



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:44 PM GMT

PDB ID : 1SA1
Title : Tubulin-podophyllotoxin:stathmin-like domain complex
Authors : Ravelli, R.B.; Gigant, B.; Curmi, P.A.; Jourdain, I.; Lachkar, S.; Sobel, A.; Knossow, M.
Deposited on : 2004-02-06
Resolution : 4.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

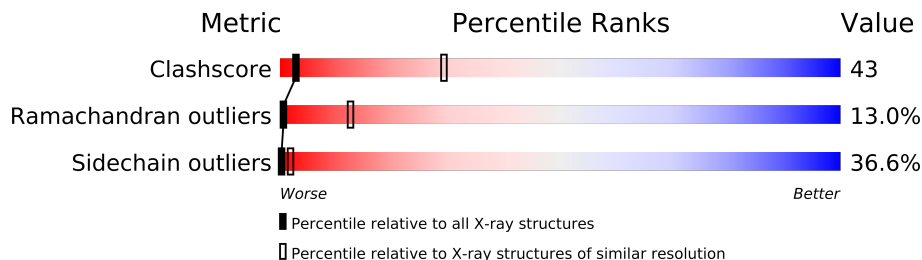
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 4.20 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))
Clashscore	79885	1259 (4.84-3.50)
Ramachandran outliers	78287	1192 (4.84-3.50)
Sidechain outliers	78261	1175 (4.84-3.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	451	
1	C	451	
2	B	445	
2	D	445	
3	E	142	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14180 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Tubulin alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	0	0
			3299	2089	559	631	20			
1	C	430	Total	C	N	O	S	0	0	0
			3275	2072	555	628	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	ILE	ALA	SEE REMARK 999	UNP P02550
C	265	ILE	ALA	SEE REMARK 999	UNP P02550

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	422	Total	C	N	O	S	0	0	0
			3241	2040	545	631	25			
2	D	426	Total	C	N	O	S	0	0	0
			3278	2059	556	638	25			

- Molecule 3 is a protein called Stathmin 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	134	Total	C	N	O	S	0	0	0
			905	555	169	176	5			

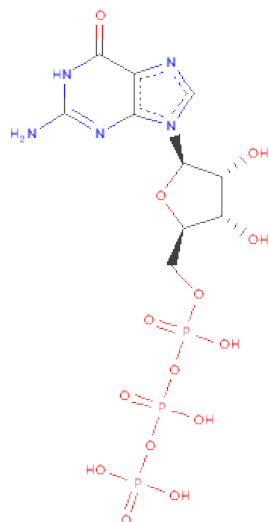
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	4	ALA	-	SEE REMARK 999	UNP P02554

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

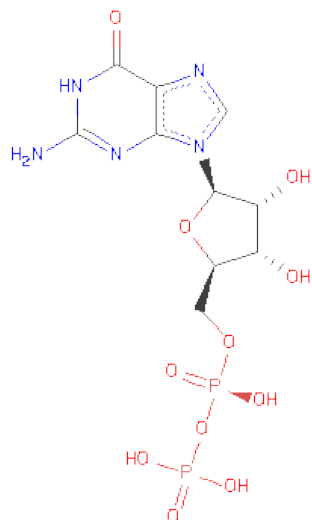
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



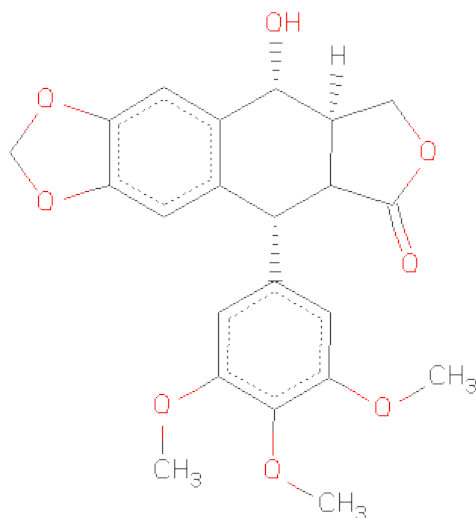
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
6	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 7 is 9-HYDROXY-5-(3,4,5-TRIMETHOXYPHENYL)-5,8,8A,9-TETRAHYDROFURO[3',4':6,7]NAPHTHO[2,3-D][1,3]DIOXOL-6(5AH)-ONE (three-letter code: POD) (formula: C₂₂H₂₂O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			30	22	8		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			30	22	8		

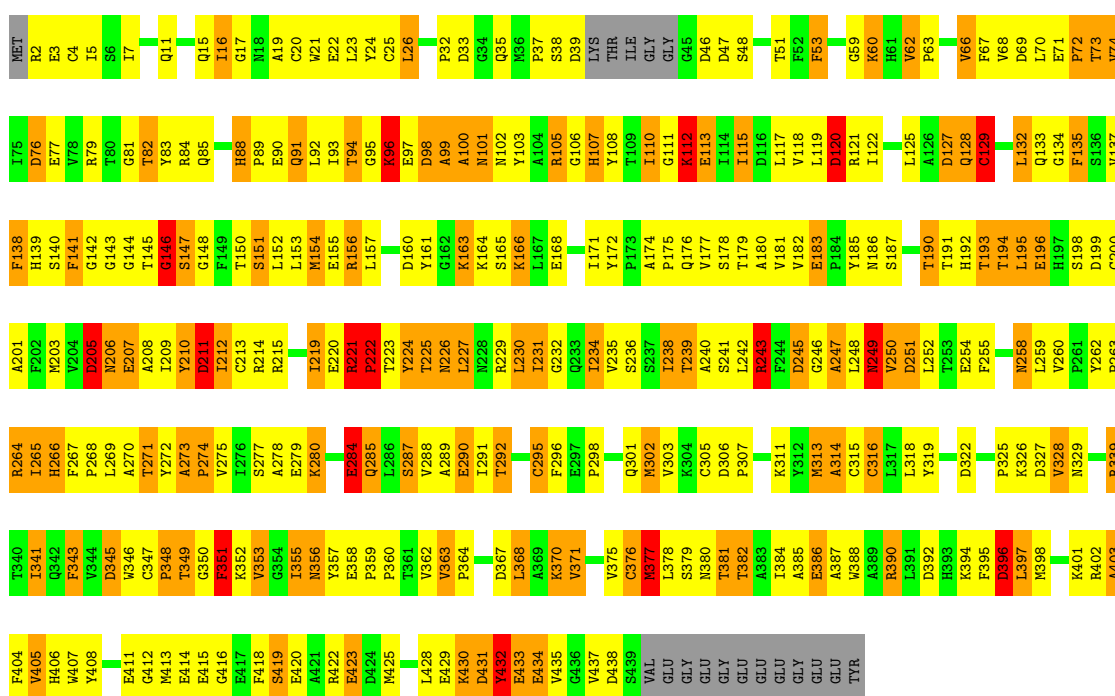
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

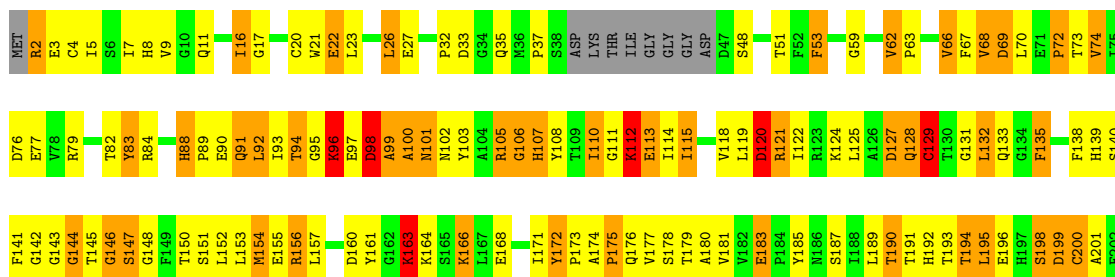
• Molecule 1: Tubulin alpha chain

Chain A:



• Molecule 1: Tubulin alpha chain

Chain C:



V409	D345	L269	M203
G410	W346	A270	V204
E411	C347	A271	D205
G412	P348	Y272	N206
M413	T349	A273	E207
E414	G350	P274	A208
E415	F351	V275	I209
G416	K352	L276	T210
E417	V353	S277	D211
F418	G354	A278	L212
S419	L355	E279	C213
N356	K280	K280	R214
A421	V357	A281	
R422	E358		L219
E423	P359	E284	E220
M425	P360	Q285	R221
	T361	L286	P222
L428	V362	S287	T223
E429	V363	V288	Y224
R430	P364	E289	T225
D431	D367	E290	N226
Y432	L368	T292	N227
E433	A369		N228
E434	K370	C295	R229
V435	V371		L230
G436	V375	Q301	L231
D437	V376	M302	G232
D438	C376	V303	Q233
S439	N377	K304	T234
VAL	L378	G365	V235
GLY	S379	D306	S236
GLY	N380	P307	E237
GLY	T381		L238
GLY	L383	K311	T239
GLY	L384	M313	A240
GLY	A385	M312	S241
GLY	E386	A314	L242
GLY	A387	C316	R243
GLY	L388		
TYR	R390	L318	L248
	L391	Y319	V250
	D392	R320	D251
	H393	P325	L252
	F395	K326	T253
	D396	F327	Q256
	L397	V328	T257
	K398		V258
	K401	A333	L259
	P402	K336	V260
	A403		P261
	F404	T339	Y262
	V405	R340	P263
	H406	I341	R264
	W407	Q342	L265
	F408	V344	H266
			P267
			P268

• Molecule 2: Tubulin beta chain

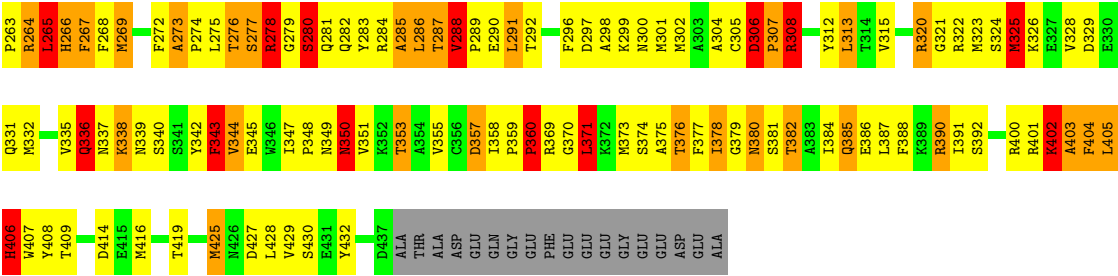
Chain B:

MET	L70	T138	Y202	P263		R401
R2	E71	H139	C203	R264	M332	R402
E3	P72	S140	I204	L265	V335	A403
I4	G73	L141	N206	H266	V336	F404
H5	T74	G142	N207	F267	N337	L405
V6	M75	G143	A208	F268	K338	H406
I7	D76	G144	L209	H269	N339	H407
Q8		T145	Y210	A273	S340	Y408
	S80	G146	D211	P274	S341	T409
	G81	G147	I212	L275	Y342	G410
	P82	G148	C213	T276	F343	D414
	F83	M149		ARG	V344	E415
	I86	G150	T216	ARG		M416
	F87	T151	L217	GLY	I347	
	R88	L152	K218	GLY	P348	T419
	P89	L153	L219	GLN	N349	
	D90	T220	S155	Q282	N350	N424
	N91	K156	T221	Y283	V351	M425
	F92	T157	P222	R284	K352	H426
	E23	R158	T223	A285	T353	D427
	V22	E159	G225	L286	V355	L428
	E22		D226	V288	G356	Y429
			D227	P289	C357	G430
			N228	E290	D357	E431
			H229	L291	F358	Y432
			L230	T292	P359	A438
			S231	F296	R369	THR
			Q232	D297	G370	ALA
			A233	A298	L371	ASP
			T234	K299	K372	GLU
			M235		M373	GLN
			S236		S374	GLY
			G237		A375	GLU
			V238		T376	PHE
			T239		F377	GIU
			D240		I378	GIU
			C241		G379	GIU
			L242		N380	GLY
			R243		S381	GLY
			P244		T382	GLU
			G245		A383	ASP
			P246		L384	GLU
			Q247		Q385	GLU
			L248		E386	ALA
			A250		L387	
			N249		F388	
			D251		V315	
			L252		A316	
			R253		L313	
			K254		T314	
			G255		V316	
			L256		A317	
			P257		V318	
			T258		F319	
			M259		R320	
			V260		I391	
			F261		S392	
			L262		E393	
			H263		Q394	
			P264		F395	
			L265		T396	
			H266		K326	
			P267		A397	
			F268		M398	
					E327	
					V328	
					R400	

• Molecule 2: Tubulin beta chain

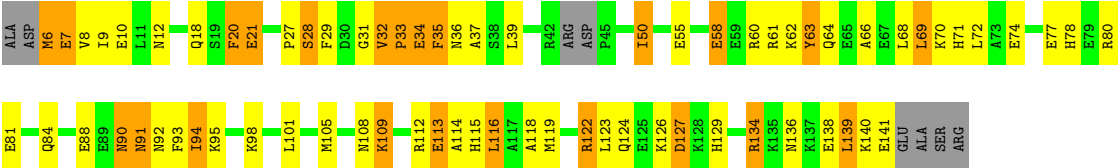
Chain D:

MET	D69	Q136	P169	T234	A233	R238	F20
	L70	L137	S170	T235	G234	H229	W21
	E71	T138	V171	S236	P235	L230	E22
	P72	H139	P173	G237	R236	V231	E23
	G73	S140	S174	T238	S232	S232	I24
	T74	L141	E175	C241	L242	D241	I24
	M75	G142	K176	R241	R243	R242	S25
	D76	G143	V177	L242	E243	E244	S26
		T145	D179	L243	P244	P245	D26
		S80	L180	L244	R246	G246	E27
	G81	L181	L245	V182	Q247	D31	
	P82	E183	L246	E184	L248	P32	
	F83	M166	L247	Y185	N249	T33	
			P175	N186	D249	G34	
			T169	K176	E250	S35	
			E110	V177	D251	Y36	
			G111	S178	R252	H37	
			H112	D179	R253	G38	
			E113	T180	K254	D39	
			L114	V181	L255	S40	
			V115	L182	P256	L41	
			D116	E183	L257	D42	
			S117	L184	E258	R43	
			V118	P184	N259	E44	
			L119	Y185	D260	L45	
			D120	L186	E261	E47	
			V121	A187	L262	R48	
			V122	T188	K264	I49	
					A265	N50	
					V267	V51	
					N268		
					E269	N54	
					L270	E55	
					P271	N59	
					E272	K60	
					L273	Y61	
					A274	E62	
					V275	P63	
					N276	R64	
					E277	A65	
					L278	L66	
					P279	L67	
					E280	V69	



• Molecule 3: Stathmin 4

Chain E:



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	328.06Å 328.06Å 54.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 4.20	Depositor
% Data completeness (in resolution range)	98.3 (20.00-4.20)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.204 , 0.259	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14180	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.89	1/3374 (0.0%)	1.09	19/4593 (0.4%)
1	C	0.74	0/3349	1.00	11/4561 (0.2%)
2	B	0.86	3/3314 (0.1%)	1.08	25/4506 (0.6%)
2	D	0.76	2/3352 (0.1%)	1.04	20/4556 (0.4%)
3	E	0.87	0/914	0.95	2/1238 (0.2%)
All	All	0.82	6/14303 (0.0%)	1.05	77/19454 (0.4%)

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	4
1	C	0	3
2	B	0	3
2	D	0	2
3	E	0	3
All	All	0	15

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	44	LEU	C-N	11.14	1.59	1.34
2	B	44	LEU	C-N	9.19	1.55	1.34
2	B	360	PRO	C-N	8.02	1.52	1.34
2	D	360	PRO	C-N	6.55	1.49	1.34
2	B	2	ARG	NE-CZ	5.14	1.39	1.33
1	A	98	ASP	CB-CG	5.13	1.62	1.51

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	427	ASP	CB-CG-OD2	8.82	126.24	118.30
2	D	205	ASP	CB-CG-OD2	8.78	126.20	118.30
2	D	163	ASP	CB-CG-OD2	8.20	125.68	118.30
2	B	205	ASP	CB-CG-OD2	7.81	125.33	118.30
1	C	211	ASP	CB-CG-OD2	7.70	125.22	118.30
1	A	160	ASP	CB-CG-OD2	7.47	125.02	118.30
2	B	308	ARG	NE-CZ-NH1	7.45	124.03	120.30
2	B	306	ASP	CB-CG-OD2	7.29	124.86	118.30
2	B	199	ASP	CB-CG-OD2	7.26	124.84	118.30
1	C	160	ASP	CB-CG-OD2	7.26	124.83	118.30
2	D	360	PRO	CA-C-N	-7.19	101.38	117.20
1	A	211	ASP	CB-CG-OD2	7.17	124.76	118.30
2	B	163	ASP	CB-CG-OD2	7.12	124.71	118.30
1	C	392	ASP	CB-CG-OD2	7.06	124.65	118.30
1	A	69	ASP	CB-CG-OD2	7.02	124.62	118.30
1	A	243	ARG	NE-CZ-NH1	7.01	123.81	120.30
3	E	69	LEU	CA-CB-CG	6.73	130.78	115.30
2	B	211	ASP	CB-CG-OD2	6.72	124.35	118.30
2	B	130	ASP	CB-CG-OD2	6.62	124.25	118.30
2	D	427	ASP	CB-CG-OD2	6.62	124.25	118.30
2	D	306	ASP	CB-CG-OD2	6.55	124.19	118.30
2	B	251	ASP	CB-CG-OD2	6.47	124.13	118.30
1	A	199	ASP	CB-CG-OD2	6.39	124.06	118.30
2	D	199	ASP	CB-CG-OD2	6.38	124.05	118.30
2	B	2	ARG	NE-CZ-NH1	6.38	123.49	120.30
2	D	211	ASP	CB-CG-OD2	6.38	124.04	118.30
2	D	308	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	A	76	ASP	CB-CG-OD2	6.28	123.95	118.30
1	C	120	ASP	CB-CG-OD2	6.27	123.94	118.30
2	B	179	ASP	CB-CG-OD2	6.20	123.88	118.30
2	B	297	ASP	CB-CG-OD2	6.10	123.79	118.30
2	B	162	PRO	N-CD-CG	-6.09	94.06	103.20
2	D	297	ASP	CB-CG-OD2	6.09	123.78	118.30
1	A	196	GLU	CA-CB-CG	6.09	126.80	113.40
2	D	357	ASP	CB-CG-OD2	6.06	123.75	118.30
1	C	76	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	397	LEU	CA-CB-CG	5.92	128.92	115.30
2	D	26	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	245	ASP	CB-CG-OD2	5.87	123.59	118.30
3	E	127	ASP	CB-CG-OD2	5.86	123.57	118.30
1	C	397	LEU	CA-CB-CG	5.86	128.77	115.30
1	A	322	ASP	CB-CG-OD2	5.83	123.54	118.30
1	A	264	ARG	C-N-CA	5.72	136.00	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	ASP	CB-CG-OD2	5.69	123.42	118.30
2	D	179	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	431	ASP	CB-CG-OD2	5.58	123.32	118.30
1	C	264	ARG	C-N-CA	5.53	135.53	121.70
2	D	31	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	98	ASP	CB-CG-OD2	5.44	123.19	118.30
1	A	127	ASP	CB-CG-OD2	5.39	123.15	118.30
1	C	69	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	146	GLY	N-CA-C	-5.38	99.64	113.10
1	C	146	GLY	N-CA-C	-5.37	99.67	113.10
1	C	199	ASP	CB-CG-OD2	5.35	123.11	118.30
2	B	26	ASP	CB-CG-OD2	5.34	123.11	118.30
2	B	69	ASP	CB-CG-OD2	5.32	123.09	118.30
2	D	329	ASP	CB-CG-OD2	5.31	123.08	118.30
2	B	44	LEU	O-C-N	-5.31	114.21	122.70
2	D	282	GLN	CB-CA-C	5.30	121.00	110.40
2	B	120	ASP	CB-CG-OD2	5.29	123.06	118.30
2	B	360	PRO	CA-C-N	-5.28	105.58	117.20
1	C	127	ASP	CB-CG-OD2	5.28	123.05	118.30
2	B	41	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	120	ASP	CB-CG-OD2	5.27	123.04	118.30
2	D	130	ASP	CB-CG-OD2	5.24	123.02	118.30
2	D	276	THR	N-CA-C	5.24	125.15	111.00
2	B	31	ASP	CB-CG-OD2	5.23	123.01	118.30
2	B	387	LEU	CA-CB-CG	5.21	127.29	115.30
2	B	255	LEU	CA-CB-CG	5.13	127.10	115.30
2	B	329	ASP	CB-CG-OD2	5.10	122.89	118.30
2	D	162	PRO	N-CD-CG	-5.09	95.56	103.20
2	B	144	GLY	N-CA-C	5.07	125.78	113.10
1	A	269	LEU	CA-CB-CG	5.05	126.92	115.30
2	D	69	ASP	CB-CG-OD2	5.04	122.83	118.30
1	A	222	PRO	N-CD-CG	-5.03	95.66	103.20
2	D	242	LEU	CA-CB-CG	5.03	126.87	115.30
2	B	51	VAL	CB-CA-C	-5.02	101.87	111.40

