



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:56 PM UTC

PDB ID : 1CR6 / pdb_00001cr6
Title : CRYSTAL STRUCTURE OF MURINE SOLUBLE EPOXIDE HYDROLASE
COMPLEXED WITH CPU INHIBITOR
Authors : Argiriadi, M.A.; Morisseau, C.; Hammock, B.D.; Christianson, D.W.
Deposited on : 1999-08-13
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

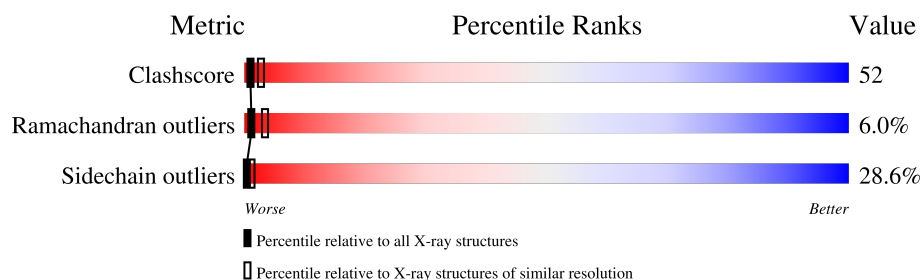
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	554	
1	B	554	

2 Entry composition [i](#)

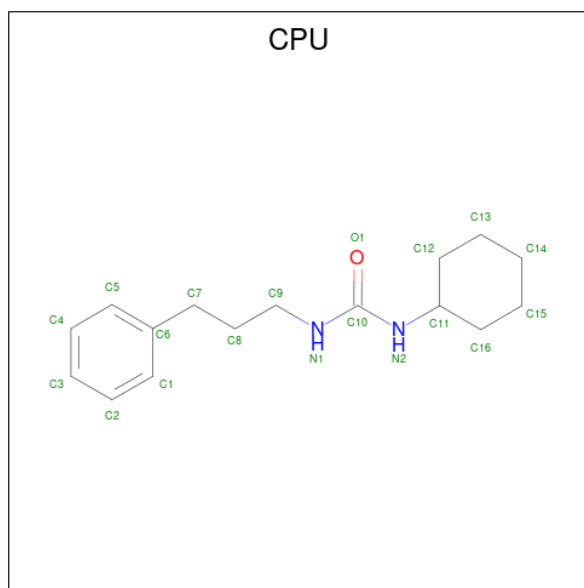
There are 3 unique types of molecules in this entry. The entry contains 8237 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 EPOXIDE HYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	61	0	0
			3879	2501	648	701	29			
1	B	541	Total	C	N	O	S	71	0	0
			4299	2766	719	783	31			

- Molecule 2 is N-CYCLOHEXYL-N'-(PROPYL)PHENYL UREA (CCD ID: CPU) (formula: $C_{16}H_{24}N_2O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	16	2	1		
2	B	1	Total	C	N	O	0	0
			19	16	2	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total 12	O 12	0	0
3	B	9	Total 9	O 9	0	0



W524	R459	K382	G312	F250	G187	N125	V64
	P461	L383	E314	M253	S188	W126	P65
	L462	Q386	M315	G254	N189	L127	L66
	E528	E387		S255	L190	D128	M67
	K529	E396	D320	G256	K191	D129	D68
	P530	K397	K321	P257	A193	G130	E69
	E532	N398	L322	A258	R194	D131	S70
	V533		G323	L259	D195	K132	Y71
	N534	R401	I324		M196	R133	R72
	K539		P325		G197	D134	K73
D542	R470	T402	V328	H263	G197	S135	S74
	N471	F403	F329	G264	M198	L136	S75
	D535	K404		F265	V199	A137	K76
	L536	S405		T200	Q138	Q138	A77
	I537	F406	H332	P266	I201	M139	G78
	V538	F407	D333	E267	L202	M140	G79
	K539	R408	W334	S268	V203	C141	A80
				W269	H204	E142	N81
				F270	N205	L143	L82
				S271	T206	S144	P83
VAL	R481	G414	V339	R273	S208	Q145	E84
	L488	F415		Y274	A209	H146	N85
	N489	I416	M342	Q275	L210	D148	S87
	V490	A417	I276	P277	F149	F149	I88
	T491	V418	Y346	A278	E212	L150	S89
		H419	P347	L279	L213	I151	Q90
		K420	E348	K280	E214	E152	I91
		A421	R349	A280	K215	F92	S92
		V422	V350	Q281	V216	C154	S93
		E423	R351	A282	T217	Q155	Q94
K494	I424	A352	G283	F284	V156	A95	A95
	G425	V353	G283	T218	G157	M96	
	G426		R285	Q220	M158		
	L496	L356	V286	F221	E159		R99
	V497	N357	L287	P222	K160	S100	
	L498	V429	T358	E223	P161	I101	
	R499	N430	P359	A288	E162	N102	
	P500	T431	F360	D290	P163	R103	
	E501	P432	M361	M291	Q164	P104	
	M502	E433	P362	K292	F227	M105	
K504	S503	D434	P363	G293	V166	L106	
	K504	P435	D364	Y294	P228	Q107	
	N505	N436	P365	G295	F168	A108	
	M506	L437	D366	D296	N231	L169	
	E507	S438	V367	S297	C230	L170	
		R508	P368	S298	P232	L170	
		K449	P369	S299	N233	D171	
	W509	T440	M370	D234	T172	A111	
	L510	T441	K371	V235	K173	L112	
	P511			S236	A174	K113	
F512	L513	E447	V372	E302	K174	K114	
	K514	P448	R374	I303	G238	K115	
	D515	Y449	S375	E305	H237	G116	
	G516	L450	R376	A307	K175	F117	
	H517	Q451	P377	M308	P177	T118	
			V378	R307		T119	
			F379	A308	V180	C120	
			N380	L310	F182	I121	
			G457	L248	L183	V122	
	D520	F458	Y381	L311	F186	T123	

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	151.90Å 143.00Å 60.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	91.0 (20.00-2.80)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.201 , 0.312	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8237	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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: CPU

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	0.72	0/3981	1.27	60/5397 (1.1%)
1	B	0.70	0/4413	1.25	62/5984 (1.0%)
All	All	0.71	0/8394	1.26	122/11381 (1.1%)

There are no bond length outliers.

