



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 3S7Y / pdb_00003s7y
Title : Crystal structure of mmNAGS in Space Group P3121 at 4.3 Å resolution
Authors : Shi, D.; Li, Y.; Cabrera-Luque, J.; Jin, Z.; Yu, X.; Allewell, N.M.; Tuchman, M.
Deposited on : 2011-05-27
Resolution : 4.31 Å (reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

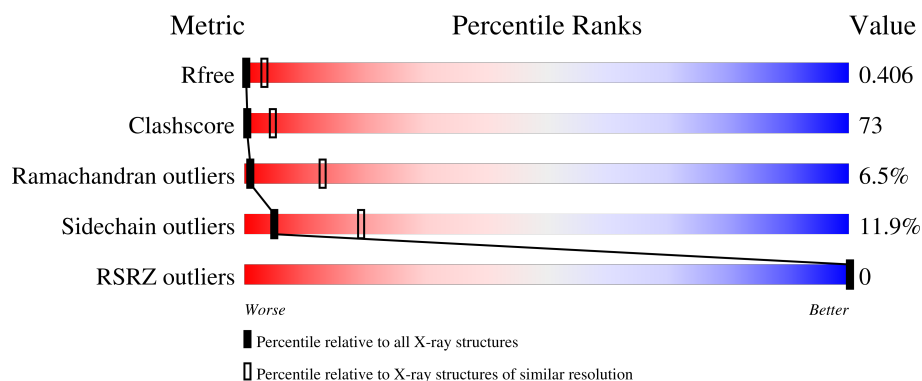
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.31 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	1052 (4.70-3.90)
Clashscore	190562	1097 (4.70-3.90)
Ramachandran outliers	187476	1001 (4.70-3.90)
Sidechain outliers	187428	1007 (4.72-3.88)
RSRZ outliers	180081	1049 (4.70-3.90)

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	461	
1	X	461	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 6683 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called N-acetylglutamate kinase / N-acetylglutamate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	1	0
			3349	2107	605	631	6			
1	X	435	Total	C	N	O	S	0	0	0
			3334	2097	601	630	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q0ASS9
A	-18	GLY	-	expression tag	UNP Q0ASS9
A	-17	SER	-	expression tag	UNP Q0ASS9
A	-16	SER	-	expression tag	UNP Q0ASS9
A	-15	HIS	-	expression tag	UNP Q0ASS9
A	-14	HIS	-	expression tag	UNP Q0ASS9
A	-13	HIS	-	expression tag	UNP Q0ASS9
A	-12	HIS	-	expression tag	UNP Q0ASS9
A	-11	HIS	-	expression tag	UNP Q0ASS9
A	-10	HIS	-	expression tag	UNP Q0ASS9
A	-9	SER	-	expression tag	UNP Q0ASS9
A	-8	SER	-	expression tag	UNP Q0ASS9
A	-7	GLY	-	expression tag	UNP Q0ASS9
A	-6	LEU	-	expression tag	UNP Q0ASS9
A	-5	VAL	-	expression tag	UNP Q0ASS9
A	-4	PRO	-	expression tag	UNP Q0ASS9
A	-3	ARG	-	expression tag	UNP Q0ASS9
A	-2	GLY	-	expression tag	UNP Q0ASS9
A	-1	SER	-	expression tag	UNP Q0ASS9
A	0	HIS	-	expression tag	UNP Q0ASS9
X	-19	MET	-	expression tag	UNP Q0ASS9
X	-18	GLY	-	expression tag	UNP Q0ASS9
X	-17	SER	-	expression tag	UNP Q0ASS9
X	-16	SER	-	expression tag	UNP Q0ASS9
X	-15	HIS	-	expression tag	UNP Q0ASS9

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Chain	Residue	Modelled	Actual	Comment	Reference
X	-14	HIS	-	expression tag	UNP Q0ASS9
X	-13	HIS	-	expression tag	UNP Q0ASS9
X	-12	HIS	-	expression tag	UNP Q0ASS9
X	-11	HIS	-	expression tag	UNP Q0ASS9
X	-10	HIS	-	expression tag	UNP Q0ASS9
X	-9	SER	-	expression tag	UNP Q0ASS9
X	-8	SER	-	expression tag	UNP Q0ASS9
X	-7	GLY	-	expression tag	UNP Q0ASS9
X	-6	LEU	-	expression tag	UNP Q0ASS9
X	-5	VAL	-	expression tag	UNP Q0ASS9
X	-4	PRO	-	expression tag	UNP Q0ASS9
X	-3	ARG	-	expression tag	UNP Q0ASS9
X	-2	GLY	-	expression tag	UNP Q0ASS9
X	-1	SER	-	expression tag	UNP Q0ASS9
X	0	HIS	-	expression tag	UNP Q0ASS9

GLN	V372	L308	A173	Q238	I106
	V373	D309	I174	A239	P107
	N374	N310	L175		I108
	R375	L311		V242	I109
				N243	
	A380	A315	L178	G244	L113
	P381	F316	G245	G246	T114
	Q382	G317	E180	R247	Q115
	L383	R318	T181	L248	A116
	L384		P182	K249	N117
V385	E322	D183	L250	L118	
R386	G323	G184	E251	A119	
S387	Y324	T185		L120	
R388	W325	L186		V121	
T389	R326		K254		
N390	R327	R255	R256	I124	
N391	L328	L256			
P392	R329	A191	N190	R130	
V393	R330	D192	A191	A131	
N394	D331	D259	V193	A132	
G395	R332	L260	A194	A133	
	A333	P261	V195	V134	
	F334	L262	R196	P135	
	V335	S263	A197	R136	
F398	T336	S264			
C401	E337	S265	H200	G137	
D402	R338	V266	A201	V138	
G403	S338	S267	E140	F139	
A404	V339		L202	E140	
V405	R340	L268	Q203	A141	
R406	A341	T269	P204	D142	
R407	A342	R270	Y205	I143	
D408	A343		K206	V144	
E409	R344		V207	D145	
W410	T345	L274	V208	D146	
T411	R346	A275	F209	D147	
V412	R347	R276	L210	K148	
F413	L348	E277	T211	L148	
W414	D349	L278	L149	G150	
	G350	F279	G212	G150	
			T213	R151	
P420	W351		G214	V152	
V421	V352	T286	G215	G153	
E422	V353	L287	L216	E154	
V423	L354	L288	L217	P155	
A424	D355	R289		R156	
D425	K356	R290	G221	H157	
V426	F357	G291	D222		
E427	A358	E292	I223	I158	
V428	V359	R293	L224	H159	
K429	L360		S225	D161	
A430	D361	A296	S226	L162	
F431	D362	T297	N227	V163	
A432	A363	D298	N228	G164	
L433	R364	D299	L229	S165	
P434	G365	K300	A230	A166	
P435	E366	S301	T231	A167	
T436	G367	S302	D232	R168	
L437	L368	L303	F233	A169	
E438	G369	D304		G170	
A439	R370		L236	Q171	
PR40	T371	R307	M237	A172	

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	95.11Å 95.11Å 253.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.13 – 4.31 31.13 – 4.31	Depositor EDS
% Data completeness (in resolution range)	92.1 (31.13-4.31) 89.1 (31.13-4.31)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 4.29Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.274 , 0.419 0.259 , 0.406	Depositor DCC
R_{free} test set	949 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	192.6	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 436.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.067 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6683	wwPDB-VP
Average B, all atoms (Å ²)	456.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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 [i](#)

5.1 Standard geometry [i](#)

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	1.05	7/3412 (0.2%)	1.87	123/4639 (2.7%)
1	X	0.91	7/3393 (0.2%)	1.44	53/4613 (1.1%)
All	All	0.98	14/6805 (0.2%)	1.67	176/9252 (1.9%)

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	2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	404	ALA	CA-CB	-8.54	1.38	1.53
1	X	352	VAL	C-O	-8.33	1.15	1.24
1	A	174	ILE	CA-CB	-7.39	1.44	1.54
1	A	43	ILE	CA-CB	-7.22	1.44	1.54
1	A	95	VAL	CA-CB	6.92	1.63	1.54
1	X	413	PHE	C-O	-6.83	1.14	1.23
1	X	330	VAL	CA-CB	-6.18	1.46	1.54
1	X	297	THR	N-CA	5.63	1.52	1.45
1	X	208	VAL	C-O	-5.61	1.18	1.24
1	A	404	ALA	C-O	-5.39	1.17	1.23
1	A	133	ALA	CA-C	-5.15	1.46	1.52
1	X	124	ILE	CA-CB	5.10	1.60	1.54
1	X	353	TYR	C-O	-5.05	1.18	1.24
1	A	96	ASP	N-CA	5.01	1.52	1.46