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	GLY	Peptide
1	A	220	GLU	Peptide
1	A	221	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	A	339	ARG	Peptide
2	B	244	PHE	Peptide
2	B	286	LEU	Peptide
2	B	49	ILE	Peptide
1	C	221	ARG	Peptide
1	C	254	GLU	Peptide
1	C	339	ARG	Peptide
2	D	244	PHE	Peptide
2	D	288	VAL	Peptide
3	E	32	VAL	Peptide
3	E	39	LEU	Peptide
3	E	50	ILE	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3299	0	3129	275	0
1	C	3275	0	3104	271	0
2	B	3241	0	3033	321	0
2	D	3278	0	3074	297	0
3	E	905	0	730	59	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	32	0	12	3	0
5	C	32	0	12	2	0
6	B	28	0	12	1	0
6	D	28	0	12	2	0
7	B	30	0	19	5	0
7	D	30	0	19	4	0
All	All	14180	0	13156	1177	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 43.

All (1177) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:E:33:PRO:HB3	3:E:35:PHE:CZ	1.64	1.33
1:C:240:ALA:HB2	1:C:243:ARG:NH1	1.39	1.33
2:D:273:ALA:CB	2:D:274:PRO:HD3	1.74	1.18
2:B:191:VAL:HG11	2:B:425:MET:HE3	1.22	1.15
2:D:191:VAL:HG11	2:D:425:MET:HE3	1.22	1.14
1:A:273:ALA:CB	1:A:274:PRO:HD3	1.78	1.13
1:C:273:ALA:HB3	1:C:274:PRO:HD3	1.24	1.11
1:C:240:ALA:HA	1:C:243:ARG:HG2	1.19	1.10
1:A:133:GLN:HE21	1:A:252:LEU:HG	1.02	1.10
1:C:191:THR:HG23	1:C:425:MET:HE1	1.29	1.08
2:B:273:ALA:CB	2:B:274:PRO:HD3	1.81	1.08
1:A:240:ALA:HA	1:A:243:ARG:CG	1.84	1.07
1:A:240:ALA:HA	1:A:243:ARG:HG3	1.09	1.07
2:B:11:GLN:HG3	2:B:74:THR:HG21	1.30	1.07
2:D:332:MET:HG3	2:D:353:THR:HG21	1.34	1.07
1:C:240:ALA:CB	1:C:243:ARG:HH11	1.69	1.05
1:A:191:THR:HG23	1:A:425:MET:HE1	1.38	1.04
2:D:273:ALA:HB3	2:D:274:PRO:HD3	1.34	1.04
1:A:128:GLN:O	1:A:129:CYS:HB2	1.56	1.04
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.07	1.02
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	1.95	1.02
1:A:348:PRO:HG3	3:E:27:PRO:HD3	1.41	1.02
2:B:147:SER:O	2:B:151:THR:OG1	1.76	1.01
2:B:273:ALA:HB3	2:B:274:PRO:HD3	1.40	1.00
2:D:11:GLN:HG3	2:D:74:THR:HG21	1.38	1.00
1:A:191:THR:HG23	1:A:425:MET:CE	1.92	1.00
2:D:191:VAL:HG11	2:D:425:MET:CE	1.93	0.98
2:B:251:ASP:O	2:B:253:ARG:N	1.96	0.97
3:E:33:PRO:HB3	3:E:35:PHE:CE2	1.98	0.97
1:A:24:TYR:CE2	1:A:243:ARG:NH2	2.31	0.97
1:A:16:ILE:HD13	1:A:171:ILE:HD11	1.44	0.97
1:A:353:VAL:HG21	3:E:20:PHE:CE2	1.99	0.97
2:B:158:ARG:O	2:B:159:GLU:HB2	1.63	0.96
1:C:209:ILE:HG22	1:C:227:LEU:HD12	1.44	0.96
1:A:273:ALA:HB3	1:A:274:PRO:CD	1.95	0.96
2:D:291:LEU:HD21	2:D:375:ALA:CB	1.94	0.96
2:D:291:LEU:HD21	2:D:375:ALA:HB3	1.47	0.96
1:C:191:THR:HG23	1:C:425:MET:CE	1.96	0.96
2:D:307:PRO:O	2:D:308:ARG:HB2	1.66	0.96
3:E:33:PRO:CB	3:E:35:PHE:CZ	2.48	0.96
1:C:273:ALA:CB	1:C:274:PRO:HD3	1.96	0.95
1:A:347:CYS:O	1:A:348:PRO:O	1.85	0.94
2:D:251:ASP:O	2:D:253:ARG:N	2.00	0.94