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	387	GLU	CA-C-N	12.31	133.10	119.93
1	A	387	GLU	C-N-CA	12.31	133.10	119.93
1	B	231	ASN	C-N-CD	-11.76	94.72	120.60
1	B	231	ASN	CA-C-N	10.61	152.46	127.00
1	B	231	ASN	C-N-CA	10.61	152.46	127.00
1	B	387	GLU	CA-C-N	10.47	132.93	119.84
1	B	387	GLU	C-N-CA	10.47	132.93	119.84
1	A	92	PHE	N-CA-C	-9.42	103.89	114.62
1	B	246	ILE	N-CA-C	9.17	121.37	107.99
1	A	246	ILE	N-CA-C	8.89	120.96	107.99
1	A	209	ALA	N-CA-C	-8.64	101.99	112.54
1	A	53	LEU	N-CA-C	-8.48	102.04	111.28
1	B	427	ILE	N-CA-C	-8.18	104.78	112.96
1	A	50	THR	N-CA-C	-7.41	104.48	113.97
1	B	422	THR	N-CA-C	7.39	120.27	111.33
1	B	299	SER	CA-C-N	-7.18	112.98	120.38
1	B	299	SER	C-N-CA	-7.18	112.98	120.38
1	B	263	HIS	N-CA-C	7.08	119.66	110.53
1	A	299	SER	CA-C-N	-7.04	113.13	120.38
1	A	299	SER	C-N-CA	-7.04	113.13	120.38
1	B	529	LYS	CA-C-N	7.04	126.29	118.97
1	B	529	LYS	C-N-CA	7.04	126.29	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	213	LEU	N-CA-C	-6.86	105.03	113.19
1	A	351	ARG	N-CA-C	-6.84	103.88	111.82
1	B	364	ASP	CA-C-N	6.79	126.25	118.85
1	B	364	ASP	C-N-CA	6.79	126.25	118.85
1	A	263	HIS	N-CA-C	6.59	119.03	110.53
1	A	220	GLN	N-CA-C	6.58	120.22	109.76
1	B	231	ASN	N-CA-C	6.56	121.04	108.12
1	A	234	ASP	N-CA-C	-6.49	105.32	112.72
1	B	9	ASP	N-CA-C	-6.47	100.90	110.48
1	B	328	VAL	N-CA-C	-6.47	98.54	107.99
1	A	100	SER	N-CA-C	6.41	116.53	108.45
1	A	529	LYS	CA-C-N	6.39	125.62	118.97
1	A	529	LYS	C-N-CA	6.39	125.62	118.97
1	B	106	LEU	N-CA-C	-6.37	104.34	111.28
1	B	114	LYS	N-CA-C	-6.36	104.26	111.07
1	B	351	ARG	N-CA-C	-6.31	103.92	111.69
1	A	422	THR	N-CA-C	-6.24	99.11	109.46
1	B	32	LEU	CA-C-N	6.22	127.20	119.98
1	B	32	LEU	C-N-CA	6.22	127.20	119.98
1	A	328	VAL	N-CA-C	-6.21	98.92	107.99
1	A	333	ASP	CB-CA-C	-6.17	109.47	116.63
1	A	423	GLU	N-CA-C	-6.15	97.71	110.80
1	B	333	ASP	CB-CA-C	-6.14	109.51	116.63
1	A	289	ILE	N-CA-C	6.12	118.00	109.55
1	A	497	VAL	N-CA-C	-6.11	101.12	109.55
1	A	233	ASN	N-CA-C	-6.07	103.37	112.54
1	B	226	LEU	CA-C-N	6.02	126.03	119.89
1	B	226	LEU	C-N-CA	6.02	126.03	119.89
1	B	420	LYS	N-CA-C	6.01	118.73	111.40
1	B	71	TYR	N-CA-C	-6.00	104.66	111.14
1	B	132	LYS	N-CA-C	-5.95	104.62	112.72
1	B	100	SER	N-CA-C	5.93	117.60	109.18
1	A	364	ASP	CA-C-N	5.92	125.62	119.05
1	A	364	ASP	C-N-CA	5.92	125.62	119.05
1	A	300	PRO	CA-C-N	5.90	125.60	119.05
1	A	300	PRO	C-N-CA	5.90	125.60	119.05
1	B	210	LEU	N-CA-C	-5.89	105.94	113.01
1	A	258	ALA	N-CA-C	5.88	119.49	110.20
1	B	101	ILE	N-CA-C	5.86	117.13	109.58
1	A	471	ASN	N-CA-C	-5.83	104.11	111.11
1	B	258	ALA	N-CA-C	5.83	119.42	110.20
1	B	289	ILE	N-CA-C	5.83	117.60	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	CYS	N-CA-C	5.81	117.08	108.60
1	B	113	LYS	N-CA-C	-5.80	104.33	111.40
1	B	233	ASN	N-CA-C	-5.79	105.71	112.89
1	B	200	THR	N-CA-C	5.78	118.50	107.75
1	B	57	LYS	N-CA-C	-5.77	104.42	112.45
1	A	14	LEU	N-CA-C	-5.76	105.92	113.17
1	A	213	LEU	N-CA-C	-5.75	106.11	113.01
1	B	471	ASN	N-CA-C	-5.73	104.24	111.11
1	A	280	ALA	N-CA-C	-5.72	104.95	111.07
1	A	376	ILE	CA-C-N	5.71	125.24	119.19
1	A	376	ILE	C-N-CA	5.71	125.24	119.19
1	A	48	GLY	CA-C-N	5.70	125.80	119.87
1	A	48	GLY	C-N-CA	5.70	125.80	119.87
1	B	142	GLU	N-CA-C	5.70	118.26	111.71
1	A	494	LYS	N-CA-C	5.69	119.99	112.25
1	B	204	HIS	N-CA-C	-5.67	103.16	110.19
1	A	528	GLU	N-CA-C	5.66	118.65	111.69
1	B	280	ALA	N-CA-C	-5.64	105.04	111.07
1	B	528	GLU	N-CA-C	5.63	118.62	111.69
1	B	120	CYS	N-CA-C	5.62	117.38	108.79
1	A	439	LYS	N-CA-C	-5.60	106.43	113.20
1	B	376	ILE	CA-C-N	5.57	125.10	119.19
1	B	376	ILE	C-N-CA	5.57	125.10	119.19
1	A	515	ARG	N-CA-C	5.53	117.59	109.24
1	A	129	ASP	N-CA-C	-5.52	106.13	112.92
1	A	194	ARG	N-CA-C	-5.48	105.38	111.36
1	B	296	ASP	N-CA-C	5.48	119.95	113.16
1	B	497	VAL	N-CA-C	-5.46	100.50	109.12
1	A	536	ILE	N-CA-C	5.45	115.65	110.42
1	B	300	PRO	CA-C-N	5.45	125.10	119.05
1	B	300	PRO	C-N-CA	5.45	125.10	119.05
1	A	296	ASP	N-CA-C	5.45	119.91	113.16
1	A	142	GLU	N-CA-C	5.42	117.00	111.14
1	B	12	GLY	CA-C-N	-5.41	117.42	123.16
1	B	12	GLY	C-N-CA	-5.41	117.42	123.16
1	A	189	ASN	N-CA-C	-5.40	106.74	113.38
1	B	439	LYS	N-CA-C	-5.39	106.67	113.20
1	B	189	ASN	N-CA-C	-5.38	106.68	113.18
1	A	106	LEU	N-CA-C	-5.36	105.44	111.28
1	B	494	LYS	N-CA-C	5.35	119.53	112.25
1	A	228	VAL	CA-C-N	5.33	126.50	119.84
1	A	228	VAL	C-N-CA	5.33	126.50	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	MET	N-CA-C	-5.32	105.38	111.07
1	A	368	SER	CA-C-N	5.29	124.92	119.05
1	A	368	SER	C-N-CA	5.29	124.92	119.05
1	A	176	LYS	CA-C-N	5.27	124.88	119.56
1	A	176	LYS	C-N-CA	5.27	124.88	119.56
1	A	188	SER	N-CA-C	-5.26	106.70	113.01
1	B	515	ARG	N-CA-C	5.26	117.38	109.23
1	B	368	SER	CA-C-N	5.24	124.86	119.05
1	B	368	SER	C-N-CA	5.24	124.86	119.05
1	B	536	ILE	N-CA-C	5.24	115.45	110.42
1	A	132	LYS	N-CA-C	-5.23	105.14	112.25
1	B	415	PHE	N-CA-C	5.19	121.86	110.80
1	A	151	ILE	N-CA-C	5.19	111.76	106.21
1	A	415	PHE	N-CA-C	5.13	121.74	110.80
1	B	55	LYS	N-CA-C	-5.09	107.06	113.28
1	A	269	TRP	N-CA-C	-5.02	106.42	112.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3879	0	3863	397	0
1	B	4299	0	4270	460	0
2	A	19	0	24	5	0
2	B	19	0	24	5	0
3	A	12	0	0	0	0
3	B	9	0	0	0	0
All	All	8237	0	8181	839	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 52.