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	134	VAL	CA-C-N	16.01	137.16	120.83
1	X	134	VAL	C-N-CA	16.01	137.16	120.83
1	A	344	ILE	N-CA-C	14.99	129.63	107.75
1	A	134	VAL	CA-C-N	14.06	137.91	120.89
1	A	134	VAL	C-N-CA	14.06	137.91	120.89
1	A	138	VAL	N-CA-C	-13.15	101.23	111.62
1	A	290	ARG	N-CA-C	-11.15	99.18	113.12
1	A	439	ALA	N-CA-C	10.59	125.36	110.01
1	X	344	ILE	N-CA-C	10.32	123.05	107.77
1	A	277	GLU	N-CA-C	10.31	122.28	111.14
1	A	177	CYS	N-CA-C	10.14	123.43	110.65
1	A	318	ARG	CA-C-N	-9.81	107.57	119.84
1	A	318	ARG	C-N-CA	-9.81	107.57	119.84
1	A	115	GLN	CB-CG-CD	9.72	129.12	112.60
1	A	158	ILE	N-CA-C	9.36	121.22	107.37
1	X	290	ARG	N-CA-C	-9.21	101.61	113.12
1	A	374	ASN	N-CA-C	9.06	121.24	111.36
1	A	248	LEU	N-CA-C	9.00	121.17	111.36
1	A	207	VAL	N-CA-C	8.97	120.84	107.75
1	A	433	LEU	CA-C-N	8.94	129.58	120.38
1	A	433	LEU	C-N-CA	8.94	129.58	120.38
1	A	118	LEU	N-CA-C	-8.84	101.73	111.36
1	A	373	TRP	N-CA-C	-8.61	101.90	111.28
1	A	249	LYS	N-CA-C	-8.56	101.94	111.28
1	A	324	TYR	N-CA-C	8.50	120.16	111.07
1	X	154	GLU	CA-C-N	8.45	130.40	119.84
1	X	154	GLU	C-N-CA	8.45	130.40	119.84
1	X	433	LEU	CA-C-N	8.44	129.07	120.38
1	X	433	LEU	C-N-CA	8.44	129.07	120.38
1	X	374	ASN	N-CA-C	8.40	120.06	111.07
1	X	208	VAL	N-CA-C	8.38	119.99	107.75
1	X	45	VAL	N-CA-C	8.38	120.40	108.17
1	A	380	ALA	CA-C-N	8.37	129.18	119.47
1	A	380	ALA	C-N-CA	8.37	129.18	119.47
1	A	154	GLU	CA-C-N	8.36	130.29	119.84
1	A	154	GLU	C-N-CA	8.36	130.29	119.84
1	A	370	ARG	N-CA-C	8.34	120.45	111.36
1	A	309	ASP	N-CA-C	-8.24	102.23	111.71
1	A	368	LEU	N-CA-C	8.19	123.83	112.45
1	A	208	VAL	N-CA-C	8.09	120.27	108.53
1	A	87	ALA	N-CA-C	-7.97	102.54	111.07
1	A	266	VAL	N-CA-C	7.97	118.26	108.06
1	X	115	GLN	CB-CG-CD	7.78	125.83	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	VAL	N-CA-CB	7.76	118.01	111.64
1	A	95	VAL	N-CA-C	7.76	125.47	109.34
1	A	215	GLY	N-CA-C	-7.63	100.94	111.09
1	A	217	LEU	N-CA-C	7.61	121.89	109.72
1	X	138	VAL	N-CA-C	-7.54	105.79	112.12
1	A	241	TRP	N-CA-C	-7.51	103.09	111.28
1	A	291	GLY	N-CA-C	-7.49	95.99	112.17
1	A	224	LEU	N-CA-C	7.46	120.24	108.67
1	A	363	ALA	N-CA-C	7.45	119.05	111.07
1	A	112	THR	N-CA-C	7.45	119.18	111.14
1	X	380	ALA	CA-C-N	7.43	128.09	119.47
1	X	380	ALA	C-N-CA	7.43	128.09	119.47
1	A	162	LEU	N-CA-C	7.43	119.46	111.36
1	A	260	LEU	CA-C-N	-7.38	112.18	119.78
1	A	260	LEU	C-N-CA	-7.38	112.18	119.78
1	A	189	ILE	N-CA-C	-7.36	97.74	108.71
1	X	297	THR	N-CA-C	7.34	120.51	108.99
1	X	318	ARG	CA-C-N	-7.31	110.70	119.84
1	X	318	ARG	C-N-CA	-7.31	110.70	119.84
1	A	140	GLU	N-CA-C	-7.30	97.69	109.96
1	A	190	ASN	N-CA-C	-7.30	99.48	110.28
1	A	202	LEU	N-CA-C	7.17	122.30	112.90
1	A	312	VAL	N-CA-C	7.11	117.87	110.62
1	X	212	GLY	N-CA-C	-7.04	104.28	112.73
1	A	276	ARG	N-CA-C	7.02	119.78	111.71
1	X	402	ASP	N-CA-C	-7.00	102.33	111.71
1	A	137	GLY	N-CA-C	6.92	126.98	114.46
1	A	17	SER	N-CA-C	6.86	118.75	111.28
1	A	48	ALA	N-CA-C	6.85	119.38	111.02
1	A	181	THR	N-CA-C	-6.78	98.88	109.87
1	A	160	LEU	N-CA-C	-6.75	104.79	113.16
1	A	49	VAL	N-CA-C	6.74	118.31	110.62
1	A	344	ILE	CB-CA-C	-6.66	101.31	110.77
1	X	215	GLY	N-CA-C	-6.65	102.24	111.09
1	A	273	GLU	N-CA-C	-6.63	104.33	112.88
1	A	347	ARG	CA-CB-CG	-6.60	100.90	114.10
1	X	158	ILE	N-CA-C	6.54	117.29	107.75
1	X	35	ILE	N-CA-C	-6.51	103.46	110.23
1	A	9	ARG	N-CA-C	6.50	118.91	111.11
1	A	334	PHE	N-CA-C	6.48	120.39	107.62
1	A	266	VAL	N-CA-CB	-6.44	102.50	111.19
1	A	28	TYR	N-CA-C	-6.42	104.29	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	118	LEU	N-CA-C	-6.41	104.37	111.36
1	X	207	VAL	N-CA-C	6.38	117.21	107.77
1	A	289	ARG	CA-C-N	-6.37	110.31	122.53
1	A	289	ARG	C-N-CA	-6.37	110.31	122.53
1	X	344	ILE	CB-CA-C	-6.37	101.83	110.42
1	A	191	ALA	N-CA-C	6.36	119.03	111.71
1	A	156	ARG	CG-CD-NE	6.33	125.93	112.00
1	A	119	ALA	N-CA-C	-6.29	104.43	111.28
1	A	98	LEU	N-CA-C	6.25	118.25	107.93
1	A	236	LEU	CA-CB-CG	-6.24	94.45	116.30
1	A	60	ALA	N-CA-C	6.24	117.77	110.97
1	X	115	GLN	CA-CB-CG	-6.23	101.63	114.10
1	A	40	PHE	N-CA-C	6.21	117.92	111.03
1	A	338	SER	N-CA-C	6.17	120.67	113.20
1	A	198	LEU	N-CA-C	6.13	117.63	111.07
1	X	277	GLU	N-CA-C	6.10	119.20	111.69
1	A	250	LEU	N-CA-C	-6.09	104.55	111.07
1	X	156	ARG	CG-CD-NE	5.95	125.10	112.00
1	A	427	VAL	N-CA-C	5.93	116.58	110.36
1	A	32	PHE	N-CA-C	-5.90	104.47	112.26
1	A	304	ASP	N-CA-C	5.88	119.05	108.17
1	X	95	VAL	CB-CA-C	-5.88	102.93	110.98
1	X	190	ASN	N-CA-C	-5.87	101.59	110.28
1	X	353	TYR	CA-C-N	-5.85	112.82	121.24
1	X	353	TYR	C-N-CA	-5.85	112.82	121.24
1	A	146	ALA	N-CA-C	5.82	123.20	110.80
1	A	406	ARG	N-CA-C	5.82	118.44	109.07
1	A	188	ASN	CA-C-N	-5.81	114.60	122.91
1	A	188	ASN	C-N-CA	-5.81	114.60	122.91
1	A	342	ALA	N-CA-C	5.79	117.93	108.55
1	A	278	LEU	N-CA-C	5.73	119.45	112.23
1	A	268	ILE	N-CA-C	-5.71	97.47	109.34
1	A	280	THR	N-CA-C	5.67	118.48	109.81
1	X	156	ARG	CD-NE-CZ	-5.66	116.48	124.40
1	A	233	PHE	N-CA-C	5.62	117.86	111.11
1	A	286	THR	N-CA-C	5.62	117.89	108.73
1	A	336	THR	N-CA-C	-5.61	101.33	110.20
1	X	248	LEU	N-CA-C	5.59	117.18	111.14
1	A	142	ASP	N-CA-C	5.58	118.72	109.46
1	A	260	LEU	CA-CB-CG	5.57	135.81	116.30
1	X	270	ARG	N-CA-C	-5.56	103.17	110.39
1	X	286	THR	CB-CA-C	-5.54	101.91	110.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	ILE	N-CA-C	5.54	115.74	110.53
1	A	286	THR	CB-CA-C	-5.52	101.24	110.19
1	A	76	GLY	N-CA-C	-5.52	102.90	112.06
1	A	137	GLY	CA-C-N	-5.51	117.31	123.16
1	A	137	GLY	C-N-CA	-5.51	117.31	123.16
1	A	346	THR	N-CA-C	-5.47	101.31	109.96
1	A	274	LEU	N-CA-C	-5.42	105.28	111.07
1	X	370	ARG	N-CA-C	5.41	119.04	112.23
1	A	142	ASP	N-CA-CB	-5.40	101.24	110.16
1	A	399	GLU	N-CA-C	5.38	119.33	112.34
1	A	402	ASP	N-CA-C	-5.37	104.29	111.87
1	A	174	ILE	N-CA-C	5.36	120.49	109.34
1	A	422	GLU	N-CA-C	-5.36	105.13	110.97
1	X	332	ARG	N-CA-C	5.34	117.20	108.76
1	A	380	ALA	N-CA-C	5.34	118.89	108.21
1	A	330	VAL	N-CA-C	5.33	120.42	109.34
1	X	318	ARG	CB-CG-CD	5.33	123.55	111.30
1	A	314	ALA	N-CA-C	5.32	118.23	111.69
1	A	305	LEU	N-CA-C	5.32	116.76	111.07
1	A	434	PRO	CA-C-N	-5.31	114.45	119.76
1	A	434	PRO	C-N-CA	-5.31	114.45	119.76
1	A	51	GLN	N-CA-C	5.30	116.91	111.03
1	A	270	ARG	N-CA-C	-5.29	102.99	110.29
1	A	368	LEU	CB-CG-CD1	-5.28	94.86	110.70
1	X	260	LEU	CA-C-N	-5.28	114.34	119.78
1	X	260	LEU	C-N-CA	-5.28	114.34	119.78
1	A	126	ASP	N-CA-C	-5.27	105.53	111.28
1	A	13	VAL	N-CA-C	5.25	116.32	111.81
1	A	354	LEU	CA-CB-CG	-5.23	98.01	116.30
1	A	68	GLY	N-CA-C	-5.22	107.80	114.85
1	A	396	PHE	N-CA-C	-5.20	105.69	111.36
1	X	32	PHE	N-CA-C	-5.20	107.11	112.93
1	X	181	THR	N-CA-C	-5.18	102.50	110.01
1	X	233	PHE	N-CA-C	5.13	117.27	111.11
1	X	49	VAL	N-CA-C	5.13	115.74	110.36
1	X	342	ALA	N-CA-C	5.12	116.85	108.76
1	A	177	CYS	CB-CA-C	-5.11	104.74	111.74
1	X	434	PRO	CA-C-N	-5.11	114.47	119.99
1	X	434	PRO	C-N-CA	-5.11	114.47	119.99
1	X	140	GLU	N-CA-C	-5.10	101.64	109.76
1	A	421	VAL	CB-CA-C	-5.08	105.29	112.14
1	A	19	MET	N-CA-C	5.07	118.02	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	309	ASP	N-CA-C	-5.06	105.89	111.71
1	A	170	GLY	N-CA-C	-5.03	107.87	115.32
1	A	55	PRO	N-CA-C	5.03	120.44	113.65
1	X	354	LEU	CA-CB-CG	-5.02	98.72	116.30
1	X	330	VAL	N-CA-C	5.01	119.77	109.34
1	A	357	PHE	N-CA-C	5.01	116.94	108.02
1	A	386	ARG	CA-CB-CG	-5.01	104.08	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	GLN	Sidechain
1	A	413	PHE	Mainchain

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	3349	0	3352	549	0
1	X	3334	0	3332	473	0
All	All	6683	0	6684	982	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 73.