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:240:ALA:HA	1:C:243:ARG:CG	1.98	0.94
2:D:273:ALA:HB3	2:D:274:PRO:CD	1.97	0.94
3:E:88:GLU:O	3:E:92:ASN:HB2	1.68	0.94
1:A:209:ILE:HG22	1:A:227:LEU:HD12	1.48	0.94
1:C:240:ALA:HB2	1:C:243:ARG:HH11	0.79	0.93
1:C:301:GLN:HE22	1:C:307:PRO:HD3	1.34	0.93
2:B:403:ALA:O	2:B:405:LEU:N	2.01	0.93
2:D:247:GLN:C	2:D:248:LEU:HG	1.87	0.92
2:D:277:SER:O	2:D:278:ARG:HG3	1.68	0.92
2:D:273:ALA:CB	2:D:274:PRO:CD	2.47	0.92
2:B:244:PHE:HB3	2:B:245:PRO:HD3	1.52	0.91
2:B:332:MET:HG3	2:B:353:THR:HG21	1.50	0.91
2:D:147:SER:O	2:D:151:THR:OG1	1.90	0.90
1:C:128:GLN:O	1:C:129:CYS:HB2	1.67	0.90
2:D:32:PRO:O	2:D:86:ILE:HG13	1.72	0.89
1:A:273:ALA:CB	1:A:375:VAL:H	1.84	0.89
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.08	0.88
2:B:36:TYR:OH	2:B:40:SER:O	1.91	0.88
2:B:191:VAL:HG11	2:B:425:MET:CE	2.03	0.88
1:A:375:VAL:HG12	1:A:376:CYS:H	1.39	0.87
1:A:133:GLN:NE2	1:A:252:LEU:HG	1.88	0.87
2:D:405:LEU:O	2:D:407:TRP:N	2.07	0.87
2:B:68:VAL:HG13	2:B:118:VAL:HG21	1.56	0.87
2:B:247:GLN:OE1	2:B:247:GLN:HA	1.74	0.87
2:D:273:ALA:HB1	2:D:274:PRO:HD3	1.55	0.86
2:B:308:ARG:HH11	2:B:308:ARG:HA	1.39	0.86
2:B:32:PRO:O	2:B:86:ILE:HG13	1.75	0.86
2:D:388:PHE:HD2	2:D:425:MET:HE1	1.40	0.86
2:D:158:ARG:O	2:D:159:GLU:HB2	1.72	0.86
2:B:273:ALA:HB3	2:B:274:PRO:CD	2.05	0.85
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.58	0.85
1:C:240:ALA:CB	1:C:243:ARG:NH1	2.32	0.85
1:A:301:GLN:HE22	1:A:307:PRO:HD3	1.38	0.85
1:A:198:SER:OG	1:A:265:ILE:HD11	1.75	0.85
2:D:244:PHE:HB3	2:D:245:PRO:HD3	1.58	0.85
2:B:273:ALA:CB	2:B:274:PRO:CD	2.54	0.85
2:B:265:LEU:O	2:B:266:HIS:O	1.96	0.84
1:C:390:ARG:HH11	1:C:390:ARG:HG3	1.43	0.84
2:B:265:LEU:HD12	2:B:265:LEU:O	1.78	0.83
2:B:388:PHE:HD2	2:B:425:MET:HE1	1.43	0.83
2:D:351:VAL:O	2:D:351:VAL:HG13	1.76	0.83
2:B:247:GLN:C	2:B:248:LEU:HG	1.99	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:265:LEU:O	2:D:266:HIS:O	1.97	0.83
1:A:70:LEU:HD13	1:A:145:THR:HB	1.60	0.83
1:A:292:THR:O	1:A:295:CYS:HB2	1.78	0.82
2:B:244:PHE:CB	2:B:245:PRO:HD3	2.08	0.82
2:D:36:TYR:OH	2:D:40:SER:O	1.97	0.82
2:B:11:GLN:HG3	2:B:74:THR:CG2	2.09	0.82
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.60	0.82
1:C:70:LEU:HD13	1:C:145:THR:HB	1.63	0.81
2:D:205:ASP:OD2	2:D:207:GLU:HG3	1.81	0.81
2:D:247:GLN:O	2:D:248:LEU:HG	1.81	0.80
2:B:259:MET:HE1	2:B:378:ILE:HG22	1.64	0.80
2:B:336:GLN:OE1	2:B:351:VAL:HG11	1.80	0.80
2:B:273:ALA:HB1	2:B:274:PRO:HD3	1.62	0.80
2:B:133:GLN:HE21	2:B:252:LEU:HB2	1.45	0.80
1:A:191:THR:CG2	1:A:425:MET:HE3	2.12	0.79
1:A:191:THR:CG2	1:A:425:MET:CE	2.60	0.79
2:B:401:ARG:O	1:C:262:TYR:OH	2.00	0.79
2:B:291:LEU:HD21	2:B:375:ALA:HB3	1.65	0.79
2:D:320:ARG:HG2	2:D:360:PRO:HD3	1.64	0.79
2:B:244:PHE:HB3	2:B:245:PRO:CD	2.12	0.79
2:D:405:LEU:C	2:D:407:TRP:H	1.84	0.79
2:B:287:THR:CG2	2:B:289:PRO:HD2	2.14	0.78
1:A:240:ALA:HB2	1:A:243:ARG:NH1	1.98	0.78
2:B:351:VAL:O	2:B:351:VAL:HG13	1.82	0.78
2:B:291:LEU:HD21	2:B:375:ALA:CB	2.13	0.78
2:B:12:CYS:SG	2:B:171:VAL:HG21	2.23	0.78
1:A:98:ASP:HB3	1:A:105:ARG:HH21	1.47	0.78
1:A:88:HIS:HB2	1:A:91:GLN:HE21	1.48	0.78
1:C:16:ILE:HD13	1:C:171:ILE:HD11	1.66	0.78
2:D:244:PHE:CB	2:D:245:PRO:HD3	2.15	0.77
1:A:99:ALA:O	1:A:100:ALA:HB2	1.84	0.77
2:D:205:ASP:OD1	2:D:207:GLU:HB2	1.85	0.77
2:B:102:ASN:OD1	2:B:105:LYS:HB2	1.84	0.77
2:D:279:GLY:O	2:D:280:SER:HB2	1.83	0.77
1:C:209:ILE:CG2	1:C:227:LEU:HD12	2.14	0.77
1:C:273:ALA:HB3	1:C:375:VAL:H	1.49	0.77
1:C:273:ALA:CB	1:C:375:VAL:H	1.97	0.77
2:D:12:CYS:SG	2:D:171:VAL:HG21	2.24	0.77
1:C:95:GLY:O	1:C:97:GLU:N	2.19	0.76
2:B:133:GLN:NE2	2:B:252:LEU:HB2	2.00	0.76
1:A:419:SER:O	1:A:423:GLU:HB2	1.86	0.76
2:D:140:SER:HA	2:D:171:VAL:HG23	1.67	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:405:VAL:HG13	1:C:406:HIS:N	1.99	0.76
2:B:320:ARG:HG2	2:B:360:PRO:HD3	1.67	0.76
1:A:198:SER:OG	1:A:265:ILE:CD1	2.33	0.76
1:A:249:ASN:HB2	1:A:254:GLU:HB3	1.68	0.76
1:C:132:LEU:HG	1:C:133:GLN:N	2.01	0.75
2:B:234:THR:O	2:B:238:VAL:HG23	1.86	0.75
2:D:238:VAL:HG13	2:D:378:ILE:HD11	1.68	0.75
2:D:11:GLN:HG3	2:D:74:THR:CG2	2.15	0.75
2:B:259:MET:CE	2:B:378:ILE:HG22	2.16	0.75
2:D:382:THR:HA	2:D:432:TYR:HD2	1.51	0.75
1:A:191:THR:HA	1:A:194:THR:HG22	1.67	0.75
1:A:273:ALA:HB2	1:A:375:VAL:H	1.50	0.75
1:A:273:ALA:CB	1:A:274:PRO:CD	2.54	0.74
2:B:4:ILE:HG23	2:B:51:VAL:HG12	1.69	0.74
1:A:132:LEU:HG	1:A:133:GLN:N	2.02	0.74
2:B:405:LEU:C	2:B:407:TRP:H	1.91	0.74
1:A:239:THR:O	1:A:241:SER:N	2.19	0.74
1:A:70:LEU:HD13	1:A:145:THR:CB	2.17	0.74
1:C:273:ALA:HB3	1:C:274:PRO:CD	2.12	0.74
1:A:355:ILE:HD11	3:E:18:GLN:HB3	1.70	0.74
1:C:171:ILE:CG2	1:C:206:ASN:HD21	2.01	0.74
1:A:210:TYR:HE1	1:A:214:ARG:HE	1.34	0.74
2:B:312:TYR:HD2	2:B:381:SER:HB3	1.53	0.73
1:A:353:VAL:HG21	3:E:20:PHE:HE2	1.49	0.73
1:C:108:TYR:HD2	3:E:108:ASN:CG	1.91	0.73
1:C:205:ASP:C	1:C:205:ASP:OD1	2.24	0.73
1:A:79:ARG:HH22	1:A:94:THR:CG2	2.02	0.73
2:B:312:TYR:CD2	2:B:381:SER:HB3	2.24	0.73
1:A:265:ILE:HG23	1:A:267:PHE:CZ	2.24	0.72
1:A:240:ALA:CA	1:A:243:ARG:HG3	2.05	0.72
1:C:88:HIS:HB2	1:C:91:GLN:HE21	1.53	0.72
1:A:273:ALA:HB3	1:A:375:VAL:H	1.54	0.72
1:A:16:ILE:HD13	1:A:171:ILE:CD1	2.18	0.72
2:B:93:VAL:HG11	2:B:118:VAL:HG23	1.72	0.72
1:A:119:LEU:HD11	1:A:156:ARG:HB3	1.72	0.72
2:D:287:THR:HB	2:D:290:GLU:HG3	1.71	0.72
1:A:5:ILE:HD12	1:A:132:LEU:HD13	1.70	0.72
1:C:48:SER:O	1:C:243:ARG:O	2.07	0.71
2:B:140:SER:HA	2:B:171:VAL:HG23	1.72	0.71
2:D:68:VAL:HG13	2:D:118:VAL:HG21	1.72	0.71
1:C:265:ILE:HG23	1:C:267:PHE:CZ	2.24	0.71
2:B:67:LEU:HD12	2:B:92:PHE:CD2	2.24	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:68:VAL:CG1	2:B:118:VAL:HG21	2.19	0.71
2:D:291:LEU:CD2	2:D:375:ALA:HB3	2.21	0.71
2:D:6:HIS:HE1	2:D:8:GLN:HE21	1.39	0.71
1:C:98:ASP:HB3	1:C:105:ARG:HH21	1.55	0.71
1:A:223:THR:O	1:A:226:ASN:HB2	1.91	0.71
2:B:287:THR:O	2:B:288:VAL:HB	1.89	0.71
2:D:312:TYR:CD2	2:D:381:SER:HB3	2.26	0.71
2:B:405:LEU:O	2:B:407:TRP:N	2.23	0.70
2:D:247:GLN:OE1	2:D:247:GLN:HA	1.91	0.70
2:D:336:GLN:OE1	2:D:351:VAL:HG11	1.91	0.70
2:B:70:LEU:HA	2:B:95:GLY:HA3	1.72	0.70
1:C:208:ALA:O	1:C:212:ILE:HD12	1.91	0.70
1:A:95:GLY:O	1:A:97:GLU:N	2.24	0.70
1:C:191:THR:CG2	1:C:425:MET:CE	2.69	0.70
1:C:405:VAL:CG1	1:C:406:HIS:N	2.53	0.70
1:C:20:CYS:HB3	1:C:232:GLY:HA2	1.73	0.70
1:C:339:ARG:CB	1:C:341:ILE:HG22	2.22	0.70
2:B:59:ASN:O	2:B:60:LYS:O	2.10	0.70
1:A:209:ILE:CG2	1:A:227:LEU:HD12	2.22	0.70
1:A:405:VAL:HG13	1:A:406:HIS:N	2.05	0.70
1:A:185:TYR:OH	1:A:403:ALA:HB3	1.91	0.70
2:B:404:PHE:CD2	1:C:261:PRO:HA	2.25	0.70
2:D:312:TYR:HD2	2:D:381:SER:HB3	1.56	0.70
2:B:7:ILE:O	2:B:137:LEU:HA	1.92	0.70
2:D:244:PHE:HB3	2:D:245:PRO:CD	2.20	0.69
1:C:107:HIS:HD2	1:C:108:TYR:CE1	2.10	0.69
2:D:107:HIS:CE1	2:D:193:GLN:NE2	2.61	0.69
2:B:308:ARG:HH11	2:B:308:ARG:CA	2.06	0.69
1:C:179:THR:HG22	1:C:180:ALA:N	2.06	0.69
1:A:67:PHE:HB2	1:A:92:LEU:CD2	2.23	0.69
2:B:347:ILE:O	2:B:347:ILE:HG22	1.92	0.69
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.73	0.69
2:D:321:GLY:HA2	2:D:359:PRO:HD3	1.73	0.69
2:B:221:THR:HG21	1:C:325:PRO:HG2	1.75	0.69
1:C:99:ALA:O	1:C:100:ALA:HB2	1.93	0.69
1:C:115:ILE:HG13	1:C:152:LEU:HG	1.75	0.69
1:A:99:ALA:O	1:A:100:ALA:CB	2.41	0.68
1:A:353:VAL:CG2	3:E:20:PHE:CE2	2.76	0.68
1:A:201:ALA:HB3	1:A:267:PHE:HD2	1.59	0.68
2:B:88:ARG:O	2:B:91:ASN:HB2	1.94	0.68
2:D:143:GLY:O	2:D:147:SER:HB3	1.93	0.68
1:A:405:VAL:CG1	1:A:406:HIS:N	2.56	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:234:THR:O	2:D:238:VAL:HG23	1.93	0.68
2:B:287:THR:HG23	2:B:289:PRO:HD2	1.75	0.68
1:C:70:LEU:N	1:C:70:LEU:HD12	2.09	0.68
2:D:351:VAL:CG1	2:D:351:VAL:O	2.42	0.68
1:C:70:LEU:HD13	1:C:145:THR:CB	2.24	0.68
1:C:288:VAL:HA	1:C:291:ILE:HD11	1.76	0.68
2:D:13:GLY:O	2:D:16:ILE:HG22	1.94	0.68
2:B:404:PHE:HD2	1:C:261:PRO:HA	1.58	0.68
3:E:60:ARG:O	3:E:63:TYR:HB3	1.94	0.68
1:C:240:ALA:CA	1:C:243:ARG:HG2	2.10	0.68
2:B:209:LEU:HD21	2:B:231:VAL:HG22	1.76	0.68
2:D:209:LEU:HD21	2:D:231:VAL:HG22	1.75	0.67
1:A:205:ASP:C	1:A:205:ASP:OD1	2.33	0.67
2:D:67:LEU:HD12	2:D:92:PHE:CD2	2.29	0.67
2:D:102:ASN:HB2	2:D:408:TYR:CE2	2.30	0.67
1:A:105:ARG:HD2	1:A:411:GLU:OE1	1.94	0.67
1:C:79:ARG:HH22	1:C:94:THR:CG2	2.07	0.67
2:B:225:GLY:O	2:B:227:LEU:N	2.27	0.67
2:B:158:ARG:HD2	2:B:197:ASN:HB3	1.75	0.67
1:C:180:ALA:CB	2:D:258:ASN:HD21	2.07	0.67
1:A:375:VAL:HG12	1:A:376:CYS:N	2.09	0.67
2:B:33:THR:O	2:B:34:GLY:O	2.13	0.67
2:B:11:GLN:CG	2:B:74:THR:HG21	2.19	0.67
1:C:128:GLN:O	1:C:129:CYS:CB	2.41	0.67
2:D:347:ILE:O	2:D:347:ILE:HG22	1.95	0.67
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.76	0.67
2:D:16:ILE:HD11	2:D:231:VAL:HG11	1.78	0.66
2:D:287:THR:CG2	2:D:289:PRO:HD2	2.25	0.66
1:A:288:VAL:HA	1:A:291:ILE:HD11	1.77	0.66
1:A:107:HIS:HD2	1:A:108:TYR:CE1	2.12	0.66
2:B:107:HIS:CE1	2:B:193:GLN:NE2	2.64	0.66
1:A:102:ASN:OD1	1:A:105:ARG:HB2	1.96	0.66
1:C:100:ALA:O	1:C:101:ASN:HB2	1.94	0.66
2:B:70:LEU:HD13	2:B:145:THR:HB	1.78	0.66
2:B:239:THR:O	2:B:240:THR:C	2.34	0.66
1:C:67:PHE:HB2	1:C:92:LEU:HD22	1.78	0.66
1:A:128:GLN:O	1:A:129:CYS:CB	2.36	0.66
1:C:375:VAL:HG12	1:C:376:CYS:H	1.59	0.66
1:C:191:THR:HA	1:C:194:THR:HG22	1.78	0.66
1:A:147:SER:O	1:A:190:THR:OG1	2.12	0.66
1:C:105:ARG:NH2	2:D:2:ARG:HH21	1.93	0.66
2:D:225:GLY:O	2:D:227:LEU:N	2.29	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:247:GLN:O	2:B:248:LEU:HG	1.96	0.66
2:B:158:ARG:O	2:B:159:GLU:CB	2.39	0.65
1:A:67:PHE:HB2	1:A:92:LEU:HD22	1.77	0.65
2:B:67:LEU:HD12	2:B:92:PHE:CE2	2.32	0.65
1:A:271:THR:HG23	1:A:301:GLN:HA	1.78	0.65
2:B:349:ASN:O	2:B:351:VAL:N	2.28	0.65
2:D:298:ALA:HB1	2:D:306:ASP:HB3	1.79	0.65
1:A:115:ILE:HG13	1:A:152:LEU:HG	1.79	0.65
2:D:269:MET:HE1	2:D:301:MET:HG3	1.78	0.65
2:B:238:VAL:CG1	2:B:378:ILE:HD11	2.27	0.65
2:D:180:THR:HB	2:D:183:GLU:OE2	1.96	0.65
2:D:33:THR:O	2:D:34:GLY:O	2.15	0.64
2:D:4:ILE:HG23	2:D:51:VAL:HG12	1.77	0.64
2:B:87:PHE:H	2:B:87:PHE:HD2	1.46	0.64
1:C:336:LYS:HE3	1:C:341:ILE:HD12	1.79	0.64
2:D:204:ILE:HG21	2:D:231:VAL:HG13	1.77	0.64
2:D:238:VAL:CG1	2:D:378:ILE:HD11	2.27	0.64
1:A:368:LEU:H	1:A:368:LEU:HD12	1.63	0.64
2:B:387:LEU:O	2:B:390:ARG:HG2	1.98	0.64
2:D:6:HIS:CE1	2:D:21:TRP:HE1	2.16	0.64
2:B:287:THR:HG22	2:B:289:PRO:HD2	1.79	0.64
2:B:221:THR:CG2	1:C:325:PRO:HG2	2.27	0.64
2:D:59:ASN:O	2:D:60:LYS:O	2.16	0.64
1:A:236:SER:HA	1:A:243:ARG:HH22	1.62	0.64
1:C:252:LEU:O	1:C:254:GLU:N	2.31	0.64
2:D:141:LEU:HD13	2:D:170:SER:HB3	1.78	0.64
2:B:406:HIS:CE1	2:B:407:TRP:CD1	2.86	0.64
1:C:5:ILE:HD12	1:C:132:LEU:HD13	1.80	0.64
2:B:336:GLN:CD	2:B:351:VAL:HG11	2.18	0.64
2:B:16:ILE:HD11	2:B:231:VAL:HG11	1.79	0.63
2:B:115:VAL:HG12	2:B:116:ASP:N	2.13	0.63
2:B:180:THR:HB	2:B:183:GLU:OE2	1.97	0.63
1:A:412:GLY:O	3:E:60:ARG:NH1	2.31	0.63
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.32	0.63
1:C:238:ILE:HD13	1:C:378:LEU:HD11	1.81	0.63
1:A:250:VAL:O	1:A:251:ASP:HB3	1.98	0.63
2:B:141:LEU:HD13	2:B:170:SER:HB3	1.79	0.63
2:D:336:GLN:CD	2:D:351:VAL:HG11	2.19	0.63
1:C:265:ILE:HG12	1:C:265:ILE:O	1.99	0.63
1:A:339:ARG:CB	1:A:341:ILE:HG22	2.28	0.63
1:A:24:TYR:CD2	1:A:243:ARG:NH2	2.66	0.63
2:B:287:THR:HB	2:B:290:GLU:HG3	1.79	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:403:ALA:C	2:B:405:LEU:H	2.01	0.63
2:D:165:ILE:HG13	2:D:252:LEU:HD23	1.80	0.63
2:B:237:GLY:HA3	2:B:376:THR:HG21	1.80	0.63
2:B:116:ASP:O	2:B:120:ASP:HB3	1.98	0.63
2:D:265:LEU:HD12	2:D:265:LEU:O	1.99	0.63
1:A:70:LEU:HD12	1:A:70:LEU:N	2.14	0.63
1:C:145:THR:N	5:C:601:GTP:O2B	2.32	0.63
2:D:382:THR:HA	2:D:432:TYR:CD2	2.34	0.63
1:A:7:ILE:HA	1:A:66:VAL:HG23	1.79	0.63
2:B:102:ASN:HB2	2:B:408:TYR:CE2	2.34	0.62
1:C:343:PHE:CD1	1:C:349:THR:HG22	2.34	0.62
2:D:291:LEU:CD2	2:D:375:ALA:CB	2.75	0.62
1:C:210:TYR:HE1	1:C:214:ARG:HE	1.44	0.62
1:C:191:THR:CG2	1:C:425:MET:HE1	2.17	0.62
1:C:171:ILE:HG23	1:C:206:ASN:HD21	1.63	0.62
2:D:118:VAL:O	2:D:122:VAL:HG13	1.99	0.62
1:C:356:ASN:O	1:C:358:GLU:N	2.28	0.62
2:D:387:LEU:O	2:D:390:ARG:HG2	1.99	0.62
1:C:271:THR:HG23	1:C:301:GLN:HA	1.82	0.62
1:A:201:ALA:HB3	1:A:267:PHE:CD2	2.33	0.62
1:A:396:ASP:OD1	1:A:422:ARG:NE	2.30	0.62
1:A:292:THR:O	1:A:295:CYS:CB	2.46	0.62
1:A:265:ILE:CG2	1:A:267:PHE:CZ	2.82	0.62
2:D:349:ASN:O	2:D:351:VAL:N	2.33	0.62
2:D:388:PHE:HD2	2:D:425:MET:CE	2.13	0.62
2:B:255:LEU:HD22	2:B:259:MET:HG3	1.81	0.62
2:D:291:LEU:HD21	2:D:375:ALA:HB2	1.81	0.62
2:D:115:VAL:HG12	2:D:116:ASP:N	2.14	0.62
2:B:267:PHE:CD1	2:B:267:PHE:N	2.67	0.62
2:B:388:PHE:HD2	2:B:425:MET:CE	2.12	0.62
1:A:346:TRP:CE3	1:A:347:CYS:HB2	2.35	0.61
1:C:368:LEU:H	1:C:368:LEU:HD12	1.64	0.61
3:E:77:GLU:OE2	3:E:80:ARG:CB	2.47	0.61
1:A:273:ALA:HB2	1:A:375:VAL:N	2.15	0.61
1:A:265:ILE:HG12	1:A:265:ILE:O	2.01	0.61
1:C:180:ALA:HB2	2:D:258:ASN:HD21	1.65	0.61
2:B:238:VAL:HG13	2:B:378:ILE:HD11	1.83	0.61
1:C:99:ALA:O	1:C:100:ALA:CB	2.48	0.61
1:A:119:LEU:HD22	1:A:156:ARG:HE	1.65	0.61
1:C:185:TYR:OH	1:C:403:ALA:HB3	2.00	0.61
1:C:390:ARG:NH1	1:C:390:ARG:HG3	2.09	0.61
1:A:145:THR:N	5:A:600:GTP:O2B	2.34	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:419:SER:O	1:C:423:GLU:HB2	1.99	0.61
2:D:93:VAL:HG11	2:D:118:VAL:HG23	1.82	0.61
1:A:385:ALA:O	1:A:388:TRP:N	2.34	0.61
2:D:67:LEU:HD12	2:D:92:PHE:CE2	2.35	0.60
2:B:351:VAL:O	2:B:351:VAL:CG1	2.48	0.60
2:D:70:LEU:HD13	2:D:145:THR:HB	1.82	0.60
1:C:265:ILE:CG2	1:C:267:PHE:CZ	2.83	0.60
2:D:287:THR:O	2:D:288:VAL:HB	2.00	0.60
1:C:377:MET:HG3	1:C:377:MET:O	2.00	0.60
3:E:90:ASN:O	3:E:92:ASN:N	2.35	0.60
2:D:191:VAL:CG1	2:D:425:MET:CE	2.76	0.60
1:C:266:HIS:O	1:C:268:PRO:HD3	2.01	0.60
2:B:102:ASN:O	2:B:105:LYS:N	2.34	0.60
2:D:259:MET:CE	2:D:378:ILE:HG22	2.31	0.60
1:A:348:PRO:HG3	3:E:27:PRO:CD	2.24	0.60
1:C:252:LEU:C	1:C:254:GLU:N	2.54	0.60
2:B:259:MET:CE	2:B:378:ILE:CG2	2.79	0.60
7:D:701:POD:O6	7:D:701:POD:C21	2.50	0.60
1:C:240:ALA:CA	1:C:243:ARG:HD3	2.31	0.60
1:A:250:VAL:O	1:A:251:ASP:CB	2.49	0.60
1:A:48:SER:O	1:A:243:ARG:O	2.20	0.60
2:B:114:LEU:O	2:B:115:VAL:C	2.40	0.60
1:A:407:TRP:CE3	2:B:257:VAL:HB	2.37	0.59
1:A:273:ALA:CB	1:A:375:VAL:N	2.63	0.59
2:B:265:LEU:O	2:B:266:HIS:C	2.40	0.59
2:B:255:LEU:CD2	2:B:259:MET:HG3	2.31	0.59
1:C:147:SER:O	1:C:190:THR:OG1	2.15	0.59
2:B:251:ASP:C	2:B:253:ARG:N	2.56	0.59
2:B:266:HIS:HB3	2:B:380:ASN:HD21	1.67	0.59
2:B:181:VAL:O	2:B:181:VAL:HG12	2.01	0.59
1:A:171:ILE:CG2	1:A:206:ASN:HD21	2.15	0.59
1:A:76:ASP:O	1:A:79:ARG:N	2.35	0.59
2:D:239:THR:O	2:D:240:THR:C	2.41	0.59
1:A:180:ALA:CB	2:B:258:ASN:HD21	2.16	0.59
2:D:165:ILE:CG1	2:D:252:LEU:HD23	2.32	0.59
2:D:185:TYR:HD1	2:D:408:TYR:HE1	1.50	0.59
2:D:241:CYS:HB2	7:D:701:POD:H203	1.85	0.59
2:B:54:ASN:HB2	2:B:64:ARG:HD3	1.84	0.59
2:B:165:ILE:HG13	2:B:252:LEU:HD23	1.85	0.59
2:D:255:LEU:HD22	2:D:259:MET:CG	2.33	0.59
1:C:207:GLU:O	1:C:211:ASP:HB2	2.03	0.59
2:D:88:ARG:O	2:D:91:ASN:HB2	2.02	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:133:GLN:HE21	1:A:252:LEU:CG	1.95	0.59
1:C:316:CYS:O	1:C:377:MET:HA	2.03	0.59
2:B:264:ARG:O	2:B:266:HIS:CD2	2.56	0.59
2:D:207:GLU:HB2	2:D:304:ALA:HB2	1.83	0.59
2:D:116:ASP:O	2:D:120:ASP:HB3	2.03	0.59
1:C:139:HIS:CD2	1:C:150:THR:HG21	2.37	0.59
1:C:273:ALA:CB	1:C:274:PRO:CD	2.70	0.58
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.36	0.58
2:D:36:TYR:HD1	2:D:37:HIS:N	2.01	0.58
2:D:259:MET:HE1	2:D:378:ILE:HG22	1.83	0.58
1:C:7:ILE:HG12	1:C:66:VAL:CG2	2.33	0.58
1:C:385:ALA:O	1:C:388:TRP:N	2.35	0.58
2:D:261:PRO:HB2	2:D:262:PHE:CD1	2.37	0.58
2:D:177:VAL:CG1	2:D:177:VAL:O	2.50	0.58
2:D:404:PHE:O	2:D:407:TRP:HB2	2.04	0.58
1:A:356:ASN:O	1:A:358:GLU:N	2.31	0.58
2:D:101:ASN:HA	2:D:144:GLY:H	1.68	0.58
1:A:252:LEU:O	1:A:255:PHE:HB2	2.02	0.58
1:C:79:ARG:HH22	1:C:94:THR:HG21	1.68	0.58
1:A:247:ALA:HB2	3:E:12:ASN:CB	2.34	0.58
2:D:7:ILE:O	2:D:137:LEU:HA	2.03	0.58
2:D:195:VAL:HG21	2:D:428:LEU:HD13	1.86	0.58
2:D:102:ASN:OD1	2:D:105:LYS:HB2	2.04	0.58
2:B:174:SER:OG	2:B:176:LYS:O	2.18	0.58
1:A:298:PRO:O	1:A:301:GLN:HG3	2.03	0.58
2:B:255:LEU:HD22	2:B:259:MET:CG	2.34	0.58
1:A:395:PHE:HD2	1:A:396:ASP:N	2.02	0.58
7:D:701:POD:O6	7:D:701:POD:H213	2.03	0.58
2:B:44:LEU:O	2:B:47:GLU:C	2.42	0.58
2:D:405:LEU:C	2:D:407:TRP:N	2.50	0.58
2:D:158:ARG:HD2	2:D:197:ASN:HB3	1.84	0.58
1:C:407:TRP:CE3	2:D:257:VAL:HB	2.39	0.58
1:A:392:ASP:OD1	1:A:429:GLU:OE1	2.22	0.58
1:C:223:THR:O	1:C:226:ASN:HB2	2.04	0.58
1:C:392:ASP:OD1	1:C:429:GLU:OE1	2.22	0.58
2:B:382:THR:HA	2:B:432:TYR:HD2	1.69	0.57
2:B:296:PHE:CE2	2:B:377:PHE:HE1	2.21	0.57
2:D:133:GLN:HE21	2:D:252:LEU:HB2	1.68	0.57
2:B:337:ASN:HA	2:B:340:SER:HB3	1.86	0.57