All (839) 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:B:232:PRO:HD2	1:B:233:ASN:H	1.11	1.11
1:B:5:VAL:HG21	1:B:173:LEU:HD21	1.35	1.08
1:A:101:ILE:HG21	1:A:106:LEU:HD12	1.38	1.06
1:B:300:PRO:HG2	1:B:305:GLU:HG2	1.36	1.05
1:B:496:ILE:H	1:B:496:ILE:HD12	1.19	1.04
1:B:424:ILE:HD13	1:B:424:ILE:H	1.19	1.04
1:A:300:PRO:HG2	1:A:305:GLU:HG2	1.36	1.02
1:A:90:GLN:HG3	1:A:91:ILE:HD13	1.37	1.02
1:B:158:MET:HE3	1:B:165:ILE:HA	1.41	1.02
1:A:496:ILE:HD12	1:A:496:ILE:H	1.20	1.01
1:A:232:PRO:HD2	1:A:233:ASN:H	1.27	0.99
1:A:166:TYR:O	1:A:170:LEU:HD12	1.60	0.98
1:A:52:GLN:HG3	1:A:58:ILE:HD11	1.44	0.98
1:B:19:ILE:HD11	1:B:96:MET:HA	1.45	0.98
1:B:263:HIS:CD2	1:B:291:MET:HG2	2.00	0.96
1:A:263:HIS:CD2	1:A:291:MET:HG2	2.01	0.94
1:A:430:ASN:HD22	1:A:430:ASN:H	1.06	0.94
1:A:193:ALA:O	1:A:198:MET:HB2	1.68	0.94
1:A:13:VAL:HG22	1:A:203:VAL:HG21	1.48	0.94
1:B:155:GLN:OE1	1:B:155:GLN:HA	1.69	0.93
1:A:155:GLN:HA	1:A:155:GLN:OE1	1.69	0.92
1:A:447:GLU:HA	1:A:450:ILE:HD13	1.51	0.92
1:B:447:GLU:HA	1:B:450:ILE:HD13	1.51	0.92
1:A:322:LEU:HB3	1:A:324:ILE:CD1	2.00	0.92
1:B:106:LEU:HD21	1:B:146:HIS:CD2	2.06	0.91
1:A:205:ASN:ND2	1:A:209:ALA:H	1.69	0.91
1:B:322:LEU:HB3	1:B:324:ILE:CD1	2.00	0.90
1:A:205:ASN:HD21	1:A:209:ALA:HB3	1.36	0.90
1:B:13:VAL:HB	1:B:203:VAL:HG11	1.54	0.88
1:B:72:ARG:HA	1:B:75:SER:HB3	1.53	0.88
1:A:17:PRO:HD2	1:A:99:ARG:HA	1.54	0.88
1:A:140:MET:HE3	1:A:140:MET:HA	1.53	0.88
1:B:232:PRO:CD	1:B:233:ASN:H	1.87	0.87
1:A:232:PRO:CD	1:A:233:ASN:H	1.87	0.87
1:A:94:GLN:CD	1:A:94:GLN:H	1.82	0.87
1:B:424:ILE:H	1:B:424:ILE:CD1	1.87	0.86
1:B:127:LEU:HD12	1:B:127:LEU:H	1.40	0.86
1:B:5:VAL:HG23	1:B:118:THR:O	1.75	0.85
1:A:230:CYS:O	1:A:231:ASN:HB3	1.75	0.85
1:B:122:VAL:HB	1:B:151:ILE:HG13	1.56	0.85
1:A:211:ARG:HA	1:A:214:GLU:HB2	1.59	0.85
1:A:48:GLY:N	1:A:51:GLU:HB2	1.91	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ASN:HD22	1:A:104:PRO:HD2	1.41	0.84
1:B:496:ILE:H	1:B:496:ILE:CD1	1.90	0.84
1:A:529:LYS:O	1:A:533:VAL:HG23	1.78	0.84
1:B:404:LYS:O	1:B:408:ARG:HD2	1.77	0.84
1:B:232:PRO:O	1:B:235:VAL:HG22	1.78	0.83
1:A:404:LYS:O	1:A:408:ARG:HD2	1.78	0.83
1:B:73:LYS:HA	1:B:73:LYS:HZ2	1.43	0.83
1:A:422:THR:O	1:A:423:GLU:HB2	1.77	0.83
1:A:215:LYS:HG2	1:A:220:GLN:HA	1.61	0.82
1:A:496:ILE:H	1:A:496:ILE:CD1	1.91	0.82
1:B:322:LEU:HB3	1:B:324:ILE:HD13	1.61	0.81
1:B:424:ILE:HD13	1:B:424:ILE:N	1.95	0.81
1:B:529:LYS:O	1:B:533:VAL:HG23	1.81	0.81
1:B:5:VAL:HG13	1:B:180:VAL:HB	1.61	0.81
1:B:339:VAL:HG13	1:B:353:VAL:HG12	1.62	0.81
1:A:369:PRO:O	1:A:372:VAL:HG22	1.80	0.81
1:B:232:PRO:HD2	1:B:233:ASN:N	1.92	0.81
1:B:58:ILE:HD12	1:B:63:TRP:HB2	1.64	0.80
1:B:369:PRO:O	1:B:372:VAL:HG22	1.80	0.80
1:A:463:ASN:HA	1:A:466:ARG:HG3	1.62	0.80
1:A:96:MET:SD	1:A:136:LEU:HD23	2.21	0.80
1:A:446:ILE:O	1:A:450:ILE:HD12	1.81	0.80
1:B:463:ASN:HA	1:B:466:ARG:HG3	1.62	0.80
1:A:535:GLN:O	1:A:539:LYS:HD3	1.82	0.80
1:B:50:THR:CG2	1:B:63:TRP:HE1	1.95	0.80
1:B:270:PHE:CE1	1:B:273:ARG:HD3	2.17	0.80
1:A:62:GLN:O	1:A:63:TRP:HD1	1.64	0.80
1:A:91:ILE:C	1:A:94:GLN:HE22	1.90	0.80
1:A:102:ASN:ND2	1:A:104:PRO:HD2	1.97	0.79
1:A:133:ARG:HG2	1:B:348:GLU:HA	1.63	0.79
1:A:339:VAL:HG13	1:A:353:VAL:HG12	1.63	0.79
1:A:205:ASN:HD21	1:A:209:ALA:CB	1.94	0.79
1:B:5:VAL:HG21	1:B:173:LEU:CD2	2.11	0.79
1:B:158:MET:O	1:B:165:ILE:HG12	1.82	0.79
1:B:535:GLN:O	1:B:539:LYS:HD3	1.83	0.79
1:B:431:THR:HG22	1:B:432:PRO:HD2	1.63	0.78
1:A:270:PHE:CE1	1:A:273:ARG:HD3	2.19	0.78
1:A:124:ASN:HA	1:A:153:SER:HB3	1.65	0.77
1:B:529:LYS:HB3	1:B:532:GLU:HG3	1.66	0.77
1:A:497:VAL:O	1:A:498:LEU:HB2	1.84	0.77
1:B:300:PRO:CG	1:B:305:GLU:HG2	2.13	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:LEU:O	1:B:117:PHE:HB2	1.85	0.77
1:A:159:ILE:HD12	1:A:159:ILE:O	1.85	0.76
1:B:50:THR:HG23	1:B:63:TRP:HE1	1.49	0.76
1:A:13:VAL:CG2	1:A:203:VAL:HG21	2.15	0.76
1:B:320:ASP:OD1	1:B:349:ARG:NH2	2.19	0.76
1:B:483:ILE:HB	1:B:510:ILE:HG12	1.67	0.76
1:B:446:ILE:O	1:B:450:ILE:HD12	1.86	0.76
