:K:24:ASP:H	1.71	0.56
3:O:356:THR:N	9:O:504:HOH:O	2.19	0.56
3:R:202:LEU:O	3:R:203:ASP:HB2	2.05	0.56
3:R:329:ILE:HG22	3:R:341:PHE:CD1	2.41	0.56
2:E:71:TRP:HA	2:E:74:CYS:SG	2.46	0.56
1:M:21:GLU:N	1:M:21:GLU:OE1	2.39	0.56
2:Q:69:ASN:ND2	2:Q:72:LYS:HD3	2.20	0.56
1:A:22:PRO:HB3	1:A:126:PRO:N	2.21	0.56
3:C:206:PRO:HA	3:C:210:GLN:NE2	2.21	0.56
2:E:121:LYS:HG2	2:E:122:PHE:H	1.69	0.56
2:H:22:TRP:HA	2:H:25:ALA:HB3	1.88	0.56
3:O:202:LEU:HB2	3:O:204:ILE:CG2	2.36	0.56
2:E:58:LEU:HA	2:E:59:LYS:HB3	1.88	0.55
3:F:300:ASN:OD1	3:F:306:ARG:NH2	2.38	0.55
3:F:353:LYS:O	3:F:356:THR:HG22	2.06	0.55
3:O:197:LYS:HG3	3:O:351:LEU:HD11	1.88	0.55
1:P:38:ARG:O	1:P:132:PRO:HD2	2.06	0.55
2:B:97:VAL:HG12	2:B:108:PHE:O	2.06	0.55
2:E:76:TRP:O	2:E:84:LEU:HD22	2.05	0.55
1:P:110:TRP:HA	3:R:245:TYR:CE2	2.41	0.55
3:R:213:LEU:HD23	3:R:223:VAL:HG11	1.88	0.55
1:A:83:SER:HA	1:A:91:ILE:HD11	1.87	0.55
1:D:133:SER:O	9:D:302:HOH:O	2.18	0.55
1:G:5:LEU:CD1	1:G:6:PRO:HD2	2.36	0.55
1:G:120:ASP:OD2	1:G:122:GLN:HB2	2.06	0.55
3:L:281:VAL:HG12	3:L:309:ILE:CB	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:47:GLU:HG2	2:Q:105:ILE:HD13	1.87	0.55
1:A:22:PRO:HB3	1:A:125:ASN:C	2.32	0.55
3:I:303:ASN:CA	3:I:304:ILE:HB	2.35	0.55
2:Q:87:LYS:O	2:Q:87:LYS:HD3	2.06	0.55
3:R:322:THR:O	3:R:326:ILE:HD13	2.07	0.55
1:A:17:GLN:O	1:A:128:VAL:HG13	2.07	0.55
2:E:110:ARG:NH1	3:F:314:TYR:HE2	2.04	0.55
3:F:199:VAL:HG13	3:F:236:ILE:HG22	1.88	0.55
2:H:55:SER:HA	2:H:61:THR:HG21	1.87	0.55
1:J:99:GLY:HA2	1:J:120:ASP:OD2	2.06	0.55
3:L:341:PHE:CG	3:L:341:PHE:O	2.60	0.55
2:Q:65:LEU:HD11	2:Q:98:MET:HB2	1.87	0.55
3:F:173:ILE:CD1	3:F:209:THR:HB	2.37	0.55
2:H:116:VAL:HG13	9:H:305:HOH:O	2.07	0.55
1:M:64:PRO:HA	1:M:65:GLU:C	2.30	0.55
3:R:173:ILE:HG12	3:R:361:ILE:HG21	1.88	0.55
1:D:118:TYR:CE1	2:E:91:ARG:HB3	2.42	0.55
3:F:233:GLU:O	3:F:236:ILE:HG13	2.06	0.55
3:I:206:PRO:HA	3:I:210:GLN:CG	2.36	0.55
3:C:236:ILE:HD12	3:C:237:VAL:N	2.22	0.55
1:J:105:GLN:HE21	1:J:118:TYR:HE1	1.54	0.55
3:O:221:ARG:HA	5:O:406:CL:CL	2.43	0.55
3:O:360:GLN:HB3	9:O:505:HOH:O	2.06	0.55
2:H:63:MET:O	2:H:97:VAL:HG23	2.07	0.55
3:I:188:TRP:NE1	9:I:507:HOH:O	2.37	0.55
1:M:20:ASN:HB2	1:M:21:GLU:OE1	2.06	0.55
1:P:8:TRP:CD2	1:P:17:GLN:HB2	2.42	0.55
2:Q:1:CYS:SG	2:Q:2:PRO:HD2	2.47	0.55
2:Q:41:ILE:HG13	2:Q:98:MET:CE	2.36	0.55
2:E:15:VAL:O	9:E:301:HOH:O	2.18	0.54
2:E:57:THR:HG21	9:E:301:HOH:O	2.06	0.54
2:E:57:THR:HB	2:E:58:LEU:HD12	1.89	0.54
3:L:335:ILE:HA	3:L:336:PRO:C	2.31	0.54
1:P:33:THR:OG1	1:P:34:GLU:OE1	2.21	0.54
2:B:58:LEU:HD13	2:B:60:TYR:C	2.33	0.54
3:C:312:LEU:HD13	3:C:345:SER:HA	1.88	0.54
3:F:363:SER:H	3:F:364:ILE:HA	1.72	0.54
3:L:300:ASN:OD1	3:L:306:ARG:NH2	2.40	0.54
3:O:233:GLU:O	3:O:237:VAL:HG23	2.07	0.54
2:Q:98:MET:HE2	2:Q:107:TRP:NE1	2.22	0.54
3:I:203:ASP:O	3:I:209:THR:OG1	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:335:ILE:HG13	3:I:336:PRO:HA	1.89	0.54
3:L:236:ILE:HD12	3:L:237:VAL:N	2.22	0.54
2:B:61:THR:OG1	2:B:100:VAL:HG22	2.07	0.54
3:I:181:GLU:O	3:I:246:GLY:HA2	2.07	0.54
2:N:46:GLU:O	2:N:50:VAL:HG22	2.07	0.54
3:C:181:GLU:OE1	3:C:245:TYR:HB3	2.05	0.54
3:I:353:LYS:O	3:I:356:THR:HG22	2.08	0.54
1:G:12:ASP:OD1	1:G:13:GLN:N	2.41	0.54
1:G:72:LEU:O	1:G:105:GLN:HG2	2.08	0.54
1:J:11:TYR:HB3	1:J:16:TYR:CE1	2.42	0.54
1:J:83:SER:O	1:J:91:ILE:HG12	2.07	0.54
2:N:65:LEU:HG	2:N:66:GLY:H	1.72	0.54
1:P:129:CYS:N	9:P:301:HOH:O	2.05	0.54
1:J:24:THR:HB	1:J:122:GLN:HA	1.88	0.54
2:N:1:CYS:SG	2:N:7:SER:HB3	2.48	0.54
2:B:63:MET:O	2:B:97:VAL:HG23	2.08	0.54
1:D:76:ARG:HG2	1:D:78:GLU:N	2.22	0.54
2:E:83:LYS:HD3	2:E:83:LYS:N	2.22	0.54
1:G:70:ILE:HG12	1:G:105:GLN:O	2.08	0.54
2:K:64:TRP:H	2:K:118:PHE:CA	2.18	0.54
3:R:338:GLU:C	3:R:340:TYR:H	2.16	0.54
1:A:2:PHE:HB2	1:A:3:ASN:HA	1.89	0.54
1:G:72:LEU:HD11	2:H:76:TRP:HB3	1.88	0.54
3:O:297:ASP:HB2	9:O:511:HOH:O	2.08	0.54
2:Q:26:GLU:HA	9:Q:306:HOH:O	2.08	0.54
3:R:228:THR:HG23	3:R:229:TYR:CD2	2.43	0.54
1:A:114:ARG:NH1	9:G:301:HOH:O	2.41	0.54
2:N:101:LYS:HG3	2:N:102:THR:H	1.72	0.54
3:O:213:LEU:HD21	9:O:510:HOH:O	2.08	0.54
1:D:102:GLN:HG3	1:D:119:SER:N	2.23	0.53
3:I:239:THR:O	3:I:242:THR:HG22	2.07	0.53
3:O:188:TRP:CD2	3:O:244:GLN:HB2	2.42	0.53
3:F:361:ILE:HG22	3:F:361:ILE:O	2.08	0.53
1:M:99:GLY:O	1:M:102:GLN:HB2	2.08	0.53
3:R:202:LEU:O	3:R:203:ASP:CB	2.57	0.53
3:R:215:GLN:HG3	3:R:223:VAL:HG21	1.90	0.53
2:B:30:TYR:CB	2:B:36:SER:HB3	2.38	0.53
2:H:67:LEU:HD23	2:H:70:PRO:HG3	1.90	0.53
1:P:16:TYR:CE2	1:P:130:LYS:HD2	2.43	0.53
1:A:72:LEU:HD23	1:A:105:GLN:OE1	2.08	0.53
2:B:58:LEU:HD13	2:B:60:TYR:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:97:ASN:OD1	1:J:98:THR:N	2.42	0.53
3:L:251:ASN:OD1	3:L:287:HIS:HB3	2.09	0.53
1:M:64:PRO:HA	1:M:65:GLU:CB	2.38	0.53
2:N:24:ASP:HA	2:N:27:SER:HB3	1.89	0.53
1:P:11:TYR:HB3	1:P:16:TYR:CE1	2.44	0.53
2:Q:110:ARG:NH1	3:R:320:LEU:HD13	2.23	0.53
3:R:185:ILE:HD11	3:R:283:ASP:HB2	1.89	0.53
3:C:206:PRO:HA	3:C:210:GLN:HE21	1.72	0.53
1:D:102:GLN:O	1:D:102:GLN:HG2	2.08	0.53
3:F:211:VAL:O	3:F:226:LEU:HA	2.08	0.53
3:F:361:ILE:O	3:F:363:SER:HA	2.08	0.53
1:G:100:GLU:O	1:G:102:GLN:HB3	2.08	0.53
3:L:281:VAL:CG1	3:L:309:ILE:HD12	2.38	0.53
3:L:335:ILE:O	3:L:340:TYR:HE2	1.92	0.53
2:B:58:LEU:CB	2:B:59:LYS:C	2.80	0.53
3:F:252:THR:O	3:F:256:ILE:HG13	2.09	0.53
1:G:70:ILE:HG12	1:G:106:GLY:HA2	1.90	0.53
3:I:228:THR:HG23	3:I:229:TYR:CD2	2.44	0.53
3:I:236:ILE:HD12	3:I:237:VAL:N	2.24	0.53
2:Q:15:VAL:HG12	2:Q:119:VAL:HG12	1.91	0.53
3:R:179:CYS:HA	3:R:281:VAL:HG13	1.89	0.53
2:E:67:LEU:HD12	2:E:67:LEU:O	2.09	0.53
1:G:12:ASP:OD1	1:G:14:HIS:ND1	2.29	0.53
1:P:102:GLN:HA	1:P:120:ASP:HA	1.91	0.53
2:Q:22:TRP:CZ2	2:Q:68:ASN:HB3	2.43	0.53
1:A:100:GLU:O	1:A:102:GLN:HB3	2.09	0.53
2:B:18:GLU:OE1	2:B:18:GLU:N	2.38	0.53
3:C:339:ARG:NH2	5:C:407:CL:CL	2.79	0.53
1:D:99:GLY:O	1:D:100:GLU:HB2	2.09	0.53
3:F:175:VAL:O	3:F:211:VAL:HA	2.09	0.53
1:G:116:TRP:HB2	2:H:88:VAL:O	2.09	0.53
3:I:225:ASN:O	3:I:228:THR:HG22	2.09	0.53
3:L:233:GLU:O	3:L:236:ILE:HG13	2.08	0.53
2:B:98:MET:HG3	2:B:107:TRP:CD1	2.44	0.53
3:F:210:GLN:HG3	3:F:271:ARG:HH22	1.74	0.53
3:F:294:ALA:O	3:F:298:GLN:HG3	2.09	0.53
3:F:335:ILE:HA	3:F:337:THR:H	1.73	0.53
3:C:175:VAL:HG23	3:C:211:VAL:CG2	2.37	0.53
3:C:271:ARG:HB3	3:C:272:ARG:HB2	1.91	0.53
2:E:69:ASN:N	2:E:94:TYR:O	2.39	0.53
3:F:192:LYS:O	3:F:196:GLU:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:85:TRP:CE2	1:G:91:ILE:HD13	2.44	0.53
3:L:310:ALA:HB1	3:L:325:LEU:HD21	1.90	0.53
3:C:312:LEU:HD23	3:C:322:THR:CB	2.39	0.52
3:F:363:SER:CB	3:F:364:ILE:HA	2.38	0.52
1:G:82:SER:HB2	2:H:70:PRO:HA	1.91	0.52
1:M:34:GLU:CG	1:M:35:GLN:HA	2.38	0.52
3:I:303:ASN:HA	3:I:304:ILE:CB	2.38	0.52
2:K:71:TRP:HA	2:K:74:CYS:SG	2.48	0.52
2:N:63:MET:O	2:N:97:VAL:HG13	2.09	0.52
2:N:110:ARG:NE	2:N:114:LYS:HG3	2.24	0.52
1:P:79:GLN:O	1:P:103:MET:HG3	2.09	0.52
2:B:47:GLU:OE1	2:B:107:TRP:NE1	2.43	0.52
3:F:173:ILE:HA	3:F:274:ALA:O	2.08	0.52
3:I:322:THR:O	3:I:326:ILE:HD13	2.10	0.52
2:N:5:TRP:CD2	2:N:14:ARG:HB2	2.45	0.52
2:B:26:GLU:OE1	2:B:38:LEU:HG	2.10	0.52
3:F:188:TRP:HD1	3:F:192:LYS:HE3	1.75	0.52
2:Q:22:TRP:CH2	2:Q:68:ASN:HB3	2.45	0.52