All (982) 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:296:ALA:O	1:A:297:THR:HG22	1.21	1.26
1:A:398:PHE:CD1	1:X:398:PHE:CD1	2.33	1.15
1:A:95:VAL:H	1:A:100:VAL:CG1	1.59	1.14
1:A:295:VAL:HG22	1:A:335:VAL:O	1.46	1.14
1:A:266:VAL:O	1:A:287:LEU:HA	1.47	1.14
1:A:267:SER:HA	1:A:286:THR:O	1.48	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:PHE:CE2	1:X:406:ARG:HD2	1.85	1.10
1:X:266:VAL:O	1:X:287:LEU:HA	1.51	1.09
1:A:95:VAL:HG23	1:A:100:VAL:HG11	1.31	1.07
1:A:292:GLU:CD	1:A:368:LEU:HD11	1.78	1.07
1:A:292:GLU:OE2	1:A:368:LEU:HD11	1.52	1.06
1:X:332:ARG:HH11	1:X:332:ARG:HG3	1.24	1.02
1:A:292:GLU:CD	1:A:368:LEU:CD1	2.33	1.02
1:A:29:LEU:HD21	1:A:68:GLY:HA3	1.41	1.02
1:A:37:GLN:O	1:A:40:PHE:HD2	1.41	1.02
1:X:267:SER:HA	1:X:286:THR:O	1.59	1.01
1:X:86:GLU:O	1:X:91:PRO:HD2	1.59	1.01
1:A:232:ASP:HB3	1:A:236:LEU:CD1	1.91	1.01
1:A:29:LEU:CD2	1:A:68:GLY:HA3	1.90	1.00
1:A:65:GLN:HE22	1:A:130:ARG:HB2	1.25	0.99
1:A:420:PRO:HB3	1:X:420:PRO:HB3	1.44	0.99
1:A:95:VAL:HB	1:A:149:LEU:HD23	1.43	0.99
1:A:173:ALA:C	1:A:174:ILE:HD13	1.88	0.99
1:X:65:GLN:HE22	1:X:130:ARG:HB2	1.22	0.98
1:A:296:ALA:O	1:A:297:THR:CG2	2.11	0.98
1:A:398:PHE:CD1	1:X:398:PHE:HD1	1.78	0.98
1:X:95:VAL:HG22	1:X:99:ARG:H	1.24	0.98
1:A:90:ILE:N	1:A:91:PRO:HD3	1.76	0.97
1:X:133:ALA:C	1:X:135:PRO:HD3	1.89	0.97
1:A:13:VAL:CG1	1:A:26:ARG:HD3	1.94	0.96
1:X:232:ASP:HB3	1:X:236:LEU:HD23	1.46	0.96
1:A:95:VAL:CG1	1:A:148:LYS:HE2	1.94	0.95
1:A:95:VAL:CG2	1:A:100:VAL:HG11	1.97	0.95
1:A:196:ARG:HD3	1:A:255:ARG:HD2	1.48	0.95
1:A:406:ARG:HD2	1:X:398:PHE:CE2	2.00	0.95
1:A:95:VAL:H	1:A:100:VAL:HG13	1.32	0.95
1:A:331:ASP:HB3	1:A:345:THR:OG1	1.66	0.94
1:X:36:ASP:HB2	1:X:39:ARG:HB2	1.47	0.94
1:A:50:ILE:HG13	1:A:80:GLN:HE22	1.30	0.94
1:X:297:THR:H	1:X:332:ARG:HH12	1.17	0.93
1:A:297:THR:N	1:A:332:ARG:HH12	1.65	0.92
1:A:258:ASP:OD1	1:A:290:ARG:HD2	1.69	0.92
1:A:297:THR:H	1:A:332:ARG:HH12	1.02	0.92
1:X:50:ILE:HG13	1:X:80:GLN:HE22	1.30	0.91
1:A:13:VAL:HG11	1:A:26:ARG:HD3	1.52	0.91
1:A:121:VAL:HG21	1:A:133:ALA:HB2	1.51	0.91
1:A:37:GLN:O	1:A:40:PHE:CD2	2.25	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ASP:O	1:A:236:LEU:HD12	1.73	0.89
1:A:406:ARG:NH1	1:X:398:PHE:HE2	1.69	0.89
1:X:65:GLN:NE2	1:X:130:ARG:HB2	1.87	0.89
1:X:328:LEU:HG	1:X:330:VAL:HG23	1.54	0.89
1:X:258:ASP:OD1	1:X:290:ARG:HD2	1.71	0.89
1:A:404:ALA:HB3	1:X:404:ALA:HB3	1.56	0.88
1:A:406:ARG:HD2	1:X:398:PHE:CZ	2.09	0.88
1:A:372:VAL:HG12	1:A:373:TRP:N	1.89	0.88
1:A:133:ALA:C	1:A:135:PRO:HD3	1.98	0.88
1:A:143:ILE:HD12	1:A:152:VAL:O	1.74	0.88
1:A:77:GLY:O	1:A:81:LEU:HG	1.73	0.87
1:A:157:HIS:C	1:A:158:ILE:HD13	1.98	0.87
1:A:29:LEU:HD21	1:A:67:VAL:O	1.74	0.87
1:A:398:PHE:CE1	1:X:398:PHE:HD1	1.93	0.87
1:X:296:ALA:HB1	1:X:332:ARG:NH2	1.89	0.87
1:A:328:LEU:HG	1:A:330:VAL:HG23	1.55	0.87
1:A:203:GLN:OE1	1:A:261:PRO:HD3	1.75	0.86
1:X:64:LEU:HD22	1:X:69:LEU:HD12	1.56	0.86
1:A:404:ALA:O	1:A:405:VAL:HG23	1.73	0.86
1:A:229:LEU:HD22	1:A:254:LYS:HB2	1.58	0.86
1:X:232:ASP:HB3	1:X:236:LEU:CD2	2.04	0.86
1:A:82:ASP:OD1	1:A:99:ARG:NH2	2.08	0.86
1:X:332:ARG:HH11	1:X:332:ARG:CG	1.89	0.86
1:A:65:GLN:NE2	1:A:130:ARG:HB2	1.89	0.85
1:X:82:ASP:OD1	1:X:99:ARG:NH2	2.08	0.85
1:X:143:ILE:HD12	1:X:152:VAL:O	1.75	0.85
1:X:28:TYR:O	1:X:32:PHE:HB2	1.74	0.85
1:A:265:SER:C	1:A:266:VAL:HG23	2.01	0.85
1:A:64:LEU:HD12	1:A:71:PRO:HG3	1.57	0.85
1:A:97:GLY:O	1:A:98:LEU:HD23	1.76	0.85
1:X:353:TYR:CE2	1:X:355:ASP:HA	2.11	0.85
1:X:121:VAL:HG21	1:X:133:ALA:HB2	1.57	0.84
1:X:292:GLU:OE1	1:X:337:GLU:HB3	1.77	0.84
1:A:85:LEU:HD21	1:A:108:ILE:HG21	1.59	0.84
1:X:12:ILE:O	1:X:16:LEU:HG	1.76	0.84
1:X:353:TYR:HE2	1:X:355:ASP:HA	1.43	0.84
1:A:51:GLN:OE1	1:A:80:GLN:HG3	1.77	0.84
1:A:229:LEU:HD12	1:A:289:ARG:O	1.78	0.84
1:X:157:HIS:C	1:X:158:ILE:HD13	2.03	0.84
1:A:85:LEU:CD2	1:A:108:ILE:HG21	2.08	0.83
1:X:29:LEU:HD22	1:X:69:LEU:HD21	1.57	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:232:ASP:CB	1:X:236:LEU:HD23	2.08	0.83
1:A:398:PHE:HD1	1:X:398:PHE:CD1	1.90	0.83
1:X:401:CYS:SG	1:X:403:GLY:O	2.37	0.83
1:A:12:ILE:HA	1:X:15:LEU:HD11	1.60	0.83
1:X:43:ILE:HG22	1:X:43:ILE:O	1.78	0.83
1:A:95:VAL:HG12	1:A:148:LYS:HE2	1.59	0.82
1:X:296:ALA:HB1	1:X:332:ARG:HH22	1.44	0.82
1:X:134:VAL:N	1:X:135:PRO:HD3	1.86	0.82
1:A:214:GLY:HA2	1:A:269:THR:C	2.05	0.82
1:X:196:ARG:HD3	1:X:255:ARG:HD2	1.61	0.82
1:A:47:GLY:HA3	1:A:78:GLY:N	1.95	0.82
1:X:89:ASP:C	1:X:91:PRO:HD3	2.04	0.82
1:A:398:PHE:HD1	1:X:398:PHE:CE1	1.97	0.82
1:X:51:GLN:OE1	1:X:80:GLN:HG3	1.79	0.81
1:X:214:GLY:HA2	1:X:269:THR:C	2.06	0.81
1:A:42:VAL:HG23	1:A:204:PRO:HG2	1.60	0.81
1:X:42:VAL:HB	1:X:207:VAL:HG22	1.63	0.81
1:A:95:VAL:N	1:A:100:VAL:CG1	2.42	0.81
1:A:96:ASP:OD1	1:A:148:LYS:NZ	2.13	0.81
1:X:173:ALA:C	1:X:174:ILE:HD13	2.06	0.81
1:A:95:VAL:HG11	1:A:148:LYS:HG2	1.63	0.81
1:X:77:GLY:O	1:X:81:LEU:HG	1.81	0.81
1:A:265:SER:O	1:A:266:VAL:HG23	1.80	0.80
1:A:174:ILE:HD13	1:A:174:ILE:N	1.90	0.80
1:A:371:THR:O	1:A:374:ASN:HB2	1.80	0.80
1:X:297:THR:N	1:X:332:ARG:HH12	1.79	0.80
1:X:398:PHE:O	1:X:398:PHE:CD2	2.34	0.80
1:A:93:GLU:OE2	1:A:102:ARG:CZ	2.30	0.80
1:A:348:LEU:HD11	1:A:429:LYS:HD3	1.64	0.79
1:X:203:GLN:OE1	1:X:261:PRO:HD3	1.81	0.79
1:X:372:VAL:HG12	1:X:373:TRP:N	1.95	0.79
1:A:45:VAL:HG22	1:A:210:LEU:HB2	1.64	0.79
1:A:106:ILE:HD13	1:A:186:LEU:HD23	1.63	0.79
1:A:398:PHE:HE2	1:X:406:ARG:HH11	1.30	0.79
1:A:64:LEU:HD22	1:A:69:LEU:HD12	1.64	0.79
1:A:42:VAL:HG23	1:A:204:PRO:CG	2.12	0.79
1:X:94:ARG:O	1:X:100:VAL:N	2.16	0.79
1:A:42:VAL:HB	1:A:207:VAL:HG22	1.64	0.78
1:X:67:VAL:HG12	1:X:69:LEU:HG	1.65	0.78
1:A:63:PHE:O	1:A:67:VAL:HG13	1.82	0.78
1:A:95:VAL:HB	1:A:149:LEU:CD2	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:GLU:HB3	1:A:100:VAL:HG22	1.65	0.78
1:A:404:ALA:O	1:A:405:VAL:CG2	2.31	0.78
1:A:48:ALA:N	1:A:79:PRO:HD2	1.98	0.78
1:A:94:ARG:HG2	1:A:99:ARG:HA	1.65	0.78
1:A:411:THR:HG22	1:A:413:PHE:CE2	2.19	0.78
1:X:214:GLY:HA3	1:X:270:ARG:HB3	1.63	0.77
1:X:37:GLN:HG2	1:X:38:GLU:OE2	1.84	0.77
1:A:42:VAL:C	1:A:43:ILE:HG13	2.09	0.77
1:A:67:VAL:CG2	1:A:69:LEU:HG	2.14	0.77
1:A:214:GLY:HA3	1:A:270:ARG:HB3	1.65	0.77
1:A:372:VAL:CG1	1:A:373:TRP:N	2.48	0.77
1:X:318:ARG:CG	1:X:437:LEU:HB3	2.14	0.77
1:X:42:VAL:HG23	1:X:204:PRO:CG	2.15	0.76
1:X:348:LEU:HD11	1:X:429:LYS:HD3	1.67	0.76
1:X:404:ALA:O	1:X:405:VAL:HG23	1.84	0.76
1:A:134:VAL:N	1:A:135:PRO:HD3	1.93	0.76
1:A:42:VAL:O	1:A:43:ILE:HG13	1.86	0.76
1:X:136:ARG:HH22	1:X:180:GLU:HB3	1.51	0.76
1:A:15:LEU:HD21	1:X:15:LEU:C	2.11	0.75
1:X:75:HIS:NE2	1:X:117:ASN:OD1	2.14	0.75
1:X:95:VAL:HG22	1:X:99:ARG:N	2.01	0.75
1:A:88:ALA:O	1:A:89:ASP:HB2	1.87	0.75
1:A:266:VAL:O	1:A:287:LEU:CA	2.32	0.75
1:X:42:VAL:HG23	1:X:204:PRO:HG2	1.67	0.75
1:A:38:GLU:C	1:A:40:PHE:H	1.95	0.75
1:X:38:GLU:C	1:X:40:PHE:H	1.92	0.75
1:A:265:SER:O	1:A:266:VAL:CG2	2.35	0.75
1:A:353:TYR:CE2	1:A:355:ASP:HA	2.22	0.75
1:A:246:MET:HG3	1:A:246:MET:O	1.87	0.74
1:X:36:ASP:HB3	1:X:39:ARG:HG3	1.69	0.74
1:A:13:VAL:HG13	1:A:26:ARG:HD3	1.70	0.74
1:A:232:ASP:C	1:A:236:LEU:HD12	2.12	0.74
1:A:75:HIS:NE2	1:A:117:ASN:OD1	2.18	0.74
1:X:353:TYR:O	1:X:353:TYR:CD2	2.41	0.74
1:A:47:GLY:C	1:A:79:PRO:HD2	2.13	0.74
1:X:37:GLN:HB3	1:X:38:GLU:OE2	1.87	0.73
1:A:206:LYS:HZ1	1:A:287:LEU:HD22	1.54	0.73
1:A:406:ARG:HH11	1:X:398:PHE:HE2	1.35	0.73
1:A:32:PHE:CD1	1:A:36:ASP:OD2	2.42	0.73
1:A:95:VAL:HG23	1:A:100:VAL:CG1	2.17	0.73
1:X:411:THR:CG2	1:X:413:PHE:CE2	2.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ALA:O	1:A:200:HIS:HB3	1.89	0.73
1:A:390:ASN:O	1:A:392:PRO:N	2.22	0.73
1:A:311:LEU:CD1	1:A:360:LEU:HD11	2.19	0.73
1:X:47:GLY:HA3	1:X:78:GLY:N	2.04	0.73
1:X:357:PHE:HE1	1:X:372:VAL:HG11	1.53	0.73
1:A:136:ARG:HB3	1:A:136:ARG:HH11	1.54	0.72
1:A:292:GLU:CD	1:A:368:LEU:HD13	2.13	0.72
1:X:132:ALA:HB2	1:X:171:GLN:OE1	1.88	0.72
1:X:239:ALA:HB3	1:X:242:VAL:HG23	1.70	0.72
1:A:85:LEU:HD21	1:A:108:ILE:CG2	2.19	0.72
1:X:106:ILE:HD13	1:X:186:LEU:HD23	1.71	0.72
1:X:229:LEU:HD12	1:X:289:ARG:O	1.90	0.72
1:A:357:PHE:HE1	1:A:372:VAL:HG11	1.53	0.72
1:A:398:PHE:HE2	1:X:406:ARG:NH1	1.87	0.72
1:A:401:CYS:SG	1:A:403:GLY:O	2.44	0.72
1:X:329:ARG:O	1:X:330:VAL:HB	1.89	0.72
1:X:411:THR:HG22	1:X:413:PHE:CE2	2.25	0.71
1:X:64:LEU:HD12	1:X:71:PRO:HG3	1.71	0.71
1:A:398:PHE:CZ	1:X:406:ARG:HD2	2.23	0.71
1:X:296:ALA:CB	1:X:332:ARG:HH22	2.02	0.71
1:A:136:ARG:HH22	1:A:180:GLU:HB3	1.56	0.71
1:A:155:PRO:HD3	1:A:189:ILE:HD12	1.73	0.71
1:A:232:ASP:CB	1:A:236:LEU:CD1	2.69	0.71
1:A:131:ALA:HA	1:A:171:GLN:HB3	1.71	0.71
1:A:267:SER:CA	1:A:286:THR:O	2.35	0.70
1:A:292:GLU:OE2	1:A:368:LEU:CD1	2.33	0.70
1:X:351:TRP:CD1	1:X:426:VAL:HG11	2.26	0.70
1:A:132:ALA:HB2	1:A:171:GLN:OE1	1.90	0.70
1:X:48:ALA:N	1:X:79:PRO:HD2	2.07	0.70
1:X:136:ARG:HH11	1:X:136:ARG:HB3	1.56	0.70
1:X:157:HIS:O	1:X:158:ILE:HD13	1.92	0.70
1:X:47:GLY:C	1:X:79:PRO:HD2	2.16	0.70
1:X:67:VAL:CG1	1:X:69:LEU:HG	2.21	0.70
1:X:318:ARG:HG3	1:X:437:LEU:HB3	1.72	0.70
1:A:36:ASP:HB2	1:A:39:ARG:HB2	1.74	0.70
1:X:197:ALA:O	1:X:200:HIS:HB3	1.91	0.70
1:A:51:GLN:HB2	1:A:80:GLN:NE2	2.07	0.70
1:A:328:LEU:CG	1:A:330:VAL:HG23	2.21	0.70
1:A:406:ARG:HG2	1:A:411:THR:OG1	1.92	0.70
1:A:163:VAL:HG22	1:A:175:LEU:HD11	1.74	0.69
1:A:229:LEU:HD12	1:A:290:ARG:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:155:PRO:HD3	1:X:189:ILE:HD12	1.74	0.69
1:X:412:VAL:HG23	1:X:431:PHE:CE1	2.27	0.69
1:A:90:ILE:HD12	1:A:104:GLU:OE1	1.92	0.69
1:X:37:GLN:CB	1:X:38:GLU:OE2	2.40	0.69
1:X:51:GLN:HB2	1:X:80:GLN:NE2	2.08	0.69
1:A:29:LEU:HD21	1:A:68:GLY:CA	2.19	0.69
1:A:81:LEU:CD1	1:A:99:ARG:HH22	2.05	0.69
1:A:145:ASP:OD2	1:A:149:LEU:HD12	1.93	0.69
1:A:411:THR:CG2	1:A:413:PHE:CE2	2.75	0.69
1:A:95:VAL:HG11	1:A:148:LYS:HE2	1.72	0.69
1:A:324:TYR:CD1	1:A:324:TYR:C	2.70	0.69
1:X:64:LEU:CD2	1:X:69:LEU:HD12	2.21	0.69
1:A:32:PHE:HB2	1:A:40:PHE:CZ	2.28	0.69
1:A:420:PRO:HB3	1:X:420:PRO:CB	2.21	0.69
1:X:297:THR:N	1:X:332:ARG:NH1	2.39	0.69
1:A:5:ALA:HB3	1:A:6:PRO:HD3	1.75	0.69
1:X:265:SER:HB2	1:X:287:LEU:HD21	1.74	0.69
1:A:85:LEU:HD21	1:A:108:ILE:CB	2.23	0.69
1:A:196:ARG:O	1:A:197:ALA:C	2.36	0.69
1:A:295:VAL:HG22	1:A:335:VAL:C	2.16	0.69
1:A:332:ARG:HG3	1:A:332:ARG:HH11	1.57	0.69
1:X:81:LEU:O	1:X:86:GLU:HB2	1.92	0.69
1:X:113:LEU:O	1:X:117:ASN:N	2.26	0.69
1:A:132:ALA:HB2	1:A:171:GLN:CD	2.18	0.68
1:X:328:LEU:CG	1:X:330:VAL:HG23	2.23	0.68
1:A:121:VAL:HG21	1:A:133:ALA:CB	2.24	0.68
1:A:229:LEU:HD22	1:A:254:LYS:CB	2.23	0.68
1:A:43:ILE:HG22	1:A:43:ILE:O	1.93	0.68
1:A:353:TYR:HE2	1:A:355:ASP:HA	1.56	0.68
1:X:117:ASN:OD1	1:X:176:ALA:HB2	1.93	0.68
1:A:42:VAL:CG2	1:A:204:PRO:HG2	2.24	0.68
1:A:100:VAL:HB	1:A:149:LEU:O	1.94	0.68