1:A:322:LEU:HB3	1:A:324:ILE:HD13	1.66	0.75
1:A:52:GLN:CG	1:A:58:ILE:HD11	2.17	0.75
1:A:529:LYS:HB3	1:A:532:GLU:HG3	1.66	0.75
1:B:424:ILE:HB	1:B:429:VAL:HG11	1.67	0.75
1:A:162:GLU:HB3	1:A:164:GLN:HE21	1.51	0.75
1:A:292:LYS:NZ	1:A:305:GLU:HG3	2.03	0.74
1:B:49:PRO:HD2	1:B:67:MET:HE2	1.68	0.74
1:A:446:ILE:HG22	1:A:450:ILE:HD11	1.68	0.74
1:B:292:LYS:NZ	1:B:305:GLU:HG3	2.02	0.74
1:B:446:ILE:HG22	1:B:450:ILE:HD11	1.69	0.74
1:B:9:ASP:O	1:B:13:VAL:HG22	1.87	0.74
1:A:499:ARG:O	1:A:502:MET:HG3	1.88	0.74
1:A:320:ASP:OD1	1:A:349:ARG:NH2	2.19	0.73
1:B:177:PRO:O	1:B:198:MET:HA	1.89	0.73
1:A:300:PRO:CG	1:A:305:GLU:HG2	2.14	0.73
1:A:231:ASN:HB2	1:A:232:PRO:HA	1.69	0.73
1:A:158:MET:HE3	1:A:165:ILE:HA	1.69	0.73
1:A:205:ASN:ND2	1:A:209:ALA:HB3	2.03	0.73
1:A:483:ILE:HB	1:A:510:ILE:HG12	1.69	0.73
1:B:127:LEU:HD12	1:B:127:LEU:N	2.03	0.73
1:B:497:VAL:O	1:B:498:LEU:HB2	1.86	0.73
1:B:177:PRO:O	1:B:198:MET:HG3	1.87	0.72
1:B:499:ARG:O	1:B:502:MET:HG3	1.89	0.72
1:B:510:ILE:HG22	1:B:513:LEU:HB2	1.71	0.72
1:B:64:VAL:HB	1:B:65:PRO:CD	2.19	0.72
1:B:8:PHE:CD1	1:B:8:PHE:N	2.57	0.72
1:B:58:ILE:CD1	1:B:63:TRP:HB2	2.19	0.72
1:B:359:PRO:HD2	1:B:361:MET:HE2	1.71	0.72
1:A:159:ILE:HD12	1:A:159:ILE:C	2.15	0.72
1:B:121:ILE:O	1:B:151:ILE:HG12	1.89	0.71
1:A:348:GLU:HA	1:B:133:ARG:CG	2.19	0.71
1:B:83:PRO:HG2	1:B:86:PHE:HB2	1.69	0.71
1:B:201:ILE:HD12	1:B:201:ILE:N	2.05	0.71
1:B:420:LYS:HB3	1:B:424:ILE:HD12	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ILE:O	1:A:165:ILE:HD11	1.91	0.71
1:B:8:PHE:CE1	1:B:147:PHE:HE2	2.08	0.71
1:B:158:MET:HE3	1:B:165:ILE:CA	2.18	0.71
1:A:162:GLU:O	1:A:165:ILE:HG13	1.90	0.71
1:A:10:LEU:O	1:A:12:GLY:N	2.24	0.70
1:A:360:PHE:HB3	1:A:506:MET:HE3	1.73	0.70
1:B:232:PRO:HD2	1:B:233:ASN:HD22	1.55	0.70
1:A:359:PRO:HD2	1:A:361:MET:HE2	1.72	0.70
1:B:531:THR:HG23	1:B:532:GLU:OE2	1.90	0.70
1:B:103:ARG:O	1:B:107:GLN:HB2	1.92	0.70
1:A:58:ILE:HG22	1:A:62:GLN:HB3	1.73	0.70
1:B:360:PHE:HB3	1:B:506:MET:HE3	1.72	0.70
1:B:5:VAL:HG11	1:B:173:LEU:HD23	1.74	0.70
1:B:158:MET:CE	1:B:165:ILE:HA	2.22	0.70
1:A:136:LEU:O	1:A:140:MET:HG2	1.92	0.69
1:B:496:ILE:HD12	1:B:496:ILE:N	2.01	0.69
1:A:324:ILE:HD12	1:A:324:ILE:N	2.08	0.69
1:B:7:ALA:HA	1:B:120:CYS:O	1.91	0.69
1:B:128:ASP:O	1:B:133:ARG:HG3	1.92	0.69
1:B:181:VAL:HG23	1:B:201:ILE:CD1	2.22	0.69
1:B:259:LEU:HD12	1:B:259:LEU:O	1.92	0.69
1:A:187:GLY:HA2	1:A:190:LEU:HD12	1.74	0.69
1:A:416:ILE:HG23	1:A:427:ILE:CG1	2.23	0.69
1:B:497:VAL:HG13	2:B:1200:CPU:C12	2.21	0.69
1:B:77:ALA:O	1:B:78:CYS:HB2	1.92	0.69
1:B:212:GLU:C	1:B:214:GLU:H	2.00	0.69
1:B:229:PRO:HB2	1:B:231:ASN:HD21	1.56	0.69
1:A:348:GLU:HA	1:B:133:ARG:HG2	1.72	0.69
1:A:360:PHE:CB	1:A:506:MET:HE3	2.23	0.69
1:B:124:ASN:HA	1:B:153:SER:HB3	1.75	0.69
1:B:529:LYS:HB3	1:B:532:GLU:CG	2.22	0.69
1:B:420:LYS:C	1:B:424:ILE:HD11	2.18	0.69
1:A:510:ILE:HG22	1:A:513:LEU:HB2	1.74	0.69
1:A:216:VAL:CG1	1:A:217:THR:N	2.56	0.68
1:B:49:PRO:HB2	1:B:67:MET:HG2	1.74	0.68
1:B:103:ARG:HB2	1:B:104:PRO:HD3	1.75	0.68
1:A:52:GLN:HG3	1:A:58:ILE:CD1	2.22	0.68
1:A:430:ASN:H	1:A:430:ASN:ND2	1.84	0.68
1:B:159:ILE:O	1:B:165:ILE:HD11	1.92	0.68
1:B:222:PRO:HG2	1:B:225:PRO:HG3	1.73	0.68
1:A:8:PHE:CD1	1:A:147:PHE:HE2	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:ILE:HD12	1:A:496:ILE:N	2.03	0.68
1:B:360:PHE:CB	1:B:506:MET:HE3	2.23	0.68
1:B:427:ILE:HG13	1:B:428:LEU:HD13	1.75	0.68
1:A:214:GLU:HA	1:A:214:GLU:OE1	1.91	0.68
1:A:5:VAL:HB	1:A:118:THR:HB	1.76	0.68
1:B:458:PHE:C	1:B:461:PRO:HD2	2.19	0.68
1:A:458:PHE:C	1:A:461:PRO:HD2	2.19	0.68
1:B:93:SER:HB2	1:B:132:LYS:HE2	1.76	0.68
1:A:92:PHE:N	1:A:94:GLN:HE22	1.90	0.67
1:A:529:LYS:HB3	1:A:532:GLU:CG	2.23	0.67
1:A:157:GLY:O	1:A:158:MET:HG2	1.95	0.67
1:B:72:ARG:CA	1:B:75:SER:HB3	2.25	0.67
1:A:206:THR:O	1:A:207:ALA:HB3	1.95	0.67
1:A:223:GLU:O	1:A:225:PRO:HD3	1.94	0.67
1:A:513:LEU:HD22	1:A:514:LYS:O	1.93	0.67
1:A:205:ASN:ND2	1:A:209:ALA:N	2.43	0.67
1:A:216:VAL:HG12	1:A:217:THR:HG23	1.76	0.67