1:G:65:GLU:CG	1:G:126:PRO:HD3	2.36	0.52
1:J:72:LEU:HD11	2:K:76:TRP:HB3	1.91	0.52
3:L:279:VAL:HG22	3:L:307:PHE:HB2	1.92	0.52
3:R:225:ASN:O	3:R:228:THR:HG22	2.09	0.52
3:C:356:THR:O	3:C:359:GLU:HB2	2.10	0.52
3:C:362:PHE:O	3:C:363:SER:OG	2.23	0.52
1:D:63:ARG:HB2	9:D:307:HOH:O	2.10	0.52
3:I:211:VAL:O	3:I:226:LEU:HA	2.08	0.52
1:J:16:TYR:HE2	1:J:130:LYS:HD2	1.75	0.52
3:O:236:ILE:HD12	3:O:237:VAL:N	2.25	0.52
1:P:5:LEU:CD1	1:P:6:PRO:HD2	2.39	0.52
1:A:84:GLU:HG2	1:A:85:TRP:N	2.24	0.52
2:H:98:MET:HE2	2:H:107:TRP:NE1	2.24	0.52
3:L:272:ARG:N	3:L:273:SER:HA	2.19	0.52
2:N:29:CYS:HA	2:N:30:TYR:C	2.34	0.52
1:D:102:GLN:HG3	1:D:119:SER:C	2.35	0.52
2:E:58:LEU:CB	2:E:59:LYS:HB3	2.40	0.52
2:K:100:VAL:HG22	2:K:105:ILE:HG23	1.92	0.52
1:M:41:LEU:CD1	1:M:71:GLY:HA2	2.39	0.52
2:N:63:MET:HA	2:N:117:SER:O	2.09	0.52
2:B:83:LYS:HD3	2:B:83:LYS:N	2.20	0.52
1:D:105:GLN:HG3	2:E:76:TRP:CZ3	2.44	0.52
2:H:18:GLU:OE1	2:H:18:GLU:N	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:49:GLU:O	1:J:53:VAL:HG12	2.09	0.52
1:J:100:GLU:O	1:J:102:GLN:HB3	2.09	0.52
1:A:99:GLY:HA2	1:A:120:ASP:HB2	1.92	0.52
3:C:349:ALA:O	3:C:352:GLU:HG3	2.09	0.52
2:E:92:ARG:HD2	2:E:113:GLU:OE2	2.11	0.52
3:F:296:ILE:HA	3:F:299:CYS:SG	2.50	0.52
3:F:326:ILE:HG23	3:F:341:PHE:CZ	2.45	0.52
2:K:54:ALA:HB2	9:K:204:HOH:O	2.10	0.52
2:N:73:GLU:N	2:N:73:GLU:OE1	2.43	0.52
3:O:173:ILE:O	3:O:209:THR:HA	2.10	0.52
3:O:178:VAL:CG1	3:O:214:ILE:HD11	2.30	0.52
1:P:86:SER:C	2:Q:37:ARG:HD2	2.35	0.52
3:R:185:ILE:CD1	3:R:283:ASP:HB2	2.40	0.52
3:C:264:TYR:OH	3:C:277:VAL:O	2.26	0.51
1:P:64:PRO:HA	1:P:65:GLU:CB	2.22	0.51
1:A:66:LEU:HD13	1:A:126:PRO:CD	2.40	0.51
3:C:342:PHE:O	3:C:344:VAL:HG23	2.10	0.51
1:D:2:PHE:N	9:D:302:HOH:O	2.43	0.51
1:J:5:LEU:CD1	1:J:6:PRO:HD2	2.37	0.51
1:M:9:SER:O	1:M:15:CYS:HA	2.09	0.51
1:M:30:ARG:O	1:M:33:THR:OG1	2.25	0.51
3:O:202:LEU:HB2	3:O:204:ILE:HG22	1.91	0.51
2:E:59:LYS:HG2	2:E:60:TYR:CD2	2.46	0.51
2:H:29:CYS:HB3	2:H:32:GLN:HB3	1.92	0.51
1:M:7:GLY:O	1:M:17:GLN:NE2	2.42	0.51
1:M:25:TRP:HB3	1:M:121:CYS:CB	2.33	0.51
1:M:55:GLN:HB2	9:R:510:HOH:O	2.09	0.51
1:M:64:PRO:HB2	1:M:66:LEU:HD12	1.91	0.51
2:Q:15:VAL:HG12	2:Q:119:VAL:CG1	2.41	0.51
1:A:32:CYS:SG	1:A:41:LEU:HD23	2.50	0.51
1:G:107:LEU:HD23	1:G:116:TRP:CD1	2.45	0.51
3:I:178:VAL:HG13	3:I:214:ILE:CD1	2.40	0.51
1:P:14:HIS:CD2	1:P:132:PRO:HB3	2.46	0.51
1:D:111:THR:HG21	2:E:90:LEU:CD2	2.41	0.51
3:F:178:VAL:HG12	3:F:216:TYR:CD1	2.46	0.51
3:I:173:ILE:HD13	3:I:175:VAL:HG13	1.93	0.51
1:J:53:VAL:O	1:J:57:VAL:HG23	2.11	0.51
3:R:292:LEU:C	3:R:292:LEU:HD23	2.36	0.51
3:C:184:SER:HB3	5:C:408:CL:CL	2.48	0.51
2:H:26:GLU:OE2	2:H:27:SER:N	2.43	0.51
2:H:47:GLU:HG2	2:H:105:ILE:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:62:SER:O	2:K:117:SER:HB2	2.11	0.51
3:C:176:VAL:HG22	3:C:264:TYR:OH	2.10	0.51
1:G:23:LYS:CA	1:G:124:LYS:HB3	2.41	0.51
1:G:101:SER:HA	1:G:102:GLN:CB	2.25	0.51
3:L:181:GLU:O	3:L:246:GLY:HA2	2.11	0.51
3:R:355:GLY:O	3:R:359:GLU:HB2	2.10	0.51
3:C:199:VAL:HG13	3:C:236:ILE:HG22	1.92	0.51
2:E:113:GLU:OE1	2:E:113:GLU:N	2.44	0.51
3:O:264:TYR:CE1	3:O:276:LYS:HB3	2.44	0.51
1:D:64:PRO:HB2	1:D:65:GLU:O	2.10	0.51
2:H:62:SER:O	2:H:117:SER:HB2	2.11	0.51
3:I:316:ASN:ND2	3:I:345:SER:O	2.43	0.51
1:M:24:THR:OG1	1:M:27:GLU:N	2.38	0.51
1:M:67:TYR:O	1:M:125:ASN:HB3	2.11	0.51
1:P:74:ASP:HB3	1:P:103:MET:HE1	1.92	0.51
3:F:204:ILE:HD11	3:F:231:THR:CA	2.41	0.51
2:H:55:SER:HA	2:H:61:THR:CG2	2.40	0.51
3:L:199:VAL:CG2	3:L:235:MET:HE3	2.41	0.51
1:P:86:SER:HB3	2:Q:26:GLU:OE2	2.10	0.51
3:R:356:THR:HB	9:R:501:HOH:O	2.10	0.51
2:E:58:LEU:HD12	2:E:58:LEU:N	2.26	0.50
2:E:100:VAL:HA	2:E:105:ILE:HG12	1.93	0.50
2:N:39:ALA:HA	2:N:121:LYS:HB2	1.93	0.50
3:O:335:ILE:CG1	3:O:336:PRO:HA	2.40	0.50
3:C:175:VAL:HG12	3:C:277:VAL:HB	1.92	0.50
3:L:330:LYS:HG2	3:L:341:PHE:CZ	2.46	0.50
3:O:203:ASP:CB	3:O:204:ILE:CA	2.88	0.50
3:O:333:ALA:O	9:O:506:HOH:O	2.19	0.50
3:R:178:VAL:HA	3:R:214:ILE:O	2.11	0.50
9:A:305:HOH:O	2:B:91:ARG:HB2	2.10	0.50
3:L:229:TYR:CD1	3:L:234:GLU:HB3	2.46	0.50
1:M:15:CYS:O	1:M:130:LYS:HG3	2.10	0.50
2:N:23:GLU:HA	2:N:26:GLU:OE2	2.11	0.50
3:O:224:PHE:HB2	3:O:228:THR:HG21	1.93	0.50
1:A:110:TRP:CG	3:C:247:GLY:HA2	2.45	0.50
3:C:317:ARG:NH2	3:C:347:GLU:OE1	2.44	0.50
3:C:361:ILE:HA	3:C:362:PHE:C	2.37	0.50
3:F:174:ASP:OD1	3:F:274:ALA:HB1	2.12	0.50
3:F:178:VAL:HG12	3:F:216:TYR:CE1	2.47	0.50
3:L:225:ASN:O	3:L:228:THR:HG22	2.11	0.50
2:N:64:TRP:CZ3	2:N:95:CYS:HB2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:72:LEU:HD11	2:Q:76:TRP:HB3	1.93	0.50
3:R:207:THR:HG22	3:R:208:LYS:HB2	1.93	0.50
1:A:117:ASP:HA	9:A:305:HOH:O	2.12	0.50
3:C:313:GLY:N	3:C:345:SER:O	2.44	0.50
2:E:19:LEU:HB3	2:E:115:THR:HB	1.94	0.50
1:G:35:GLN:H	1:G:35:GLN:CD	2.16	0.50
1:J:102:GLN:H	1:J:120:ASP:HA	1.76	0.50
1:M:91:ILE:O	1:M:94:VAL:HG13	2.11	0.50
3:O:313:GLY:O	3:O:317:ARG:HG3	2.11	0.50
1:D:89:ALA:HB3	2:E:42:HIS:CE1	2.47	0.50
3:I:174:ASP:HB3	3:I:226:LEU:HD13	1.93	0.50
3:I:192:LYS:O	3:I:196:GLU:HG3	2.12	0.50
3:R:279:VAL:HG11	3:R:357:LEU:HD21	1.94	0.50
1:A:68:VAL:HB	1:A:107:LEU:HB2	1.92	0.50
1:D:16:TYR:CE1	1:D:42:VAL:HG23	2.44	0.50
2:E:67:LEU:HD11	2:E:96:ALA:HB2	1.94	0.50
3:I:305:LEU:HB2	3:I:334:SER:OG	2.12	0.50
2:N:92:ARG:NE	3:O:249:LEU:HD21	2.26	0.50
2:Q:67:LEU:HB2	2:Q:96:ALA:HB3	1.93	0.50
2:Q:100:VAL:HG23	2:Q:104:ARG:O	2.11	0.50
3:R:224:PHE:HB2	3:R:228:THR:HG21	1.93	0.50
2:B:8:TYR:N	2:B:11:TYR:O	2.45	0.50
1:D:16:TYR:OH	1:D:49:GLU:OE2	2.22	0.50
2:E:58:LEU:CA	2:E:59:LYS:HB3	2.42	0.50
2:E:104:ARG:NE	9:E:305:HOH:O	2.45	0.50
1:G:22:PRO:C	1:G:124:LYS:HB3	2.37	0.50
3:I:178:VAL:HG22	3:I:214:ILE:HD11	1.93	0.50
1:J:5:LEU:HD12	1:J:6:PRO:CD	2.39	0.50
3:L:196:GLU:O	3:L:199:VAL:HG12	2.12	0.50
2:N:100:VAL:HG13	2:N:105:ILE:CG1	2.37	0.50
1:A:5:LEU:CD1	1:A:6:PRO:HD2	2.42	0.50
2:B:65:LEU:CD1	2:B:98:MET:HE3	2.42	0.50
1:J:70:ILE:HG13	1:J:71:GLY:N	2.27	0.50
1:M:3:ASN:O	1:M:4:CYS:HB2	2.11	0.50
2:N:37:ARG:HG3	9:N:305:HOH:O	2.10	0.50
3:O:172:LEU:HD13	3:O:207:THR:C	2.37	0.50
3:O:206:PRO:O	3:O:207:THR:HB	2.12	0.50
1:D:43:SER:HA	2:E:78:TRP:CZ3	2.47	0.49
2:N:101:LYS:HG3	2:N:102:THR:N	2.26	0.49
3:O:361:ILE:CG2	3:O:362:PHE:HA	2.42	0.49
2:Q:58:LEU:N	2:Q:58:LEU:HD12	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:344:VAL:HG12	3:R:349:ALA:HB3	1.94	0.49
1:A:15:CYS:HB2	1:A:131:PHE:CE2	2.47	0.49
3:C:200:GLN:N	3:C:201:GLY:CA	2.74	0.49
1:D:15:CYS:HB2	1:D:131:PHE:CE2	2.47	0.49
1:G:69:TRP:HE3	9:G:304:HOH:O	1.95	0.49
2:K:59:LYS:HG2	2:K:60:TYR:CD2	2.48	0.49
2:Q:3:LEU:CG	2:Q:4:HIS:H	2.18	0.49
2:Q:59:LYS:HG2	2:Q:60:TYR:H	1.75	0.49
2:B:78:TRP:HB3	2:B:80:ASP:OD1	2.12	0.49
3:C:197:LYS:HA	3:C:200:GLN:HG2	1.93	0.49
3:C:214:ILE:HB	3:C:221:ARG:O	2.12	0.49
2:E:3:LEU:HD13	3:O:359:GLU:OE1	2.13	0.49
2:E:24:ASP:HA	2:E:27:SER:OG	2.12	0.49
2:E:58:LEU:CA	2:E:59:LYS:CB	2.91	0.49
3:F:213:LEU:HD21	9:F:502:HOH:O	2.11	0.49
3:I:184:SER:OG	3:I:283:ASP:OD2	2.30	0.49
1:M:111:THR:HG21	2:N:90:LEU:HD21	1.94	0.49
1:M:123:ALA:HB1	1:M:124:LYS:CB	2.40	0.49
2:N:39:ALA:HB3	2:N:119:VAL:HG23	1.93	0.49
2:N:57:THR:HG22	2:N:58:LEU:N	2.27	0.49
3:R:173:ILE:HD13	3:R:175:VAL:HG13	1.94	0.49