1:C:119:LEU:CD1	1:C:156:ARG:HB3	2.35	0.57
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.39	0.57
2:D:44:LEU:O	2:D:47:GLU:C	2.41	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:346:TRP:O	1:A:346:TRP:HE3	1.88	0.57
2:B:204:ILE:HG21	2:B:231:VAL:HG13	1.87	0.57
2:B:118:VAL:O	2:B:122:VAL:HG13	2.05	0.57
1:C:260:VAL:O	1:C:260:VAL:HG23	2.04	0.57
2:B:269:MET:HG2	2:B:384:ILE:HG12	1.85	0.57
2:D:133:GLN:NE2	2:D:252:LEU:HB2	2.19	0.57
2:D:287:THR:HG23	2:D:289:PRO:HD2	1.87	0.57
1:A:435:VAL:HG22	3:E:35:PHE:CE1	2.39	0.57
1:C:7:ILE:HA	1:C:66:VAL:HG23	1.87	0.57
2:D:68:VAL:CG1	2:D:118:VAL:HG21	2.33	0.57
2:B:6:HIS:CE1	2:B:21:TRP:HE1	2.22	0.57
1:C:16:ILE:HD13	1:C:171:ILE:CD1	2.34	0.57
1:C:266:HIS:HB3	1:C:380:ASN:OD1	2.04	0.57
2:B:337:ASN:C	2:B:339:ASN:H	2.06	0.57
1:C:213:CYS:HB3	1:C:219:ILE:HD11	1.86	0.57
2:D:237:GLY:HA3	2:D:376:THR:HG21	1.85	0.57
1:A:206:ASN:HD22	1:A:206:ASN:N	2.03	0.57
1:C:252:LEU:C	1:C:254:GLU:H	2.08	0.57
2:B:312:TYR:HD1	2:B:343:PHE:CE2	2.23	0.57
1:C:168:GLU:HG2	1:C:201:ALA:HB2	1.86	0.57
2:B:154:ILE:C	2:B:156:LYS:H	2.08	0.56
1:A:238:ILE:HD13	1:A:378:LEU:HD11	1.85	0.56
2:D:54:ASN:HB2	2:D:64:ARG:HD3	1.87	0.56
1:A:407:TRP:CG	2:B:257:VAL:HG23	2.39	0.56
1:C:100:ALA:HB2	1:C:105:ARG:HG2	1.88	0.56
2:B:244:PHE:CB	2:B:245:PRO:CD	2.78	0.56
2:D:118:VAL:HG11	2:D:153:LEU:HD11	1.87	0.56
2:D:185:TYR:HD1	2:D:408:TYR:CE1	2.24	0.56
1:C:264:ARG:O	1:C:266:HIS:CD2	2.58	0.56
3:E:119:MET:HA	3:E:122:ARG:NH2	2.20	0.56
2:B:151:THR:HG22	2:B:193:GLN:HB3	1.86	0.56
2:B:87:PHE:CD2	2:B:87:PHE:N	2.73	0.56
2:B:200:GLU:OE2	2:B:255:LEU:HD13	2.05	0.56
1:C:292:THR:O	1:C:295:CYS:HB2	2.06	0.56
2:B:388:PHE:CD2	2:B:425:MET:HE1	2.33	0.56
2:D:388:PHE:CD2	2:D:425:MET:HE1	2.30	0.56
2:D:283:TYR:HD2	2:D:285:ALA:HB3	1.71	0.56
1:C:67:PHE:HB2	1:C:92:LEU:CD2	2.36	0.56
1:A:263:PRO:HG3	3:E:37:ALA:HA	1.88	0.56
7:B:700:POD:H213	7:B:700:POD:O6	2.06	0.56
2:B:132:LEU:HD23	2:B:164:ARG:HG3	1.86	0.56
1:A:246:GLY:O	1:A:247:ALA:O	2.23	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:119:LEU:HD11	2:D:156:LYS:HB3	1.86	0.56
1:C:368:LEU:H	1:C:368:LEU:CD1	2.19	0.56
1:C:240:ALA:HA	1:C:243:ARG:CD	2.36	0.55
2:D:388:PHE:CD2	2:D:425:MET:CE	2.89	0.55
2:D:256:ALA:C	2:D:258:ASN:H	2.09	0.55
2:B:111:GLY:HA2	2:B:149:MET:HE1	1.88	0.55
1:A:24:TYR:HE2	1:A:243:ARG:NH2	1.97	0.55
2:D:287:THR:HG22	2:D:289:PRO:HD2	1.87	0.55
1:C:213:CYS:HB3	1:C:219:ILE:CD1	2.36	0.55
2:B:101:ASN:HA	2:B:144:GLY:H	1.71	0.55
1:C:206:ASN:N	1:C:206:ASN:HD22	2.05	0.55
2:B:269:MET:HE1	2:B:307:PRO:HG3	1.88	0.55
1:C:198:SER:HB2	1:C:265:ILE:CD1	2.37	0.55
1:A:143:GLY:O	1:A:147:SER:HB3	2.05	0.55
1:A:7:ILE:HG12	1:A:66:VAL:CG2	2.37	0.55
1:A:213:CYS:HB3	1:A:219:ILE:HD11	1.88	0.55
2:B:263:PRO:C	2:B:265:LEU:H	2.08	0.55
2:D:265:LEU:O	2:D:266:HIS:C	2.45	0.55
2:D:145:THR:HG23	6:D:603:GDP:O3B	2.06	0.55
2:D:195:VAL:HA	2:D:265:LEU:HD23	1.88	0.55
2:B:136:GLN:HG3	2:B:136:GLN:O	2.06	0.55
2:B:6:HIS:HE1	2:B:8:GLN:HE21	1.55	0.55
3:E:114:ALA:C	3:E:116:LEU:H	2.10	0.55
1:C:100:ALA:CB	1:C:105:ARG:HG2	2.37	0.55
2:D:107:HIS:CE1	2:D:193:GLN:HE22	2.25	0.55
2:B:255:LEU:CD2	2:B:259:MET:CG	2.85	0.55
2:D:70:LEU:HA	2:D:95:GLY:HA3	1.89	0.55
2:B:205:ASP:OD2	2:B:207:GLU:HG3	2.07	0.55
2:B:13:GLY:O	2:B:16:ILE:HG22	2.07	0.55
2:B:119:LEU:O	2:B:122:VAL:HG22	2.07	0.55
1:A:430:LYS:O	1:A:434:GLU:HB2	2.07	0.55
2:B:321:GLY:HA2	2:B:359:PRO:HD3	1.89	0.55
2:D:11:GLN:CG	2:D:74:THR:HG21	2.26	0.54
1:C:260:VAL:CG2	1:C:260:VAL:O	2.55	0.54
2:D:165:ILE:HD11	2:D:252:LEU:HD23	1.89	0.54
1:C:95:GLY:C	1:C:97:GLU:H	2.11	0.54
2:B:165:ILE:CG1	2:B:252:LEU:HD23	2.37	0.54
1:A:353:VAL:CG2	3:E:20:PHE:CD2	2.91	0.54
1:C:168:GLU:HG2	1:C:201:ALA:CB	2.38	0.54
1:A:219:ILE:C	1:A:221:ARG:H	2.11	0.54
1:A:213:CYS:HB3	1:A:219:ILE:CD1	2.37	0.54
2:B:138:THR:HG22	2:B:169:PHE:HB2	1.89	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:3:GLU:HB2	1:A:129:CYS:SG	2.47	0.54
1:C:402:ARG:O	1:C:403:ALA:C	2.45	0.54
2:B:166:MET:HE2	2:B:166:MET:HA	1.89	0.54
1:A:60:LYS:NZ	1:A:85:GLN:O	2.27	0.54
2:B:38:GLY:O	2:B:40:SER:N	2.37	0.54
2:D:336:GLN:NE2	2:D:351:VAL:HG11	2.22	0.54
2:B:135:PHE:HB2	2:B:166:MET:CE	2.38	0.54
2:D:111:GLY:HA2	2:D:149:MET:CE	2.38	0.54
1:A:72:PRO:HD3	1:A:96:LYS:HA	1.89	0.54
1:A:174:ALA:HB1	1:A:207:GLU:HB2	1.90	0.54
2:D:343:PHE:O	2:D:344:VAL:C	2.46	0.54
2:D:267:PHE:N	2:D:267:PHE:CD1	2.76	0.54
2:B:241:CYS:HB2	7:B:700:POD:H203	1.89	0.54
1:A:51:THR:CB	1:A:243:ARG:HA	2.37	0.54
2:D:177:VAL:O	2:D:177:VAL:HG12	2.08	0.54
1:A:154:MET:HE1	1:A:166:LYS:HD2	1.90	0.54
3:E:27:PRO:HG2	3:E:29:PHE:CB	2.38	0.54
1:A:179:THR:HG22	1:A:180:ALA:N	2.23	0.54
1:A:265:ILE:O	1:A:266:HIS:O	2.26	0.54
1:C:198:SER:HB2	1:C:265:ILE:HD12	1.89	0.54
1:A:395:PHE:C	1:A:395:PHE:CD2	2.80	0.54
2:D:151:THR:HG22	2:D:193:GLN:HB3	1.90	0.54
3:E:114:ALA:O	3:E:116:LEU:N	2.41	0.54
1:A:325:PRO:HB3	3:E:20:PHE:CE1	2.42	0.53
1:C:256:GLN:C	1:C:258:ASN:N	2.61	0.53
1:A:119:LEU:CD1	1:A:156:ARG:HB3	2.38	0.53
1:C:66:VAL:HG11	1:C:122:ILE:HG22	1.90	0.53
2:B:336:GLN:OE1	2:B:351:VAL:CG1	2.52	0.53
2:D:180:THR:HG21	2:D:182:VAL:HG22	1.90	0.53
2:B:298:ALA:HB1	2:B:306:ASP:HB3	1.89	0.53
2:D:254:LYS:O	2:D:258:ASN:HB2	2.08	0.53
2:D:371:LEU:HD13	2:D:371:LEU:H	1.73	0.53
2:B:207:GLU:HB2	2:B:304:ALA:HB2	1.89	0.53
3:E:139:LEU:HG	3:E:140:LYS:N	2.24	0.53
1:C:139:HIS:CG	1:C:150:THR:HG21	2.43	0.53
1:A:135:PHE:CD1	1:A:135:PHE:N	2.76	0.53
1:A:234:ILE:HG22	1:A:235:VAL:N	2.24	0.53
1:C:240:ALA:HA	1:C:243:ARG:HD3	1.91	0.53
1:A:180:ALA:HB2	2:B:258:ASN:HD21	1.74	0.53
2:B:405:LEU:C	2:B:407:TRP:N	2.57	0.53
1:C:253:THR:O	1:C:257:THR:HB	2.09	0.53
2:D:255:LEU:HD22	2:D:255:LEU:O	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:312:TYR:HB2	2:D:343:PHE:CD2	2.44	0.53
2:D:227:LEU:O	2:D:230:LEU:HB2	2.09	0.53
1:C:102:ASN:OD1	1:C:105:ARG:HB2	2.09	0.53
2:D:403:ALA:O	2:D:405:LEU:N	2.41	0.53
1:A:35:GLN:O	1:A:37:PRO:HD3	2.09	0.53
1:C:224:TYR:O	1:C:228:ASN:ND2	2.36	0.53
1:A:20:CYS:HB3	1:A:232:GLY:HA2	1.91	0.53
2:B:251:ASP:OD1	2:B:254:LYS:HG3	2.09	0.53
1:C:90:GLU:O	1:C:121:ARG:HD2	2.08	0.53
1:C:219:ILE:C	1:C:221:ARG:H	2.12	0.53
3:E:94:ILE:O	3:E:98:LYS:CB	2.56	0.53
2:B:66:ILE:HD11	2:B:121:VAL:HG12	1.91	0.53
1:A:88:HIS:CD2	1:A:89:PRO:HD2	2.43	0.53
2:B:371:LEU:H	2:B:371:LEU:HD13	1.73	0.53
2:D:165:ILE:CD1	2:D:252:LEU:HD23	2.39	0.53
2:B:38:GLY:C	2:B:40:SER:H	2.11	0.53
1:A:79:ARG:HH22	1:A:94:THR:HG21	1.73	0.53
2:D:312:TYR:HD1	2:D:343:PHE:CE2	2.27	0.53
2:D:66:ILE:HD11	2:D:121:VAL:HG12	1.89	0.53
1:C:239:THR:O	1:C:241:SER:N	2.37	0.53
1:C:256:GLN:O	1:C:258:ASN:N	2.41	0.52
2:D:209:LEU:HD21	2:D:231:VAL:CG2	2.39	0.52
2:D:87:PHE:CD2	2:D:87:PHE:N	2.77	0.52
1:C:333:ALA:O	1:C:336:LYS:HB2	2.10	0.52
1:C:35:GLN:O	1:C:37:PRO:HD3	2.09	0.52
1:A:98:ASP:HB2	1:A:110:ILE:HD13	1.91	0.52
2:D:180:THR:CG2	2:D:182:VAL:HG22	2.40	0.52
2:D:174:SER:OG	2:D:176:LYS:O	2.20	0.52
1:A:347:CYS:O	1:A:348:PRO:C	2.44	0.52
2:D:274:PRO:HB3	2:D:286:LEU:HD21	1.90	0.52
1:C:105:ARG:NH2	2:D:2:ARG:NH2	2.57	0.52
1:A:415:GLU:O	1:A:418:PHE:HB2	2.09	0.52
2:D:62:VAL:O	2:D:62:VAL:HG22	2.09	0.52
2:B:66:ILE:HD13	2:B:122:VAL:HG12	1.91	0.52
2:D:255:LEU:HD22	2:D:259:MET:HG3	1.91	0.52
2:B:325:MET:HG2	2:B:355:VAL:HG11	1.92	0.52
2:D:259:MET:HE2	2:D:378:ILE:CG2	2.39	0.52
2:B:12:CYS:HG	2:B:171:VAL:HG21	1.74	0.52
1:C:133:GLN:HE21	1:C:252:LEU:HG	1.75	0.52
2:D:87:PHE:HD2	2:D:87:PHE:H	1.55	0.52
2:D:255:LEU:CD2	2:D:259:MET:CG	2.88	0.52
1:A:211:ASP:O	1:A:214:ARG:HB2	2.10	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:346:TRP:HZ2	1:C:435:VAL:HG13	1.75	0.52
2:D:284:ARG:O	2:D:286:LEU:HD12	2.09	0.52
1:C:9:VAL:HG11	1:C:150:THR:OG1	2.10	0.52
2:B:177:VAL:CG1	2:B:177:VAL:O	2.57	0.52
1:C:407:TRP:CG	2:D:257:VAL:HG23	2.44	0.52
2:D:296:PHE:CE2	2:D:377:PHE:HE1	2.27	0.52
3:E:119:MET:HA	3:E:122:ARG:HH21	1.75	0.52
2:B:135:PHE:CD1	2:B:135:PHE:N	2.77	0.52
1:A:278:ALA:O	1:A:279:GLU:CB	2.58	0.52
2:B:154:ILE:O	2:B:156:LYS:N	2.43	0.52
1:C:102:ASN:HB2	1:C:408:TYR:CE2	2.45	0.52
2:B:180:THR:HG23	1:C:258:ASN:ND2	2.25	0.52
2:B:198:THR:OG1	2:B:265:LEU:HD22	2.10	0.52
1:A:395:PHE:CD2	1:A:396:ASP:N	2.78	0.52
2:B:111:GLY:HA2	2:B:149:MET:CE	2.39	0.52
2:D:142:GLY:HA3	2:D:173:PRO:HG3	1.92	0.52
1:A:432:TYR:O	1:A:433:GLU:C	2.47	0.51
1:A:53:PHE:CD1	1:A:53:PHE:N	2.78	0.51
2:D:244:PHE:CB	2:D:245:PRO:CD	2.85	0.51
2:B:195:VAL:CG1	2:B:196:GLU:HG2	2.40	0.51
1:A:161:TYR:HB3	1:A:164:LYS:HG3	1.91	0.51
2:B:406:HIS:HE1	2:B:407:TRP:CD1	2.28	0.51
2:B:195:VAL:HG21	2:B:428:LEU:HD13	1.93	0.51
1:A:137:VAL:O	1:A:137:VAL:HG12	2.11	0.51
2:D:38:GLY:C	2:D:40:SER:H	2.13	0.51
2:D:255:LEU:CD2	2:D:259:MET:HG3	2.40	0.51
2:B:205:ASP:OD1	2:B:207:GLU:HB2	2.11	0.51
2:B:284:ARG:O	2:B:286:LEU:N	2.44	0.51
1:C:191:THR:CG2	1:C:425:MET:HE3	2.40	0.51
2:D:251:ASP:C	2:D:253:ARG:N	2.62	0.51
1:C:180:ALA:N	1:C:183:GLU:OE1	2.44	0.51
2:B:388:PHE:CD2	2:B:425:MET:CE	2.91	0.51
1:A:11:GLN:HB3	5:A:600:GTP:O2A	2.11	0.51
2:D:205:ASP:OD1	2:D:207:GLU:CB	2.56	0.51
1:C:346:TRP:CE3	1:C:347:CYS:HB2	2.46	0.51
1:A:142:GLY:HA3	1:A:183:GLU:HG3	1.93	0.51
1:C:101:ASN:H	1:C:144:GLY:HA3	1.74	0.51
2:D:264:ARG:O	2:D:266:HIS:CD2	2.64	0.51
2:D:337:ASN:C	2:D:339:ASN:H	2.14	0.51
1:A:313:MET:O	1:A:314:ALA:HB2	2.10	0.51
2:D:264:ARG:O	2:D:266:HIS:N	2.27	0.51
1:A:402:ARG:O	1:A:403:ALA:C	2.49	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:313:MET:O	1:C:314:ALA:HB2	2.10	0.51
1:A:404:PHE:O	1:A:405:VAL:C	2.49	0.50
2:D:315:VAL:HG22	2:D:379:GLY:HA2	1.92	0.50
2:D:138:THR:HG22	2:D:169:PHE:HB2	1.94	0.50
2:B:343:PHE:O	2:B:344:VAL:C	2.49	0.50
2:D:48:ARG:O	2:D:49:ILE:C	2.48	0.50
3:E:61:ARG:O	3:E:62:LYS:C	2.49	0.50
1:A:343:PHE:CD1	1:A:349:THR:HG22	2.46	0.50
2:D:263:PRO:C	2:D:265:LEU:H	2.14	0.50
1:A:249:ASN:HA	1:A:254:GLU:CD	2.31	0.50
2:B:3:GLU:O	2:B:133:GLN:N	2.43	0.50
1:C:227:LEU:O	1:C:231:ILE:HG12	2.11	0.50
1:A:368:LEU:H	1:A:368:LEU:CD1	2.11	0.50
2:B:177:VAL:HG12	2:B:177:VAL:O	2.10	0.50
1:A:100:ALA:CB	1:A:105:ARG:HG2	2.41	0.50
3:E:70:LYS:C	3:E:72:LEU:H	2.15	0.50
1:C:406:HIS:HA	1:C:409:VAL:HG23	1.93	0.50
1:C:395:PHE:C	1:C:395:PHE:CD2	2.85	0.50
1:A:278:ALA:C	1:A:280:LYS:H	2.14	0.50
1:A:236:SER:HA	1:A:243:ARG:NH2	2.27	0.50
1:A:325:PRO:HB3	3:E:20:PHE:HE1	1.76	0.50
2:B:259:MET:HE2	2:B:378:ILE:CG2	2.40	0.50
1:A:106:GLY:O	1:A:108:TYR:N	2.43	0.50
2:B:139:HIS:HE1	2:B:170:SER:OG	1.94	0.50
2:D:114:LEU:O	2:D:115:VAL:C	2.49	0.50
2:B:143:GLY:O	2:B:147:SER:HB3	2.11	0.50
1:C:174:ALA:HB1	1:C:207:GLU:HB2	1.94	0.50
1:A:270:ALA:HB3	1:A:302:MET:HG2	1.93	0.50
1:C:68:VAL:HG11	1:C:118:VAL:HG21	1.94	0.50
2:B:107:HIS:CE1	2:B:193:GLN:HE22	2.29	0.50
1:A:181:VAL:HG23	2:B:258:ASN:OD1	2.12	0.50
2:D:158:ARG:O	2:D:159:GLU:CB	2.51	0.50
2:D:38:GLY:O	2:D:40:SER:N	2.43	0.50
2:B:287:THR:O	2:B:288:VAL:CB	2.58	0.50
1:A:207:GLU:O	1:A:211:ASP:HB2	2.11	0.50
1:A:210:TYR:CD1	1:A:210:TYR:C	2.85	0.50
7:B:700:POD:O6	7:B:700:POD:C21	2.59	0.50
1:A:348:PRO:CG	3:E:27:PRO:HD3	2.27	0.49
1:A:102:ASN:HB2	1:A:408:TYR:CE2	2.46	0.49
1:C:3:GLU:HB2	1:C:129:CYS:SG	2.51	0.49
1:C:185:TYR:O	1:C:189:LEU:HB2	2.11	0.49
2:B:291:LEU:CD2	2:B:375:ALA:HB3	2.40	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:115:ILE:O	1:C:119:LEU:HB2	2.11	0.49
2:B:135:PHE:HB2	2:B:166:MET:HE1	1.93	0.49
2:B:31:ASP:HB3	2:B:32:PRO:HD2	1.94	0.49
2:D:255:LEU:HD22	2:D:259:MET:HG2	1.94	0.49
2:B:191:VAL:CG1	2:B:425:MET:HE3	2.16	0.49
1:A:255:PHE:O	1:A:259:LEU:HB2	2.13	0.49
1:A:398:MET:CE	2:B:348:PRO:HD2	2.41	0.49
1:A:112:LYS:HD2	3:E:58:GLU:OE1	2.12	0.49
1:A:287:SER:C	1:A:289:ALA:N	2.63	0.49
2:B:2:ARG:HB2	2:B:133:GLN:HG3	1.95	0.49
1:A:387:ALA:HA	1:A:390:ARG:HD3	1.93	0.49
2:B:385:GLN:HG3	2:B:429:VAL:HG13	1.94	0.49
2:D:284:ARG:O	2:D:286:LEU:N	2.45	0.49
1:A:133:GLN:CD	1:A:251:ASP:HA	2.32	0.49
1:A:191:THR:HA	1:A:194:THR:CG2	2.40	0.49
2:B:140:SER:O	2:B:147:SER:HB2	2.13	0.49
2:B:408:TYR:O	2:B:409:THR:C	2.50	0.49
2:D:199:ASP:N	2:D:199:ASP:OD1	2.46	0.49
2:B:199:ASP:N	2:B:199:ASP:OD1	2.46	0.49
2:B:407:TRP:CH2	1:C:256:GLN:HB3	2.47	0.49
2:D:36:TYR:HD1	2:D:37:HIS:H	1.60	0.49
2:B:69:ASP:OD1	2:B:71:GLU:HG2	2.11	0.49
1:A:346:TRP:HZ2	1:A:435:VAL:HG13	1.77	0.49
1:C:111:GLY:O	1:C:113:GLU:N	2.46	0.49
2:B:336:GLN:NE2	2:B:351:VAL:HG11	2.27	0.49
2:B:48:ARG:O	2:B:51:VAL:HG23	2.13	0.49
2:D:152:LEU:O	2:D:153:LEU:C	2.51	0.49
1:C:161:TYR:HB3	1:C:164:LYS:HG3	1.94	0.49
2:D:31:ASP:HB3	2:D:32:PRO:HD2	1.94	0.49
1:C:287:SER:C	1:C:289:ALA:N	2.66	0.49
2:B:395:PHE:O	2:B:398:MET:N	2.45	0.49
1:A:240:ALA:HB2	1:A:243:ARG:CZ	2.42	0.48
2:D:198:THR:OG1	2:D:265:LEU:HD22	2.13	0.48
2:D:337:ASN:HA	2:D:340:SER:HB3	1.94	0.48
1:A:102:ASN:N	1:A:102:ASN:OD1	2.46	0.48
2:B:256:ALA:O	2:B:258:ASN:N	2.41	0.48
2:B:68:VAL:HG13	2:B:118:VAL:CG2	2.36	0.48
1:C:240:ALA:HB2	1:C:243:ARG:CZ	2.30	0.48
1:A:101:ASN:ND2	2:B:254:LYS:HE2	2.28	0.48
2:B:256:ALA:C	2:B:258:ASN:H	2.15	0.48
2:B:36:TYR:HD1	2:B:37:HIS:N	2.09	0.48
2:D:140:SER:O	2:D:147:SER:HB2	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:295:CYS:HB3	1:A:296:PHE:HD1	1.78	0.48
2:D:188:THR:HG23	2:D:391:ILE:CD1	2.44	0.48
2:B:195:VAL:HG13	2:B:196:GLU:HG2	1.94	0.48
2:D:408:TYR:O	2:D:409:THR:C	2.52	0.48
1:A:164:LYS:HG2	1:A:164:LYS:H	1.46	0.48
1:A:360:PRO:HD2	1:A:371:VAL:O	2.14	0.48
2:B:11:GLN:HG2	2:B:11:GLN:O	2.12	0.48
1:A:180:ALA:N	1:A:183:GLU:OE1	2.45	0.48
1:C:98:ASP:HB2	1:C:110:ILE:HD13	1.96	0.48
1:C:198:SER:CB	1:C:265:ILE:CD1	2.92	0.48
2:D:102:ASN:O	2:D:105:LYS:N	2.46	0.48
1:A:174:ALA:HB2	1:A:207:GLU:H	1.78	0.48
2:D:154:ILE:C	2:D:156:LYS:H	2.17	0.48
3:E:114:ALA:C	3:E:116:LEU:N	2.66	0.48
3:E:140:LYS:O	3:E:141:GLU:C	2.52	0.48
1:C:360:PRO:HD2	1:C:371:VAL:O	2.13	0.48
1:C:415:GLU:O	1:C:418:PHE:HB2	2.13	0.48
2:B:335:VAL:C	2:B:337:ASN:H	2.17	0.48
1:A:327:ASP:O	1:A:328:VAL:C	2.51	0.48
1:C:306:ASP:HA	1:C:307:PRO:HD3	1.69	0.48
2:D:135:PHE:HB2	2:D:166:MET:CE	2.42	0.48
2:D:102:ASN:O	2:D:103:TRP:C	2.52	0.47
2:D:225:GLY:O	2:D:228:ASN:N	2.47	0.47
2:B:132:LEU:HD23	2:B:164:ARG:CG	2.44	0.47
2:B:401:ARG:NH2	1:C:434:GLU:O	2.43	0.47
2:B:382:THR:HA	2:B:432:TYR:CD2	2.49	0.47
2:D:42:LEU:O	2:D:44:LEU:N	2.47	0.47
1:A:72:PRO:O	1:A:74:VAL:N	2.48	0.47
2:D:324:SER:C	2:D:326:LYS:N	2.68	0.47
1:C:250:VAL:O	1:C:251:ASP:HB3	2.14	0.47
1:A:81:GLY:O	1:A:82:THR:C	2.51	0.47
2:D:195:VAL:HA	2:D:265:LEU:CD2	2.44	0.47
1:C:119:LEU:HD22	1:C:156:ARG:HE	1.78	0.47
3:E:116:LEU:C	3:E:118:ALA:H	2.16	0.47
1:C:191:THR:O	1:C:195:LEU:HB3	2.14	0.47
1:A:100:ALA:O	1:A:101:ASN:HB2	2.13	0.47
2:B:251:ASP:OD1	2:B:254:LYS:HE3	2.13	0.47
2:B:157:ILE:O	2:B:158:ARG:C	2.51	0.47
2:D:248:LEU:O	2:D:249:ASN:HB2	2.13	0.47
1:C:430:LYS:O	1:C:434:GLU:HB2	2.15	0.47
2:B:381:SER:C	2:B:383:ALA:H	2.18	0.47
2:B:306:ASP:O	2:B:307:PRO:C	2.53	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:97:SER:OG	2:B:98:GLY:O	2.32	0.47
1:C:273:ALA:HB2	1:C:375:VAL:H	1.78	0.47
1:A:98:ASP:O	1:A:99:ALA:C	2.52	0.47
3:E:90:ASN:C	3:E:92:ASN:N	2.68	0.47
2:B:313:LEU:HB2	2:B:380:ASN:O	2.14	0.47
2:D:336:GLN:OE1	2:D:351:VAL:CG1	2.62	0.47
1:C:404:PHE:O	1:C:405:VAL:C	2.52	0.47
2:B:381:SER:C	2:B:383:ALA:N	2.67	0.47
1:C:72:PRO:HD3	1:C:96:LYS:HA	1.96	0.47
1:A:231:ILE:HG12	1:A:231:ILE:H	1.36	0.47
2:D:96:GLN:HA	2:D:96:GLN:OE1	2.15	0.47
3:E:127:ASP:C	3:E:129:HIS:H	2.18	0.47
1:A:416:GLY:O	1:A:420:GLU:HB3	2.15	0.47
3:E:33:PRO:CB	3:E:35:PHE:CE1	2.97	0.47
1:C:198:SER:CB	1:C:265:ILE:HD11	2.44	0.47
1:C:281:ALA:HB2	1:C:369:ALA:CB	2.45	0.47
2:B:251:ASP:O	2:B:253:ARG:HB2	2.15	0.47
1:A:350:GLY:O	1:A:351:PHE:CG	2.67	0.47
2:B:159:GLU:HG3	3:E:72:LEU:HD23	1.97	0.47
1:A:219:ILE:C	1:A:221:ARG:N	2.69	0.47
1:A:302:MET:HA	1:A:302:MET:HE2	1.96	0.47
1:C:51:THR:CB	1:C:243:ARG:HA	2.45	0.46
1:A:176:GLN:HG2	1:A:177:VAL:N	2.30	0.46
2:B:6:HIS:HD2	2:B:136:GLN:HG3	1.80	0.46
1:C:102:ASN:O	1:C:105:ARG:N	2.46	0.46
2:B:248:LEU:O	2:B:249:ASN:HB2	2.15	0.46
2:B:47:GLU:HG2	2:B:47:GLU:H	1.60	0.46
1:C:390:ARG:H	1:C:390:ARG:HG2	1.54	0.46
1:C:108:TYR:CD2	3:E:108:ASN:CG	2.80	0.46
1:A:95:GLY:C	1:A:97:GLU:H	2.17	0.46
2:D:48:ARG:C	2:D:50:ASN:N	2.68	0.46
1:A:66:VAL:HG11	1:A:122:ILE:HG22	1.97	0.46
2:D:132:LEU:HD23	2:D:164:ARG:HG3	1.97	0.46
1:C:355:ILE:H	1:C:355:ILE:HG13	1.54	0.46
1:C:132:LEU:CG	1:C:133:GLN:N	2.76	0.46
2:B:86:ILE:HG22	2:B:87:PHE:N	2.30	0.46
1:A:224:TYR:CE2	5:A:600:GTP:C5	3.03	0.46
2:B:202:TYR:CE2	2:B:238:VAL:HG11	2.51	0.46
2:B:6:HIS:CE1	2:B:8:GLN:HB2	2.50	0.46
7:D:701:POD:C20	7:D:701:POD:H213	2.45	0.46
2:B:337:ASN:C	2:B:339:ASN:N	2.68	0.46
2:B:269:MET:CE	2:B:307:PRO:HG3	2.46	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:106:GLY:O	2:B:149:MET:HA	2.15	0.46