1:A:294:ILE:CD1	1:A:372:VAL:HA	2.23	0.68
1:A:295:VAL:CG2	1:A:335:VAL:O	2.35	0.68
1:X:181:THR:HG23	1:X:185:THR:O	1.94	0.68
1:A:304:ASP:CG	1:A:307:ARG:HB2	2.18	0.68
1:X:266:VAL:O	1:X:287:LEU:CA	2.37	0.68
1:A:81:LEU:HD12	1:A:99:ARG:HH22	1.59	0.67
1:A:95:VAL:CB	1:A:149:LEU:HD23	2.23	0.67
1:A:232:ASP:HB3	1:A:236:LEU:HD13	1.75	0.67
1:X:81:LEU:CD1	1:X:99:ARG:HH12	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:132:ALA:HB2	1:X:171:GLN:CD	2.20	0.66
1:X:23:LYS:HE3	1:X:27:GLU:OE2	1.94	0.66
1:X:398:PHE:CD2	1:X:398:PHE:C	2.73	0.66
1:X:404:ALA:O	1:X:405:VAL:CG2	2.43	0.66
1:X:37:GLN:CG	1:X:38:GLU:OE2	2.43	0.66
1:X:120:LEU:HD12	1:X:120:LEU:O	1.95	0.66
1:A:216:LEU:O	1:A:217:LEU:HD23	1.96	0.66
1:A:311:LEU:HD12	1:A:360:LEU:HD11	1.76	0.66
1:A:331:ASP:OD1	1:A:347:ARG:NE	2.28	0.66
1:X:42:VAL:C	1:X:43:ILE:HG13	2.20	0.66
1:X:81:LEU:HD12	1:X:99:ARG:HH22	1.61	0.66
1:X:265:SER:C	1:X:266:VAL:HG23	2.20	0.66
1:X:61:LEU:HD22	1:X:73:VAL:HG21	1.77	0.66
1:X:227:ILE:HG22	1:X:228:ASN:N	2.11	0.66
1:X:229:LEU:HD12	1:X:290:ARG:HA	1.77	0.66
1:X:372:VAL:CG1	1:X:373:TRP:N	2.59	0.65
1:X:353:TYR:CD2	1:X:353:TYR:C	2.74	0.65
1:A:28:TYR:OH	1:A:205:TYR:HE2	1.78	0.65
1:A:77:GLY:O	1:A:78:GLY:C	2.38	0.65
1:A:81:LEU:CD1	1:A:99:ARG:HH12	2.10	0.65
1:X:77:GLY:O	1:X:78:GLY:C	2.39	0.65
1:X:232:ASP:C	1:X:236:LEU:HD23	2.20	0.65
1:X:292:GLU:CD	1:X:337:GLU:HB3	2.21	0.65
1:A:93:GLU:CB	1:A:100:VAL:HG22	2.26	0.65
1:X:356:LYS:NZ	1:X:436:THR:HG21	2.12	0.65
1:A:404:ALA:CB	1:X:404:ALA:HB3	2.25	0.65
1:X:100:VAL:HB	1:X:149:LEU:O	1.96	0.65
1:X:239:ALA:HB3	1:X:242:VAL:CG2	2.26	0.65
1:X:332:ARG:CG	1:X:332:ARG:NH1	2.53	0.65
1:A:61:LEU:HD22	1:A:73:VAL:HG21	1.79	0.65
1:A:426:VAL:O	1:A:429:LYS:HB2	1.97	0.65
1:X:292:GLU:OE1	1:X:338:SER:N	2.29	0.65
1:A:292:GLU:HG3	1:A:336:THR:OG1	1.96	0.65
1:A:9:ARG:HA	1:A:12:ILE:HG22	1.78	0.65
1:A:329:ARG:O	1:A:330:VAL:HB	1.96	0.65
1:X:81:LEU:CD1	1:X:99:ARG:HH22	2.09	0.65
1:A:15:LEU:CD2	1:X:15:LEU:HG	2.27	0.64
1:X:239:ALA:O	1:X:242:VAL:HB	1.97	0.64
1:X:133:ALA:O	1:X:135:PRO:HD3	1.97	0.64
1:X:175:LEU:N	1:X:175:LEU:HD12	2.11	0.64
1:X:318:ARG:HG2	1:X:437:LEU:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:136:ARG:NH2	1:X:180:GLU:HB3	2.12	0.64
1:A:292:GLU:OE1	1:A:336:THR:HG21	1.98	0.64
1:X:13:VAL:C	1:X:15:LEU:H	2.05	0.64
1:X:368:LEU:C	1:X:370:ARG:N	2.54	0.64
1:A:140:GLU:HG2	1:A:182:PRO:HG3	1.80	0.64
1:X:88:ALA:C	1:X:90:ILE:H	2.03	0.64
1:A:265:SER:C	1:A:266:VAL:CG2	2.71	0.64
1:X:174:ILE:O	1:X:174:ILE:HG22	1.97	0.64
1:A:9:ARG:HA	1:A:12:ILE:CG2	2.28	0.63
1:A:322:GLU:HG2	1:A:323:GLY:N	2.13	0.63
1:A:29:LEU:HD22	1:A:68:GLY:HA3	1.78	0.63
1:A:242:VAL:HG13	1:A:246:MET:HG2	1.78	0.63
1:A:334:PHE:CE1	1:A:375:ARG:HB3	2.34	0.63
1:A:136:ARG:NH2	1:A:180:GLU:HB3	2.13	0.63
1:A:109:ILE:HG22	1:A:178:LEU:HD21	1.80	0.63
1:A:181:THR:HG23	1:A:185:THR:O	1.99	0.63
1:A:229:LEU:CD2	1:A:254:LYS:HB2	2.29	0.63
1:A:157:HIS:O	1:A:158:ILE:HD13	1.98	0.63
1:X:311:LEU:CD1	1:X:360:LEU:HD11	2.29	0.63
1:X:42:VAL:O	1:X:43:ILE:HG13	1.99	0.63
1:X:390:ASN:O	1:X:392:PRO:N	2.32	0.63
1:A:9:ARG:NH2	1:A:33:SER:HB2	2.13	0.62
1:A:28:TYR:OH	1:A:205:TYR:CE2	2.51	0.62
1:A:295:VAL:N	1:A:335:VAL:O	2.29	0.62
1:A:351:TRP:CD1	1:A:426:VAL:HG11	2.33	0.62
1:A:113:LEU:HD12	1:A:178:LEU:CD1	2.30	0.62
1:A:351:TRP:HD1	1:A:426:VAL:HB	1.64	0.62
1:A:95:VAL:CB	1:A:100:VAL:HG11	2.29	0.62
1:A:106:ILE:HG22	1:A:107:PRO:CD	2.30	0.62
1:A:144:VAL:HG13	1:A:144:VAL:O	2.00	0.62
1:A:196:ARG:NH1	1:A:255:ARG:HD2	2.15	0.62
1:X:174:ILE:HD13	1:X:174:ILE:N	2.11	0.62
1:X:334:PHE:CE1	1:X:375:ARG:HB3	2.35	0.62
1:A:5:ALA:C	1:A:7:GLY:H	2.08	0.62
1:X:304:ASP:CG	1:X:307:ARG:HB2	2.25	0.62
1:A:354:LEU:HB3	1:A:385:TRP:HB3	1.82	0.62
1:A:414:TRP:CE3	1:A:423:VAL:HG11	2.35	0.61
1:X:145:ASP:OD2	1:X:149:LEU:HD12	2.00	0.61
1:A:44:LYS:HG3	1:A:45:VAL:N	2.15	0.61
1:X:63:PHE:CE2	1:X:67:VAL:HG21	2.35	0.61
1:X:426:VAL:O	1:X:429:LYS:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ASP:HB3	1:A:236:LEU:HD12	1.80	0.61
1:X:106:ILE:HG23	1:X:186:LEU:HD23	1.82	0.61
1:X:414:TRP:CE3	1:X:423:VAL:HG11	2.35	0.61
1:A:412:VAL:HG23	1:A:431:PHE:CE1	2.35	0.61
1:X:121:VAL:HG21	1:X:133:ALA:CB	2.27	0.61
1:X:296:ALA:C	1:X:332:ARG:HH22	2.08	0.61
1:A:34:GLY:O	1:A:36:ASP:N	2.34	0.61
1:X:132:ALA:HB3	1:X:166:ALA:CB	2.31	0.61
1:X:346:THR:HG23	1:X:355:ASP:HB2	1.83	0.61
1:X:368:LEU:O	1:X:369:GLY:C	2.43	0.61
1:A:106:ILE:HG22	1:A:107:PRO:HD3	1.82	0.61
1:A:293:ARG:CZ	1:A:337:GLU:OE2	2.49	0.61
1:A:131:ALA:CA	1:A:171:GLN:HB3	2.30	0.61
1:A:404:ALA:C	1:A:405:VAL:HG23	2.25	0.61
1:X:10:GLN:C	1:X:12:ILE:H	2.09	0.61
1:A:16:LEU:HD23	1:X:19:MET:SD	2.41	0.60
1:A:38:GLU:C	1:A:40:PHE:N	2.59	0.60
1:A:63:PHE:CE2	1:A:67:VAL:HG11	2.35	0.60
1:A:120:LEU:O	1:A:120:LEU:HD12	2.02	0.60
1:X:140:GLU:HG2	1:X:182:PRO:HG3	1.82	0.60
1:X:246:MET:O	1:X:246:MET:HG3	1.98	0.60
1:X:383:LEU:C	1:X:384:ILE:HD12	2.26	0.60
1:A:25:ILE:HG12	1:A:279:PHE:CE1	2.36	0.60
1:A:164:GLY:O	1:A:168:ARG:HB2	2.01	0.60
1:A:173:ALA:O	1:A:174:ILE:HD13	2.02	0.60
1:A:33:SER:O	1:A:37:GLN:NE2	2.34	0.60
1:A:196:ARG:CD	1:A:255:ARG:HD2	2.28	0.60
1:X:75:HIS:HE2	1:X:176:ALA:HB2	1.66	0.60
1:A:406:ARG:NH1	1:X:398:PHE:CE2	2.61	0.60
1:A:90:ILE:N	1:A:91:PRO:CD	2.52	0.60
1:X:38:GLU:C	1:X:40:PHE:N	2.60	0.60
1:X:94:ARG:O	1:X:100:VAL:HG13	2.01	0.60
1:A:32:PHE:HD1	1:A:36:ASP:CG	2.10	0.60
1:A:65:GLN:NE2	1:A:170:GLY:O	2.35	0.60
1:A:77:GLY:O	1:A:78:GLY:O	2.18	0.60
1:A:90:ILE:CD1	1:A:104:GLU:OE1	2.50	0.60
1:A:356:LYS:NZ	1:A:436:THR:HG21	2.17	0.60
1:A:138:VAL:HG21	1:A:175:LEU:HG	1.84	0.60
1:X:32:PHE:C	1:X:34:GLY:H	2.09	0.60
1:X:356:LYS:CE	1:X:436:THR:OG1	2.50	0.60
1:A:106:ILE:HG23	1:A:186:LEU:HD23	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:LEU:C	1:A:384:ILE:HD12	2.26	0.59
1:X:42:VAL:CG2	1:X:204:PRO:HG2	2.32	0.59
1:X:371:THR:O	1:X:374:ASN:HB2	2.02	0.59
1:A:15:LEU:CD1	1:X:15:LEU:HG	2.32	0.59
1:A:227:ILE:HG22	1:A:228:ASN:N	2.16	0.59
1:X:75:HIS:NE2	1:X:176:ALA:HB2	2.17	0.59
1:A:113:LEU:O	1:A:117:ASN:N	2.21	0.59
1:X:26:ARG:O	1:X:30:HIS:CG	2.55	0.59
1:X:37:GLN:HB3	1:X:38:GLU:CD	2.27	0.59
1:X:144:VAL:O	1:X:145:ASP:HB3	2.02	0.59
1:X:228:ASN:N	1:X:232:ASP:OD2	2.35	0.59
1:X:106:ILE:HG22	1:X:107:PRO:N	2.17	0.59
1:A:53:ASP:O	1:A:54:LEU:C	2.44	0.59
1:A:113:LEU:HD12	1:A:178:LEU:HD11	1.85	0.59
1:X:138:VAL:HG11	1:X:175:LEU:HD23	1.83	0.59
1:A:64:LEU:CD2	1:A:69:LEU:HD12	2.31	0.59
1:A:95:VAL:N	1:A:100:VAL:HG13	2.12	0.59
1:A:15:LEU:HD21	1:X:16:LEU:N	2.18	0.59
1:A:362:ASP:OD2	1:A:362:ASP:N	2.33	0.59
1:X:391:ASN:C	1:X:393:VAL:H	2.09	0.59
1:X:116:ALA:O	1:X:119:ALA:HB3	2.02	0.58
1:X:164:GLY:O	1:X:168:ARG:HB2	2.03	0.58
1:X:77:GLY:O	1:X:78:GLY:O	2.21	0.58
1:A:26:ARG:O	1:A:29:LEU:HB2	2.03	0.58
1:X:42:VAL:HG12	1:X:43:ILE:N	2.18	0.58
1:A:133:ALA:O	1:A:135:PRO:HD3	2.03	0.58
1:A:175:LEU:HD12	1:A:175:LEU:N	2.18	0.58
1:A:356:LYS:CE	1:A:436:THR:OG1	2.52	0.58
1:A:390:ASN:O	1:A:391:ASN:C	2.45	0.58
1:A:47:GLY:O	1:A:50:ILE:HG12	2.04	0.58
1:A:297:THR:N	1:A:332:ARG:NH1	2.47	0.58
1:X:29:LEU:CD1	1:X:67:VAL:HG13	2.34	0.58
1:X:113:LEU:HD12	1:X:178:LEU:HD11	1.83	0.58
1:A:131:ALA:C	1:A:171:GLN:HB3	2.29	0.58
1:A:214:GLY:HA2	1:A:270:ARG:N	2.18	0.58
1:X:36:ASP:CB	1:X:39:ARG:HG3	2.34	0.58
1:X:191:ALA:O	1:X:194:ALA:HB3	2.03	0.58
1:X:214:GLY:HA2	1:X:270:ARG:N	2.19	0.57
1:X:331:ASP:HB3	1:X:345:THR:OG1	2.04	0.57
1:A:47:GLY:HA3	1:A:78:GLY:H	1.68	0.57
1:X:44:LYS:HG2	1:X:209:PHE:CD1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ILE:H	1:A:91:PRO:HD3	1.64	0.57
1:A:174:ILE:HG22	1:A:174:ILE:O	2.03	0.57
1:X:229:LEU:HD22	1:X:254:LYS:HB2	1.86	0.57
1:A:340:ARG:O	1:A:360:LEU:HD12	2.04	0.57
1:X:254:LYS:O	1:X:258:ASP:CG	2.47	0.57
1:A:94:ARG:HG2	1:A:99:ARG:H	1.70	0.57
1:A:203:GLN:N	1:A:204:PRO:HD3	2.19	0.57
1:A:138:VAL:HG11	1:A:175:LEU:HD23	1.86	0.57
1:A:44:LYS:HG2	1:A:209:PHE:CD1	2.40	0.57
1:A:48:ALA:CA	1:A:79:PRO:HG2	2.35	0.57
1:A:28:TYR:CE1	1:A:205:TYR:CD2	2.93	0.57
1:X:322:GLU:HG2	1:X:323:GLY:N	2.19	0.57
1:X:351:TRP:HD1	1:X:426:VAL:CB	2.18	0.57
1:A:94:ARG:HA	1:A:99:ARG:HA	1.86	0.56
1:A:132:ALA:HB3	1:A:166:ALA:CB	2.35	0.56
1:A:239:ALA:O	1:A:242:VAL:HB	2.05	0.56
1:X:48:ALA:CA	1:X:79:PRO:HG2	2.35	0.56
1:X:163:VAL:HG13	1:X:173:ALA:CB	2.35	0.56
1:A:228:ASN:N	1:A:232:ASP:OD2	2.36	0.56
1:A:353:TYR:CD2	1:A:353:TYR:C	2.83	0.56
1:X:54:LEU:HB3	1:X:55:PRO:HD3	1.88	0.56
1:X:64:LEU:HD22	1:X:69:LEU:CD1	2.31	0.56
1:X:109:ILE:HG22	1:X:178:LEU:HD21	1.87	0.56
1:X:307:ARG:O	1:X:310:ASN:HB2	2.05	0.56
1:A:42:VAL:O	1:A:43:ILE:CG1	2.52	0.56
1:A:94:ARG:HG2	1:A:99:ARG:CA	2.34	0.56
1:X:48:ALA:HA	1:X:79:PRO:HG2	1.88	0.56
1:X:106:ILE:HG22	1:X:107:PRO:CD	2.35	0.56
1:X:13:VAL:C	1:X:15:LEU:N	2.64	0.56
1:X:81:LEU:HD13	1:X:99:ARG:HH12	1.70	0.56
1:X:225:SER:O	1:X:226:SER:HB3	2.04	0.56
1:A:18:HIS:CE1	1:X:275:ALA:HB1	2.41	0.56
1:A:351:TRP:HD1	1:A:426:VAL:CB	2.17	0.56
1:X:139:PHE:CZ	1:X:194:ALA:HB1	2.40	0.56
1:A:48:ALA:HB2	1:A:79:PRO:HG2	1.88	0.56
1:A:232:ASP:CB	1:A:236:LEU:HD13	2.34	0.56
1:X:47:GLY:O	1:X:50:ILE:HG12	2.06	0.56
1:X:348:LEU:HD21	1:X:429:LYS:HB3	1.86	0.56
1:A:254:LYS:HG2	1:A:258:ASP:OD2	2.05	0.56
1:X:311:LEU:HD12	1:X:360:LEU:HD11	1.87	0.56
1:A:54:LEU:N	1:A:55:PRO:CD	2.68	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ARG:HH11	1:A:255:ARG:HD2	1.70	0.55
1:A:254:LYS:O	1:A:258:ASP:CG	2.50	0.55
1:X:113:LEU:HD12	1:X:178:LEU:CD1	2.36	0.55
1:X:351:TRP:HD1	1:X:426:VAL:HB	1.70	0.55
1:X:175:LEU:H	1:X:175:LEU:CD1	2.19	0.55
1:X:292:GLU:OE1	1:X:337:GLU:CB	2.50	0.55
1:A:13:VAL:HG13	1:A:26:ARG:CD	2.35	0.55
1:X:216:LEU:O	1:X:217:LEU:HD23	2.05	0.55
1:X:328:LEU:HG	1:X:330:VAL:CG2	2.31	0.55
1:A:112:THR:O	1:A:115:GLN:HB3	2.07	0.55
1:A:132:ALA:HB3	1:A:166:ALA:HB2	1.89	0.55
1:A:145:ASP:O	1:A:147:ASP:N	2.39	0.55
1:A:331:ASP:CB	1:A:345:THR:OG1	2.49	0.55
1:X:138:VAL:HG21	1:X:175:LEU:HG	1.87	0.55
1:X:391:ASN:O	1:X:393:VAL:N	2.38	0.55
1:X:196:ARG:NH1	1:X:255:ARG:HD2	2.22	0.55
1:A:120:LEU:O	1:A:124:ILE:HG13	2.06	0.55
1:A:136:ARG:HH11	1:A:136:ARG:CB	2.19	0.55
1:X:136:ARG:HH11	1:X:136:ARG:CB	2.20	0.55
1:A:309:ASP:HA	1:A:325:TRP:HZ2	1.72	0.55
1:A:13:VAL:HA	1:A:16:LEU:HD12	1.88	0.55
1:A:15:LEU:HD22	1:X:15:LEU:HG	1.87	0.55
1:A:196:ARG:HD3	1:A:255:ARG:CD	2.32	0.55
1:X:5:ALA:N	1:X:6:PRO:CD	2.70	0.54
1:X:175:LEU:N	1:X:175:LEU:CD1	2.71	0.54
1:X:351:TRP:HZ3	1:X:382:GLN:OE1	1.90	0.54
1:X:432:ALA:O	1:X:433:LEU:C	2.49	0.54
1:A:214:GLY:CA	1:A:270:ARG:N	2.70	0.54
1:A:405:VAL:HG11	1:A:431:PHE:HE2	1.72	0.54
1:X:145:ASP:O	1:X:147:ASP:N	2.39	0.54
1:A:357:PHE:CE1	1:A:372:VAL:HG11	2.37	0.54
1:X:159:HIS:HB3	1:X:161:ASP:OD2	2.07	0.54
1:A:19:MET:HE2	1:X:19:MET:HB2	1.89	0.54