1:A:5:VAL:HG22	1:A:180:VAL:HB	1.77	0.66
1:B:19:ILE:HD11	1:B:96:MET:CA	2.23	0.66
1:A:205:ASN:C	1:A:207:ALA:H	2.04	0.66
1:B:513:LEU:HD22	1:B:514:LYS:O	1.95	0.66
1:A:157:GLY:C	1:A:158:MET:HG2	2.20	0.66
1:A:531:THR:HG23	1:A:532:GLU:OE2	1.95	0.66
1:A:124:ASN:HD21	1:A:160:LYS:HB2	1.60	0.66
1:B:181:VAL:HA	1:B:199:VAL:HB	1.76	0.66
1:A:259:LEU:HD12	1:A:259:LEU:O	1.96	0.66
1:B:532:GLU:O	1:B:536:ILE:HG13	1.96	0.65
1:A:137:ALA:O	1:A:141:CYS:N	2.27	0.65
1:A:15:ALA:O	1:A:16:LEU:HD23	1.97	0.65
1:A:108:ALA:O	1:A:111:ALA:HB3	1.96	0.65
1:A:292:LYS:HZ3	1:A:305:GLU:HG3	1.60	0.65
1:B:499:ARG:HB3	1:B:501:GLU:HG3	1.79	0.65
1:A:272:TRP:HA	1:A:275:GLN:HE21	1.60	0.65
1:B:272:TRP:HA	1:B:275:GLN:HE21	1.61	0.65
1:B:497:VAL:HG13	2:B:1200:CPU:H121	1.79	0.65
1:B:324:ILE:N	1:B:324:ILE:HD12	2.10	0.65
1:A:264:GLY:HA3	1:A:333:ASP:HB3	1.78	0.65
1:A:416:ILE:HG23	1:A:427:ILE:HG13	1.77	0.64
1:A:532:GLU:O	1:A:536:ILE:HG13	1.97	0.64
1:B:25:ARG:O	1:B:29:ALA:HB2	1.97	0.64
1:B:264:GLY:HA3	1:B:333:ASP:HB3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:PRO:O	1:A:198:MET:HG3	1.97	0.64
1:A:211:ARG:CA	1:A:214:GLU:HB2	2.26	0.64
1:A:255:SER:O	1:A:256:GLY:O	2.16	0.64
1:B:64:VAL:HB	1:B:65:PRO:HD3	1.79	0.64
1:A:101:ILE:CG2	1:A:106:LEU:HD12	2.21	0.64
1:A:499:ARG:HB3	1:A:501:GLU:HG3	1.80	0.64
1:B:158:MET:HE1	1:B:168:PHE:CB	2.28	0.64
1:B:255:SER:O	1:B:256:GLY:O	2.16	0.64
1:A:169:LEU:O	1:A:173:LEU:HB2	1.97	0.64
1:B:119:THR:HG23	1:B:148:ASP:H	1.61	0.63
1:B:469:GLU:O	1:B:472:TRP:HB3	1.98	0.63
1:A:5:VAL:HG21	1:A:173:LEU:CD2	2.28	0.63
1:A:190:LEU:HD22	1:A:200:THR:HG22	1.79	0.63
1:B:72:ARG:HD3	1:B:73:LYS:NZ	2.13	0.63
1:B:158:MET:HE1	1:B:168:PHE:HB2	1.81	0.63
1:A:9:ASP:OD1	1:A:11:ASP:HB2	1.98	0.63
1:B:248:LEU:HA	1:B:297:SER:HB3	1.79	0.63
1:A:106:LEU:HD22	1:A:110:ILE:HD11	1.80	0.63
1:B:124:ASN:HA	1:B:153:SER:CB	2.29	0.63
1:B:292:LYS:CE	1:B:305:GLU:HG3	2.28	0.63
1:A:205:ASN:ND2	1:A:209:ALA:CB	2.61	0.63
1:A:248:LEU:HA	1:A:297:SER:HB3	1.79	0.63
1:B:535:GLN:HB3	1:B:539:LYS:HZ2	1.64	0.63
1:A:125:ASN:OD1	1:A:152:GLU:HB3	1.99	0.63
1:A:214:GLU:HB3	1:A:221:PHE:CZ	2.33	0.63
1:A:292:LYS:CE	1:A:305:GLU:HG3	2.29	0.62
1:A:158:MET:O	1:A:165:ILE:HG12	1.99	0.62
1:B:32:LEU:HB3	1:B:33:PRO:HD2	1.82	0.62
1:A:193:ALA:HA	1:A:198:MET:HE3	1.80	0.62
1:A:232:PRO:CD	1:A:233:ASN:N	2.60	0.62
1:A:497:VAL:HG13	2:A:1100:CPU:H122	1.81	0.62
1:B:26:SER:HA	1:B:29:ALA:HB3	1.81	0.62
1:B:75:SER:OG	1:B:76:LYS:N	2.31	0.62
1:B:232:PRO:HG2	1:B:233:ASN:ND2	2.14	0.62
1:A:62:GLN:HE22	1:B:481:ARG:HA	1.63	0.62
1:B:180:VAL:HG22	1:B:198:MET:CG	2.30	0.62
1:B:181:VAL:HG23	1:B:201:ILE:HD13	1.80	0.62
1:A:216:VAL:HG12	1:A:217:THR:N	2.14	0.62
1:A:230:CYS:HB3	1:A:277:PRO:HG3	1.82	0.62
1:B:292:LYS:HZ3	1:B:305:GLU:HG3	1.62	0.62
1:A:206:THR:O	1:A:207:ALA:CB	2.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ILE:HD11	1:A:288:ALA:CB	2.29	0.61
1:A:190:LEU:CD2	1:A:200:THR:HG22	2.30	0.61
1:A:433:GLU:HA	1:A:433:GLU:OE1	1.99	0.61
1:A:124:ASN:ND2	1:A:160:LYS:HB2	2.14	0.61
1:A:205:ASN:HD21	1:A:209:ALA:N	1.98	0.61
1:B:524:TRP:HB3	1:B:527:ILE:HD12	1.81	0.61
1:B:32:LEU:HD22	1:B:36:PHE:CD2	2.35	0.61
1:B:141:CYS:O	1:B:144:SER:OG	2.17	0.61
1:B:380:ASN:ND2	1:B:422:THR:OG1	2.32	0.61
1:A:163:PRO:O	1:A:167:ASN:ND2	2.34	0.61
1:A:183:LEU:HD13	1:A:201:ILE:HB	1.82	0.61
1:A:193:ALA:O	1:A:198:MET:HE3	2.00	0.61
1:A:294:TYR:CZ	1:A:461:PRO:HB3	2.36	0.61
1:B:62:GLN:O	1:B:65:PRO:HD2	2.01	0.61
1:B:119:THR:HG23	1:B:147:PHE:HA	1.83	0.61
1:B:276:ILE:HD11	1:B:288:ALA:CB	2.30	0.61
1:A:339:VAL:CG1	1:A:353:VAL:HG12	2.30	0.60
1:A:469:GLU:O	1:A:472:TRP:HB3	2.01	0.60
1:A:153:SER:OG	1:A:154:CYS:N	2.31	0.60
1:A:205:ASN:HD21	1:A:209:ALA:H	1.48	0.60
1:A:524:TRP:HB3	1:A:527:ILE:HD12	1.84	0.60
1:B:339:VAL:CG1	1:B:353:VAL:HG12	2.31	0.60
1:B:194:ARG:HB2	1:B:200:THR:HG21	1.84	0.60
1:B:39:GLY:HA2	1:B:43:THR:CG2	2.31	0.60
1:B:107:GLN:HA	1:B:107:GLN:NE2	2.17	0.60
1:A:4:ARG:HA	1:A:179:GLU:O	2.01	0.60