1:A:171:ILE:HG23	1:A:206:ASN:HD21	1.80	0.46
2:D:171:VAL:HA	2:D:204:ILE:O	2.15	0.46
1:A:406:HIS:CE1	2:B:263:PRO:HD3	2.50	0.46
1:A:223:THR:CG2	1:A:225:THR:HG23	2.46	0.46
1:A:367:ASP:H	1:A:368:LEU:HD12	1.81	0.46
1:C:143:GLY:O	1:C:147:SER:HB3	2.15	0.46
1:C:105:ARG:NH1	1:C:411:GLU:OE1	2.37	0.46
1:A:221:ARG:N	1:A:222:PRO:HD2	2.31	0.46
2:D:111:GLY:HA2	2:D:149:MET:HE1	1.98	0.46
2:D:132:LEU:HD23	2:D:164:ARG:CD	2.46	0.46
1:C:416:GLY:O	1:C:420:GLU:HB3	2.15	0.46
1:C:278:ALA:C	1:C:280:LYS:H	2.19	0.46
1:A:21:TRP:CH2	1:A:63:PRO:HB3	2.46	0.46
2:D:308:ARG:CA	2:D:308:ARG:HH11	2.29	0.46
2:D:6:HIS:CE1	2:D:8:GLN:HB2	2.51	0.46
2:B:296:PHE:CE2	2:B:377:PHE:CE1	3.04	0.46
2:B:100:GLY:O	2:B:101:ASN:HB2	2.15	0.46
1:A:103:TYR:CD1	1:A:148:GLY:HA2	2.50	0.46
1:C:27:GLU:CD	1:C:320:ARG:HH22	2.19	0.46
2:B:306:ASP:C	2:B:307:PRO:O	2.50	0.46
2:B:424:ASN:O	2:B:427:ASP:HB2	2.15	0.46
1:A:316:CYS:O	1:A:377:MET:HA	2.15	0.46
2:D:325:MET:HG2	2:D:355:VAL:HG11	1.98	0.46
1:A:311:LYS:H	1:A:382:THR:HG23	1.81	0.46
2:B:83:PHE:HD2	2:B:83:PHE:HA	1.71	0.46
2:D:266:HIS:HB3	2:D:380:ASN:HD21	1.81	0.46
2:D:238:VAL:HG13	2:D:378:ILE:CD1	2.44	0.46
2:B:132:LEU:HD23	2:B:164:ARG:CD	2.46	0.46
1:A:163:LYS:H	1:A:163:LYS:HE3	1.80	0.46
1:C:256:GLN:HB3	1:C:257:THR:H	1.58	0.46
2:D:277:SER:O	2:D:278:ARG:CG	2.52	0.46
2:D:6:HIS:CE1	2:D:8:GLN:HE21	2.26	0.46
2:B:255:LEU:HD22	2:B:255:LEU:O	2.15	0.46
2:B:60:LYS:O	2:B:61:TYR:HD2	1.99	0.46
1:A:288:VAL:HA	1:A:291:ILE:CD1	2.45	0.46
1:A:221:ARG:N	1:A:222:PRO:CD	2.79	0.46
1:A:151:SER:OG	1:A:193:THR:HB	2.16	0.46
1:A:240:ALA:CA	1:A:243:ARG:CG	2.75	0.45
2:B:165:ILE:HG21	2:B:253:ARG:HD3	1.98	0.45
2:B:118:VAL:HG11	2:B:153:LEU:HD11	1.98	0.45
2:D:2:ARG:HB2	2:D:133:GLN:HG3	1.97	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:174:ALA:O	1:C:176:GLN:N	2.49	0.45
2:D:48:ARG:O	2:D:50:ASN:N	2.50	0.45
2:B:320:ARG:NH1	2:B:360:PRO:HG3	2.30	0.45
2:D:195:VAL:HG12	2:D:196:GLU:HG2	1.99	0.45
2:B:253:ARG:HG3	2:B:253:ARG:HH11	1.81	0.45
2:D:12:CYS:HG	2:D:171:VAL:HG21	1.81	0.45
1:C:189:LEU:HD23	1:C:189:LEU:HA	1.84	0.45
1:A:358:GLU:HA	1:A:359:PRO:HD3	1.81	0.45
3:E:33:PRO:O	3:E:34:GLU:CB	2.65	0.45
2:B:312:TYR:HB2	2:B:343:PHE:CD2	2.51	0.45
2:D:119:LEU:CD1	2:D:156:LYS:HB3	2.46	0.45
1:A:21:TRP:CZ3	1:A:63:PRO:CB	2.83	0.45
1:A:100:ALA:HB2	1:A:105:ARG:HG2	1.98	0.45
2:B:180:THR:HG22	2:B:182:VAL:H	1.81	0.45
2:B:86:ILE:HG22	2:B:87:PHE:CD2	2.51	0.45
1:C:62:VAL:CG2	1:C:91:GLN:HE22	2.30	0.45
2:B:347:ILE:O	2:B:348:PRO:C	2.55	0.45
2:B:8:GLN:NE2	2:B:17:GLY:HA3	2.32	0.45
1:A:287:SER:O	1:A:289:ALA:N	2.50	0.45
1:A:287:SER:O	1:A:290:GLU:N	2.49	0.45
1:C:233:GLN:O	1:C:236:SER:HB3	2.17	0.45
2:B:191:VAL:CG1	2:B:425:MET:CE	2.86	0.45
1:C:406:HIS:HA	1:C:409:VAL:CG2	2.47	0.45
1:C:11:GLN:HB3	5:C:601:GTP:O2A	2.17	0.45
2:B:185:TYR:HD1	2:B:408:TYR:CE1	2.35	0.45
1:C:107:HIS:CD2	1:C:108:TYR:CE1	2.99	0.45
1:C:108:TYR:CD2	3:E:108:ASN:ND2	2.85	0.45
2:D:93:VAL:HG21	2:D:118:VAL:HG22	1.99	0.45
1:A:185:TYR:CD1	1:A:418:PHE:HE2	2.34	0.45
2:D:104:ALA:HB2	2:D:408:TYR:HD2	1.82	0.45
1:C:7:ILE:HG12	1:C:66:VAL:HG23	1.99	0.45
2:B:393:GLU:O	2:B:393:GLU:HG3	2.15	0.45
2:B:133:GLN:HE21	2:B:252:LEU:CB	2.24	0.45
3:E:136:ASN:ND2	3:E:139:LEU:HD23	2.32	0.45
2:B:96:GLN:O	2:B:97:SER:O	2.35	0.45
3:E:27:PRO:O	3:E:28:SER:CB	2.64	0.45
2:B:171:VAL:HA	2:B:204:ILE:O	2.17	0.45
1:C:53:PHE:CD1	1:C:53:PHE:N	2.84	0.45
1:C:386:GLU:O	1:C:390:ARG:HG2	2.16	0.45
1:A:90:GLU:O	1:A:121:ARG:HD2	2.17	0.45
2:D:259:MET:CE	2:D:378:ILE:CG2	2.94	0.45
2:D:255:LEU:CD2	2:D:259:MET:HG2	2.47	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:359:PRO:HB3	2:D:371:LEU:O	2.17	0.45
1:C:168:GLU:CG	1:C:201:ALA:HB1	2.47	0.45
1:C:398:MET:CE	2:D:348:PRO:HD2	2.46	0.45
1:A:208:ALA:O	1:A:212:ILE:HD12	2.16	0.44
3:E:90:ASN:O	3:E:91:ASN:C	2.54	0.44
1:A:198:SER:OG	1:A:265:ILE:HD12	2.16	0.44
1:C:405:VAL:CG1	1:C:406:HIS:H	2.28	0.44
2:B:316:ALA:HB1	7:B:700:POD:C22	2.47	0.44
1:A:234:ILE:HG13	1:A:272:TYR:HB2	1.98	0.44
1:C:68:VAL:CG1	1:C:118:VAL:HG21	2.46	0.44
1:C:432:TYR:O	1:C:433:GLU:C	2.55	0.44
2:D:245:PRO:HB2	2:D:246:GLY:H	1.58	0.44
2:B:260:VAL:HG12	2:B:266:HIS:HB2	1.98	0.44
1:C:176:GLN:HE22	1:C:207:GLU:HG3	1.82	0.44
1:A:392:ASP:O	1:A:395:PHE:HB3	2.17	0.44
2:D:112:ALA:CB	3:E:134:ARG:HH22	2.30	0.44
2:B:158:ARG:HD2	2:B:197:ASN:CB	2.47	0.44
1:C:70:LEU:N	1:C:70:LEU:CD1	2.79	0.44
2:B:227:LEU:O	2:B:230:LEU:HB2	2.18	0.44
1:C:392:ASP:O	1:C:395:PHE:HB3	2.16	0.44
2:B:335:VAL:O	2:B:339:ASN:HB2	2.17	0.44
3:E:136:ASN:OD1	3:E:139:LEU:CD2	2.65	0.44
2:B:153:LEU:O	2:B:157:ILE:HG12	2.16	0.44
2:D:402:LYS:O	2:D:403:ALA:O	2.34	0.44
2:D:406:HIS:CE1	2:D:407:TRP:CD1	3.05	0.44
2:B:263:PRO:O	2:B:265:LEU:N	2.35	0.44
2:D:306:ASP:OD2	2:D:306:ASP:N	2.50	0.44
1:C:120:ASP:O	1:C:122:ILE:N	2.51	0.44
2:B:32:PRO:HA	2:B:83:PHE:CD2	2.53	0.44
2:B:262:PHE:O	2:B:263:PRO:C	2.56	0.44
2:D:195:VAL:CG1	2:D:196:GLU:HG2	2.48	0.44
1:A:88:HIS:O	1:A:91:GLN:HG3	2.17	0.44
1:C:16:ILE:HG22	1:C:17:GLY:N	2.32	0.44
1:C:176:GLN:HG2	1:C:177:VAL:N	2.33	0.44
1:C:350:GLY:O	1:C:351:PHE:CG	2.70	0.44
2:B:347:ILE:CG2	2:B:347:ILE:O	2.63	0.44
2:B:291:LEU:HD21	2:B:375:ALA:HB2	1.95	0.44
2:B:427:ASP:O	2:B:430:SER:N	2.51	0.44
2:D:6:HIS:HD2	2:D:136:GLN:HG3	1.83	0.44
1:C:405:VAL:O	1:C:407:TRP:N	2.51	0.44
2:D:236:SER:OG	2:D:237:GLY:N	2.51	0.44
2:D:135:PHE:CD1	2:D:135:PHE:N	2.86	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:284:GLU:O	1:C:285:GLN:CB	2.65	0.44
2:B:375:ALA:C	2:B:376:THR:HG22	2.37	0.44
2:D:287:THR:O	2:D:288:VAL:CB	2.66	0.44
2:D:335:VAL:O	2:D:339:ASN:HB2	2.18	0.44
2:B:324:SER:C	2:B:326:LYS:N	2.71	0.44
1:A:258:ASN:OD1	1:A:352:LYS:HG3	2.18	0.44
1:C:154:MET:HE1	1:C:166:LYS:HD2	1.99	0.44
2:B:194:LEU:HD22	2:B:194:LEU:HA	1.89	0.44
2:D:134:GLY:HA3	2:D:165:ILE:O	2.18	0.43
2:D:36:TYR:CE1	2:D:38:GLY:O	2.71	0.43
1:A:107:HIS:CD2	1:A:108:TYR:CE1	2.99	0.43
3:E:6:MET:O	3:E:7:GLU:O	2.34	0.43
1:A:353:VAL:HG23	3:E:20:PHE:CD2	2.54	0.43
2:B:402:LYS:O	2:B:403:ALA:O	2.36	0.43
2:D:204:ILE:N	2:D:204:ILE:HD12	2.34	0.43
2:B:315:VAL:O	2:B:351:VAL:HA	2.19	0.43
1:C:142:GLY:HA3	1:C:183:GLU:HG3	2.00	0.43
1:C:346:TRP:CZ3	1:C:347:CYS:HB2	2.52	0.43
2:B:154:ILE:C	2:B:156:LYS:N	2.71	0.43
2:B:93:VAL:HG21	2:B:118:VAL:HG22	2.00	0.43
3:E:70:LYS:O	3:E:74:GLU:HB2	2.18	0.43
2:D:242:LEU:HA	2:D:249:ASN:O	2.18	0.43
2:D:206:ASN:HA	2:D:209:LEU:HB2	2.00	0.43
2:B:195:VAL:HA	2:B:265:LEU:HD23	2.00	0.43
2:B:102:ASN:O	2:B:103:TRP:C	2.57	0.43
2:B:169:PHE:CE2	2:B:235:MET:HG2	2.53	0.43
1:C:304:LYS:O	1:C:305:CYS:HB3	2.19	0.43
2:D:20:PHE:CZ	2:D:24:ILE:HG21	2.52	0.43
2:B:217:LEU:O	2:B:219:LEU:N	2.50	0.43
1:A:21:TRP:CH2	1:A:63:PRO:CB	3.02	0.43
2:B:406:HIS:C	2:B:406:HIS:ND1	2.72	0.43
1:C:259:LEU:HD23	1:C:259:LEU:HA	1.80	0.43
1:C:206:ASN:H	1:C:206:ASN:HD22	1.65	0.43
2:B:104:ALA:HB2	2:B:408:TYR:HD2	1.82	0.43
2:D:347:ILE:CG2	2:D:350:ASN:HB3	2.46	0.43
1:C:163:LYS:O	1:C:164:LYS:C	2.57	0.43
1:C:72:PRO:O	1:C:74:VAL:N	2.51	0.43
2:B:232:SER:OG	2:B:233:ALA:N	2.50	0.43
1:A:134:GLY:HA3	1:A:165:SER:O	2.18	0.43
1:A:25:CYS:O	1:A:26:LEU:C	2.56	0.43
1:C:270:ALA:O	1:C:302:MET:HB2	2.19	0.43
3:E:33:PRO:HB2	3:E:34:GLU:H	1.63	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:252:LEU:O	1:C:253:THR:C	2.57	0.43
2:D:86:ILE:HG22	2:D:87:PHE:CD2	2.53	0.43
1:A:70:LEU:HB2	1:A:145:THR:HG21	2.01	0.43
2:D:312:TYR:CD1	2:D:343:PHE:CE2	3.06	0.43
1:C:375:VAL:HG12	1:C:376:CYS:N	2.30	0.43
1:A:191:THR:O	1:A:195:LEU:HB3	2.19	0.43
1:A:206:ASN:C	1:A:208:ALA:N	2.72	0.43
1:A:168:GLU:HG2	1:A:201:ALA:CB	2.49	0.43
2:B:185:TYR:HD1	2:B:408:TYR:HE1	1.67	0.43
1:C:106:GLY:O	1:C:108:TYR:N	2.51	0.43
1:C:377:MET:O	1:C:377:MET:CG	2.66	0.43
1:A:38:SER:O	1:A:39:ASP:C	2.56	0.43
2:D:273:ALA:CB	2:D:375:ALA:H	2.31	0.43
1:C:288:VAL:HA	1:C:291:ILE:CD1	2.47	0.43
3:E:90:ASN:C	3:E:92:ASN:H	2.21	0.43
2:B:261:PRO:HB2	2:B:262:PHE:CD1	2.54	0.43
1:C:406:HIS:CE1	2:D:263:PRO:HD3	2.54	0.43
1:C:262:TYR:O	1:C:263:PRO:C	2.55	0.43
1:C:177:VAL:HG12	1:C:177:VAL:O	2.19	0.43
2:B:88:ARG:HG2	2:B:89:PRO:HD2	2.00	0.43
2:D:325:MET:HA	2:D:328:VAL:HB	2.01	0.43
1:C:302:MET:HE2	1:C:302:MET:HA	2.01	0.43
2:B:407:TRP:HH2	1:C:256:GLN:HB3	1.84	0.43
2:D:139:HIS:HD2	2:D:146:GLY:O	2.00	0.43
1:A:226:ASN:HD22	1:A:226:ASN:HA	1.66	0.43
2:B:205:ASP:HB3	2:B:303:ALA:HA	2.01	0.43
2:D:96:GLN:HB3	2:D:97:SER:H	1.66	0.43
2:D:158:ARG:HD2	2:D:197:ASN:CB	2.46	0.43
1:A:266:HIS:O	1:A:268:PRO:HD3	2.19	0.43
1:C:387:ALA:HA	1:C:390:ARG:HH11	1.84	0.43
1:A:139:HIS:CG	1:A:150:THR:HG21	2.54	0.43
2:B:306:ASP:OD2	2:B:306:ASP:N	2.51	0.43
1:A:387:ALA:HA	1:A:390:ARG:HH11	1.84	0.43
1:C:281:ALA:HB2	1:C:369:ALA:HB3	2.01	0.43
3:E:109:LYS:O	3:E:113:GLU:HB2	2.19	0.43
2:B:109:THR:HB	2:B:110:GLU:H	1.72	0.43
1:C:103:TYR:CD1	1:C:148:GLY:HA2	2.53	0.43
2:D:273:ALA:HB2	2:D:375:ALA:H	1.84	0.42
2:D:269:MET:CE	2:D:307:PRO:HG3	2.49	0.42
2:D:315:VAL:O	2:D:351:VAL:HA	2.18	0.42
2:D:67:LEU:HD12	2:D:92:PHE:HD2	1.82	0.42
2:B:174:SER:CB	2:B:207:GLU:HG2	2.49	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:273:ALA:CB	2:B:375:ALA:H	2.32	0.42
2:D:151:THR:CG2	2:D:193:GLN:HB3	2.49	0.42
2:B:165:ILE:HD11	2:B:252:LEU:HD23	2.00	0.42
1:C:8:HIS:HE1	1:C:21:TRP:HE1	1.67	0.42
1:C:88:HIS:CD2	1:C:89:PRO:HD2	2.54	0.42
2:B:339:ASN:HD22	2:B:339:ASN:HA	1.68	0.42
1:C:287:SER:O	1:C:290:GLU:N	2.53	0.42
2:D:164:ARG:HG2	2:D:164:ARG:H	1.51	0.42
2:D:112:ALA:HB2	3:E:134:ARG:HH22	1.83	0.42
2:D:332:MET:CG	2:D:353:THR:HG21	2.25	0.42
1:A:328:VAL:HG11	1:A:353:VAL:HG11	2.01	0.42
2:D:253:ARG:HH11	2:D:253:ARG:HG3	1.85	0.42
2:B:317:ALA:O	2:B:353:THR:HA	2.19	0.42
2:B:315:VAL:HG22	2:B:379:GLY:HA2	2.02	0.42
2:B:67:LEU:HD12	2:B:92:PHE:HD2	1.82	0.42
1:C:22:GLU:HB2	1:C:83:TYR:CE1	2.53	0.42
2:B:152:LEU:HD12	2:B:152:LEU:O	2.19	0.42
1:A:174:ALA:O	1:A:176:GLN:N	2.52	0.42
2:D:347:ILE:CG2	2:D:347:ILE:O	2.65	0.42
2:D:273:ALA:HB2	2:D:375:ALA:O	2.20	0.42
2:B:391:ILE:HD11	2:B:425:MET:CE	2.50	0.42
1:C:168:GLU:HG3	1:C:201:ALA:HB1	2.02	0.42
2:D:54:ASN:O	2:D:62:VAL:O	2.38	0.42
1:A:287:SER:C	1:A:289:ALA:H	2.21	0.42
1:C:327:ASP:O	1:C:328:VAL:C	2.57	0.42
1:C:172:TYR:HA	1:C:173:PRO:HD3	1.85	0.42
1:C:236:SER:O	1:C:243:ARG:NH1	2.52	0.42
2:B:183:GLU:O	2:B:184:PRO:C	2.58	0.42
2:B:408:TYR:C	2:B:410:GLY:N	2.69	0.42
1:C:205:ASP:OD1	1:C:207:GLU:N	2.52	0.42
3:E:63:TYR:O	3:E:66:ALA:N	2.53	0.42
2:D:7:ILE:HA	2:D:66:ILE:HG22	2.02	0.42
1:A:154:MET:HE2	1:A:154:MET:HB3	1.97	0.42
2:D:385:GLN:HG3	2:D:429:VAL:HG13	2.01	0.42
1:A:347:CYS:C	1:A:348:PRO:O	2.53	0.42
2:D:274:PRO:HB3	2:D:286:LEU:CD2	2.50	0.42
1:A:190:THR:HG22	1:A:191:THR:N	2.34	0.42
2:B:312:TYR:CD1	2:B:343:PHE:CE2	3.07	0.42
2:B:225:GLY:O	2:B:228:ASN:N	2.52	0.42
1:C:428:LEU:O	1:C:431:ASP:HB2	2.20	0.42
1:A:132:LEU:CG	1:A:133:GLN:N	2.78	0.42
2:B:151:THR:CG2	2:B:193:GLN:HB3	2.49	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:254:LYS:O	2:B:258:ASN:HB2	2.19	0.42
1:C:105:ARG:HD2	1:C:411:GLU:OE1	2.19	0.42
2:B:21:TRP:O	2:B:25:SER:HB2	2.20	0.42
2:D:47:GLU:HG2	2:D:47:GLU:H	1.56	0.42
2:D:377:PHE:C	2:D:377:PHE:CD2	2.93	0.42
2:D:132:LEU:HD23	2:D:164:ARG:CG	2.50	0.42
1:A:17:GLY:O	1:A:19:ALA:N	2.53	0.42
1:A:117:LEU:O	1:A:120:ASP:HB3	2.19	0.42
2:D:272:PHE:CD2	2:D:273:ALA:N	2.88	0.42
2:B:119:LEU:HD11	2:B:156:LYS:HB3	2.02	0.42
2:D:380:ASN:HD22	2:D:380:ASN:HA	1.55	0.42
1:A:92:LEU:HA	1:A:92:LEU:HD23	1.58	0.42
1:C:174:ALA:HA	1:C:175:PRO:HD2	1.75	0.42
2:D:287:THR:CB	2:D:290:GLU:HG3	2.46	0.42
1:C:210:TYR:C	1:C:210:TYR:CD1	2.92	0.42
1:C:219:ILE:C	1:C:221:ARG:N	2.73	0.42
1:C:328:VAL:HG11	1:C:353:VAL:HG11	2.02	0.42
1:A:428:LEU:O	1:A:431:ASP:HB2	2.20	0.42
1:C:135:PHE:CD1	1:C:135:PHE:N	2.87	0.42
1:C:138:PHE:N	1:C:138:PHE:CD1	2.88	0.42
2:D:256:ALA:C	2:D:258:ASN:N	2.73	0.41
1:A:407:TRP:CD2	2:B:257:VAL:HG23	2.54	0.41
3:E:94:ILE:HG22	3:E:95:LYS:N	2.35	0.41
2:B:20:PHE:CZ	2:B:24:ILE:HG21	2.55	0.41
2:D:274:PRO:HG3	2:D:286:LEU:HD22	2.02	0.41
2:D:403:ALA:C	2:D:405:LEU:H	2.23	0.41
2:B:31:ASP:HB2	2:B:34:GLY:HA3	2.00	0.41
1:A:88:HIS:H	1:A:91:GLN:NE2	2.18	0.41
2:D:119:LEU:O	2:D:122:VAL:HG22	2.20	0.41
2:B:145:THR:HG23	6:B:602:GDP:O3B	2.20	0.41
1:C:396:ASP:OD1	1:C:422:ARG:NE	2.46	0.41
1:A:138:PHE:N	1:A:138:PHE:CD1	2.89	0.41
1:A:381:THR:HG23	1:A:381:THR:O	2.19	0.41
1:C:273:ALA:CB	1:C:375:VAL:N	2.76	0.41
2:D:16:ILE:CG2	2:D:17:GLY:N	2.83	0.41
1:A:306:ASP:HA	1:A:307:PRO:HD3	1.78	0.41
2:D:298:ALA:C	2:D:300:ASN:H	2.23	0.41
2:D:298:ALA:CB	2:D:306:ASP:HB3	2.50	0.41
1:C:395:PHE:HD2	1:C:396:ASP:N	2.18	0.41
2:D:111:GLY:O	2:D:149:MET:HE1	2.19	0.41
3:E:58:GLU:HB2	3:E:61:ARG:NH2	2.34	0.41
2:D:269:MET:HE1	2:D:307:PRO:HG3	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:256:GLN:O	1:C:257:THR:C	2.59	0.41
1:C:21:TRP:HZ3	1:C:53:PHE:CZ	2.38	0.41
1:C:69:ASP:C	1:C:70:LEU:HD12	2.40	0.41
1:A:210:TYR:C	1:A:210:TYR:HD1	2.23	0.41
1:A:398:MET:HE3	2:B:348:PRO:HD2	2.01	0.41
1:A:205:ASP:HB3	1:A:303:VAL:HA	2.03	0.41
2:D:224:TYR:OH	6:D:603:GDP:H2'	2.19	0.41
1:C:9:VAL:CG1	1:C:150:THR:OG1	2.69	0.41
1:C:311:LYS:H	1:C:382:THR:HG23	1.86	0.41
1:A:346:TRP:CZ3	1:A:347:CYS:HB2	2.55	0.41
2:D:2:ARG:HD3	2:D:133:GLN:HG3	2.02	0.41
1:A:62:VAL:CG2	1:A:91:GLN:HE22	2.34	0.41
2:B:318:VAL:HG11	7:B:700:POD:H211	2.02	0.41
1:A:270:ALA:HB3	1:A:302:MET:CG	2.49	0.41
1:C:242:LEU:HA	1:C:250:VAL:HG21	2.03	0.41
1:A:182:VAL:HG23	1:A:186:ASN:ND2	2.35	0.41
2:D:131:CYS:O	2:D:131:CYS:SG	2.79	0.41
2:B:165:ILE:HG21	2:B:253:ARG:CD	2.51	0.41
2:B:118:VAL:O	2:B:120:ASP:N	2.54	0.41
2:D:13:GLY:HA3	2:D:139:HIS:HA	2.02	0.41
2:D:204:ILE:H	2:D:204:ILE:HD12	1.85	0.41
1:C:287:SER:HB2	1:C:290:GLU:H	1.85	0.41
2:D:82:PRO:HB2	2:D:83:PHE:H	1.49	0.41
1:A:284:GLU:O	1:A:285:GLN:CB	2.69	0.41
1:C:277:SER:HA	1:C:367:ASP:O	2.21	0.41
1:A:141:PHE:CE2	1:A:191:THR:HB	2.56	0.41
1:C:8:HIS:CE1	1:C:21:TRP:HE1	2.38	0.41
2:B:308:ARG:NH1	2:B:308:ARG:HA	2.19	0.41
1:A:385:ALA:O	1:A:386:GLU:C	2.58	0.41
1:A:262:TYR:O	1:A:263:PRO:C	2.58	0.41
1:C:345:ASP:HB3	1:C:346:TRP:CD1	2.55	0.41
1:A:377:MET:HE3	1:A:377:MET:HA	2.03	0.41
1:A:111:GLY:O	1:A:113:GLU:N	2.54	0.41
1:C:21:TRP:CH2	1:C:63:PRO:HB3	2.54	0.41
2:B:41:ASP:O	2:B:42:LEU:C	2.59	0.41
1:A:345:ASP:HB3	1:A:346:TRP:CD1	2.56	0.41
1:C:240:ALA:HB2	1:C:243:ARG:HD3	2.03	0.41
2:B:188:THR:HG23	2:B:391:ILE:CD1	2.51	0.41
1:C:105:ARG:HH12	2:D:253:ARG:HH22	1.69	0.41
2:B:245:PRO:HB2	2:B:246:GLY:H	1.65	0.41
2:D:10:GLY:O	2:D:13:GLY:N	2.53	0.41
1:A:91:GLN:O	1:A:92:LEU:HD23	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:355:ILE:H	1:A:355:ILE:HG13	1.45	0.41
1:C:108:TYR:O	1:C:112:LYS:HB2	2.21	0.41
2:B:164:ARG:H	2:B:164:ARG:HG2	1.70	0.41
2:D:135:PHE:HB2	2:D:166:MET:HE1	2.03	0.41
1:C:278:ALA:O	1:C:279:GLU:CB	2.69	0.41
2:B:146:GLY:HA2	2:B:150:GLY:H	1.85	0.41
1:C:98:ASP:O	1:C:99:ALA:C	2.59	0.41
2:B:264:ARG:C	2:B:266:HIS:CD2	2.95	0.41
2:D:3:GLU:HA	2:D:51:VAL:HG13	2.03	0.41
1:C:266:HIS:CB	1:C:380:ASN:OD1	2.67	0.41
1:C:26:LEU:HD21	1:C:364:PRO:HD3	2.03	0.41
1:C:180:ALA:O	1:C:181:VAL:C	2.57	0.40
2:B:224:TYR:O	2:B:228:ASN:ND2	2.54	0.40
2:B:139:HIS:CE1	2:B:170:SER:OG	2.74	0.40
2:B:325:MET:HA	2:B:328:VAL:HB	2.02	0.40
2:B:325:MET:CG	2:B:355:VAL:HG11	2.51	0.40
1:C:2:ARG:HB2	1:C:131:GLY:O	2.21	0.40
1:A:363:VAL:HA	1:A:364:PRO:HD3	1.85	0.40
2:B:75:MET:HG2	2:B:75:MET:H	1.69	0.40
2:D:313:LEU:HB2	2:D:380:ASN:O	2.22	0.40
2:B:141:LEU:O	2:B:187:ALA:HA	2.22	0.40
3:E:8:VAL:HA	3:E:21:GLU:O	2.21	0.40
2:B:210:TYR:O	2:B:213:CYS:HB2	2.21	0.40
2:B:165:ILE:CD1	2:B:252:LEU:HD23	2.51	0.40
1:A:265:ILE:O	1:A:266:HIS:C	2.59	0.40
1:A:118:VAL:HG12	1:A:119:LEU:N	2.35	0.40
2:D:109:THR:HB	2:D:110:GLU:H	1.73	0.40
2:B:392:SER:O	2:B:396:THR:N	2.44	0.40
1:A:230:LEU:O	1:A:230:LEU:HD12	2.21	0.40
2:B:391:ILE:HD11	2:B:425:MET:SD	2.61	0.40
2:D:187:ALA:O	2:D:191:VAL:HB	2.22	0.40
1:C:291:ILE:HB	1:C:375:VAL:HG23	2.03	0.40
2:B:209:LEU:HD21	2:B:231:VAL:CG2	2.49	0.40
2:D:165:ILE:HG21	2:D:253:ARG:HD3	2.03	0.40
1:C:256:GLN:O	1:C:259:LEU:N	2.41	0.40
1:A:319:TYR:HB2	1:A:355:ILE:HA	2.02	0.40
1:A:177:VAL:HG12	1:A:177:VAL:O	2.22	0.40
2:D:63:PRO:CD	2:D:86:ILE:HG23	2.51	0.40
1:C:180:ALA:HB1	2:D:258:ASN:HD21	1.84	0.40
2:D:50:ASN:HB3	2:D:51:VAL:H	1.73	0.40
2:D:106:GLY:O	2:D:149:MET:HA	2.22	0.40
3:E:81:GLU:HA	3:E:84:GLN:HB3	2.04	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	429/451 (95%)	288 (67%)	88 (20%)	53 (12%)	1	14
1	C	426/451 (94%)	289 (68%)	90 (21%)	47 (11%)	1	17
2	B	418/445 (94%)	274 (66%)	87 (21%)	57 (14%)	0	11
2	D	424/445 (95%)	276 (65%)	87 (20%)	61 (14%)	0	10
3	E	130/142 (92%)	81 (62%)	29 (22%)	20 (15%)	0	8
All	All	1827/1934 (94%)	1208 (66%)	381 (21%)	238 (13%)	0	12