1:X:29:LEU:CD2	1:X:69:LEU:HD21	2.34	0.54
1:X:404:ALA:C	1:X:405:VAL:HG23	2.32	0.54
1:A:40:PHE:CE1	1:A:69:LEU:HD22	2.43	0.54
1:A:163:VAL:HG13	1:A:173:ALA:CB	2.38	0.54
1:X:36:ASP:HB2	1:X:39:ARG:CB	2.29	0.54
1:X:132:ALA:HB3	1:X:166:ALA:HB2	1.90	0.54
1:X:351:TRP:CD1	1:X:426:VAL:CG1	2.90	0.54
1:X:134:VAL:HG11	1:X:162:LEU:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:390:ASN:O	1:X:391:ASN:C	2.50	0.54
1:A:206:LYS:NZ	1:A:287:LEU:HD22	2.23	0.54
1:X:47:GLY:CA	1:X:79:PRO:HD2	2.38	0.54
1:X:203:GLN:N	1:X:204:PRO:HD3	2.22	0.54
1:X:411:THR:HG21	1:X:413:PHE:CE2	2.42	0.54
1:A:28:TYR:CE1	1:A:205:TYR:HD2	2.24	0.54
1:A:307:ARG:O	1:A:310:ASN:HB2	2.07	0.54
1:A:28:TYR:CZ	1:A:205:TYR:CE2	2.96	0.53
1:A:94:ARG:CG	1:A:99:ARG:HA	2.35	0.53
1:X:65:GLN:NE2	1:X:170:GLY:O	2.41	0.53
1:X:35:ILE:C	1:X:37:GLN:N	2.61	0.53
1:A:34:GLY:C	1:A:35:ILE:HG12	2.32	0.53
1:A:295:VAL:O	1:A:334:PHE:HA	2.08	0.53
1:X:183:ASP:OD2	1:X:183:ASP:C	2.52	0.53
1:X:356:LYS:HZ3	1:X:436:THR:HG21	1.74	0.53
1:A:29:LEU:CD2	1:A:68:GLY:CA	2.77	0.53
1:X:43:ILE:CD1	1:X:71:PRO:HB3	2.38	0.53
1:X:53:ASP:O	1:X:54:LEU:C	2.50	0.53
1:X:167:ALA:O	1:X:170:GLY:N	2.29	0.53
1:X:217:LEU:HD22	1:X:222:ASP:C	2.34	0.53
1:X:292:GLU:OE1	1:X:337:GLU:CA	2.57	0.53
1:X:120:LEU:HD12	1:X:120:LEU:C	2.31	0.53
1:X:262:LEU:HD21	1:X:290:ARG:CZ	2.39	0.53
1:X:406:ARG:HG2	1:X:411:THR:OG1	2.08	0.53
1:A:191:ALA:O	1:A:194:ALA:HB3	2.08	0.53
1:X:163:VAL:HG22	1:X:175:LEU:HD11	1.90	0.53
1:X:254:LYS:HG2	1:X:258:ASP:OD2	2.07	0.53
1:X:265:SER:C	1:X:266:VAL:CG2	2.82	0.53
1:A:106:ILE:CB	1:A:107:PRO:HD3	2.38	0.53
1:X:354:LEU:HB3	1:X:385:TRP:CB	2.39	0.53
1:X:383:LEU:O	1:X:384:ILE:HD12	2.08	0.53
1:A:432:ALA:O	1:A:433:LEU:C	2.51	0.53
1:X:296:ALA:CA	1:X:332:ARG:HH22	2.22	0.53
1:A:116:ALA:O	1:A:119:ALA:HB3	2.09	0.53
1:A:368:LEU:O	1:A:369:GLY:C	2.52	0.53
1:A:196:ARG:O	1:A:198:LEU:N	2.42	0.53
1:A:352:VAL:O	1:A:383:LEU:HD12	2.09	0.53
1:X:13:VAL:HG12	1:X:14:GLN:N	2.24	0.53
1:X:242:VAL:HG13	1:X:246:MET:HG2	1.90	0.53
1:X:391:ASN:CG	1:X:393:VAL:HG23	2.34	0.53
1:A:81:LEU:HD13	1:A:99:ARG:HH12	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:138:VAL:HG11	1:X:175:LEU:CD2	2.39	0.52
1:X:287:LEU:HD23	1:X:288:ILE:N	2.23	0.52
1:A:106:ILE:CG2	1:A:107:PRO:HD3	2.39	0.52
1:A:351:TRP:CD1	1:A:426:VAL:HB	2.44	0.52
1:A:372:VAL:HG12	1:A:373:TRP:H	1.73	0.52
1:A:106:ILE:HG22	1:A:107:PRO:N	2.24	0.52
1:A:311:LEU:HD13	1:A:360:LEU:HD11	1.92	0.52
1:X:84:ALA:O	1:X:88:ALA:N	2.42	0.52
1:X:265:SER:O	1:X:266:VAL:CG2	2.58	0.52
1:X:289:ARG:HD2	1:X:366:GLU:HB3	1.90	0.52
1:A:351:TRP:HZ3	1:A:382:GLN:OE1	1.92	0.52
1:A:354:LEU:HB3	1:A:385:TRP:CB	2.40	0.52
1:X:214:GLY:CA	1:X:270:ARG:N	2.72	0.52
1:X:292:GLU:OE1	1:X:337:GLU:N	2.42	0.52
1:A:38:GLU:O	1:A:40:PHE:N	2.43	0.52
1:X:262:LEU:C	1:X:264:SER:H	2.17	0.52
1:A:348:LEU:HD21	1:A:429:LYS:HB3	1.91	0.52
1:X:196:ARG:O	1:X:197:ALA:C	2.52	0.52
1:X:262:LEU:C	1:X:264:SER:N	2.67	0.52
1:X:324:TYR:CD1	1:X:324:TYR:C	2.87	0.52
1:A:73:VAL:HB	1:A:174:ILE:HD12	1.92	0.52
1:A:106:ILE:HD13	1:A:186:LEU:CD2	2.38	0.52
1:A:144:VAL:O	1:A:145:ASP:HB3	2.10	0.52
1:A:217:LEU:HD22	1:A:222:ASP:C	2.35	0.52
1:A:294:ILE:HA	1:A:336:THR:HA	1.92	0.52
1:A:295:VAL:CG2	1:A:335:VAL:HB	2.40	0.52
1:A:340:ARG:CA	1:A:360:LEU:HD12	2.39	0.52
1:X:217:LEU:HD13	1:X:221:GLY:O	2.10	0.51
1:X:231:THR:CG2	1:X:293:ARG:HA	2.39	0.51
1:X:391:ASN:C	1:X:393:VAL:N	2.68	0.51
1:X:409:GLU:OE1	1:X:410:TRP:HD1	1.94	0.51
1:A:315:ALA:CB	1:A:358:ALA:HB1	2.41	0.51
1:A:189:ILE:HG22	1:A:190:ASN:O	2.10	0.51
1:A:217:LEU:HD13	1:A:221:GLY:O	2.10	0.51
1:A:47:GLY:CA	1:A:79:PRO:HD2	2.40	0.51
1:A:81:LEU:HD11	1:A:99:ARG:HH12	1.76	0.51
1:X:44:LYS:HE2	1:X:191:ALA:HB3	1.91	0.51
1:A:294:ILE:HD11	1:A:372:VAL:HA	1.92	0.51
1:X:383:LEU:HD12	1:X:384:ILE:H	1.76	0.51
1:X:27:GLU:O	1:X:31:ARG:HB3	2.10	0.51
1:A:32:PHE:HA	1:A:36:ASP:OD1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:38:GLU:O	1:X:40:PHE:N	2.44	0.51
1:X:389:THR:O	1:X:394:ASN:ND2	2.43	0.51
1:X:54:LEU:N	1:X:55:PRO:CD	2.74	0.51
1:X:106:ILE:CB	1:X:107:PRO:HD3	2.41	0.51
1:X:297:THR:H	1:X:332:ARG:NH1	1.94	0.51
1:A:174:ILE:N	1:A:174:ILE:CD1	2.56	0.51
1:A:19:MET:HA	1:X:21:ASP:HB2	1.93	0.51
1:X:289:ARG:NE	1:X:366:GLU:HB3	2.25	0.51
1:X:405:VAL:HG11	1:X:431:PHE:HE2	1.76	0.51
1:A:17:SER:HA	1:A:26:ARG:HH21	1.75	0.50
1:A:140:GLU:OE2	1:A:182:PRO:HB3	2.11	0.50
1:A:205:TYR:O	1:A:264:SER:HA	2.11	0.50
1:A:409:GLU:OE1	1:A:410:TRP:HD1	1.94	0.50
1:X:332:ARG:N	1:X:345:THR:OG1	2.44	0.50
1:A:183:ASP:C	1:A:183:ASP:OD2	2.53	0.50
1:X:353:TYR:CE2	1:X:355:ASP:CA	2.92	0.50
1:A:140:GLU:CG	1:A:182:PRO:HG3	2.41	0.50
1:A:403:GLY:HA3	1:A:414:TRP:CE2	2.46	0.50
1:A:15:LEU:HD13	1:X:15:LEU:HG	1.92	0.50
1:A:32:PHE:HD1	1:A:36:ASP:OD2	1.87	0.50
1:A:57:LEU:O	1:A:60:ALA:HB3	2.10	0.50
1:A:423:VAL:O	1:A:424:ALA:C	2.54	0.50
1:X:39:ARG:HD3	1:X:202:LEU:O	2.11	0.50
1:X:42:VAL:O	1:X:43:ILE:CG1	2.60	0.50
1:A:398:PHE:CD2	1:A:398:PHE:C	2.89	0.50
1:X:40:PHE:CE1	1:X:69:LEU:HD22	2.47	0.50
1:X:227:ILE:CG2	1:X:228:ASN:N	2.74	0.50
1:A:88:ALA:O	1:A:89:ASP:CB	2.56	0.50
1:X:106:ILE:HB	1:X:107:PRO:HD3	1.92	0.50
1:X:120:LEU:O	1:X:124:ILE:HG13	2.12	0.50
1:X:47:GLY:HA3	1:X:79:PRO:HD2	1.93	0.50
1:A:39:ARG:HD3	1:A:202:LEU:O	2.12	0.50
1:A:139:PHE:CZ	1:A:194:ALA:HB1	2.47	0.50
1:X:43:ILE:HD12	1:X:71:PRO:HB3	1.94	0.50
1:X:131:ALA:HA	1:X:171:GLN:HB3	1.94	0.50
1:X:357:PHE:CE1	1:X:372:VAL:HG11	2.41	0.50
1:A:48:ALA:N	1:A:79:PRO:CD	2.73	0.49
1:A:94:ARG:HG2	1:A:99:ARG:N	2.27	0.49
1:X:353:TYR:O	1:X:353:TYR:HD2	1.92	0.49
1:A:398:PHE:CD1	1:X:398:PHE:CE1	2.78	0.49
1:X:132:ALA:HB3	1:X:166:ALA:HB1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:LYS:O	1:A:258:ASP:N	2.42	0.49
1:A:266:VAL:H	1:A:287:LEU:HD13	1.76	0.49
1:A:296:ALA:C	1:A:297:THR:HG22	2.21	0.49
1:A:351:TRP:CD1	1:A:426:VAL:CG1	2.95	0.49
1:A:54:LEU:HB3	1:A:55:PRO:HD3	1.95	0.49
1:A:80:GLN:O	1:A:84:ALA:CB	2.61	0.49
1:A:405:VAL:HG12	1:A:431:PHE:CZ	2.48	0.49
1:X:141:ALA:HB1	1:X:154:GLU:C	2.38	0.49
1:X:401:CYS:O	1:X:402:ASP:OD1	2.31	0.49
1:A:9:ARG:HG3	1:A:29:LEU:HD13	1.95	0.49
1:A:61:LEU:CD2	1:A:73:VAL:HG21	2.42	0.49
1:A:354:LEU:HG	1:A:355:ASP:N	2.24	0.49
1:A:356:LYS:HZ3	1:A:436:THR:HG21	1.76	0.49
1:X:88:ALA:C	1:X:90:ILE:N	2.71	0.49
1:X:140:GLU:CG	1:X:182:PRO:HG3	2.42	0.49
1:X:196:ARG:HH11	1:X:255:ARG:HD2	1.76	0.49
1:X:227:ILE:HG22	1:X:228:ASN:H	1.75	0.49
1:X:354:LEU:HB3	1:X:385:TRP:HB3	1.95	0.49
1:A:12:ILE:O	1:A:16:LEU:HG	2.12	0.49
1:A:196:ARG:O	1:A:199:VAL:N	2.46	0.49
1:A:106:ILE:CD1	1:A:186:LEU:HD23	2.36	0.49
1:A:138:VAL:HG11	1:A:175:LEU:CD2	2.43	0.49
1:A:64:LEU:HD22	1:A:69:LEU:CD1	2.37	0.48
1:A:89:ASP:C	1:A:91:PRO:HD3	2.36	0.48
1:A:141:ALA:HB1	1:A:154:GLU:C	2.38	0.48
1:A:414:TRP:CZ3	1:A:423:VAL:HG11	2.48	0.48
1:X:289:ARG:CD	1:X:366:GLU:HB3	2.44	0.48
1:A:232:ASP:CB	1:A:236:LEU:HD12	2.41	0.48
1:A:64:LEU:CD1	1:A:71:PRO:HG3	2.37	0.48
1:A:262:LEU:HD21	1:A:290:ARG:CZ	2.43	0.48
1:A:324:TYR:CD1	1:A:325:TRP:N	2.80	0.48
1:X:296:ALA:CB	1:X:332:ARG:NH2	2.67	0.48
1:X:423:VAL:O	1:X:424:ALA:C	2.55	0.48
1:A:232:ASP:O	1:A:236:LEU:CD1	2.56	0.48
1:X:35:ILE:O	1:X:37:GLN:N	2.47	0.48
1:X:65:GLN:NE2	1:X:130:ARG:O	2.44	0.48
1:X:232:ASP:CA	1:X:236:LEU:HD23	2.43	0.48
1:X:387:SER:OG	1:X:388:ARG:N	2.45	0.48
1:A:65:GLN:NE2	1:A:130:ARG:O	2.44	0.48
1:A:117:ASN:O	1:A:121:VAL:HG23	2.13	0.48
1:A:391:ASN:O	1:A:393:VAL:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:37:GLN:CD	1:X:168:ARG:HG3	2.38	0.48
1:A:19:MET:CE	1:X:19:MET:HB2	2.43	0.48
1:A:93:GLU:HB3	1:A:100:VAL:CG2	2.42	0.48
1:X:412:VAL:HG23	1:X:431:PHE:CZ	2.49	0.48
1:A:63:PHE:CZ	1:A:67:VAL:HG11	2.49	0.48
1:X:143:ILE:HA	1:X:153:GLY:HA2	1.95	0.48
1:X:189:ILE:HG22	1:X:190:ASN:O	2.14	0.48
1:X:324:TYR:CD1	1:X:325:TRP:N	2.81	0.48
1:A:106:ILE:HB	1:A:107:PRO:HD3	1.95	0.48
1:A:405:VAL:HG12	1:A:431:PHE:HZ	1.78	0.48
1:X:94:ARG:HB3	1:X:100:VAL:HG22	1.95	0.48
1:X:414:TRP:CZ3	1:X:423:VAL:HG11	2.49	0.48
1:A:332:ARG:N	1:A:345:THR:OG1	2.46	0.48
1:X:10:GLN:O	1:X:12:ILE:N	2.39	0.48
1:A:94:ARG:HA	1:A:99:ARG:CA	2.43	0.48
1:A:237:MET:O	1:A:247:ARG:NE	2.47	0.48
1:A:311:LEU:O	1:A:360:LEU:HD21	2.14	0.48
1:X:51:GLN:HB2	1:X:80:GLN:CD	2.39	0.48
1:X:403:GLY:HA3	1:X:414:TRP:CE2	2.48	0.48
1:A:175:LEU:N	1:A:175:LEU:CD1	2.77	0.47
1:A:293:ARG:NH1	1:A:337:GLU:OE2	2.47	0.47
1:A:391:ASN:C	1:A:393:VAL:H	2.21	0.47
1:X:266:VAL:O	1:X:288:ILE:N	2.47	0.47
1:X:315:ALA:CB	1:X:358:ALA:HB1	2.44	0.47
1:X:362:ASP:OD2	1:X:362:ASP:N	2.39	0.47
1:X:227:ILE:HD12	1:X:288:ILE:CD1	2.44	0.47
1:A:78:GLY:O	1:A:82:ASP:CG	2.57	0.47
1:A:332:ARG:HG3	1:A:332:ARG:NH1	2.26	0.47
1:X:344:ILE:O	1:X:344:ILE:HG22	2.11	0.47
1:A:85:LEU:HD21	1:A:108:ILE:HG13	1.97	0.47
1:A:356:LYS:HE3	1:A:437:LEU:HD11	1.96	0.47
1:X:78:GLY:O	1:X:82:ASP:CG	2.57	0.47
1:X:81:LEU:HD11	1:X:99:ARG:HH12	1.77	0.47
1:A:12:ILE:HD13	1:X:15:LEU:CD1	2.44	0.47
1:X:29:LEU:HD13	1:X:67:VAL:HG13	1.96	0.47
1:X:65:GLN:NE2	1:X:130:ARG:CB	2.70	0.47
1:X:81:LEU:HD12	1:X:82:ASP:N	2.29	0.47
1:X:274:LEU:HD12	1:X:274:LEU:HA	1.66	0.47
1:X:409:GLU:OE1	1:X:410:TRP:CD1	2.68	0.47
1:X:212:GLY:O	1:X:213:THR:C	2.57	0.47
1:A:9:ARG:O	1:A:12:ILE:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:GLY:O	1:A:213:THR:C	2.57	0.47
1:A:232:ASP:CA	1:A:236:LEU:HD12	2.44	0.47
1:X:106:ILE:HD13	1:X:186:LEU:CD2	2.44	0.47
1:X:205:TYR:O	1:X:264:SER:HA	2.15	0.47
1:X:297:THR:O	1:X:332:ARG:NH1	2.47	0.47
1:X:315:ALA:HB3	1:X:358:ALA:HB1	1.96	0.47
1:A:26:ARG:HD2	1:A:30:HIS:HE1	1.80	0.47
1:A:262:LEU:C	1:A:264:SER:H	2.23	0.47
1:X:24:GLU:OE1	1:X:279:PHE:O	2.33	0.47
1:X:42:VAL:CG1	1:X:43:ILE:N	2.77	0.47
1:X:232:ASP:O	1:X:236:LEU:HD23	2.13	0.47
1:A:45:VAL:HG12	1:A:46:GLY:O	2.15	0.47
1:X:356:LYS:HE2	1:X:436:THR:OG1	2.15	0.47
1:A:51:GLN:HB2	1:A:80:GLN:CD	2.39	0.47
1:X:35:ILE:O	1:X:36:ASP:C	2.57	0.47
1:X:231:THR:HG22	1:X:293:ARG:HA	1.97	0.47
1:X:237:MET:O	1:X:247:ARG:NE	2.48	0.47
1:X:44:LYS:HE2	1:X:191:ALA:CB	2.44	0.46
1:X:297:THR:C	1:X:332:ARG:NH1	2.72	0.46
1:A:13:VAL:CG1	1:A:26:ARG:CD	2.81	0.46
1:A:295:VAL:O	1:A:335:VAL:N	2.49	0.46
1:X:106:ILE:HG22	1:X:107:PRO:HD3	1.96	0.46
1:A:353:TYR:CD2	1:A:353:TYR:O	2.68	0.46
1:X:48:ALA:HB2	1:X:79:PRO:HG2	1.97	0.46
1:X:154:GLU:HA	1:X:155:PRO:HD3	1.80	0.46
1:X:287:LEU:HD23	1:X:287:LEU:C	2.41	0.46
1:A:11:THR:C	1:A:13:VAL:N	2.73	0.46
1:A:13:VAL:C	1:A:15:LEU:N	2.70	0.46
1:A:48:ALA:CB	1:A:79:PRO:HG2	2.45	0.46
1:A:167:ALA:O	1:A:170:GLY:N	2.27	0.46
1:A:299:ASP:OD2	1:A:302:SER:HB3	2.15	0.46
1:X:106:ILE:CD1	1:X:186:LEU:HD23	2.40	0.46
1:A:5:ALA:C	1:A:7:GLY:N	2.74	0.46
1:A:9:ARG:CA	1:A:12:ILE:HG22	2.43	0.46
1:A:36:ASP:HB2	1:A:39:ARG:CB	2.43	0.46
1:A:113:LEU:HD12	1:A:178:LEU:HD12	1.97	0.46