1:A:71:GLY:O	2:B:79:SER:N	2.41	0.49
2:B:16:PHE:O	2:B:117:SER:HB3	2.12	0.49
3:C:215:GLN:HG3	3:C:223:VAL:CG2	2.42	0.49
3:C:228:THR:HG23	3:C:229:TYR:CD2	2.48	0.49
3:I:213:LEU:HB3	3:I:224:PHE:CE2	2.47	0.49
3:I:233:GLU:O	3:I:236:ILE:HG13	2.11	0.49
1:M:85:TRP:HZ3	2:N:65:LEU:HG	1.77	0.49
2:N:53:LEU:O	2:N:53:LEU:HD23	2.12	0.49
3:O:178:VAL:HG12	3:O:214:ILE:CD1	2.32	0.49
1:P:16:TYR:HE2	1:P:130:LYS:HD2	1.77	0.49
1:P:71:GLY:O	2:Q:79:SER:HB2	2.13	0.49
2:Q:50:VAL:O	2:Q:54:ALA:HB2	2.13	0.49
3:C:305:LEU:HB2	3:O:335:ILE:HD11	1.95	0.49
1:D:16:TYR:CE1	1:D:130:LYS:HD2	2.46	0.49
3:F:180:ASP:HB2	3:F:281:VAL:O	2.12	0.49
1:G:101:SER:CA	1:G:102:GLN:CB	2.89	0.49
3:I:233:GLU:O	3:I:237:VAL:HG23	2.13	0.49
2:K:33:HIS:CD2	2:K:34:LYS:H	2.30	0.49
1:M:5:LEU:HG	1:M:6:PRO:HD2	1.93	0.49
2:N:57:THR:C	2:N:58:LEU:HG	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:234:GLU:OE2	3:R:243:SER:HB2	2.12	0.49
3:R:272:ARG:N	3:R:273:SER:HA	2.24	0.49
1:A:62:LYS:C	1:A:64:PRO:HD3	2.37	0.49
2:B:12:CYS:H	2:B:122:PHE:HB3	1.77	0.49
3:I:281:VAL:CG2	3:I:309:ILE:HD12	2.39	0.49
2:K:36:SER:HB3	2:K:122:PHE:O	2.13	0.49
2:K:87:LYS:O	2:K:87:LYS:HG3	2.12	0.49
2:K:92:ARG:NH2	8:L:406:SO4:O2	2.44	0.49
3:L:180:ASP:HB2	3:L:282:THR:HA	1.94	0.49
3:L:310:ALA:HB1	3:L:325:LEU:CD2	2.43	0.49
1:M:87:MET:HE1	2:N:40:SER:HB3	1.95	0.49
3:I:308:GLY:C	3:I:341:PHE:HB2	2.37	0.49
2:N:13:TYR:CE1	2:N:121:LYS:HG3	2.48	0.49
2:N:21:THR:O	2:N:25:ALA:N	2.41	0.49
2:N:64:TRP:CE2	2:N:116:VAL:HG12	2.48	0.49
2:Q:64:TRP:O	2:Q:65:LEU:HD23	2.12	0.49
3:R:173:ILE:CD1	3:R:209:THR:HB	2.42	0.49
1:A:44:ILE:HB	1:A:116:TRP:HZ2	1.78	0.49
3:C:180:ASP:HB2	3:C:282:THR:HA	1.95	0.49
2:H:64:TRP:CE2	2:H:116:VAL:HG22	2.47	0.49
2:N:35:GLY:H	2:N:36:SER:HG	1.59	0.49
3:O:278:MET:HE3	3:O:304:ILE:HD13	1.93	0.49
3:R:344:VAL:HG12	3:R:346:ASP:O	2.13	0.49
2:B:21:THR:O	2:B:25:ALA:N	2.34	0.49
2:B:64:TRP:NE1	2:B:116:VAL:HG12	2.28	0.49
3:C:193:ASN:HB3	3:C:351:LEU:HD12	1.94	0.49
3:C:312:LEU:N	3:C:312:LEU:HD12	2.28	0.49
2:E:8:TYR:HB3	2:E:13:TYR:CE1	2.48	0.49
2:H:24:ASP:HA	2:H:27:SER:OG	2.12	0.49
3:I:325:LEU:CD2	3:I:329:ILE:HD13	2.42	0.49
1:A:54:ALA:O	1:A:58:THR:OG1	2.24	0.49
1:A:101:SER:CA	1:A:102:GLN:CB	2.91	0.49
1:A:69:TRP:NE1	1:A:125:ASN:HB2	2.27	0.48
3:L:178:VAL:HG23	3:L:280:VAL:HG13	1.93	0.48
2:N:29:CYS:HB2	2:N:36:SER:O	2.13	0.48
1:D:5:LEU:HB3	1:D:8:TRP:CD1	2.48	0.48
2:E:58:LEU:HD23	2:E:59:LYS:HE2	1.95	0.48
3:I:173:ILE:HA	3:I:275:THR:CG2	2.43	0.48
3:I:296:ILE:HG23	3:I:305:LEU:HD11	1.95	0.48
3:L:178:VAL:HG23	3:L:178:VAL:O	2.13	0.48
3:L:228:THR:HG23	3:L:229:TYR:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:271:ARG:HB3	3:L:272:ARG:CB	2.42	0.48
1:M:2:PHE:N	5:M:203:CL:CL	2.84	0.48
3:O:178:VAL:HG21	3:O:280:VAL:HG12	1.95	0.48
3:O:225:ASN:O	3:O:228:THR:HG22	2.13	0.48
2:Q:103:ASP:C	2:Q:104:ARG:HG3	2.37	0.48
2:B:15:VAL:HA	2:B:119:VAL:HG12	1.95	0.48
2:K:39:ALA:HB3	2:K:119:VAL:HG23	1.95	0.48
1:M:26:ASP:HB3	1:M:30:ARG:NH1	2.28	0.48
3:R:207:THR:HG23	3:R:208:LYS:HB2	1.93	0.48
2:B:24:ASP:HA	2:B:27:SER:OG	2.14	0.48
1:D:118:TYR:HE1	2:E:91:ARG:HB3	1.78	0.48
2:E:73:GLU:O	2:E:73:GLU:HG2	2.13	0.48
3:I:272:ARG:N	3:I:274:ALA:HB3	2.28	0.48
1:M:75:ARG:NH2	2:N:77:GLU:HB3	2.29	0.48
3:O:173:ILE:HD11	3:O:362:PHE:HD1	1.79	0.48
3:O:294:ALA:O	3:O:298:GLN:HG3	2.14	0.48
3:C:192:LYS:O	3:C:196:GLU:HG3	2.13	0.48
3:F:329:ILE:HD12	3:F:332:ILE:HD12	1.94	0.48
2:H:22:TRP:CH2	2:H:66:GLY:HA2	2.49	0.48
1:J:64:PRO:HG3	1:J:109:ARG:CZ	2.44	0.48
2:Q:19:LEU:O	2:Q:20:LYS:HG3	2.14	0.48
3:R:178:VAL:HG22	3:R:280:VAL:HG12	1.95	0.48
1:A:41:LEU:HB3	9:A:306:HOH:O	2.12	0.48
2:B:92:ARG:HH12	2:B:111:GLY:HA3	1.77	0.48
3:C:213:LEU:HB3	3:C:224:PHE:CE2	2.48	0.48
3:C:281:VAL:HG22	3:C:309:ILE:HD12	1.95	0.48
1:G:16:TYR:HE2	1:G:130:LYS:HD2	1.78	0.48
3:I:272:ARG:N	3:I:273:SER:C	2.71	0.48
1:J:18:ALA:HB1	1:J:61:ILE:HD11	1.95	0.48
1:J:70:ILE:HG12	1:J:105:GLN:O	2.13	0.48
2:K:100:VAL:HG13	2:K:105:ILE:HG12	1.95	0.48
2:N:23:GLU:O	2:N:27:SER:CB	2.61	0.48
1:P:74:ASP:HB3	1:P:103:MET:HE3	1.95	0.48
3:R:173:ILE:HA	3:R:275:THR:HB	1.95	0.48
2:B:110:ARG:NH2	3:C:320:LEU:HD13	2.29	0.48
1:J:64:PRO:CA	1:J:65:GLU:HB2	2.40	0.48
2:K:41:ILE:HG23	2:K:46:GLU:HB2	1.96	0.48
2:N:71:TRP:HA	2:N:74:CYS:SG	2.53	0.48
3:O:172:LEU:HD13	3:O:207:THR:HA	1.96	0.48
3:O:226:LEU:HD12	3:O:226:LEU:H	1.78	0.48
2:Q:1:CYS:SG	2:Q:5:TRP:HB2	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:180:ASP:O	3:R:185:ILE:HG13	2.14	0.48
1:D:49:GLU:O	1:D:53:VAL:HG23	2.13	0.48
3:F:250:THR:O	3:F:287:HIS:N	2.31	0.48
3:I:194:PHE:CD1	3:I:350:LEU:HG	2.48	0.48
1:J:91:ILE:CG2	1:J:94:VAL:HG13	2.43	0.48
1:M:10:ALA:HA	1:M:14:HIS:O	2.12	0.48
1:M:100:GLU:C	1:M:102:GLN:HB3	2.39	0.48
1:M:110:TRP:HA	3:O:245:TYR:CE1	2.49	0.48
2:Q:84:LEU:HD12	2:Q:84:LEU:N	2.28	0.48
1:A:118:TYR:HB2	2:B:91:ARG:HH21	1.79	0.48
2:B:19:LEU:HB3	2:B:115:THR:OG1	2.13	0.48
3:C:314:TYR:HB3	9:C:512:HOH:O	2.13	0.48
2:E:109:ASN:N	9:E:303:HOH:O	2.27	0.48
2:H:47:GLU:CG	2:H:105:ILE:HD13	2.44	0.48
3:I:333:ALA:HB2	3:I:341:PHE:HB3	1.96	0.48
1:J:22:PRO:HA	1:J:125:ASN:O	2.14	0.48
2:K:59:LYS:H	2:K:59:LYS:CD	2.19	0.48
2:Q:62:SER:O	2:Q:117:SER:HB2	2.12	0.48
3:C:233:GLU:O	3:C:237:VAL:HG23	2.14	0.48
3:C:312:LEU:HD23	3:C:322:THR:HB	1.95	0.48
1:D:76:ARG:HG2	1:D:77:LYS:N	2.29	0.48
2:E:61:THR:OG1	2:E:100:VAL:O	2.32	0.48
3:I:211:VAL:C	3:I:226:LEU:HD23	2.39	0.48
2:N:35:GLY:HA2	2:N:37:ARG:N	2.28	0.48
1:P:104:CYS:N	1:P:121:CYS:SG	2.87	0.48
2:B:122:PHE:HA	9:B:307:HOH:O	2.13	0.47
1:G:8:TRP:CD2	1:G:17:GLN:HB2	2.49	0.47
3:I:273:SER:OG	3:I:274:ALA:N	2.35	0.47
3:L:175:VAL:O	3:L:211:VAL:HG23	2.14	0.47
1:M:69:TRP:HB2	1:M:127:PHE:HB3	1.96	0.47
1:G:53:VAL:O	1:G:57:VAL:HG23	2.13	0.47
1:G:77:LYS:HD2	1:G:77:LYS:N	2.30	0.47
1:J:14:HIS:ND1	1:J:14:HIS:N	2.61	0.47
1:J:21:GLU:OE1	1:J:22:PRO:HD2	2.13	0.47
1:J:67:TYR:HA	1:J:107:LEU:O	2.14	0.47
3:L:213:LEU:HB3	3:L:224:PHE:CE2	2.49	0.47
3:R:239:THR:O	3:R:242:THR:HG22	2.13	0.47
1:D:20:ASN:ND2	8:D:208:SO4:O4	2.45	0.47
3:F:363:SER:N	3:F:364:ILE:HA	2.27	0.47
1:G:70:ILE:HG13	1:G:71:GLY:N	2.30	0.47
1:G:70:ILE:N	9:G:304:HOH:O	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:292:LEU:C	3:I:292:LEU:HD23	2.38	0.47
2:K:44:ARG:NH1	2:K:45:GLU:HB2	2.28	0.47
1:M:41:LEU:CB	1:M:71:GLY:HA3	2.44	0.47
3:C:209:THR:O	3:C:209:THR:HG23	2.13	0.47
1:D:23:LYS:NZ	9:D:309:HOH:O	2.46	0.47
2:E:84:LEU:HG	2:E:84:LEU:O	2.14	0.47
1:G:33:THR:HA	1:G:39:GLY:O	2.14	0.47
1:G:108:ALA:HB3	1:G:111:THR:CG2	2.44	0.47
2:K:115:THR:HG23	2:K:115:THR:O	2.14	0.47
3:L:181:GLU:HG3	3:L:217:ALA:HB2	1.95	0.47
1:P:42:VAL:HG23	1:P:130:LYS:HD2	1.96	0.47
2:Q:116:VAL:HG22	2:Q:117:SER:N	2.29	0.47
1:A:43:SER:HA	2:B:78:TRP:CZ3	2.50	0.47
3:C:199:VAL:CG2	3:C:235:MET:HE3	2.45	0.47
1:G:11:TYR:HB3	1:G:16:TYR:CE1	2.50	0.47
3:L:325:LEU:HD23	3:L:329:ILE:HD13	1.95	0.47
3:L:353:LYS:O	3:L:356:THR:HG22	2.15	0.47
3:C:329:ILE:HD12	3:C:329:ILE:N	2.29	0.47
2:E:16:PHE:O	2:E:117:SER:HB3	2.13	0.47
3:F:188:TRP:CD1	3:F:192:LYS:HE3	2.49	0.47
2:H:116:VAL:HG22	9:H:305:HOH:O	2.14	0.47
3:O:325:LEU:O	3:O:329:ILE:HD13	2.15	0.47
1:A:97:ASN:HB2	2:B:106:PHE:CD1	2.49	0.47
3:C:181:GLU:O	3:C:246:GLY:HA2	2.14	0.47