All (238) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	47	ASP
1	A	62	VAL
1	A	73	THR
1	A	96	LYS
1	A	99	ALA
1	A	100	ALA
1	A	112	LYS
1	A	129	CYS
1	A	247	ALA
1	A	273	ALA
1	A	284	GLU
1	A	345	ASP
1	A	348	PRO
1	A	403	ALA
1	A	437	VAL
2	B	34	GLY
2	B	39	ASP
2	B	42	LEU
2	B	43	GLN

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Mol	Chain	Res	Type
2	B	50	ASN
2	B	60	LYS
2	B	62	VAL
2	B	72	PRO
2	B	73	GLY
2	B	82	PRO
2	B	97	SER
2	B	115	VAL
2	B	145	THR
2	B	217	LEU
2	B	226	ASP
2	B	240	THR
2	B	244	PHE
2	B	265	LEU
2	B	266	HIS
2	B	273	ALA
2	B	285	ALA
2	B	288	VAL
2	B	308	ARG
2	B	343	PHE
2	B	350	ASN
2	B	360	PRO
2	B	369	ARG
2	B	371	LEU
2	B	400	ARG
2	B	403	ALA
2	B	404	PHE
2	B	406	HIS
1	C	62	VAL
1	C	73	THR
1	C	96	LYS
1	C	99	ALA
1	C	100	ALA
1	C	112	LYS
1	C	129	CYS
1	C	256	GLN
1	C	257	THR
1	C	265	ILE
1	C	273	ALA
1	C	284	GLU
1	C	345	ASP
1	C	351	PHE