1:A:118:LEU:O	1:A:119:ALA:C	2.57	0.46
1:A:292:GLU:OE1	1:A:336:THR:CG2	2.63	0.46
1:A:332:ARG:HD3	1:A:379:TYR:CE1	2.51	0.46
1:A:406:ARG:CD	1:X:398:PHE:CE2	2.88	0.46
1:A:411:THR:HG22	1:A:413:PHE:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:356:LYS:HZ1	1:X:436:THR:HG21	1.81	0.46
1:A:64:LEU:HB2	1:A:71:PRO:HG3	1.98	0.46
1:A:81:LEU:HD12	1:A:82:ASP:N	2.31	0.46
1:A:433:LEU:HA	1:A:434:PRO:HD3	1.64	0.46
1:X:229:LEU:HD22	1:X:254:LYS:CB	2.46	0.46
1:X:230:ALA:HB2	1:X:290:ARG:O	2.16	0.46
1:X:357:PHE:HE1	1:X:372:VAL:CG1	2.27	0.46
1:A:85:LEU:HD21	1:A:108:ILE:HB	1.97	0.46
1:A:93:GLU:OE2	1:A:102:ARG:NH1	2.49	0.46
1:A:37:GLN:O	1:A:70:THR:HB	2.16	0.46
1:A:47:GLY:HA3	1:A:79:PRO:HD2	1.97	0.46
1:A:151:ARG:HH21	1:A:185:THR:HG23	1.80	0.46
1:A:273:GLU:HB3	1:A:284:SER:HB3	1.98	0.46
1:X:29:LEU:HD11	1:X:67:VAL:HG13	1.97	0.46
1:X:32:PHE:C	1:X:34:GLY:N	2.74	0.46
1:A:16:LEU:HA	1:X:19:MET:HE2	1.98	0.45
1:A:40:PHE:CE1	1:A:69:LEU:CD2	2.99	0.45
1:A:292:GLU:HG2	1:A:368:LEU:CD2	2.46	0.45
1:A:351:TRP:CD1	1:A:426:VAL:CB	2.98	0.45
1:A:389:THR:O	1:A:394:ASN:ND2	2.48	0.45
1:A:270:ARG:NH1	1:A:273:GLU:CG	2.79	0.45
1:X:8:VAL:O	1:X:12:ILE:HG13	2.15	0.45
1:X:75:HIS:NE2	1:X:176:ALA:CB	2.78	0.45
1:A:36:ASP:HB2	1:A:39:ARG:HG3	1.99	0.45
1:A:120:LEU:HD12	1:A:120:LEU:C	2.41	0.45
1:A:368:LEU:C	1:A:370:ARG:N	2.68	0.45
1:X:144:VAL:O	1:X:145:ASP:CB	2.64	0.45
1:A:292:GLU:OE1	1:A:368:LEU:HD13	2.16	0.45
1:A:328:LEU:HG	1:A:330:VAL:CG2	2.37	0.45
1:X:354:LEU:HG	1:X:355:ASP:N	2.30	0.45
1:A:5:ALA:O	1:A:7:GLY:N	2.50	0.45
1:A:42:VAL:HG23	1:A:204:PRO:HG3	1.98	0.45
1:A:231:THR:OG1	1:A:232:ASP:OD1	2.26	0.45
1:X:57:LEU:HD13	1:X:210:LEU:HD12	1.99	0.45
1:X:63:PHE:CZ	1:X:67:VAL:HG21	2.52	0.45
1:X:227:ILE:CG2	1:X:228:ASN:H	2.30	0.45
1:X:433:LEU:HA	1:X:434:PRO:HD3	1.59	0.45
1:A:9:ARG:O	1:A:10:GLN:C	2.59	0.45
1:A:65:GLN:HA	1:A:69:LEU:O	2.17	0.45
1:X:117:ASN:ND2	1:X:135:PRO:HG3	2.31	0.45
1:X:190:ASN:OD1	1:X:190:ASN:C	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:243:ASN:O	1:X:244:GLY:C	2.59	0.45
1:A:13:VAL:CG2	1:A:29:LEU:HD12	2.47	0.45
1:A:270:ARG:NH1	1:A:273:GLU:HG2	2.30	0.45
1:A:292:GLU:CG	1:A:368:LEU:HD11	2.46	0.45
1:A:26:ARG:O	1:A:26:ARG:HG3	2.14	0.45
1:A:383:LEU:O	1:A:384:ILE:HD12	2.17	0.45
1:A:15:LEU:HD21	1:X:16:LEU:CA	2.47	0.45
1:A:19:MET:HE2	1:X:19:MET:CB	2.47	0.45
1:A:19:MET:HB3	1:X:21:ASP:H	1.82	0.45
1:A:42:VAL:HG12	1:A:43:ILE:N	2.31	0.45
1:A:423:VAL:CG1	1:A:427:VAL:HG23	2.47	0.45
1:A:423:VAL:HG13	1:A:427:VAL:HG23	1.99	0.45
1:X:42:VAL:HG23	1:X:204:PRO:HG3	1.93	0.45
1:A:262:LEU:C	1:A:264:SER:N	2.74	0.44
1:X:10:GLN:C	1:X:12:ILE:N	2.73	0.44
1:X:265:SER:O	1:X:266:VAL:HG23	2.16	0.44
1:A:56:GLY:O	1:A:57:LEU:C	2.59	0.44
1:A:296:ALA:C	1:A:333:ALA:O	2.61	0.44
1:A:405:VAL:HG11	1:A:431:PHE:CE2	2.51	0.44
1:X:40:PHE:CE1	1:X:69:LEU:CD2	3.00	0.44
1:X:83:ALA:O	1:X:87:ALA:HB3	2.17	0.44
1:X:124:ILE:HG21	1:X:131:ALA:HB2	1.99	0.44
1:X:309:ASP:HA	1:X:325:TRP:HZ2	1.81	0.44
1:X:423:VAL:HG13	1:X:427:VAL:HG23	1.98	0.44
1:A:86:GLU:HA	1:A:91:PRO:HG3	2.00	0.44
1:A:257:LEU:HD23	1:A:257:LEU:HA	1.77	0.44
1:A:401:CYS:HB2	1:A:414:TRP:O	2.17	0.44
1:A:85:LEU:CD2	1:A:108:ILE:HG13	2.47	0.44
1:A:97:GLY:O	1:A:98:LEU:CD2	2.55	0.44
1:A:227:ILE:CG2	1:A:228:ASN:N	2.78	0.44
1:A:156:ARG:O	1:A:156:ARG:HG2	2.17	0.44
1:A:265:SER:HB2	1:A:287:LEU:HD11	1.99	0.44
1:X:44:LYS:HG3	1:X:45:VAL:N	2.33	0.44
1:X:189:ILE:CG2	1:X:193:VAL:CG2	2.96	0.44
1:X:232:ASP:O	1:X:236:LEU:CD2	2.65	0.44
1:X:311:LEU:HD13	1:X:360:LEU:HD11	2.00	0.44
1:X:346:THR:OG1	1:X:347:ARG:N	2.44	0.44
1:A:44:LYS:HE2	1:A:191:ALA:HB3	2.00	0.44
1:A:398:PHE:CE1	1:X:398:PHE:CD1	2.79	0.44
1:A:398:PHE:CD2	1:A:398:PHE:O	2.70	0.44
1:A:409:GLU:OE1	1:A:410:TRP:CD1	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:351:TRP:CD1	1:X:426:VAL:HB	2.50	0.44
1:A:239:ALA:HB3	1:A:242:VAL:HG23	2.00	0.44
1:X:340:ARG:CA	1:X:360:LEU:HD12	2.48	0.44
1:A:48:ALA:HA	1:A:79:PRO:HG2	1.98	0.44
1:A:270:ARG:HH11	1:A:273:GLU:HG2	1.82	0.44
1:X:403:GLY:HA3	1:X:414:TRP:CD2	2.53	0.44
1:A:14:GLN:NE2	1:A:14:GLN:HA	2.32	0.44
1:A:328:LEU:HD11	1:A:346:THR:HG22	2.00	0.44
1:X:74:VAL:HG12	1:X:75:HIS:N	2.32	0.44
1:X:32:PHE:CE1	1:X:40:PHE:HD1	2.36	0.43
1:X:267:SER:CA	1:X:286:THR:O	2.47	0.43
1:X:299:ASP:OD1	1:X:301:SER:OG	2.30	0.43
1:A:44:LYS:CG	1:A:45:VAL:N	2.79	0.43
1:A:9:ARG:HH22	1:A:33:SER:HB2	1.80	0.43
1:A:356:LYS:HE2	1:A:436:THR:OG1	2.18	0.43
1:A:15:LEU:HD21	1:X:15:LEU:O	2.19	0.43
1:X:83:ALA:O	1:X:87:ALA:CB	2.66	0.43
1:X:257:LEU:HD23	1:X:257:LEU:HA	1.76	0.43
1:A:132:ALA:N	1:A:171:GLN:HB3	2.33	0.43
1:X:42:VAL:C	1:X:43:ILE:CG1	2.90	0.43
1:X:26:ARG:HG2	1:X:30:HIS:NE2	2.33	0.43
1:X:427:VAL:O	1:X:430:ALA:N	2.52	0.43
1:A:93:GLU:CD	1:A:102:ARG:CZ	2.92	0.43
1:X:44:LYS:O	1:X:45:VAL:HG12	2.19	0.43
1:X:411:THR:HG22	1:X:413:PHE:CD2	2.52	0.43
1:A:85:LEU:HA	1:A:85:LEU:HD23	1.87	0.43
1:A:144:VAL:O	1:A:144:VAL:CG1	2.66	0.43
1:A:158:ILE:HD13	1:A:158:ILE:N	2.23	0.43
1:A:243:ASN:O	1:A:244:GLY:C	2.62	0.43
1:A:9:ARG:C	1:A:12:ILE:HG22	2.44	0.42
1:X:57:LEU:O	1:X:60:ALA:HB3	2.19	0.42
1:A:13:VAL:HG22	1:A:29:LEU:HD12	2.01	0.42
1:A:67:VAL:HG23	1:A:69:LEU:HG	1.98	0.42
1:A:232:ASP:C	1:A:236:LEU:CD1	2.88	0.42
1:A:85:LEU:HD21	1:A:108:ILE:CG1	2.49	0.42
1:X:299:ASP:OD2	1:X:302:SER:HB3	2.19	0.42
1:A:120:LEU:O	1:A:124:ILE:N	2.51	0.42
1:A:163:VAL:CG2	1:A:175:LEU:HD21	2.49	0.42
1:A:166:ALA:HB1	1:A:171:GLN:HB2	2.01	0.42
1:A:327:ARG:HE	1:A:327:ARG:HB2	1.56	0.42
1:A:356:LYS:HD3	1:A:356:LYS:HA	1.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ASN:C	1:A:393:VAL:N	2.77	0.42
1:A:404:ALA:C	1:A:405:VAL:CG2	2.87	0.42
1:X:42:VAL:HG12	1:X:43:ILE:H	1.84	0.42
1:X:120:LEU:O	1:X:124:ILE:N	2.48	0.42
1:X:270:ARG:NH1	1:X:273:GLU:CG	2.83	0.42
1:A:36:ASP:HB2	1:A:39:ARG:CG	2.49	0.42
1:A:67:VAL:HG22	1:A:69:LEU:HG	1.96	0.42
1:X:232:ASP:HB3	1:X:236:LEU:HD21	1.92	0.42
1:X:423:VAL:CG1	1:X:427:VAL:HG23	2.50	0.42
1:A:91:PRO:HD2	1:A:91:PRO:O	2.19	0.42
1:A:154:GLU:CD	1:A:155:PRO:HD2	2.44	0.42
1:A:159:HIS:HB3	1:A:161:ASP:OD2	2.19	0.42
1:X:56:GLY:O	1:X:57:LEU:C	2.62	0.42
1:A:75:HIS:NE2	1:A:176:ALA:HB2	2.35	0.42
1:X:5:ALA:N	1:X:6:PRO:HD3	2.34	0.42
1:X:106:ILE:CG2	1:X:107:PRO:HD3	2.50	0.42
1:X:393:VAL:O	1:X:395:GLY:N	2.53	0.42
1:X:407:ARG:O	1:X:408:ASP:C	2.62	0.42
1:A:44:LYS:N	1:A:208:VAL:O	2.51	0.42
1:A:93:GLU:H	1:A:93:GLU:HG3	1.42	0.42
1:X:154:GLU:CD	1:X:155:PRO:HD2	2.45	0.42
1:X:270:ARG:NH1	1:X:273:GLU:HG2	2.35	0.42
1:X:351:TRP:CD1	1:X:426:VAL:CB	3.00	0.42
1:A:44:LYS:HG2	1:A:209:PHE:HD1	1.85	0.42
1:X:81:LEU:HD11	1:X:99:ARG:NH1	2.35	0.42
1:A:15:LEU:HD21	1:X:16:LEU:HA	2.02	0.41
1:A:141:ALA:O	1:A:181:THR:HG22	2.20	0.41
1:A:303:LEU:HD23	1:A:303:LEU:HA	1.88	0.41
1:A:315:ALA:HB3	1:A:358:ALA:HB1	2.02	0.41
1:A:328:LEU:HD21	1:A:330:VAL:CG2	2.49	0.41
1:X:48:ALA:CB	1:X:79:PRO:HG2	2.50	0.41
1:X:98:LEU:O	1:X:99:ARG:O	2.38	0.41
1:X:327:ARG:HE	1:X:327:ARG:HB2	1.56	0.41
1:A:95:VAL:H	1:A:100:VAL:HG11	1.65	0.41
1:A:304:ASP:OD1	1:A:307:ARG:HB2	2.20	0.41
1:X:78:GLY:O	1:X:82:ASP:OD1	2.38	0.41
1:X:262:LEU:O	1:X:264:SER:N	2.52	0.41
1:X:368:LEU:C	1:X:370:ARG:H	2.28	0.41
1:X:106:ILE:HD12	1:X:151:ARG:NH1	2.35	0.41
1:X:412:VAL:HG23	1:X:431:PHE:CD1	2.55	0.41
1:A:95:VAL:CG1	1:A:149:LEU:HD23	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:GLU:CG	1:A:336:THR:OG1	2.66	0.41
1:X:61:LEU:CD2	1:X:73:VAL:HG21	2.47	0.41
1:A:75:HIS:HE2	1:A:176:ALA:HB2	1.84	0.41
1:A:231:THR:CG2	1:A:293:ARG:HA	2.51	0.41
1:A:411:THR:HG21	1:A:413:PHE:CE2	2.55	0.41
1:X:42:VAL:CG1	1:X:43:ILE:H	2.34	0.41
1:X:332:ARG:HG3	1:X:333:ALA:H	1.84	0.41
1:A:28:TYR:CZ	1:A:205:TYR:HE2	2.37	0.41
1:A:42:VAL:C	1:A:43:ILE:CG1	2.84	0.41
1:A:47:GLY:CA	1:A:78:GLY:H	2.32	0.41
1:A:64:LEU:HD12	1:A:71:PRO:CG	2.39	0.41
1:A:91:PRO:O	1:A:92:THR:HG23	2.20	0.41
1:A:155:PRO:HG2	1:A:193:VAL:HG23	2.01	0.41
1:A:265:SER:HB2	1:A:287:LEU:CD1	2.50	0.41
1:X:159:HIS:C	1:X:161:ASP:H	2.29	0.41
1:X:383:LEU:HD12	1:X:384:ILE:N	2.36	0.41
1:A:227:ILE:HD13	1:A:250:LEU:HD21	2.02	0.41
1:A:266:VAL:O	1:A:288:ILE:N	2.54	0.41
1:X:196:ARG:CD	1:X:255:ARG:HD2	2.43	0.41
1:A:117:ASN:OD1	1:A:176:ALA:HB2	2.21	0.41
1:A:340:ARG:HA	1:A:360:LEU:HD12	2.01	0.41
1:X:90:ILE:N	1:X:91:PRO:HD3	2.33	0.41
1:X:134:VAL:N	1:X:135:PRO:CD	2.67	0.41
1:X:167:ALA:O	1:X:168:ARG:C	2.63	0.41
1:X:231:THR:OG1	1:X:232:ASP:OD1	2.29	0.41
1:X:289:ARG:HE	1:X:366:GLU:HG2	1.85	0.41
1:X:331:ASP:HB2	1:X:347:ARG:HG3	2.02	0.41
1:X:398:PHE:C	1:X:398:PHE:HD2	2.27	0.41
1:A:28:TYR:CZ	1:A:205:TYR:CD2	3.08	0.41
1:A:40:PHE:CD1	1:A:69:LEU:HD22	2.56	0.41
1:A:106:ILE:HD12	1:A:151:ARG:NH1	2.35	0.41
1:A:154:GLU:HA	1:A:155:PRO:HD3	1.84	0.41
1:A:216:LEU:C	1:A:217:LEU:HD23	2.44	0.41
1:A:253:ILE:HD12	1:A:288:ILE:HD12	2.03	0.41
1:A:273:GLU:OE1	1:A:284:SER:CB	2.69	0.41
1:X:24:GLU:HG2	1:X:28:TYR:HD2	1.86	0.41
1:X:26:ARG:O	1:X:30:HIS:CD2	2.73	0.41
1:X:32:PHE:HD1	1:X:32:PHE:O	2.03	0.41
1:X:57:LEU:HG	1:X:61:LEU:HD11	2.03	0.41
1:X:121:VAL:O	1:X:124:ILE:HB	2.20	0.41
1:X:132:ALA:N	1:X:171:GLN:HB3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:192:ASP:C	1:X:194:ALA:N	2.74	0.41
1:X:254:LYS:O	1:X:258:ASP:N	2.49	0.41
1:X:270:ARG:HH11	1:X:273:GLU:HG2	1.86	0.41
1:X:340:ARG:HB3	1:X:360:LEU:HD12	2.02	0.41
1:X:353:TYR:CE2	1:X:354:LEU:O	2.74	0.41
1:X:354:LEU:HB3	1:X:385:TRP:HB2	2.01	0.41
1:X:393:VAL:O	1:X:394:ASN:C	2.64	0.41
1:A:255:ARG:HH11	1:A:255:ARG:HD3	1.73	0.41
1:A:348:LEU:O	1:A:351:TRP:N	2.54	0.41
1:A:353:TYR:CE2	1:A:355:ASP:CA	3.00	0.41
1:X:81:LEU:CD1	1:X:99:ARG:NH1	2.81	0.41
1:X:336:THR:O	1:X:338:SER:N	2.54	0.41
1:A:91:PRO:CD	1:A:91:PRO:O	2.69	0.40
1:A:131:ALA:O	1:A:171:GLN:NE2	2.54	0.40
1:A:132:ALA:HB3	1:A:166:ALA:HB1	2.03	0.40
1:X:40:PHE:CE1	1:X:69:LEU:HA	2.56	0.40
1:A:165:SER:HA	1:A:168:ARG:HH21	1.86	0.40
1:A:196:ARG:C	1:A:198:LEU:N	2.78	0.40
1:A:331:ASP:OD2	1:A:379:TYR:OH	2.28	0.40
1:A:292:GLU:HG2	1:A:368:LEU:HD21	2.02	0.40
1:A:376:LEU:O	1:A:376:LEU:HG	2.19	0.40
1:A:394:ASN:HA	1:A:397:TYR:CD2	2.56	0.40
1:A:403:GLY:HA3	1:A:414:TRP:CD2	2.57	0.40
1:A:64:LEU:O	1:A:69:LEU:HB2	2.22	0.40
1:A:140:GLU:HA	1:A:180:GLU:O	2.21	0.40
1:A:294:ILE:HD13	1:A:372:VAL:HA	2.00	0.40
1:A:309:ASP:HA	1:A:325:TRP:CZ2	2.53	0.40
1:X:63:PHE:CD2	1:X:63:PHE:C	3.00	0.40
1:X:328:LEU:CD1	1:X:330:VAL:HG23	2.51	0.40
1:A:81:LEU:CD1	1:A:99:ARG:NH2	2.80	0.40
1:X:32:PHE:O	1:X:32:PHE:CD1	2.75	0.40
1:X:65:GLN:HG3	1:X:66:THR:N	2.36	0.40
1:X:405:VAL:HG12	1:X:431:PHE:CZ	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/461 (94%)	360 (83%)	46 (11%)	29 (7%)	1	12
1	X	433/461 (94%)	349 (81%)	57 (13%)	27 (6%)	1	13
All	All	868/922 (94%)	709 (82%)	103 (12%)	56 (6%)	1	13