3:C:200:GLN:N	3:C:201:GLY:HA3	2.28	0.47
3:C:329:ILE:HG22	3:C:341:PHE:HD1	1.80	0.47
3:C:339:ARG:HG3	9:C:504:HOH:O	2.14	0.47
3:C:342:PHE:CZ	3:C:357:LEU:HD13	2.49	0.47
1:D:110:TRP:HB3	3:F:246:GLY:O	2.14	0.47
2:E:64:TRP:CZ3	2:E:95:CYS:HB2	2.49	0.47
3:I:214:ILE:HB	3:I:221:ARG:O	2.15	0.47
3:I:362:PHE:O	3:I:363:SER:OG	2.19	0.47
2:K:64:TRP:CB	2:K:118:PHE:HB3	2.42	0.47
2:N:36:SER:H	2:N:122:PHE:C	2.22	0.47
2:N:113:GLU:OE1	2:N:113:GLU:N	2.40	0.47
1:P:24:THR:HG22	1:P:122:GLN:O	2.14	0.47
1:P:64:PRO:HG3	1:P:109:ARG:NH1	2.30	0.47
2:Q:35:GLY:HA3	2:Q:36:SER:HA	1.55	0.47
2:Q:46:GLU:OE2	2:Q:121:LYS:NZ	2.47	0.47
3:R:181:GLU:HG3	3:R:217:ALA:HB2	1.96	0.47
3:F:175:VAL:HG23	3:F:211:VAL:CG2	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:22:TRP:HH2	2:H:66:GLY:HA2	1.80	0.47
3:O:292:LEU:C	3:O:292:LEU:HD23	2.39	0.47
2:Q:47:GLU:CG	2:Q:105:ILE:HD13	2.44	0.47
1:A:17:GLN:OE1	1:A:17:GLN:HA	2.15	0.47
1:A:56:LEU:C	1:A:56:LEU:HD23	2.40	0.47
2:K:58:LEU:HB3	2:K:60:TYR:O	2.15	0.47
3:L:178:VAL:HG21	3:L:280:VAL:HG22	1.96	0.47
1:P:41:LEU:CB	1:P:71:GLY:HA3	2.44	0.47
3:R:335:ILE:C	3:R:335:ILE:HD12	2.40	0.47
1:G:38:ARG:HG3	1:G:38:ARG:O	2.15	0.47
3:I:285:GLU:OE2	3:I:324:ASN:HB2	2.14	0.47
3:L:292:LEU:HD23	3:L:292:LEU:C	2.40	0.47
3:L:326:ILE:O	3:L:330:LYS:HG3	2.15	0.47
3:C:326:ILE:HG12	3:C:341:PHE:HZ	1.80	0.46
3:I:271:ARG:HB3	3:I:272:ARG:CB	2.45	0.46
1:M:77:LYS:O	1:M:77:LYS:HG2	2.16	0.46
2:N:64:TRP:NE1	2:N:116:VAL:HG12	2.30	0.46
2:N:99:VAL:O	2:N:105:ILE:HG23	2.15	0.46
1:A:107:LEU:HB3	1:A:113:PHE:HD1	1.80	0.46
3:C:174:ASP:O	3:C:277:VAL:N	2.47	0.46
3:C:197:LYS:HA	3:C:200:GLN:HE21	1.80	0.46
3:C:344:VAL:HG12	3:C:344:VAL:O	2.13	0.46
1:D:91:ILE:O	1:D:91:ILE:HG22	2.14	0.46
2:E:55:SER:O	1:P:6:PRO:HG3	2.15	0.46
2:H:29:CYS:HA	2:H:30:TYR:C	2.41	0.46
2:N:11:TYR:HD2	2:N:122:PHE:HB3	1.79	0.46
1:P:117:ASP:OD1	2:Q:91:ARG:NE	2.48	0.46
1:A:87:MET:HE2	9:A:302:HOH:O	2.14	0.46
2:B:68:ASN:ND2	2:B:95:CYS:SG	2.88	0.46
1:G:111:THR:HG23	9:G:303:HOH:O	2.15	0.46
1:P:20:ASN:HA	1:P:126:PRO:HB3	1.97	0.46
3:R:173:ILE:HD12	3:R:173:ILE:C	2.39	0.46
3:C:199:VAL:O	3:C:199:VAL:HG22	2.15	0.46
3:I:281:VAL:HG13	3:I:309:ILE:CG2	2.45	0.46
3:L:329:ILE:CG2	3:L:341:PHE:HB2	2.45	0.46
3:L:344:VAL:HG12	3:L:346:ASP:H	1.81	0.46
1:M:52:PHE:O	1:M:55:GLN:HG2	2.15	0.46
1:M:64:PRO:HA	1:M:65:GLU:O	2.16	0.46
3:O:178:VAL:HG23	3:O:178:VAL:O	2.15	0.46
1:A:86:SER:HB3	2:B:66:GLY:O	2.15	0.46
2:B:100:VAL:HG12	2:B:105:ILE:CG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:178:VAL:CG2	3:C:280:VAL:HG12	2.45	0.46
3:C:208:LYS:HB2	3:C:208:LYS:NZ	2.31	0.46
2:E:100:VAL:HG13	2:E:105:ILE:CG1	2.45	0.46
1:G:16:TYR:CE2	1:G:130:LYS:HD2	2.51	0.46
2:K:35:GLY:HA3	2:K:36:SER:HA	1.67	0.46
3:L:176:VAL:HG12	3:L:264:TYR:OH	2.16	0.46
3:L:325:LEU:O	3:L:329:ILE:HD13	2.14	0.46
1:A:9:SER:HA	3:I:257:GLN:OE1	2.16	0.46
2:B:63:MET:HA	2:B:117:SER:O	2.16	0.46
3:C:326:ILE:HG23	3:C:341:PHE:CE2	2.50	0.46
1:D:72:LEU:HD11	2:E:76:TRP:HB3	1.97	0.46
2:H:90:LEU:HD23	2:H:90:LEU:H	1.81	0.46
3:I:271:ARG:HA	3:I:272:ARG:HA	1.74	0.46
3:I:281:VAL:HG22	3:I:309:ILE:CB	2.45	0.46
2:K:33:HIS:CG	2:K:34:LYS:H	2.33	0.46
2:K:39:ALA:CB	2:K:119:VAL:HG23	2.44	0.46
3:R:286:SER:OG	3:R:328:GLU:OE2	2.29	0.46
1:D:84:GLU:HB3	1:D:88:SER:HA	1.97	0.46
3:F:202:LEU:HD21	3:F:209:THR:OG1	2.16	0.46
1:G:95:ASN:ND2	2:H:47:GLU:OE2	2.48	0.46
1:J:84:GLU:HA	1:J:90:SER:HA	1.97	0.46
1:M:55:GLN:NE2	9:M:303:HOH:O	2.43	0.46
2:E:39:ALA:HA	2:E:121:LYS:HB2	1.98	0.46
1:G:23:LYS:HE3	1:G:27:GLU:CG	2.46	0.46
1:G:32:CYS:SG	1:G:41:LEU:HD23	2.56	0.46
1:G:68:VAL:HB	1:G:107:LEU:HB2	1.97	0.46
2:K:53:LEU:O	9:K:204:HOH:O	2.20	0.46
1:M:34:GLU:HG3	1:M:35:GLN:CA	2.46	0.46
1:M:74:ASP:OD2	2:N:75:LYS:N	2.44	0.46
3:O:361:ILE:HG23	3:O:362:PHE:HA	1.96	0.46
3:R:312:LEU:HD21	3:R:326:ILE:HD11	1.97	0.46
1:A:41:LEU:HB2	1:A:71:GLY:HA2	1.97	0.46
1:G:44:ILE:HB	1:G:116:TRP:CZ2	2.51	0.46
2:H:98:MET:SD	2:H:105:ILE:HD11	2.56	0.46
1:J:55:GLN:HA	1:J:58:THR:HG22	1.97	0.46
1:J:64:PRO:HD3	9:J:303:HOH:O	2.15	0.46
1:J:70:ILE:HD11	1:J:105:GLN:HB3	1.98	0.46
2:Q:26:GLU:HG3	9:Q:306:HOH:O	2.15	0.46
3:R:207:THR:HA	3:R:208:LYS:HA	1.52	0.46
2:B:15:VAL:HG23	2:B:53:LEU:HG	1.98	0.46
1:D:65:GLU:N	1:D:65:GLU:OE1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:46:GLU:O	2:E:50:VAL:HG22	2.16	0.46
3:F:202:LEU:HD23	3:F:203:ASP:O	2.16	0.46
3:F:314:TYR:HB3	9:F:508:HOH:O	2.15	0.46
3:I:181:GLU:HG3	3:I:217:ALA:HB2	1.97	0.46
3:I:281:VAL:HG13	3:I:309:ILE:HG22	1.97	0.46
1:J:36:ALA:O	6:J:205:GOL:H2	2.16	0.46
1:J:65:GLU:HG3	1:J:126:PRO:HD3	1.97	0.46
1:M:29:GLU:OE1	1:M:41:LEU:HG	2.15	0.46
1:M:85:TRP:CD1	1:M:91:ILE:HD13	2.51	0.46
2:B:22:TRP:N	9:B:301:HOH:O	2.49	0.45
3:C:292:LEU:C	3:C:292:LEU:HD23	2.42	0.45
2:E:110:ARG:NH1	3:F:314:TYR:CE2	2.84	0.45
3:I:325:LEU:HD23	3:I:325:LEU:C	2.41	0.45
3:I:363:SER:OG	9:I:504:HOH:O	2.20	0.45
1:J:29:GLU:O	1:J:33:THR:HG23	2.15	0.45
1:J:68:VAL:HB	1:J:107:LEU:HB2	1.97	0.45
3:L:178:VAL:CG1	3:L:214:ILE:HD11	2.39	0.45
1:M:87:MET:C	1:M:88:SER:HG	2.17	0.45
3:O:204:ILE:C	3:O:204:ILE:HD12	2.40	0.45
3:O:281:VAL:HG22	3:O:309:ILE:HD12	1.97	0.45
3:O:349:ALA:O	3:O:352:GLU:HG3	2.16	0.45
1:P:43:SER:HA	2:Q:78:TRP:CH2	2.52	0.45
2:Q:5:TRP:CE2	2:Q:14:ARG:HB2	2.51	0.45
3:R:236:ILE:HD12	3:R:236:ILE:C	2.41	0.45
1:A:16:TYR:CE1	1:A:130:LYS:HD2	2.52	0.45
3:C:202:LEU:N	3:C:202:LEU:HD12	2.30	0.45
2:E:17:SER:N	9:E:301:HOH:O	2.49	0.45
3:F:278:MET:HE3	3:F:304:ILE:HG21	1.98	0.45
2:H:39:ALA:HA	2:H:121:LYS:HB2	1.98	0.45
3:I:194:PHE:CG	3:I:350:LEU:HG	2.51	0.45
1:J:93:TYR:OH	2:K:47:GLU:OE1	2.27	0.45
2:N:35:GLY:HA2	9:N:305:HOH:O	2.15	0.45
3:R:339:ARG:HB3	3:R:360:GLN:OE1	2.16	0.45
3:C:285:GLU:OE2	3:C:324:ASN:HB2	2.16	0.45
3:F:178:VAL:CG2	3:F:214:ILE:HD11	2.45	0.45
1:J:64:PRO:CD	1:J:109:ARG:NH1	2.77	0.45
2:K:17:SER:HA	2:K:58:LEU:CD1	2.40	0.45
2:K:44:ARG:HH12	2:K:45:GLU:HB2	1.81	0.45
3:L:204:ILE:C	3:L:204:ILE:HD12	2.41	0.45
3:L:292:LEU:O	3:L:296:ILE:HG12	2.15	0.45
3:R:175:VAL:O	3:R:226:LEU:HD21	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:182:SER:OG	3:C:184:SER:OG	2.34	0.45
3:F:260:ARG:NH2	3:F:298:GLN:OE1	2.49	0.45
2:K:53:LEU:C	2:K:53:LEU:HD23	2.41	0.45
3:L:178:VAL:HG23	3:L:280:VAL:HA	1.98	0.45
3:L:358:GLY:C	3:L:360:GLN:H	2.24	0.45
1:M:28:ALA:HB1	1:M:127:PHE:CD1	2.52	0.45
2:N:61:THR:HB	9:N:301:HOH:O	2.16	0.45
3:O:185:ILE:HA	3:O:347:GLU:OE2	2.17	0.45
2:Q:62:SER:HB2	2:Q:116:VAL:CG2	2.46	0.45
3:C:196:GLU:O	3:C:200:GLN:HG2	2.17	0.45
3:C:292:LEU:O	3:C:296:ILE:HG12	2.15	0.45
3:F:199:VAL:CG1	3:F:236:ILE:HG22	2.45	0.45
3:F:335:ILE:CB	3:F:336:PRO:HA	2.46	0.45
1:G:97:ASN:HB2	2:H:106:PHE:CD2	2.51	0.45
2:H:91:ARG:HE	2:H:91:ARG:HA	1.81	0.45
2:K:78:TRP:NE1	9:K:207:HOH:O	2.49	0.45
3:R:253:PHE:CE1	3:R:292:LEU:HG	2.51	0.45
1:A:102:GLN:HA	1:A:120:ASP:HA	1.97	0.45
3:C:202:LEU:HD12	3:C:202:LEU:H	1.81	0.45
3:F:211:VAL:HG22	3:F:212:GLY:N	2.32	0.45
1:G:17:GLN:O	1:G:128:VAL:HG13	2.16	0.45
3:I:329:ILE:N	3:I:329:ILE:HD12	2.32	0.45
2:K:59:LYS:HG2	2:K:60:TYR:CE2	2.51	0.45
3:O:272:ARG:H	3:O:273:SER:CA	2.30	0.45
1:P:35:GLN:HA	1:P:36:ALA:HA	1.58	0.45
3:R:329:ILE:N	3:R:329:ILE:HD12	2.32	0.45