1:B:119:THR:HG21	1:B:146:HIS:O	2.01	0.60
1:B:122:VAL:CB	1:B:151:ILE:HG13	2.31	0.60
1:A:201:ILE:HD13	1:A:213:LEU:HB3	1.84	0.60
1:A:287:LEU:O	1:A:289:ILE:HG13	2.02	0.60
1:A:293:GLY:HA2	1:A:299:SER:HA	1.84	0.60
1:B:122:VAL:HG11	1:B:182:PHE:HE1	1.67	0.60
1:B:4:ARG:HB3	1:B:4:ARG:CZ	2.32	0.60
1:A:177:PRO:O	1:A:198:MET:HA	2.02	0.59
1:B:421:ALA:N	1:B:424:ILE:HD11	2.18	0.59
1:A:216:VAL:HG12	1:A:217:THR:H	1.67	0.59
1:B:72:ARG:HA	1:B:75:SER:CB	2.30	0.59
1:B:183:LEU:CD1	1:B:201:ILE:HB	2.33	0.59
1:B:467:ASN:OD1	1:B:470:ARG:HD2	2.02	0.59
1:B:20:ALA:O	1:B:23:PHE:HB2	2.03	0.59
1:B:45:PHE:CE1	1:B:47:GLU:HB2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:GLN:HG3	1:A:91:ILE:N	2.18	0.59
1:A:215:LYS:HG3	1:A:221:PHE:CE1	2.38	0.59
1:B:54:MET:HB2	1:B:159:ILE:CG2	2.33	0.58
1:A:232:PRO:HG2	1:A:233:ASN:OD1	2.03	0.58
1:A:213:LEU:O	1:A:216:VAL:HG12	2.03	0.58
1:B:24:ARG:C	1:B:26:SER:H	2.11	0.58
1:A:304:GLU:H	1:A:304:GLU:CD	2.12	0.58
1:A:398:ASN:C	1:A:398:ASN:OD1	2.45	0.58
1:B:201:ILE:HD12	1:B:201:ILE:H	1.69	0.58
1:B:294:TYR:CZ	1:B:461:PRO:HB3	2.38	0.58
1:A:211:ARG:C	1:A:214:GLU:HB2	2.28	0.58
1:A:236:SER:HB2	1:B:322:LEU:HD12	1.85	0.58
1:B:8:PHE:CD1	1:B:147:PHE:HE2	2.21	0.58
1:B:293:GLY:HA2	1:B:299:SER:HA	1.83	0.58
1:A:309:GLU:HB2	1:A:474:TRP:CD2	2.38	0.58
1:A:347:PRO:O	1:B:133:ARG:HD2	2.04	0.58
1:B:304:GLU:CD	1:B:304:GLU:H	2.12	0.58
1:A:535:GLN:HB3	1:A:539:LYS:HZ2	1.67	0.57
1:B:37:LEU:C	1:B:39:GLY:H	2.09	0.57
1:B:228:VAL:O	1:B:277:PRO:HG2	2.03	0.57
1:B:309:GLU:HB2	1:B:474:TRP:CD2	2.38	0.57
1:B:420:LYS:HB3	1:B:424:ILE:CD1	2.33	0.57
1:A:94:GLN:CD	1:A:94:GLN:N	2.59	0.57
1:B:287:LEU:O	1:B:289:ILE:HG13	2.03	0.57
1:B:432:PRO:HB2	1:B:434:ASP:OD1	2.04	0.57
1:B:75:SER:HB2	1:B:82:LEU:HB3	1.86	0.57
1:A:169:LEU:HD11	1:A:173:LEU:HD22	1.85	0.57
1:B:160:LYS:HA	1:B:165:ILE:CD1	2.34	0.57
1:B:272:TRP:HE3	1:B:275:GLN:HG3	1.69	0.57
1:B:102:ASN:O	1:B:105:MET:HB2	2.04	0.57
1:B:212:GLU:C	1:B:214:GLU:N	2.61	0.57
1:B:398:ASN:OD1	1:B:398:ASN:C	2.48	0.57
1:B:417:ALA:HB3	1:B:427:ILE:HA	1.85	0.57
1:B:511:PRO:C	1:B:513:LEU:H	2.12	0.57
1:B:434:ASP:N	1:B:435:PRO:CD	2.68	0.57
1:B:91:ILE:HG13	1:B:92:PHE:N	2.19	0.56
1:A:467:ASN:OD1	1:A:470:ARG:HD2	2.05	0.56
1:A:53:LEU:HD23	1:A:59:THR:O	2.05	0.56
1:B:44:GLU:O	1:B:46:PRO:HD3	2.05	0.56
1:B:46:PRO:HG2	1:B:159:ILE:HD11	1.87	0.56
1:B:51:GLU:O	1:B:55:LYS:HG3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ASN:OD1	1:B:105:MET:HG3	2.05	0.56
1:B:222:PRO:CG	1:B:225:PRO:HG3	2.35	0.56
1:A:106:LEU:HD21	1:A:146:HIS:CD2	2.40	0.56
1:A:272:TRP:HE3	1:A:275:GLN:HG3	1.70	0.56
1:B:270:PHE:CZ	1:B:273:ARG:HD3	2.40	0.56
1:B:458:PHE:HB3	1:B:462:LEU:HD12	1.87	0.56
1:A:510:ILE:O	1:A:513:LEU:HB2	2.05	0.56
1:A:230:CYS:O	1:A:231:ASN:CB	2.52	0.56
1:B:426:GLY:HA3	1:B:429:VAL:HG23	1.88	0.56
1:A:192:PRO:O	1:A:195:ASP:HB2	2.05	0.56
1:A:214:GLU:HB3	1:A:221:PHE:HZ	1.69	0.56
1:A:270:PHE:CZ	1:A:273:ARG:HD3	2.41	0.56
1:A:307:ALA:O	1:A:311:LEU:HG	2.05	0.56
1:B:72:ARG:HD3	1:B:73:LYS:HZ1	1.70	0.56
1:B:292:LYS:HE2	1:B:305:GLU:HG3	1.88	0.56
1:B:8:PHE:O	1:B:121:ILE:HG23	2.05	0.56
1:B:322:LEU:C	1:B:324:ILE:HD12	2.30	0.56
1:A:426:GLY:HA3	1:A:429:VAL:CG2	2.36	0.56
1:B:421:ALA:HA	1:B:426:GLY:O	2.05	0.56
1:B:33:PRO:O	1:B:34:ARG:C	2.48	0.55
1:A:446:ILE:HG22	1:A:450:ILE:CD1	2.36	0.55
1:B:232:PRO:CD	1:B:233:ASN:HD22	2.19	0.55
1:A:230:CYS:HB3	1:A:277:PRO:CG	2.36	0.55
1:B:26:SER:O	1:B:30:LEU:HB2	2.06	0.55
1:B:170:LEU:O	1:B:174:LYS:N	2.39	0.55
1:B:337:VAL:HG21	2:B:1200:CPU:H4	1.88	0.55
1:B:529:LYS:O	1:B:532:GLU:HG2	2.06	0.55
1:A:186:PHE:O	1:A:188:SER:N	2.39	0.55
1:B:50:THR:O	1:B:54:MET:HG2	2.06	0.55
1:A:159:ILE:C	1:A:159:ILE:CD1	2.79	0.55
1:A:407:PHE:C	1:A:408:ARG:HG2	2.30	0.55
1:A:426:GLY:HA3	1:A:429:VAL:HG23	1.89	0.55
1:A:231:ASN:HB2	1:A:232:PRO:CA	2.36	0.55
1:A:351:ARG:HD2	1:A:351:ARG:O	2.07	0.55
1:A:511:PRO:C	1:A:513:LEU:H	2.14	0.55
1:B:181:VAL:HG23	1:B:201:ILE:HD11	1.88	0.55
1:B:446:ILE:HG22	1:B:450:ILE:CD1	2.37	0.55