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	89	ASP
1	A	95	VAL
1	A	96	ASP
1	A	99	ARG
1	A	145	ASP
1	A	146	ALA
1	X	99	ARG
1	X	145	ASP
1	X	146	ALA
1	A	78	GLY
1	A	88	ALA
1	A	91	PRO
1	A	226	SER
1	A	330	VAL
1	A	405	VAL
1	X	36	ASP
1	X	39	ARG
1	X	43	ILE
1	X	78	GLY
1	X	316	PHE
1	A	23	LYS
1	A	39	ARG
1	A	92	THR
1	A	93	GLU

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Mol	Chain	Res	Type
1	A	196	ARG
1	A	297	THR
1	A	316	PHE
1	A	349	ASP
1	X	84	ALA
1	X	89	ASP
1	X	103	ASP
1	X	226	SER
1	X	330	VAL
1	X	337	GLU
1	X	349	ASP
1	A	6	PRO
1	A	438	GLU
1	X	11	THR
1	X	91	PRO
1	X	92	THR
1	X	185	THR
1	X	196	ARG
1	X	405	VAL
1	A	110	ARG
1	A	387	SER
1	X	8	VAL
1	X	33	SER
1	X	88	ALA
1	A	317	GLY
1	X	438	GLU
1	A	392	PRO
1	X	242	VAL
1	A	391	ASN
1	X	317	GLY
1	A	155	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/367 (94%)	305 (88%)	41 (12%)	5	19
1	X	344/367 (94%)	302 (88%)	42 (12%)	5	19
All	All	690/734 (94%)	607 (88%)	83 (12%)	5	19