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Mol	Chain	Res	Type
1	C	403	ALA
1	C	437	VAL
2	D	34	GLY
2	D	42	LEU
2	D	43	GLN
2	D	50	ASN
2	D	60	LYS
2	D	62	VAL
2	D	72	PRO
2	D	73	GLY
2	D	82	PRO
2	D	97	SER
2	D	115	VAL
2	D	145	THR
2	D	217	LEU
2	D	226	ASP
2	D	227	LEU
2	D	240	THR
2	D	244	PHE
2	D	265	LEU
2	D	266	HIS
2	D	273	ALA
2	D	277	SER
2	D	280	SER
2	D	285	ALA
2	D	288	VAL
2	D	308	ARG
2	D	343	PHE
2	D	344	VAL
2	D	350	ASN
2	D	360	PRO
2	D	371	LEU
2	D	400	ARG
2	D	403	ALA
2	D	406	HIS
3	E	7	GLU
3	E	28	SER
3	E	34	GLU
3	E	63	TYR
3	E	64	GLN
3	E	68	LEU
1	A	32	PRO

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Mol	Chain	Res	Type
1	A	72	PRO
1	A	101	ASN
1	A	144	GLY
1	A	222	PRO
1	A	239	THR
1	A	245	ASP
1	A	249	ASN
1	A	251	ASP
1	A	264	ARG
1	A	265	ILE
1	A	285	GLN
1	A	351	PHE
1	A	377	MET
1	A	386	GLU
1	A	405	VAL
2	B	99	ALA
2	B	103	TRP
2	B	109	THR
2	B	144	GLY
2	B	155	SER
2	B	157	ILE
2	B	159	GLU
2	B	227	LEU
2	B	245	PRO
2	B	264	ARG
2	B	344	VAL
2	B	370	GLY
1	C	72	PRO
1	C	107	HIS
1	C	120	ASP
1	C	144	GLY
1	C	175	PRO
1	C	222	PRO
1	C	239	THR
1	C	285	GLN
1	C	357	TYR
1	C	386	GLU
2	D	11	GLN
2	D	39	ASP
2	D	103	TRP
2	D	159	GLU
2	D	245	PRO

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Mol	Chain	Res	Type
2	D	257	VAL
2	D	264	ARG
2	D	276	THR
2	D	370	GLY
2	D	402	LYS
2	D	404	PHE
3	E	9	ILE
3	E	32	VAL
3	E	33	PRO
3	E	91	ASN
3	E	115	HIS
1	A	46	ASP
1	A	107	HIS
1	A	120	ASP
1	A	207	GLU
1	A	248	LEU
1	A	314	ALA
1	A	326	LYS
1	A	396	ASP
2	B	11	GLN
2	B	218	LYS
2	B	257	VAL
2	B	299	LYS
2	B	305	CYS
2	B	402	LYS
1	C	32	PRO
1	C	33	ASP
1	C	98	ASP
1	C	101	ASN
1	C	251	ASP
1	C	253	THR
1	C	264	ARG
1	C	305	CYS
1	C	314	ALA
1	C	377	MET
1	C	405	VAL
2	D	109	THR
2	D	144	GLY
2	D	218	LYS
2	D	278	ARG
2	D	299	LYS
2	D	305	CYS

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Mol	Chain	Res	Type
2	D	336	GLN
3	E	21	GLU
3	E	36	ASN
3	E	71	HIS
1	A	83	TYR
1	A	175	PRO
1	A	305	CYS
1	A	432	TYR
2	B	223	THR
2	B	248	LEU
2	B	336	GLN
1	C	59	GLY
1	C	83	TYR
1	C	163	LYS
1	C	200	CYS
1	C	248	LEU
2	D	59	ASN
2	D	99	ALA
2	D	251	ASP
2	D	325	MET
2	D	369	ARG
3	E	20	PHE
3	E	90	ASN
3	E	123	LEU
3	E	138	GLU
1	A	266	HIS
1	A	357	TYR
1	A	370	LYS
2	B	59	ASN
2	B	252	LEU
1	C	121	ARG
1	C	124	LYS
1	C	146	GLY
2	D	248	LEU
2	D	338	LYS
3	E	50	ILE
1	A	146	GLY
1	A	274	PRO
2	B	96	GLN
1	C	106	GLY
1	A	328	VAL
2	B	13	GLY

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Mol	Chain	Res	Type
1	A	250	VAL
3	E	31	GLY
1	A	59	GLY
1	C	274	PRO
2	D	13	GLY
2	D	157	ILE
1	A	221	ARG
2	D	307	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	342/378 (90%)	217 (64%)	125 (36%)	0	2
1	C	340/378 (90%)	219 (64%)	121 (36%)	0	2
2	B	343/381 (90%)	216 (63%)	127 (37%)	0	1
2	D	348/381 (91%)	214 (62%)	134 (38%)	0	1
3	E	65/126 (52%)	45 (69%)	20 (31%)	0	5
All	All	1438/1644 (88%)	911 (63%)	527 (37%)	0	2

All (527) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	4	CYS
1	A	15	GLN
1	A	16	ILE
1	A	22	GLU
1	A	23	LEU
1	A	26	LEU
1	A	53	PHE
1	A	60	LYS
1	A	66	VAL
1	A	68	VAL
1	A	71	GLU
1	A	73	THR

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Mol	Chain	Res	Type
1	A	74	VAL
1	A	77	GLU
1	A	82	THR
1	A	84	ARG
1	A	88	HIS
1	A	91	GLN
1	A	94	THR
1	A	96	LYS
1	A	105	ARG
1	A	110	ILE
1	A	112	LYS
1	A	113	GLU
1	A	115	ILE
1	A	125	LEU
1	A	127	ASP
1	A	128	GLN
1	A	129	CYS
1	A	132	LEU
1	A	135	PHE
1	A	138	PHE
1	A	140	SER
1	A	141	PHE
1	A	147	SER
1	A	151	SER
1	A	153	LEU
1	A	154	MET
1	A	155	GLU
1	A	156	ARG
1	A	157	LEU
1	A	163	LYS
1	A	166	LYS
1	A	172	TYR
1	A	178	SER
1	A	183	GLU
1	A	187	SER
1	A	190	THR
1	A	192	HIS
1	A	193	THR
1	A	194	THR
1	A	195	LEU
1	A	196	GLU
1	A	200	CYS

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Mol	Chain	Res	Type
1	A	203	MET
1	A	205	ASP
1	A	206	ASN
1	A	210	TYR
1	A	211	ASP
1	A	212	ILE
1	A	215	ARG
1	A	219	ILE
1	A	224	TYR
1	A	225	THR
1	A	226	ASN
1	A	227	LEU
1	A	229	ARG
1	A	230	LEU
1	A	231	ILE
1	A	234	ILE
1	A	238	ILE
1	A	242	LEU
1	A	243	ARG
1	A	249	ASN
1	A	258	ASN
1	A	260	VAL
1	A	271	THR
1	A	275	VAL
1	A	277	SER
1	A	280	LYS
1	A	284	GLU
1	A	287	SER
1	A	290	GLU
1	A	292	THR
1	A	295	CYS
1	A	302	MET
1	A	313	MET
1	A	315	CYS
1	A	316	CYS
1	A	318	LEU
1	A	329	ASN
1	A	341	ILE
1	A	343	PHE
1	A	349	THR
1	A	351	PHE
1	A	353	VAL

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Mol	Chain	Res	Type
1	A	355	ILE
1	A	356	ASN
1	A	362	VAL
1	A	363	VAL
1	A	368	LEU
1	A	370	LYS
1	A	371	VAL
1	A	376	CYS
1	A	377	MET
1	A	379	SER
1	A	380	ASN
1	A	381	THR
1	A	382	THR
1	A	384	ILE
1	A	390	ARG
1	A	394	LYS
1	A	396	ASP
1	A	397	LEU
1	A	401	LYS
1	A	413	MET
1	A	414	GLU
1	A	419	SER
1	A	423	GLU
1	A	430	LYS
1	A	432	TYR
1	A	433	GLU
1	A	434	GLU
1	A	438	ASP
2	B	4	ILE
2	B	15	GLN
2	B	16	ILE
2	B	23	VAL
2	B	24	ILE
2	B	25	SER
2	B	26	ASP
2	B	27	GLU
2	B	33	THR
2	B	36	TYR
2	B	41	ASP
2	B	42	LEU
2	B	44	LEU
2	B	47	GLU

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Mol	Chain	Res	Type
2	B	51	VAL
2	B	55	GLU
2	B	61	TYR
2	B	62	VAL
2	B	66	ILE
2	B	74	THR
2	B	75	MET
2	B	76	ASP
2	B	80	SER
2	B	83	PHE
2	B	86	ILE
2	B	87	PHE
2	B	88	ARG
2	B	90	ASP
2	B	94	PHE
2	B	97	SER
2	B	101	ASN
2	B	105	LYS
2	B	109	THR
2	B	110	GLU
2	B	120	ASP
2	B	122	VAL
2	B	128	SER
2	B	129	CYS
2	B	131	CYS
2	B	135	PHE
2	B	137	LEU
2	B	140	SER
2	B	145	THR
2	B	149	MET
2	B	151	THR
2	B	153	LEU
2	B	155	SER
2	B	156	LYS
2	B	159	GLU
2	B	163	ASP
2	B	164	ARG
2	B	166	MET
2	B	170	SER
2	B	171	VAL
2	B	178	SER
2	B	183	GLU

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Mol	Chain	Res	Type
2	B	188	THR
2	B	191	VAL
2	B	192	HIS
2	B	193	GLN
2	B	194	LEU
2	B	195	VAL
2	B	197	ASN
2	B	199	ASP
2	B	201	THR
2	B	203	CYS
2	B	205	ASP
2	B	212	ILE
2	B	216	THR
2	B	220	THR
2	B	223	THR
2	B	224	TYR
2	B	229	HIS
2	B	231	VAL
2	B	232	SER
2	B	236	SER
2	B	240	THR
2	B	242	LEU
2	B	248	LEU
2	B	251	ASP
2	B	252	LEU
2	B	253	ARG
2	B	255	LEU
2	B	258	ASN
2	B	265	LEU
2	B	267	PHE
2	B	269	MET
2	B	275	LEU
2	B	282	GLN
2	B	286	LEU
2	B	287	THR
2	B	291	LEU
2	B	292	THR
2	B	302	MET
2	B	305	CYS
2	B	306	ASP
2	B	308	ARG
2	B	313	LEU

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Mol	Chain	Res	Type
2	B	320	ARG
2	B	323	MET
2	B	325	MET
2	B	336	GLN
2	B	342	TYR
2	B	343	PHE
2	B	350	ASN
2	B	353	THR
2	B	357	ASP
2	B	371	LEU
2	B	373	MET
2	B	374	SER
2	B	376	THR
2	B	378	ILE
2	B	380	ASN
2	B	382	THR
2	B	384	ILE
2	B	385	GLN
2	B	386	GLU
2	B	401	ARG
2	B	402	LYS
2	B	405	LEU
2	B	406	HIS
2	B	409	THR
2	B	414	ASP
2	B	416	MET
2	B	419	THR
2	B	425	MET
2	B	430	SER
1	C	2	ARG
1	C	4	CYS
1	C	16	ILE
1	C	22	GLU
1	C	23	LEU
1	C	26	LEU
1	C	53	PHE
1	C	66	VAL
1	C	68	VAL
1	C	74	VAL
1	C	77	GLU
1	C	82	THR
1	C	84	ARG