1:D:29:GLU:OE1	2:E:79:SER:HB2	2.17	0.45
3:I:283:ASP:HA	3:I:311:VAL:O	2.17	0.45
3:L:185:ILE:CD1	3:L:283:ASP:HB2	2.44	0.45
1:M:39:GLY:O	1:M:40:HIS:ND1	2.50	0.45
1:M:70:ILE:CG2	1:M:107:LEU:HG	2.47	0.45
2:Q:5:TRP:CD2	2:Q:14:ARG:HB2	2.52	0.45
2:B:3:LEU:HG	2:B:4:HIS:H	1.81	0.45
1:D:54:ALA:O	1:D:58:THR:HG23	2.16	0.45
2:E:16:PHE:HB2	2:E:118:PHE:CE2	2.52	0.45
1:M:72:LEU:HD22	1:M:116:TRP:CZ3	2.52	0.45
3:O:273:SER:CB	3:O:274:ALA:HB2	2.40	0.45
1:A:30:ARG:O	1:A:33:THR:OG1	2.33	0.45
2:B:65:LEU:O	2:B:65:LEU:HG	2.17	0.45
2:B:100:VAL:HG12	2:B:105:ILE:HD13	1.99	0.45
3:C:225:ASN:O	3:C:228:THR:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:281:VAL:HG22	3:C:309:ILE:HB	1.98	0.45
3:F:233:GLU:O	3:F:237:VAL:HG23	2.16	0.45
2:H:29:CYS:HB3	2:H:32:GLN:CB	2.47	0.45
2:K:64:TRP:CD1	2:K:118:PHE:HB3	2.52	0.45
3:O:325:LEU:HD23	3:O:325:LEU:C	2.41	0.45
2:Q:63:MET:HA	2:Q:117:SER:O	2.16	0.45
1:A:101:SER:HG	1:A:103:MET:HG2	1.82	0.45
3:C:273:SER:HB3	3:C:274:ALA:CA	2.48	0.45
3:F:204:ILE:HD11	3:F:231:THR:C	2.42	0.45
1:G:2:PHE:HA	1:G:3:ASN:HA	1.48	0.45
3:O:228:THR:HG23	3:O:229:TYR:N	2.32	0.45
3:R:271:ARG:O	3:R:274:ALA:HB3	2.17	0.45
3:C:213:LEU:HD21	9:C:509:HOH:O	2.16	0.44
1:J:72:LEU:HD23	1:J:105:GLN:CD	2.42	0.44
2:N:63:MET:SD	2:N:98:MET:HB3	2.56	0.44
2:N:75:LYS:O	2:N:75:LYS:HG3	2.18	0.44
3:O:296:ILE:HA	3:O:299:CYS:SG	2.57	0.44
2:E:69:ASN:ND2	5:E:206:CL:CL	2.87	0.44
3:F:363:SER:CB	3:F:364:ILE:CA	2.95	0.44
1:G:5:LEU:HD23	1:G:8:TRP:CD1	2.52	0.44
2:H:30:TYR:CG	2:H:31:ALA:N	2.85	0.44
3:O:178:VAL:CG2	3:O:280:VAL:HA	2.47	0.44
3:O:336:PRO:C	3:O:337:THR:HG1	2.24	0.44
1:P:34:GLU:HA	1:P:35:GLN:HA	1.66	0.44
2:Q:34:LYS:O	2:Q:34:LYS:HD3	2.17	0.44
2:Q:56:GLN:N	2:Q:56:GLN:OE1	2.50	0.44
1:A:38:ARG:O	1:A:40:HIS:ND1	2.50	0.44
2:B:64:TRP:CE2	2:B:116:VAL:HG12	2.51	0.44
3:C:272:ARG:N	3:C:273:SER:HA	2.30	0.44
1:D:19:PHE:HE2	1:D:129:CYS:HB2	1.81	0.44
3:F:362:PHE:HA	3:F:363:SER:HA	1.67	0.44
1:G:5:LEU:HD12	1:G:6:PRO:CD	2.44	0.44
2:N:22:TRP:CZ2	2:N:68:ASN:HB2	2.52	0.44
3:O:214:ILE:C	3:O:214:ILE:HD12	2.43	0.44
1:P:109:ARG:HE	3:R:245:TYR:HA	1.82	0.44
2:B:85:ASP:O	2:B:87:LYS:HG3	2.18	0.44
3:F:338:GLU:O	3:F:339:ARG:HG3	2.16	0.44
2:N:21:THR:OG1	2:N:112:CYS:O	2.25	0.44
3:O:356:THR:O	3:O:359:GLU:HB2	2.16	0.44
1:P:5:LEU:HD12	1:P:6:PRO:CD	2.47	0.44
3:C:221:ARG:NH2	3:C:245:TYR:HB2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:THR:CG2	2:E:90:LEU:HD22	2.47	0.44
3:F:202:LEU:HD23	3:F:202:LEU:C	2.43	0.44
3:I:229:TYR:CD1	3:I:234:GLU:HB3	2.53	0.44
2:K:32:GLN:O	2:K:33:HIS:C	2.61	0.44
1:M:41:LEU:HD12	1:M:71:GLY:HA2	1.98	0.44
3:O:172:LEU:HD13	3:O:207:THR:CA	2.47	0.44
1:P:16:TYR:CD2	1:P:130:LYS:HB2	2.52	0.44
1:P:102:GLN:O	1:P:102:GLN:HG2	2.17	0.44
1:P:110:TRP:HA	3:R:245:TYR:CD2	2.53	0.44
3:F:228:THR:HG23	3:F:229:TYR:N	2.32	0.44
3:I:220:PRO:HG3	3:I:255:ALA:HA	2.00	0.44
3:I:304:ILE:HG13	3:I:305:LEU:H	1.83	0.44
2:K:59:LYS:HD3	2:K:59:LYS:N	2.20	0.44
2:K:101:LYS:O	2:K:104:ARG:N	2.51	0.44
3:L:272:ARG:H	3:L:274:ALA:N	2.16	0.44
1:A:100:GLU:C	1:A:102:GLN:HB3	2.43	0.44
3:I:207:THR:HA	3:I:208:LYS:HA	1.56	0.44
1:J:8:TRP:CH2	1:J:129:CYS:HB2	2.52	0.44
2:K:30:TYR:CB	2:K:31:ALA:HA	2.46	0.44
3:L:239:THR:O	3:L:242:THR:HG22	2.17	0.44
3:L:325:LEU:HD23	3:L:325:LEU:C	2.43	0.44
3:R:281:VAL:HA	3:R:309:ILE:HB	1.99	0.44
3:R:347:GLU:OE1	3:R:347:GLU:N	2.44	0.44
1:A:63:ARG:N	1:A:64:PRO:CD	2.81	0.44
1:A:68:VAL:HG12	1:A:69:TRP:N	2.33	0.44
3:C:208:LYS:C	3:C:209:THR:HG22	2.43	0.44
1:G:65:GLU:OE1	1:G:65:GLU:HA	2.18	0.44
2:H:116:VAL:N	9:H:305:HOH:O	2.51	0.44
3:I:271:ARG:C	3:I:274:ALA:HB3	2.43	0.44
3:I:301:HIS:C	3:I:303:ASN:N	2.76	0.44
1:J:107:LEU:CD2	6:J:204:GOL:H32	2.48	0.44
3:L:340:TYR:O	3:L:341:PHE:CD2	2.71	0.44
3:O:202:LEU:CB	3:O:204:ILE:HG22	2.48	0.44
2:Q:59:LYS:HG2	2:Q:60:TYR:N	2.33	0.44
2:Q:64:TRP:CZ3	2:Q:95:CYS:HB2	2.53	0.44
1:A:89:ALA:O	1:A:90:SER:OG	2.32	0.44
1:A:110:TRP:HB3	3:C:246:GLY:O	2.18	0.44
1:G:110:TRP:HB3	3:I:246:GLY:O	2.17	0.44
2:H:22:TRP:HA	2:H:25:ALA:CB	2.48	0.44
2:H:38:LEU:O	2:H:39:ALA:HB2	2.18	0.44
3:I:207:THR:OG1	3:I:271:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:22:TRP:HD1	2:N:64:TRP:CE3	2.36	0.44
3:O:188:TRP:HB2	3:O:244:GLN:OE1	2.18	0.44
3:O:274:ALA:C	3:O:275:THR:HG22	2.42	0.44
1:P:11:TYR:HB2	1:P:52:PHE:CZ	2.52	0.44
3:R:178:VAL:HG21	3:R:280:VAL:HG12	2.00	0.44
3:R:278:MET:O	3:R:306:ARG:HA	2.18	0.44
3:I:338:GLU:OE1	3:I:338:GLU:HA	2.18	0.43
1:J:101:SER:CA	1:J:102:GLN:CB	2.91	0.43
3:L:200:GLN:HA	3:L:202:LEU:HB3	1.99	0.43
1:M:34:GLU:CG	1:M:35:GLN:HG3	2.36	0.43
2:B:92:ARG:NE	3:C:249:LEU:HD21	2.33	0.43
1:D:93:TYR:CD1	1:J:78:GLU:HG2	2.52	0.43
2:E:30:TYR:O	2:E:31:ALA:HB3	2.17	0.43
2:E:99:VAL:HG11	2:E:106:PHE:CZ	2.53	0.43
2:E:110:ARG:NH1	8:F:401:SO4:O2	2.47	0.43
2:E:113:GLU:CD	2:E:113:GLU:H	2.26	0.43
3:F:286:SER:OG	3:F:328:GLU:OE2	2.34	0.43
3:I:173:ILE:HA	3:I:275:THR:HG23	1.99	0.43
1:J:14:HIS:HD2	1:J:130:LYS:CE	2.28	0.43
1:J:65:GLU:CG	1:J:126:PRO:HD3	2.48	0.43
3:L:277:VAL:HG12	3:L:278:MET:N	2.33	0.43
1:M:101:SER:HA	1:M:102:GLN:CB	2.25	0.43
1:P:53:VAL:O	1:P:57:VAL:HG23	2.19	0.43
3:C:197:LYS:HA	3:C:200:GLN:CG	2.47	0.43
3:C:272:ARG:H	3:C:273:SER:CA	2.25	0.43
3:F:175:VAL:HA	3:F:277:VAL:O	2.18	0.43
3:F:181:GLU:HG3	3:F:217:ALA:HB2	2.00	0.43
1:J:77:LYS:HD2	1:J:77:LYS:N	2.33	0.43
3:L:335:ILE:HA	9:L:503:HOH:O	2.18	0.43
3:L:341:PHE:O	3:L:341:PHE:CD1	2.71	0.43
1:P:43:SER:HA	2:Q:78:TRP:CZ3	2.53	0.43
2:Q:99:VAL:HG11	3:R:318:ASN:O	2.18	0.43
3:R:173:ILE:HG22	3:R:275:THR:HB	2.00	0.43
3:R:212:GLY:N	3:R:226:LEU:HD23	2.34	0.43
2:B:35:GLY:HA3	2:B:36:SER:CB	2.34	0.43
1:D:65:GLU:HB3	1:D:66:LEU:H	1.62	0.43
2:K:29:CYS:CA	2:K:30:TYR:C	2.88	0.43
1:M:130:LYS:HG2	1:M:131:PHE:N	2.33	0.43
1:P:21:GLU:OE1	1:P:22:PRO:HD2	2.18	0.43
1:P:93:TYR:OH	2:Q:47:GLU:OE2	2.25	0.43
2:E:83:LYS:H	2:E:83:LYS:CD	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:56:GLN:O	2:H:57:THR:HG23	2.19	0.43
2:H:64:TRP:CZ3	2:H:95:CYS:HB2	2.53	0.43
3:I:313:GLY:O	3:I:317:ARG:HG3	2.19	0.43
3:I:334:SER:HB2	3:I:340:TYR:CZ	2.54	0.43
1:J:85:TRP:N	9:J:301:HOH:O	2.51	0.43
2:K:110:ARG:NH1	3:L:320:LEU:HD11	2.33	0.43
3:L:192:LYS:O	3:L:196:GLU:HG3	2.18	0.43
1:M:100:GLU:O	1:M:102:GLN:HB3	2.18	0.43
3:O:283:ASP:OD2	3:O:314:TYR:HB2	2.18	0.43
2:Q:3:LEU:HG	2:Q:4:HIS:N	2.20	0.43
2:E:14:ARG:HG3	2:E:15:VAL:N	2.32	0.43
2:E:52:LYS:O	2:E:56:GLN:HG3	2.18	0.43
3:F:306:ARG:HD3	3:F:306:ARG:N	2.33	0.43
3:I:335:ILE:CG1	3:I:336:PRO:HA	2.48	0.43
3:L:178:VAL:HG12	3:L:214:ILE:CG1	2.49	0.43
3:L:207:THR:HA	3:L:208:LYS:HA	1.49	0.43
3:L:357:LEU:C	3:L:357:LEU:HD13	2.43	0.43
1:M:91:ILE:HG22	1:M:94:VAL:CG1	2.48	0.43
1:P:56:LEU:O	1:P:56:LEU:HD23	2.18	0.43
1:P:102:GLN:HA	1:P:119:SER:C	2.43	0.43
3:R:361:ILE:HA	3:R:362:PHE:HA	1.65	0.43
1:A:16:TYR:HE1	1:A:130:LYS:HD2	1.83	0.43
1:A:99:GLY:O	1:A:102:GLN:NE2	2.51	0.43
2:B:100:VAL:HG12	2:B:105:ILE:HG23	2.01	0.43
3:F:322:THR:O	3:F:326:ILE:HD13	2.18	0.43
1:G:5:LEU:HD23	1:G:8:TRP:HD1	1.84	0.43
2:K:64:TRP:CZ3	2:K:95:CYS:HB2	2.54	0.43
1:M:44:ILE:HB	1:M:116:TRP:HZ2	1.83	0.43
3:O:200:GLN:N	3:O:201:GLY:CA	2.79	0.43
1:P:20:ASN:OD1	1:P:62:LYS:N	2.52	0.43