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	20	ARG
1	A	35	ILE
1	A	65	GLN
1	A	89	ASP
1	A	92	THR
1	A	100	VAL
1	A	106	ILE
1	A	118	LEU
1	A	136	ARG
1	A	143	ILE
1	A	144	VAL
1	A	152	VAL
1	A	158	ILE
1	A	190	ASN
1	A	193	VAL
1	A	196	ARG
1	A	206	LYS
1	A	223	ILE
1	A	224	LEU
1	A	236	LEU
1	A	246	MET
1	A	249	LYS
1	A	251	GLU
1	A	254	LYS
1	A	255	ARG
1	A	287	LEU
1	A	293	ARG
1	A	318	ARG
1	A	327	ARG
1	A	332	ARG
1	A	354	LEU

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Mol	Chain	Res	Type
1	A	362	ASP
1	A	364[A]	ARG
1	A	364[B]	ARG
1	A	370	ARG
1	A	372	VAL
1	A	388	ARG
1	A	390	ASN
1	A	393	VAL
1	A	421	VAL
1	X	10	GLN
1	X	14	GLN
1	X	25	ILE
1	X	26	ARG
1	X	37	GLN
1	X	45	VAL
1	X	65	GLN
1	X	67	VAL
1	X	90	ILE
1	X	100	VAL
1	X	106	ILE
1	X	115	GLN
1	X	136	ARG
1	X	143	ILE
1	X	144	VAL
1	X	152	VAL
1	X	190	ASN
1	X	196	ARG
1	X	206	LYS
1	X	223	ILE
1	X	236	LEU
1	X	246	MET
1	X	249	LYS
1	X	251	GLU
1	X	254	LYS
1	X	255	ARG
1	X	269	THR
1	X	318	ARG
1	X	327	ARG
1	X	332	ARG
1	X	344	ILE
1	X	346	THR
1	X	353	TYR

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Mol	Chain	Res	Type
1	X	354	LEU
1	X	362	ASP
1	X	364	ARG
1	X	370	ARG
1	X	372	VAL
1	X	390	ASN
1	X	393	VAL
1	X	421	VAL
1	X	437	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	18	HIS
1	A	30	HIS
1	A	65	GLN
1	A	80	GLN
1	A	394	ASN
1	X	14	GLN
1	X	18	HIS
1	X	65	GLN
1	X	80	GLN
1	X	188	ASN
1	X	394	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	436/461 (94%)	-0.86	0 100 100	185, 421, 690, 893	1 (0%)
1	X	435/461 (94%)	-0.87	0 100 100	209, 472, 685, 784	0
All	All	871/922 (94%)	-0.87	0 100 100	185, 454, 688, 893	1 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.