1:B:186:PHE:C	1:B:188:SER:H	2.15	0.54
1:A:61:SER:C	1:A:63:TRP:H	2.15	0.54
1:A:140:MET:HE3	1:A:140:MET:CA	2.28	0.54
1:B:222:PRO:HB2	1:B:225:PRO:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:ARG:HD2	1:B:351:ARG:O	2.06	0.54
1:A:292:LYS:HE2	1:A:305:GLU:HG3	1.89	0.54
1:B:510:ILE:O	1:B:513:LEU:HB2	2.06	0.54
1:B:203:VAL:HG12	1:B:203:VAL:O	2.06	0.54
1:B:372:VAL:CG2	1:B:373:ILE:HD12	2.37	0.54
1:A:264:GLY:HA3	1:A:333:ASP:CB	2.38	0.54
1:B:186:PHE:HB2	1:B:189:ASN:HD22	1.71	0.54
1:A:458:PHE:HB3	1:A:462:LEU:HD12	1.89	0.54
1:B:407:PHE:C	1:B:408:ARG:HG2	2.32	0.54
1:B:535:GLN:CB	1:B:539:LYS:HZ2	2.21	0.54
1:A:359:PRO:HD2	1:A:361:MET:CE	2.38	0.54
1:A:92:PHE:C	1:A:92:PHE:CD2	2.86	0.54
1:B:20:ALA:O	1:B:21:GLY:C	2.51	0.54
1:B:37:LEU:C	1:B:39:GLY:N	2.63	0.54
1:A:484:LEU:HD13	1:B:61:SER:OG	2.08	0.54
1:B:136:LEU:O	1:B:140:MET:HG2	2.08	0.54
1:B:157:GLY:C	1:B:158:MET:HG2	2.33	0.54
1:A:54:MET:O	1:A:154:CYS:CA	2.56	0.53
1:B:134:ASP:O	1:B:137:ALA:N	2.41	0.53
1:B:229:PRO:C	1:B:231:ASN:HD22	2.13	0.53
1:B:264:GLY:HA3	1:B:333:ASP:CB	2.38	0.53
1:B:358:THR:HG23	1:B:361:MET:HE3	1.89	0.53
1:A:170:LEU:HD23	1:A:175:ALA:O	2.07	0.53
1:A:60:PHE:C	1:A:62:GLN:N	2.64	0.53
1:A:497:VAL:CG1	2:A:1100:CPU:H122	2.38	0.53
1:B:9:ASP:OD1	1:B:11:ASP:O	2.26	0.53
1:B:30:LEU:HB3	1:B:32:LEU:CD1	2.39	0.53
1:B:106:LEU:O	1:B:110:ILE:HG13	2.08	0.53
1:A:5:VAL:HG21	1:A:173:LEU:HD21	1.89	0.53
1:B:497:VAL:HG13	2:B:1200:CPU:H122	1.90	0.53
1:B:497:VAL:CG1	2:B:1200:CPU:H122	2.38	0.53
1:A:140:MET:HA	1:A:140:MET:CE	2.34	0.53
1:A:529:LYS:O	1:A:532:GLU:HG2	2.08	0.53
1:B:125:ASN:HB2	1:B:152:GLU:HB3	1.89	0.53
1:A:322:LEU:C	1:A:324:ILE:HD12	2.33	0.53
1:B:187:GLY:HA2	1:B:190:LEU:HD12	1.89	0.53
1:B:534:ASN:O	1:B:535:GLN:C	2.52	0.53
1:A:358:THR:HG23	1:A:361:MET:HE3	1.91	0.53
1:B:73:LYS:HA	1:B:73:LYS:NZ	2.17	0.53
1:B:212:GLU:HA	1:B:215:LYS:HG3	1.89	0.53
1:A:48:GLY:O	1:A:52:GLN:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:TRP:CZ3	2:A:1100:CPU:H4	2.44	0.53
1:B:45:PHE:CZ	1:B:47:GLU:HB2	2.44	0.53
1:B:375:SER:OG	1:B:376:ILE:N	2.42	0.53
1:B:434:ASP:O	1:B:435:PRO:C	2.51	0.53
1:B:20:ALA:O	1:B:23:PHE:N	2.42	0.52
1:A:122:VAL:HG22	1:A:122:VAL:O	2.08	0.52
1:A:156:VAL:HG23	1:A:158:MET:HG3	1.91	0.52
1:A:193:ALA:HA	1:A:198:MET:CE	2.39	0.52
1:A:236:SER:HB2	1:B:322:LEU:CD1	2.39	0.52
1:B:441:THR:OG1	1:B:446:ILE:HD11	2.09	0.52
1:A:372:VAL:CG2	1:A:373:ILE:HD12	2.39	0.52
1:B:11:ASP:HB2	1:B:99:ARG:NH1	2.24	0.52
1:B:86:PHE:CD1	1:B:87:SER:N	2.77	0.52
1:A:159:ILE:O	1:A:162:GLU:HB2	2.09	0.52
1:A:441:THR:OG1	1:A:446:ILE:HD11	2.10	0.52
1:A:160:LYS:HA	1:A:165:ILE:CD1	2.39	0.52
1:A:300:PRO:HG2	1:A:305:GLU:CG	2.26	0.52
1:B:75:SER:HB2	1:B:82:LEU:CB	2.39	0.52
1:B:125:ASN:C	1:B:154:CYS:HB3	2.35	0.52
1:B:328:VAL:HG22	1:B:352:ALA:HB3	1.92	0.52
1:A:301:PRO:HG2	1:A:302:GLU:OE1	2.10	0.52
1:A:538:ILE:O	1:A:542:GLN:HG2	2.10	0.52
1:A:54:MET:O	1:A:154:CYS:HA	2.09	0.52
1:A:211:ARG:HA	1:A:214:GLU:CB	2.37	0.52
1:A:458:PHE:O	1:A:461:PRO:HD2	2.10	0.52
1:B:356:LEU:O	1:B:357:ASN:HB2	2.10	0.52
1:A:246:ILE:N	1:A:246:ILE:HD12	2.25	0.52
1:B:276:ILE:HB	1:B:277:PRO:HD3	1.90	0.52
1:B:332:HIS:CD2	1:B:333:ASP:HB2	2.45	0.52
1:B:359:PRO:HD2	1:B:361:MET:CE	2.38	0.52
1:A:375:SER:OG	1:A:376:ILE:N	2.39	0.51
1:B:301:PRO:HG2	1:B:302:GLU:OE1	2.10	0.51
1:A:91:ILE:HA	1:A:94:GLN:OE1	2.09	0.51
1:A:381:TYR:CE1	1:A:382:GLN:HG3	2.45	0.51
1:B:77:ALA:O	1:B:78:CYS:CB	2.58	0.51
1:B:479:LEU:O	1:B:509:TRP:HZ3	1.94	0.51
1:A:112:LEU:HD23	1:A:117:PHE:CD2	2.45	0.51
1:B:64:VAL:CG1	1:B:89:SER:HB2	2.41	0.51
1:A:62:GLN:NE2	1:B:481:ARG:HA	2.25	0.51
1:B:458:PHE:O	1:B:461:PRO:HD2	2.11	0.51
1:B:381:TYR:CE1	1:B:382:GLN:HG3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:PHE:C	1:A:188:SER:H	2.18	0.51
1:A:289:ILE:HG22	1:A:290:ASP:N	2.25	0.51
1:B:39:GLY:HA2	1:B:43:THR:HG23	1.91	0.51
1:A:91:ILE:HD13	1:A:91:ILE:H	1.75	0.51
1:A:192:PRO:HA	1:A:195:ASP:HB2	1.92	0.51
1:A:363:PRO:HB2	1:A:472:TRP:CD1	2.46	0.51