2:Q:21:THR:HA	2:Q:114:LYS:O	2.19	0.43
3:C:197:LYS:HA	3:C:200:GLN:CD	2.44	0.43
3:C:344:VAL:HG23	3:C:353:LYS:HG3	2.00	0.43
1:D:96:TRP:HA	2:E:107:TRP:HB2	2.01	0.43
2:E:116:VAL:HG22	2:E:117:SER:N	2.33	0.43
3:F:285:GLU:OE2	3:F:324:ASN:HB2	2.19	0.43
3:F:308:GLY:O	3:F:341:PHE:HA	2.18	0.43
1:G:16:TYR:CD2	1:G:130:LYS:HB2	2.53	0.43
1:J:118:TYR:CD2	2:K:91:ARG:HG2	2.53	0.43
3:L:211:VAL:HG13	3:L:235:MET:SD	2.58	0.43
3:L:233:GLU:HA	3:L:236:ILE:CG1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:271:ARG:HB3	3:L:272:ARG:CA	2.49	0.43
1:M:84:GLU:HB2	1:M:88:SER:CA	2.47	0.43
2:N:90:LEU:HD22	9:O:520:HOH:O	2.19	0.43
2:N:99:VAL:HG11	2:N:106:PHE:CZ	2.54	0.43
3:O:294:ALA:HA	9:O:511:HOH:O	2.19	0.43
1:P:122:GLN:N	1:P:122:GLN:OE1	2.52	0.43
3:R:344:VAL:CG1	3:R:349:ALA:HB3	2.49	0.43
1:G:74:ASP:CG	1:G:76:ARG:HD2	2.43	0.43
2:H:41:ILE:CG2	2:H:47:GLU:HB2	2.47	0.43
3:L:272:ARG:CB	3:L:273:SER:C	2.92	0.43
1:M:102:GLN:HA	1:M:120:ASP:CA	2.33	0.43
2:B:61:THR:HG23	2:B:61:THR:O	2.18	0.43
2:E:32:GLN:OE1	3:O:356:THR:HB	2.19	0.43
2:K:65:LEU:HG	9:K:203:HOH:O	2.19	0.43
3:L:175:VAL:O	3:L:211:VAL:HA	2.19	0.43
3:L:179:CYS:SG	3:L:191:VAL:HG11	2.59	0.43
3:L:200:GLN:HA	3:L:201:GLY:HA3	1.65	0.43
3:O:197:LYS:HG3	3:O:351:LEU:CD1	2.49	0.43
1:P:33:THR:HG22	1:P:40:HIS:ND1	2.33	0.43
2:Q:34:LYS:HD3	2:Q:34:LYS:C	2.44	0.43
3:R:277:VAL:HA	3:R:305:LEU:O	2.19	0.43
2:E:108:PHE:HB2	9:E:303:HOH:O	2.18	0.42
3:I:281:VAL:HG22	3:I:309:ILE:CD1	2.46	0.42
1:J:102:GLN:CA	1:J:120:ASP:HA	2.49	0.42
2:K:97:VAL:HG11	2:K:108:PHE:CE2	2.54	0.42
3:L:281:VAL:HG12	3:L:309:ILE:CD1	2.47	0.42
3:R:196:GLU:O	3:R:199:VAL:HG12	2.19	0.42
2:B:71:TRP:HA	2:B:74:CYS:SG	2.58	0.42
1:D:57:VAL:O	1:D:61:ILE:HB	2.19	0.42
3:F:204:ILE:C	3:F:204:ILE:HD12	2.43	0.42
1:G:20:ASN:HA	1:G:126:PRO:HB3	2.00	0.42
3:L:233:GLU:O	3:L:237:VAL:HG23	2.19	0.42
3:R:356:THR:O	3:R:359:GLU:HB3	2.19	0.42
3:R:361:ILE:HA	9:R:511:HOH:O	2.17	0.42
2:E:17:SER:HA	2:E:117:SER:OG	2.20	0.42
3:F:200:GLN:N	3:F:201:GLY:CA	2.75	0.42
3:I:338:GLU:C	3:I:340:TYR:H	2.26	0.42
1:J:102:GLN:H	1:J:121:CYS:H	1.68	0.42
1:J:107:LEU:HD22	6:J:204:GOL:C3	2.49	0.42
2:K:44:ARG:HH11	2:K:45:GLU:H	1.66	0.42
3:L:178:VAL:CG2	3:L:280:VAL:HA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:17:GLN:NE2	5:M:202:CL:CL	2.89	0.42
2:N:45:GLU:CD	2:N:45:GLU:H	2.27	0.42
3:O:175:VAL:O	3:O:211:VAL:HA	2.20	0.42
3:O:228:THR:HG23	3:O:229:TYR:CD2	2.55	0.42
3:R:233:GLU:O	3:R:237:VAL:HG23	2.19	0.42
3:C:194:PHE:CD1	3:C:354:ALA:HB2	2.55	0.42
3:C:233:GLU:O	3:C:236:ILE:HG13	2.19	0.42
1:D:69:TRP:NE1	1:D:125:ASN:HB2	2.34	0.42
2:E:41:ILE:HG21	2:E:47:GLU:CB	2.47	0.42
3:F:220:PRO:HG3	3:F:255:ALA:HA	2.01	0.42
3:F:351:LEU:C	3:F:351:LEU:HD23	2.44	0.42
3:L:281:VAL:HG23	3:L:281:VAL:O	2.19	0.42
1:M:70:ILE:HG12	1:M:106:GLY:HA2	2.01	0.42
3:O:174:ASP:HB3	3:O:226:LEU:CD2	2.49	0.42
3:O:274:ALA:O	3:O:275:THR:CG2	2.66	0.42
3:R:335:ILE:HD12	3:R:335:ILE:O	2.19	0.42
2:B:95:CYS:N	2:B:112:CYS:SG	2.93	0.42
3:F:195:LEU:HB2	3:F:239:THR:CG2	2.50	0.42
1:G:4:CYS:SG	1:G:10:ALA:HB2	2.60	0.42
3:I:198:PHE:O	3:I:199:VAL:O	2.37	0.42
1:J:70:ILE:CD1	1:J:72:LEU:HB3	2.49	0.42
1:M:107:LEU:HD13	1:M:113:PHE:HB3	2.01	0.42
3:O:225:ASN:HB3	3:O:268:SER:O	2.19	0.42
1:P:100:GLU:C	1:P:102:GLN:HB3	2.43	0.42
3:C:220:PRO:HG3	3:C:255:ALA:HA	2.01	0.42
1:D:111:THR:HG21	2:E:90:LEU:HD22	2.01	0.42
3:F:281:VAL:HG22	3:F:309:ILE:HB	2.02	0.42
3:F:314:TYR:O	3:F:318:ASN:ND2	2.45	0.42
1:J:118:TYR:HD2	2:K:91:ARG:NH1	2.18	0.42
2:N:90:LEU:C	2:N:90:LEU:HD12	2.44	0.42
1:P:79:GLN:HG3	1:P:80:GLN:OE1	2.19	0.42
3:R:337:THR:O	3:R:338:GLU:HG2	2.20	0.42
3:C:181:GLU:HG3	3:C:217:ALA:HB2	2.01	0.42
2:E:41:ILE:CG2	2:E:47:GLU:HB2	2.50	0.42
3:F:341:PHE:O	3:F:341:PHE:CG	2.73	0.42
3:F:344:VAL:CG1	3:F:349:ALA:HB3	2.50	0.42
3:I:272:ARG:CB	3:I:273:SER:CB	2.94	0.42
2:K:64:TRP:CE2	2:K:116:VAL:HG22	2.55	0.42
1:M:24:THR:HG1	1:M:27:GLU:H	1.63	0.42
1:M:49:GLU:O	1:M:53:VAL:HG12	2.19	0.42
1:M:78:GLU:OE1	1:M:78:GLU:N	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:101:SER:CA	1:P:102:GLN:CB	2.92	0.42
3:R:172:LEU:O	3:R:274:ALA:HB1	2.20	0.42
3:R:325:LEU:HD23	3:R:329:ILE:HD13	2.02	0.42
2:B:67:LEU:HB3	2:B:96:ALA:HB3	2.02	0.42
2:E:51:GLY:HA2	2:E:100:VAL:HG21	2.02	0.42
3:F:173:ILE:HD12	3:F:173:ILE:C	2.45	0.42
3:F:236:ILE:HD12	3:F:236:ILE:C	2.44	0.42
3:F:277:VAL:HG22	3:F:305:LEU:HB2	2.01	0.42
1:G:64:PRO:O	1:G:65:GLU:C	2.63	0.42
1:G:102:GLN:HE21	1:G:118:TYR:HB2	1.85	0.42
2:H:30:TYR:O	2:H:31:ALA:HB3	2.20	0.42
2:H:51:GLY:HA2	2:H:100:VAL:HG11	2.00	0.42
2:H:95:CYS:N	2:H:112:CYS:SG	2.92	0.42
3:I:185:ILE:O	3:I:186:TYR:HB2	2.20	0.42
3:L:272:ARG:H	3:L:274:ALA:H	1.65	0.42
2:N:57:THR:HG22	2:N:58:LEU:H	1.85	0.42
3:O:213:LEU:HB3	3:O:224:PHE:CE2	2.55	0.42
3:C:199:VAL:O	3:C:201:GLY:HA3	2.20	0.42
1:G:21:GLU:O	1:G:21:GLU:HG3	2.20	0.42
1:G:84:GLU:O	1:G:91:ILE:HG12	2.19	0.42
1:J:25:TRP:CZ2	1:J:71:GLY:HA2	2.55	0.42
2:K:63:MET:HG2	2:K:119:VAL:HG13	2.02	0.42
3:L:175:VAL:HG23	3:L:211:VAL:CG2	2.47	0.42
1:M:79:GLN:OE1	1:M:96:TRP:HD1	2.03	0.42
1:M:87:MET:HE1	2:N:40:SER:OG	2.20	0.42
2:N:41:ILE:HG21	2:N:47:GLU:HB2	2.01	0.42
1:A:108:ALA:O	1:A:111:THR:HG22	2.20	0.42
2:B:116:VAL:HG22	2:B:117:SER:N	2.34	0.42
3:C:280:VAL:CG2	3:C:308:GLY:HA2	2.50	0.42
3:C:339:ARG:N	9:C:504:HOH:O	2.15	0.42
2:E:67:LEU:HD12	2:E:67:LEU:C	2.44	0.42
2:H:39:ALA:HB2	2:H:119:VAL:HG23	2.02	0.42
3:L:211:VAL:HG22	3:L:212:GLY:N	2.35	0.42
3:O:261:LYS:NZ	8:O:407:SO4:O2	2.53	0.42
3:O:280:VAL:HG22	3:O:307:PHE:O	2.19	0.42
2:Q:11:TYR:HD2	2:Q:122:PHE:HB3	1.80	0.42
3:C:352:GLU:CD	3:C:353:LYS:HG2	2.45	0.41
3:F:180:ASP:HB2	3:F:282:THR:HA	2.01	0.41
3:I:214:ILE:C	3:I:214:ILE:HD12	2.45	0.41
1:J:114:ARG:O	6:J:204:GOL:H11	2.20	0.41
2:K:84:LEU:HA	9:K:207:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:206:PRO:O	3:L:207:THR:HB	2.19	0.41
3:O:225:ASN:OD1	3:O:268:SER:HB2	2.20	0.41
2:Q:87:LYS:HE3	2:Q:89:TRP:CE2	2.55	0.41
2:E:3:LEU:HB3	2:E:4:HIS:H	1.58	0.41
3:I:344:VAL:HG12	3:I:346:ASP:O	2.19	0.41
3:L:185:ILE:O	3:L:186:TYR:HB2	2.20	0.41
3:L:335:ILE:CB	3:L:336:PRO:HA	2.49	0.41
1:P:35:GLN:HB3	1:P:36:ALA:HB2	2.02	0.41
1:A:81:CYS:HB2	2:B:70:PRO:O	2.20	0.41
3:F:178:VAL:CG1	3:F:214:ILE:HD11	2.42	0.41
3:F:202:LEU:HG	3:F:362:PHE:CE1	2.55	0.41
1:G:23:LYS:HG3	1:G:127:PHE:HE1	1.85	0.41
3:I:340:TYR:HA	3:I:341:PHE:C	2.44	0.41
2:N:59:LYS:CG	2:N:60:TYR:H	2.29	0.41
1:A:42:VAL:N	9:A:306:HOH:O	2.47	0.41
3:C:185:ILE:HD13	3:C:283:ASP:HB3	2.01	0.41
3:C:264:TYR:CE1	3:C:276:LYS:HB3	2.55	0.41
1:D:101:SER:N	1:D:102:GLN:HB3	2.36	0.41
2:E:29:CYS:HA	2:E:30:TYR:C	2.45	0.41
2:H:71:TRP:HA	2:H:74:CYS:SG	2.60	0.41
1:J:63:ARG:HE	1:J:63:ARG:HA	1.85	0.41
1:M:111:THR:HG21	2:N:90:LEU:CD2	2.50	0.41
3:R:304:ILE:O	3:R:306:ARG:NH1	2.51	0.41
1:A:66:LEU:HD13	1:A:67:TYR:O	2.21	0.41
2:B:8:TYR:HB2	2:B:49:PHE:CZ	2.55	0.41
3:F:282:THR:HG21	3:F:329:ILE:HD11	2.02	0.41
1:G:72:LEU:CD1	2:H:76:TRP:HB3	2.49	0.41
3:I:173:ILE:HD12	3:I:173:ILE:C	2.45	0.41
1:J:70:ILE:HD11	1:J:105:GLN:HB2	2.01	0.41
1:J:115:LYS:HA	2:K:88:VAL:CG1	2.51	0.41
3:L:253:PHE:CE1	3:L:292:LEU:HG	2.55	0.41
3:O:236:ILE:HD12	3:O:236:ILE:C	2.45	0.41
3:O:335:ILE:HG22	9:O:501:HOH:O	2.20	0.41