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Mol	Chain	Res	Type
1	C	88	HIS
1	C	91	GLN
1	C	92	LEU
1	C	94	THR
1	C	96	LYS
1	C	98	ASP
1	C	105	ARG
1	C	110	ILE
1	C	112	LYS
1	C	113	GLU
1	C	114	ILE
1	C	115	ILE
1	C	125	LEU
1	C	127	ASP
1	C	128	GLN
1	C	129	CYS
1	C	132	LEU
1	C	135	PHE
1	C	140	SER
1	C	141	PHE
1	C	147	SER
1	C	151	SER
1	C	153	LEU
1	C	154	MET
1	C	155	GLU
1	C	156	ARG
1	C	157	LEU
1	C	163	LYS
1	C	166	LYS
1	C	172	TYR
1	C	178	SER
1	C	183	GLU
1	C	187	SER
1	C	190	THR
1	C	192	HIS
1	C	193	THR
1	C	194	THR
1	C	195	LEU
1	C	196	GLU
1	C	198	SER
1	C	199	ASP
1	C	200	CYS

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Mol	Chain	Res	Type
1	C	203	MET
1	C	205	ASP
1	C	206	ASN
1	C	210	TYR
1	C	211	ASP
1	C	212	ILE
1	C	219	ILE
1	C	224	TYR
1	C	225	THR
1	C	226	ASN
1	C	227	LEU
1	C	229	ARG
1	C	231	ILE
1	C	234	ILE
1	C	242	LEU
1	C	243	ARG
1	C	249	ASN
1	C	250	VAL
1	C	251	ASP
1	C	252	LEU
1	C	256	GLN
1	C	257	THR
1	C	258	ASN
1	C	275	VAL
1	C	280	LYS
1	C	284	GLU
1	C	287	SER
1	C	290	GLU
1	C	292	THR
1	C	295	CYS
1	C	302	MET
1	C	305	CYS
1	C	313	MET
1	C	316	CYS
1	C	318	LEU
1	C	341	ILE
1	C	343	PHE
1	C	344	VAL
1	C	349	THR
1	C	353	VAL
1	C	355	ILE
1	C	356	ASN

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Mol	Chain	Res	Type
1	C	362	VAL
1	C	363	VAL
1	C	368	LEU
1	C	370	LYS
1	C	371	VAL
1	C	377	MET
1	C	379	SER
1	C	380	ASN
1	C	382	THR
1	C	384	ILE
1	C	390	ARG
1	C	394	LYS
1	C	396	ASP
1	C	397	LEU
1	C	401	LYS
1	C	413	MET
1	C	414	GLU
1	C	419	SER
1	C	423	GLU
1	C	430	LYS
1	C	432	TYR
1	C	433	GLU
1	C	434	GLU
1	C	438	ASP
2	D	4	ILE
2	D	12	CYS
2	D	15	GLN
2	D	16	ILE
2	D	23	VAL
2	D	24	ILE
2	D	25	SER
2	D	26	ASP
2	D	27	GLU
2	D	33	THR
2	D	36	TYR
2	D	41	ASP
2	D	42	LEU
2	D	44	LEU
2	D	47	GLU
2	D	51	VAL
2	D	55	GLU
2	D	61	TYR

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Mol	Chain	Res	Type
2	D	62	VAL
2	D	66	ILE
2	D	75	MET
2	D	76	ASP
2	D	80	SER
2	D	83	PHE
2	D	86	ILE
2	D	87	PHE
2	D	88	ARG
2	D	90	ASP
2	D	94	PHE
2	D	97	SER
2	D	101	ASN
2	D	105	LYS
2	D	109	THR
2	D	110	GLU
2	D	120	ASP
2	D	122	VAL
2	D	128	SER
2	D	129	CYS
2	D	131	CYS
2	D	135	PHE
2	D	137	LEU
2	D	140	SER
2	D	145	THR
2	D	149	MET
2	D	151	THR
2	D	153	LEU
2	D	155	SER
2	D	156	LYS
2	D	163	ASP
2	D	164	ARG
2	D	166	MET
2	D	170	SER
2	D	171	VAL
2	D	177	VAL
2	D	178	SER
2	D	181	VAL
2	D	183	GLU
2	D	188	THR
2	D	191	VAL
2	D	192	HIS

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Mol	Chain	Res	Type
2	D	193	GLN
2	D	194	LEU
2	D	195	VAL
2	D	197	ASN
2	D	199	ASP
2	D	201	THR
2	D	203	CYS
2	D	205	ASP
2	D	216	THR
2	D	220	THR
2	D	223	THR
2	D	224	TYR
2	D	229	HIS
2	D	232	SER
2	D	236	SER
2	D	240	THR
2	D	242	LEU
2	D	248	LEU
2	D	251	ASP
2	D	252	LEU
2	D	253	ARG
2	D	255	LEU
2	D	258	ASN
2	D	265	LEU
2	D	267	PHE
2	D	268	PHE
2	D	269	MET
2	D	275	LEU
2	D	278	ARG
2	D	280	SER
2	D	281	GLN
2	D	286	LEU
2	D	287	THR
2	D	291	LEU
2	D	292	THR
2	D	302	MET
2	D	306	ASP
2	D	308	ARG
2	D	313	LEU
2	D	320	ARG
2	D	322	ARG
2	D	323	MET

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Mol	Chain	Res	Type
2	D	325	MET
2	D	331	GLN
2	D	336	GLN
2	D	338	LYS
2	D	342	TYR
2	D	343	PHE
2	D	345	GLU
2	D	350	ASN
2	D	353	THR
2	D	357	ASP
2	D	358	ILE
2	D	371	LEU
2	D	373	MET
2	D	374	SER
2	D	376	THR
2	D	378	ILE
2	D	380	ASN
2	D	382	THR
2	D	384	ILE
2	D	385	GLN
2	D	386	GLU
2	D	390	ARG
2	D	392	SER
2	D	401	ARG
2	D	402	LYS
2	D	405	LEU
2	D	406	HIS
2	D	414	ASP
2	D	416	MET
2	D	419	THR
2	D	425	MET
2	D	430	SER
3	E	6	MET
3	E	10	GLU
3	E	35	PHE
3	E	55	GLU
3	E	58	GLU
3	E	69	LEU
3	E	78	HIS
3	E	93	PHE
3	E	94	ILE
3	E	101	LEU

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Mol	Chain	Res	Type
3	E	105	MET
3	E	109	LYS
3	E	112	ARG
3	E	113	GLU
3	E	116	LEU
3	E	122	ARG
3	E	124	GLN
3	E	126	LYS
3	E	134	ARG
3	E	139	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	88	HIS
1	A	91	GLN
1	A	101	ASN
1	A	107	HIS
1	A	133	GLN
1	A	139	HIS
1	A	176	GLN
1	A	206	ASN
1	A	216	ASN
1	A	301	GLN
1	A	329	ASN
2	B	6	HIS
2	B	8	GLN
2	B	14	ASN
2	B	107	HIS
2	B	133	GLN
2	B	136	GLN
2	B	139	HIS
2	B	206	ASN
2	B	266	HIS
2	B	294	GLN
2	B	300	ASN
2	B	339	ASN
2	B	350	ASN
2	B	380	ASN
2	B	406	HIS
1	C	8	HIS

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Mol	Chain	Res	Type
1	C	11	GLN
1	C	88	HIS
1	C	91	GLN
1	C	107	HIS
1	C	133	GLN
1	C	139	HIS
1	C	176	GLN
1	C	206	ASN
1	C	216	ASN
1	C	258	ASN
1	C	301	GLN
2	D	6	HIS
2	D	8	GLN
2	D	14	ASN
2	D	43	GLN
2	D	107	HIS
2	D	133	GLN
2	D	136	GLN
2	D	139	HIS
2	D	193	GLN
2	D	206	ASN
2	D	258	ASN
2	D	266	HIS
2	D	294	GLN
2	D	300	ASN
2	D	309	HIS
2	D	339	ASN
2	D	350	ASN
2	D	380	ASN
3	E	78	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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$
5	GTP	A	600	4	34,34,34	1.28	3 (8%)	51,54,54	2.00	14 (27%)
6	GDP	B	602	-	30,30,30	0.95	1 (3%)	44,47,47	2.06	13 (29%)
7	POD	B	700	-	34,34,34	3.14	11 (32%)	51,51,51	4.15	23 (45%)
5	GTP	C	601	4	34,34,34	1.13	4 (11%)	51,54,54	1.68	10 (19%)
6	GDP	D	603	-	30,30,30	1.03	2 (6%)	44,47,47	1.87	12 (27%)
7	POD	D	701	-	34,34,34	3.10	11 (32%)	51,51,51	3.93	22 (43%)

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
5	GTP	A	600	4	-	0/22/38/38	0/1/3/3
6	GDP	B	602	-	-	0/16/32/32	0/1/3/3
7	POD	B	700	-	1/1/5/5	0/10/45/45	0/1/5/5
5	GTP	C	601	4	-	0/22/38/38	0/1/3/3
6	GDP	D	603	-	-	0/16/32/32	0/1/3/3
7	POD	D	701	-	1/1/5/5	0/10/45/45	0/1/5/5

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	701	POD	C7-C6	-9.80	1.21	1.39
7	D	701	POD	C7-C2	-8.95	1.21	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	700	POD	C7-C6	-8.72	1.23	1.39
7	B	700	POD	C7-C2	-8.49	1.22	1.38
7	B	700	POD	C10-C11	-6.52	1.45	1.56
7	B	700	POD	C10-C13	-6.25	1.42	1.51
7	D	701	POD	C10-C11	-4.94	1.48	1.56
7	D	701	POD	C10-C13	-4.77	1.44	1.51
7	B	700	POD	O1-C3	4.72	1.45	1.38
7	D	701	POD	O1-C3	4.62	1.45	1.38
7	D	701	POD	O4-C13	4.47	1.45	1.34
7	B	700	POD	O4-C13	3.77	1.43	1.34
7	B	700	POD	O2-C2	3.76	1.43	1.38
7	D	701	POD	C3-C2	-3.66	1.29	1.39
7	B	700	POD	C14-C11	-3.59	1.47	1.52
6	D	603	GDP	C2-N3	3.42	1.37	1.33
7	B	700	POD	C3-C2	-3.37	1.30	1.39
7	D	701	POD	O2-C2	3.16	1.42	1.38
5	A	600	GTP	C2-N3	3.15	1.37	1.33
5	A	600	GTP	PA-O3A	2.87	1.65	1.59
7	D	701	POD	C14-C11	-2.77	1.48	1.52
6	B	602	GDP	C2-N3	2.62	1.36	1.33
7	B	700	POD	C10-C9	-2.54	1.49	1.54
5	C	601	GTP	C2-N3	2.37	1.36	1.33
5	C	601	GTP	O4'-C4'	-2.32	1.39	1.45
5	A	600	GTP	PB-O3A	2.31	1.64	1.59
7	B	700	POD	C16-C17	-2.26	1.35	1.40
5	C	601	GTP	PA-O3A	2.24	1.63	1.59
7	D	701	POD	C16-C17	-2.23	1.35	1.40
7	D	701	POD	C6-C5	-2.11	1.37	1.40
5	C	601	GTP	C2'-C1'	-2.08	1.50	1.53
6	D	603	GDP	PA-O3A	2.06	1.63	1.59

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	700	POD	C2-C7-C6	13.51	149.06	119.53
7	D	701	POD	C2-C7-C6	12.96	147.85	119.53
7	D	701	POD	C7-C6-C5	-12.11	103.81	120.16
7	B	700	POD	C7-C6-C5	-11.80	104.22	120.16
7	B	700	POD	C7-C2-C3	-10.72	107.77	122.06
7	B	700	POD	C9-C10-C11	9.50	131.61	112.68
7	D	701	POD	C7-C2-C3	-9.45	109.47	122.06
7	D	701	POD	C9-C10-C11	9.04	130.69	112.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	700	POD	O2-C2-C7	7.67	138.97	127.85
7	D	701	POD	O2-C2-C7	7.56	138.81	127.85
7	D	701	POD	O4-C13-O5	5.98	128.22	121.40
7	B	700	POD	C20-O6-C16	5.96	126.40	117.59
7	B	700	POD	O4-C13-O5	5.86	128.09	121.40
6	B	602	GDP	N2-C2-N3	-5.80	112.45	120.30
6	D	603	GDP	C6-C5-N7	-5.50	133.40	134.14
5	A	600	GTP	C6-C5-N7	5.47	134.88	134.14
5	A	600	GTP	O4'-C1'-N9	5.25	113.33	108.44
7	B	700	POD	C21-O7-C17	5.17	129.02	114.90
7	D	701	POD	C21-O7-C17	4.92	128.34	114.90
5	A	600	GTP	C2-N3-C4	4.66	121.63	115.09
7	B	700	POD	O5-C13-C10	-4.65	123.42	129.43
6	B	602	GDP	C6-C5-N7	-4.60	133.52	134.14
7	D	701	POD	C6-C5-C11	4.47	124.96	114.18
7	D	701	POD	C14-C11-C10	-4.42	106.73	113.49
6	B	602	GDP	O4'-C1'-N9	4.25	112.39	108.44
7	B	700	POD	C6-C5-C11	4.23	124.38	114.18
6	D	603	GDP	C2-N3-C4	4.14	120.91	115.09
7	B	700	POD	C14-C11-C10	-4.04	107.32	113.49
6	B	602	GDP	C2-N3-C4	3.94	120.63	115.09
7	D	701	POD	C9-C10-C13	3.93	108.87	103.19
5	C	601	GTP	N2-C2-N1	3.81	122.06	117.86
5	C	601	GTP	O4'-C1'-N9	3.80	111.98	108.44
7	B	700	POD	C10-C9-C8	3.65	117.66	110.30
6	D	603	GDP	C5-C4-N3	-3.62	120.70	125.94
5	C	601	GTP	C2-N3-C4	3.58	120.13	115.09
7	D	701	POD	O5-C13-C10	-3.58	124.80	129.43
5	C	601	GTP	PB-O3B-PG	-3.57	121.20	131.68
7	B	700	POD	C9-C10-C13	3.57	108.34	103.19
5	A	600	GTP	PB-O3B-PG	-3.54	121.29	131.68
6	D	603	GDP	N2-C2-N3	-3.52	115.53	120.30
5	A	600	GTP	C1'-N9-C4	-3.52	120.56	126.64
7	D	701	POD	C12-O4-C13	3.47	113.57	110.19
5	A	600	GTP	N2-C2-N1	3.44	121.65	117.86
7	B	700	POD	C12-C9-C8	3.43	127.07	116.60
7	D	701	POD	C10-C9-C8	3.40	117.15	110.30
6	B	602	GDP	PA-O3A-PB	-3.40	121.71	131.68
7	B	700	POD	O1-C3-C4	3.38	132.75	127.85
5	C	601	GTP	C1'-N9-C4	-3.30	120.93	126.64
7	D	701	POD	C5-C6-C8	3.26	131.08	121.62
7	B	700	POD	C5-C6-C8	3.24	131.01	121.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	701	POD	C12-C9-C8	3.14	126.20	116.60
5	A	600	GTP	C5-C4-N3	-3.12	121.42	125.94
6	D	603	GDP	N3-C4-N9	3.06	131.39	126.91
7	B	700	POD	C19-C14-C11	3.05	125.41	120.25
7	B	700	POD	C12-C9-C10	3.01	106.75	101.79
6	B	602	GDP	O4'-C1'-C2'	2.99	111.35	106.77
5	A	600	GTP	C8-N9-C1'	2.97	132.24	126.38
6	D	603	GDP	C4-C5-N7	-2.92	107.02	109.52
7	D	701	POD	C19-C14-C11	2.91	125.17	120.25
7	D	701	POD	C12-C9-C10	2.86	106.51	101.79
5	C	601	GTP	C2'-C3'-C4'	2.85	108.33	102.65
7	D	701	POD	C7-C6-C8	2.84	125.04	118.93
6	B	602	GDP	C5-C4-N3	-2.75	121.96	125.94
7	B	700	POD	O2-C2-C3	2.73	113.26	109.78
5	C	601	GTP	C8-N9-C1'	2.71	131.72	126.38
7	B	700	POD	C7-C6-C8	2.69	124.72	118.93
7	D	701	POD	O1-C3-C4	2.68	131.74	127.85
6	B	602	GDP	C2'-C1'-N9	-2.62	106.54	113.27
5	C	601	GTP	C5-C4-N3	-2.62	122.15	125.94
7	D	701	POD	C4-C3-C2	-2.60	118.59	122.06
6	B	602	GDP	C1'-N9-C4	-2.55	122.22	126.64
7	B	700	POD	C12-O4-C13	2.53	112.66	110.19
6	D	603	GDP	C3'-C2'-C1'	2.51	104.83	100.91
5	A	600	GTP	O3A-PB-O3B	2.49	106.73	101.66
6	B	602	GDP	C2'-C3'-C4'	2.46	107.55	102.65
6	B	602	GDP	N3-C4-N9	2.45	130.50	126.91
6	B	602	GDP	N1-C2-N3	-2.44	118.36	121.78
5	A	600	GTP	C2'-C3'-C4'	2.42	107.47	102.65
5	A	600	GTP	C5-C6-N1	2.38	122.35	115.39
6	D	603	GDP	N7-C8-N9	-2.32	107.79	114.36
5	A	600	GTP	N3-C4-N9	2.24	130.19	126.91
7	D	701	POD	O4-C13-C10	-2.18	106.47	109.66
6	D	603	GDP	O4'-C1'-N9	2.18	110.46	108.44
5	A	600	GTP	N7-C8-N9	-2.14	108.31	114.36
5	A	600	GTP	N1-C2-N3	-2.09	118.86	121.78
7	D	701	POD	C15-C14-C11	-2.08	116.72	120.25
5	C	601	GTP	N3-C4-N9	2.06	129.93	126.91
6	B	602	GDP	N7-C8-N9	-2.05	108.55	114.36
7	B	700	POD	C4-C3-C2	-2.04	119.33	122.06
6	D	603	GDP	O4'-C4'-C3'	2.03	109.29	105.17
5	C	601	GTP	N7-C8-N9	-2.03	108.61	114.36
6	D	603	GDP	O3B-PB-O3A	2.01	114.65	105.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	603	GDP	N1-C2-N3	-2.00	118.98	121.78
7	B	700	POD	O3-C8-C6	2.00	114.58	110.35

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	D	701	POD	C10
7	B	700	POD	C10

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.