2:Q:87:LYS:HE3	2:Q:89:TRP:NE1	2.35	0.41
3:R:185:ILE:O	3:R:186:TYR:HB2	2.21	0.41
1:A:108:ALA:HB3	1:A:111:THR:HG22	2.01	0.41
1:G:23:LYS:HB3	1:G:27:GLU:CG	2.50	0.41
1:G:110:TRP:HB3	3:I:245:TYR:O	2.21	0.41
2:H:67:LEU:CD2	2:H:70:PRO:HG3	2.51	0.41
1:P:41:LEU:HB2	1:P:71:GLY:HA3	2.03	0.41
1:D:101:SER:HA	1:D:102:GLN:CB	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3:LEU:HD13	3:O:359:GLU:CD	2.45	0.41
3:F:173:ILE:HD13	3:F:175:VAL:HG13	2.03	0.41
1:G:115:LYS:HG3	2:H:88:VAL:HG11	2.02	0.41
3:I:174:ASP:OD1	3:I:271:ARG:NH2	2.53	0.41
3:I:176:VAL:CG2	3:I:278:MET:HB3	2.50	0.41
3:I:206:PRO:O	3:I:207:THR:HB	2.21	0.41
3:I:329:ILE:HG22	3:I:341:PHE:CG	2.55	0.41
1:J:87:MET:SD	2:K:40:SER:HB2	2.59	0.41
3:L:198:PHE:CD1	3:L:357:LEU:HD12	2.56	0.41
2:N:116:VAL:HG22	2:N:117:SER:N	2.36	0.41
2:K:78:TRP:HB2	2:K:82:ALA:HB2	2.03	0.41
2:N:110:ARG:NH1	3:O:314:TYR:HE2	2.19	0.41
3:O:214:ILE:HB	3:O:221:ARG:O	2.20	0.41
1:P:41:LEU:HB3	1:P:71:GLY:HA3	2.01	0.41
2:Q:5:TRP:HE3	2:Q:12:CYS:HB3	1.86	0.41
1:A:14:HIS:CD2	1:A:132:PRO:HA	2.56	0.41
1:A:22:PRO:CB	1:A:125:ASN:C	2.94	0.41
1:A:62:LYS:HD2	1:A:62:LYS:HA	1.87	0.41
2:E:59:LYS:HG2	2:E:60:TYR:H	1.85	0.41
2:H:15:VAL:HA	2:H:119:VAL:HG12	2.03	0.41
2:H:58:LEU:CA	2:H:59:LYS:HG2	2.43	0.41
2:H:100:VAL:HG12	2:H:105:ILE:HG13	2.01	0.41
3:I:236:ILE:HD12	3:I:236:ILE:C	2.46	0.41
3:I:325:LEU:O	3:I:329:ILE:HD13	2.21	0.41
1:J:61:ILE:HG22	1:J:62:LYS:N	2.36	0.41
1:J:102:GLN:HA	1:J:119:SER:C	2.44	0.41
2:K:95:CYS:N	2:K:112:CYS:SG	2.94	0.41
2:K:113:GLU:H	2:K:113:GLU:CD	2.28	0.41
3:L:311:VAL:HG11	3:L:347:GLU:HG2	2.02	0.41
1:M:24:THR:HG22	1:M:122:GLN:O	2.21	0.41
2:N:34:LYS:C	2:N:34:LYS:HD3	2.46	0.41
3:O:253:PHE:CZ	3:O:292:LEU:HG	2.56	0.41
3:O:361:ILE:HA	3:O:362:PHE:HA	1.80	0.41
1:P:110:TRP:HE1	2:Q:90:LEU:CD2	2.30	0.41
2:Q:8:TYR:CE1	2:Q:45:GLU:HG2	2.56	0.41
3:R:251:ASN:HB3	9:R:502:HOH:O	2.20	0.41
3:R:264:TYR:OH	3:R:277:VAL:O	2.39	0.41
3:R:283:ASP:HA	3:R:311:VAL:HB	2.03	0.41
3:C:325:LEU:C	3:C:325:LEU:HD23	2.46	0.41
1:D:5:LEU:HD23	1:D:5:LEU:C	2.46	0.41
1:G:14:HIS:HB2	1:G:16:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:23:LYS:HD3	1:J:27:GLU:HG2	2.03	0.41
3:L:214:ILE:HB	3:L:221:ARG:O	2.21	0.41
1:M:41:LEU:HB3	1:M:71:GLY:HA3	2.03	0.41
1:M:69:TRP:HH2	1:M:120:ASP:O	2.04	0.41
3:O:194:PHE:CD2	3:O:195:LEU:HD23	2.56	0.41
2:Q:18:GLU:OE1	2:Q:18:GLU:N	2.52	0.41
2:B:58:LEU:HB3	2:B:60:TYR:N	2.37	0.40
1:D:83:SER:N	9:D:306:HOH:O	2.38	0.40
3:F:292:LEU:O	3:F:293:LYS:C	2.61	0.40
2:H:38:LEU:HD23	9:H:304:HOH:O	2.20	0.40
3:I:243:SER:OG	9:I:505:HOH:O	2.21	0.40
1:J:116:TRP:HE1	6:J:204:GOL:H12	1.86	0.40
3:O:186:TYR:N	3:O:347:GLU:OE2	2.55	0.40
2:E:52:LYS:HE2	2:E:56:GLN:HE21	1.86	0.40
2:E:98:MET:O	2:E:98:MET:HG3	2.21	0.40
3:I:188:TRP:HB2	3:I:244:GLN:NE2	2.36	0.40
3:L:313:GLY:O	3:L:317:ARG:HG3	2.21	0.40
1:M:16:TYR:HA	1:M:130:LYS:HB2	2.04	0.40
1:M:34:GLU:HA	1:M:35:GLN:HA	1.74	0.40
3:O:178:VAL:HG22	3:O:280:VAL:HG12	2.03	0.40
1:P:85:TRP:CZ3	2:Q:40:SER:HA	2.55	0.40
2:Q:110:ARG:HE	2:Q:114:LYS:CB	2.34	0.40
2:B:16:PHE:HB2	2:B:118:PHE:CE1	2.56	0.40
2:B:90:LEU:HD12	2:B:90:LEU:C	2.45	0.40
2:E:115:THR:O	2:E:116:VAL:HB	2.22	0.40
3:I:199:VAL:C	3:I:201:GLY:N	2.66	0.40
1:J:97:ASN:O	1:J:100:GLU:HG2	2.22	0.40
2:K:23:GLU:OE2	2:K:113:GLU:HA	2.22	0.40
2:N:19:LEU:HD22	2:N:116:VAL:HA	2.03	0.40
3:R:236:ILE:HD12	3:R:237:VAL:N	2.36	0.40
3:R:253:PHE:N	9:R:502:HOH:O	2.54	0.40
3:R:361:ILE:HG12	9:R:511:HOH:O	2.22	0.40
1:D:47:ASP:OD1	2:E:86:TYR:OH	2.36	0.40
3:F:197:LYS:HA	3:F:200:GLN:HG2	2.03	0.40
2:H:23:GLU:O	2:H:26:GLU:OE2	2.38	0.40
1:M:20:ASN:HB3	1:M:61:ILE:HD12	2.01	0.40
2:N:1:CYS:HB3	2:N:5:TRP:HB2	2.03	0.40
2:Q:110:ARG:NH2	2:Q:114:LYS:HD2	2.35	0.40
1:A:65:GLU:C	1:A:66:LEU:HG	2.47	0.40
1:D:2:PHE:HA	1:D:3:ASN:HA	1.78	0.40
1:G:67:TYR:HA	1:G:107:LEU:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:75:ARG:O	1:G:75:ARG:HG2	2.22	0.40
1:J:23:LYS:HD2	1:J:127:PHE:CE1	2.57	0.40
2:K:69:ASN:ND2	2:K:72:LYS:HB2	2.36	0.40
3:L:271:ARG:HA	3:L:272:ARG:HA	1.96	0.40
1:M:110:TRP:CG	3:O:247:GLY:HA2	2.56	0.40
2:Q:63:MET:O	2:Q:97:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	125/135 (93%)	106 (85%)	19 (15%)	0	100	100
1	D	126/135 (93%)	108 (86%)	18 (14%)	0	100	100
1	G	130/135 (96%)	118 (91%)	12 (9%)	0	100	100
1	J	129/135 (96%)	114 (88%)	15 (12%)	0	100	100
1	M	130/135 (96%)	113 (87%)	17 (13%)	0	100	100
1	P	130/135 (96%)	122 (94%)	8 (6%)	0	100	100
2	B	113/124 (91%)	103 (91%)	10 (9%)	0	100	100
2	E	120/124 (97%)	111 (92%)	8 (7%)	1 (1%)	16	50
2	H	116/124 (94%)	101 (87%)	15 (13%)	0	100	100
2	K	106/124 (86%)	94 (89%)	12 (11%)	0	100	100
2	N	120/124 (97%)	111 (92%)	9 (8%)	0	100	100
2	Q	120/124 (97%)	109 (91%)	10 (8%)	1 (1%)	16	50
3	C	186/217 (86%)	174 (94%)	11 (6%)	1 (0%)	24	60
3	F	191/217 (88%)	168 (88%)	22 (12%)	1 (0%)	24	60
3	I	189/217 (87%)	167 (88%)	19 (10%)	3 (2%)	7	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	187/217 (86%)	168 (90%)	18 (10%)	1 (0%)	24	60
3	O	187/217 (86%)	169 (90%)	17 (9%)	1 (0%)	24	60
3	R	179/217 (82%)	166 (93%)	13 (7%)	0	100	100
All	All	2584/2856 (90%)	2322 (90%)	253 (10%)	9 (0%)	36	70

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	199	VAL
3	I	200	GLN
3	I	304	ILE
2	E	116	VAL
2	Q	116	VAL
3	C	344	VAL
3	F	336	PRO
3	L	336	PRO
3	O	336	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	102/118 (86%)	100 (98%)	2 (2%)	48	76
1	D	103/118 (87%)	103 (100%)	0	100	100
1	G	111/118 (94%)	108 (97%)	3 (3%)	39	71
1	J	109/118 (92%)	107 (98%)	2 (2%)	51	77
1	M	107/118 (91%)	104 (97%)	3 (3%)	38	70
1	P	110/118 (93%)	107 (97%)	3 (3%)	39	71
2	B	102/112 (91%)	101 (99%)	1 (1%)	68	84
2	E	105/112 (94%)	103 (98%)	2 (2%)	50	76
2	H	94/112 (84%)	93 (99%)	1 (1%)	65	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	91/112 (81%)	87 (96%)	4 (4%)	25	60
2	N	110/112 (98%)	109 (99%)	1 (1%)	70	85
2	Q	109/112 (97%)	108 (99%)	1 (1%)	70	85
3	C	149/181 (82%)	147 (99%)	2 (1%)	61	81
3	F	149/181 (82%)	144 (97%)	5 (3%)	32	66
3	I	138/181 (76%)	137 (99%)	1 (1%)	76	86
3	L	140/181 (77%)	140 (100%)	0	100	100
3	O	148/181 (82%)	147 (99%)	1 (1%)	76	86
3	R	146/181 (81%)	146 (100%)	0	100	100
All	All	2123/2466 (86%)	2091 (98%)	32 (2%)	57	80

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	MET
1	A	121	CYS
2	B	29	CYS
3	C	338	GLU
3	C	343	ASN
2	E	3	LEU
2	E	23	GLU
3	F	228	THR
3	F	288	ASP
3	F	291	MET
3	F	362	PHE
3	F	363	SER
1	G	2	PHE
1	G	13	GLN
1	G	111	THR
2	H	26	GLU
3	I	305	LEU
1	J	14	HIS
1	J	63	ARG
2	K	53	LEU
2	K	63	MET
2	K	97	VAL
2	K	98	MET
1	M	21	GLU
1	M	24	THR

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Mol	Chain	Res	Type
1	M	121	CYS
2	N	26	GLU
3	O	273	SER
1	P	4	CYS
1	P	15	CYS
1	P	81	CYS
2	Q	32	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
3	C	200	GLN
3	C	210	GLN
3	C	219	ASN
3	C	318	ASN
3	C	360	GLN
1	D	13	GLN
1	D	40	HIS
1	D	125	ASN
2	E	56	GLN
2	E	68	ASN
3	F	210	GLN
3	F	257	GLN
1	G	102	GLN
1	G	105	GLN
3	I	215	GLN
3	I	244	GLN
3	I	303	ASN
1	J	14	HIS
1	J	102	GLN
1	J	125	ASN
2	K	109	ASN
3	L	257	GLN
3	L	287	HIS
1	M	13	GLN
3	O	183	ASN
3	O	200	GLN
3	O	318	ASN
1	P	3	ASN
2	Q	33	HIS
2	Q	42	HIS

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Mol	Chain	Res	Type
2	Q	69	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 90 ligands modelled in this entry, 72 are monoatomic - leaving 18 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	$\# Z > 2$
6	GOL	P	204	-	5,5,5	0.36	0	5,5,5	0.30	0
8	SO4	F	401	7	4,4,4	0.23	0	6,6,6	0.07	0
8	SO4	I	407	7	4,4,4	0.23	0	6,6,6	0.08	0
6	GOL	G	205	-	5,5,5	0.37	0	5,5,5	0.24	0
8	SO4	D	208	-	4,4,4	0.24	0	6,6,6	0.07	0
8	SO4	F	406	-	4,4,4	0.23	0	6,6,6	0.07	0
8	SO4	R	404	7	4,4,4	0.23	0	6,6,6	0.07	0
8	SO4	C	409	-	4,4,4	0.23	0	6,6,6	0.08	0
6	GOL	J	204	-	5,5,5	0.39	0	5,5,5	0.39	0
6	GOL	J	205	-	5,5,5	0.39	0	5,5,5	0.27	0
8	SO4	L	406	-	4,4,4	0.23	0	6,6,6	0.07	0
6	GOL	C	410	-	5,5,5	0.37	0	5,5,5	0.31	0
6	GOL	A	203	-	5,5,5	0.38	0	5,5,5	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	G	204	-	5,5,5	0.36	0	5,5,5	0.32	0
8	SO4	O	407	-	4,4,4	0.24	0	6,6,6	0.07	0
6	GOL	H	204	-	5,5,5	0.37	0	5,5,5	0.33	0
8	SO4	E	207	4	4,4,4	0.23	0	6,6,6	0.08	0
8	SO4	O	402	4	4,4,4	0.24	0	6,6,6	0.08	0

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
6	GOL	P	204	-	-	2/4/4/4	-
6	GOL	G	205	-	-	1/4/4/4	-
6	GOL	J	204	-	-	2/4/4/4	-
6	GOL	J	205	-	-	2/4/4/4	-
6	GOL	C	410	-	-	2/4/4/4	-
6	GOL	A	203	-	-	2/4/4/4	-
6	GOL	G	204	-	-	2/4/4/4	-
6	GOL	H	204	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	203	GOL	O1-C1-C2-C3
6	C	410	GOL	O1-C1-C2-C3
6	H	204	GOL	O1-C1-C2-C3
6	J	204	GOL	O1-C1-C2-C3
6	G	204	GOL	O1-C1-C2-C3
6	J	205	GOL	O1-C1-C2-C3
6	P	204	GOL	O1-C1-C2-C3
6	A	203	GOL	O1-C1-C2-O2
6	G	204	GOL	O1-C1-C2-O2
6	J	204	GOL	O1-C1-C2-O2
6	J	205	GOL	O1-C1-C2-O2
6	P	204	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	C	410	GOL	O1-C1-C2-O2
6	H	204	GOL	O1-C1-C2-O2
6	G	205	GOL	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	401	SO4	1	0
8	D	208	SO4	1	0
6	J	204	GOL	9	0
6	J	205	GOL	2	0
8	L	406	SO4	2	0
8	O	407	SO4	4	0
6	H	204	GOL	1	0
8	E	207	SO4	1	0
8	O	402	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	129/135 (95%)	-0.81	0 100 100	66, 99, 147, 169	0
1	D	130/135 (96%)	-1.18	0 100 100	55, 84, 129, 169	0
1	G	132/135 (97%)	-1.19	0 100 100	49, 78, 124, 149	0
1	J	131/135 (97%)	-0.92	0 100 100	59, 88, 114, 128	0
1	M	132/135 (97%)	-0.62	0 100 100	66, 113, 179, 221	0
1	P	132/135 (97%)	-0.75	0 100 100	60, 96, 157, 213	0
2	B	119/124 (95%)	-1.04	0 100 100	61, 89, 131, 204	0
2	E	122/124 (98%)	-1.03	0 100 100	64, 88, 131, 215	0
2	H	120/124 (96%)	-0.93	0 100 100	63, 93, 155, 173	0
2	K	108/124 (87%)	-0.85	0 100 100	73, 106, 185, 255	0
2	N	122/124 (98%)	-1.12	0 100 100	53, 82, 118, 154	0
2	Q	122/124 (98%)	-0.86	0 100 100	66, 99, 163, 248	0
3	C	190/217 (87%)	-1.10	0 100 100	57, 94, 147, 199	0
3	F	193/217 (88%)	-0.94	0 100 100	60, 92, 127, 151	0
3	I	191/217 (88%)	-0.95	0 100 100	60, 87, 139, 187	0
3	L	189/217 (87%)	-1.14	0 100 100	49, 87, 149, 228	0
3	O	191/217 (88%)	-1.13	0 100 100	55, 84, 130, 196	0
3	R	187/217 (86%)	-1.18	0 100 100	52, 80, 122, 156	0
All	All	2640/2856 (92%)	-1.00	0 100 100	49, 90, 149, 255	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [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(Å ²)	Q<0.9
4	NA	C	401	1/1	0.94	0.05	78,78,78,78	0
5	CL	N	204	1/1	0.94	0.05	99,99,99,99	0
4	NA	J	201	1/1	0.95	0.06	72,72,72,72	0
5	CL	C	405	1/1	0.95	0.08	116,116,116,116	0
5	CL	H	203	1/1	0.95	0.13	165,165,165,165	0
4	NA	C	403	1/1	0.95	0.11	67,67,67,67	0
4	NA	F	403	1/1	0.96	0.05	102,102,102,102	0
4	NA	D	202	1/1	0.97	0.05	52,52,52,52	0
4	NA	D	209	1/1	0.97	0.10	158,158,158,158	0
5	CL	H	202	1/1	0.97	0.04	77,77,77,77	0
4	NA	C	411	1/1	0.97	0.07	117,117,117,117	0
5	CL	I	404	1/1	0.97	0.06	137,137,137,137	0
5	CL	J	203	1/1	0.97	0.04	78,78,78,78	0
4	NA	I	401	1/1	0.97	0.10	115,115,115,115	0
5	CL	Q	203	1/1	0.97	0.03	88,88,88,88	0
5	CL	Q	204	1/1	0.97	0.03	89,89,89,89	0
6	GOL	J	205	6/6	0.97	0.06	67,72,82,83	0
6	GOL	P	204	6/6	0.97	0.06	69,78,86,87	0
8	SO4	O	402	5/5	0.97	0.08	108,118,125,130	0
4	NA	G	201	1/1	0.98	0.06	54,54,54,54	0
4	NA	E	201	1/1	0.98	0.07	103,103,103,103	0
4	NA	E	203	1/1	0.98	0.05	62,62,62,62	0
5	CL	I	405	1/1	0.98	0.05	72,72,72,72	0
4	NA	L	401	1/1	0.98	0.04	74,74,74,74	0
5	CL	M	203	1/1	0.98	0.04	92,92,92,92	0
5	CL	N	202	1/1	0.98	0.02	95,95,95,95	0
5	CL	N	203	1/1	0.98	0.08	98,98,98,98	0
4	NA	O	401	1/1	0.98	0.04	76,76,76,76	0
5	CL	P	203	1/1	0.98	0.04	70,70,70,70	0
4	NA	Q	201	1/1	0.98	0.06	95,95,95,95	0
4	NA	B	201	1/1	0.98	0.04	62,62,62,62	0
6	GOL	A	203	6/6	0.98	0.04	55,71,77,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GOL	C	410	6/6	0.98	0.03	43,66,73,81	0
6	GOL	G	204	6/6	0.98	0.04	65,70,77,87	0
5	CL	E	206	1/1	0.98	0.04	90,90,90,90	0
5	CL	G	202	1/1	0.98	0.04	91,91,91,91	0
8	SO4	E	207	5/5	0.98	0.04	119,123,130,133	0
8	SO4	I	407	5/5	0.98	0.06	101,107,112,115	0
5	CL	G	203	1/1	0.98	0.04	123,123,123,123	0
8	SO4	O	407	5/5	0.98	0.03	93,95,103,107	0
8	SO4	R	404	5/5	0.98	0.04	95,104,116,118	0
4	NA	E	202	1/1	0.99	0.03	68,68,68,68	0
4	NA	A	201	1/1	0.99	0.04	87,87,87,87	0
4	NA	J	202	1/1	0.99	0.04	60,60,60,60	0
4	NA	F	402	1/1	0.99	0.02	37,37,37,37	0
4	NA	L	402	1/1	0.99	0.03	54,54,54,54	0
4	NA	M	201	1/1	0.99	0.03	66,66,66,66	0
4	NA	N	201	1/1	0.99	0.05	81,81,81,81	0
5	CL	I	406	1/1	0.99	0.04	81,81,81,81	0
4	NA	C	402	1/1	0.99	0.02	61,61,61,61	0
5	CL	L	404	1/1	0.99	0.02	100,100,100,100	0
5	CL	L	405	1/1	0.99	0.05	86,86,86,86	0
5	CL	M	202	1/1	0.99	0.03	77,77,77,77	0
4	NA	O	404	1/1	0.99	0.04	74,74,74,74	0
4	NA	P	201	1/1	0.99	0.03	55,55,55,55	0
4	NA	D	201	1/1	0.99	0.03	90,90,90,90	0
4	NA	Q	202	1/1	0.99	0.03	40,40,40,40	0
5	CL	O	406	1/1	0.99	0.03	69,69,69,69	0
5	CL	P	202	1/1	0.99	0.04	77,77,77,77	0
4	NA	R	401	1/1	0.99	0.03	46,46,46,46	0
5	CL	A	202	1/1	0.99	0.04	89,89,89,89	0
4	NA	H	201	1/1	0.99	0.04	62,62,62,62	0
5	CL	R	403	1/1	0.99	0.04	78,78,78,78	0
5	CL	C	406	1/1	0.99	0.02	82,82,82,82	0
5	CL	C	407	1/1	0.99	0.05	84,84,84,84	0
5	CL	C	408	1/1	0.99	0.04	76,76,76,76	0
6	GOL	G	205	6/6	0.99	0.05	73,91,109,109	0
6	GOL	H	204	6/6	0.99	0.04	47,61,78,89	0
6	GOL	J	204	6/6	0.99	0.06	52,66,83,88	0
5	CL	D	203	1/1	0.99	0.04	83,83,83,83	0
5	CL	D	204	1/1	0.99	0.03	82,82,82,82	0
7	MG	I	403	1/1	0.99	0.03	51,51,51,51	0
7	MG	L	403	1/1	0.99	0.08	169,169,169,169	0
7	MG	O	405	1/1	0.99	0.05	226,226,226,226	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	SO4	C	409	5/5	0.99	0.04	105,106,113,120	0
5	CL	D	205	1/1	0.99	0.03	80,80,80,80	0
8	SO4	F	401	5/5	0.99	0.04	91,91,97,121	0
8	SO4	F	406	5/5	0.99	0.02	77,79,83,100	0
5	CL	D	206	1/1	0.99	0.04	68,68,68,68	0
8	SO4	L	406	5/5	0.99	0.04	103,108,109,118	0
5	CL	D	207	1/1	0.99	0.02	71,71,71,71	0
5	CL	E	204	1/1	0.99	0.03	82,82,82,82	0
5	CL	E	205	1/1	0.99	0.03	70,70,70,70	0
5	CL	F	405	1/1	1.00	0.03	83,83,83,83	0
4	NA	I	402	1/1	1.00	0.02	65,65,65,65	0
4	NA	O	403	1/1	1.00	0.01	60,60,60,60	0
7	MG	R	402	1/1	1.00	0.03	47,47,47,47	0
7	MG	C	404	1/1	1.00	0.03	84,84,84,84	0
8	SO4	D	208	5/5	1.00	0.02	55,55,62,85	0
7	MG	F	404	1/1	1.00	0.03	103,103,103,103	0

6.5 Other polymers [i](#)

There are no such residues in this entry.