1:B:299:SER:HB2	1:B:456:THR:HG22	1.93	0.51
1:B:434:ASP:H	1:B:435:PRO:CD	2.24	0.51
1:A:158:MET:SD	1:A:164:GLN:HB2	2.51	0.51
1:B:11:ASP:HB2	1:B:99:ARG:HH12	1.75	0.51
1:B:34:ARG:O	1:B:35:ASP:HB2	2.11	0.51
1:B:50:THR:HA	1:B:53:LEU:HB2	1.92	0.51
1:A:5:VAL:HG21	1:A:173:LEU:HD23	1.91	0.50
1:A:191:LYS:CB	1:A:192:PRO:HD3	2.41	0.50
1:B:36:PHE:HE2	1:B:82:LEU:HD13	1.75	0.50
1:B:122:VAL:HA	1:B:151:ILE:HG13	1.92	0.50
1:B:307:ALA:O	1:B:311:LEU:HG	2.12	0.50
1:A:276:ILE:HB	1:A:277:PRO:HD3	1.92	0.50
1:A:332:HIS:CD2	1:A:333:ASP:HB2	2.45	0.50
1:A:485:VAL:HB	1:B:133:ARG:NH1	2.26	0.50
1:B:8:PHE:CE1	1:B:147:PHE:CE2	2.96	0.50
1:B:72:ARG:O	1:B:72:ARG:HG2	2.11	0.50
1:B:363:PRO:HB2	1:B:472:TRP:CD1	2.46	0.50
1:A:128:ASP:O	1:A:133:ARG:HG3	2.10	0.50
1:A:328:VAL:HG22	1:A:352:ALA:HB3	1.94	0.50
1:B:155:GLN:OE1	1:B:155:GLN:CA	2.51	0.50
1:B:246:ILE:HD12	1:B:246:ILE:N	2.25	0.50
1:B:372:VAL:HG22	1:B:373:ILE:HD12	1.93	0.50
1:B:160:LYS:HA	1:B:165:ILE:HD11	1.94	0.50
1:A:90:GLN:CG	1:A:91:ILE:HD13	2.26	0.50
1:B:21:GLY:O	1:B:25:ARG:HD3	2.11	0.50
1:A:231:ASN:CB	1:A:232:PRO:HA	2.34	0.50
1:A:299:SER:HB2	1:A:456:THR:HG22	1.94	0.50
1:A:62:GLN:O	1:A:63:TRP:CD1	2.55	0.50
1:A:121:ILE:HG13	1:A:147:PHE:CD2	2.46	0.49
1:A:325:PRO:O	1:A:349:ARG:NH1	2.45	0.49
1:B:17:PRO:O	1:B:18:SER:C	2.53	0.49
1:B:43:THR:O	1:B:44:GLU:CB	2.60	0.49
1:B:180:VAL:HG23	1:B:181:VAL:N	2.26	0.49
1:B:229:PRO:O	1:B:231:ASN:ND2	2.33	0.49
1:A:60:PHE:C	1:A:62:GLN:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ASN:HA	1:A:153:SER:CB	2.37	0.49
1:B:63:TRP:O	1:B:67:MET:HB2	2.12	0.49
1:B:194:ARG:HB2	1:B:200:THR:CG2	2.42	0.49
1:B:402:THR:O	1:B:406:PHE:HD2	1.96	0.49
1:A:61:SER:HB2	1:B:484:LEU:HD13	1.95	0.49
1:A:55:LYS:HG3	1:A:159:ILE:HG23	1.93	0.49
1:A:106:LEU:CD2	1:A:110:ILE:HD11	2.41	0.49
1:A:535:GLN:CB	1:A:539:LYS:HZ2	2.24	0.49
1:B:106:LEU:HD22	1:B:110:ILE:HD11	1.94	0.49
1:B:192:PRO:O	1:B:196:MET:HB2	2.12	0.49
1:B:125:ASN:CB	1:B:152:GLU:HB3	2.43	0.49
1:B:278:ALA:HA	1:B:281:GLN:HE21	1.77	0.49
1:B:325:PRO:O	1:B:349:ARG:NH1	2.45	0.49
1:A:501:GLU:O	1:A:504:LYS:HD3	2.13	0.48
1:B:166:TYR:OH	1:B:189:ASN:O	2.29	0.48
1:B:229:PRO:HA	1:B:273:ARG:O	2.13	0.48
1:A:53:LEU:HA	1:A:58:ILE:HD12	1.95	0.48
1:B:428:LEU:CD1	1:B:428:LEU:N	2.76	0.48
1:A:356:LEU:O	1:A:357:ASN:HB2	2.13	0.48
1:A:534:ASN:O	1:A:535:GLN:C	2.54	0.48
1:B:8:PHE:HD1	1:B:8:PHE:H	1.61	0.48
1:B:186:PHE:HB3	1:B:188:SER:OG	2.12	0.48
1:A:208:SER:C	1:A:210:LEU:N	2.66	0.48
1:A:15:ALA:HA	1:A:100:SER:O	2.14	0.48
1:A:102:ASN:HD22	1:A:102:ASN:C	2.22	0.48
1:A:210:LEU:C	1:A:212:GLU:H	2.22	0.48
1:A:479:LEU:O	1:A:509:TRP:HZ3	1.97	0.48
1:B:339:VAL:O	1:B:342:MET:HB2	2.13	0.48
1:A:205:ASN:HD21	1:A:209:ALA:CA	2.26	0.48
1:B:182:PHE:HD2	1:B:190:LEU:HD23	1.78	0.48
1:B:267:GLU:HB3	1:B:271:SER:OG	2.13	0.48
1:A:339:VAL:O	1:A:342:MET:HB2	2.13	0.48
1:A:231:ASN:CB	1:A:232:PRO:CA	2.91	0.48
1:A:17:PRO:O	1:A:18:SER:O	2.32	0.48
1:A:256:GLY:N	1:A:285:ARG:HB2	2.29	0.48
1:B:238:GLY:HA3	1:B:250:PHE:CE1	2.49	0.48
1:A:474:TRP:O	1:A:477:LYS:HG3	2.14	0.48
1:B:215:LYS:NZ	1:B:221:PHE:O	2.47	0.48
1:B:290:ASP:HB3	1:B:297:SER:OG	2.14	0.48
1:B:535:GLN:HB3	1:B:539:LYS:NZ	2.27	0.48
1:B:160:LYS:HB3	1:B:189:ASN:OD1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:THR:CG2	1:B:432:PRO:HD2	2.41	0.47
1:A:193:ALA:O	1:A:198:MET:CB	2.51	0.47
1:A:290:ASP:HB3	1:A:297:SER:OG	2.14	0.47
1:A:278:ALA:HA	1:A:281:GLN:HE21	1.79	0.47
1:B:210:LEU:O	1:B:214:GLU:HB2	2.13	0.47
1:B:253:MET:HE3	1:B:253:MET:HB2	1.83	0.47
1:B:491:THR:OG1	1:B:517:HIS:HD2	1.98	0.47
1:B:538:ILE:O	1:B:542:GLN:HG2	2.15	0.47
1:A:9:ASP:O	1:A:13:VAL:HB	2.15	0.47
1:A:107:GLN:O	1:A:108:ALA:C	2.57	0.47
1:B:102:ASN:HB3	1:B:105:MET:HB2	1.96	0.47
1:B:270:PHE:HB2	1:B:448:PHE:CE2	2.50	0.47
1:A:372:VAL:HG22	1:A:373:ILE:HD12	1.95	0.47
1:B:124:ASN:HA	1:B:153:SER:OG	2.14	0.47
1:B:233:ASN:H	1:B:233:ASN:HD22	1.61	0.47
1:B:329:PHE:O	1:B:353:VAL:HA	2.15	0.47
1:B:474:TRP:O	1:B:477:LYS:HG3	2.14	0.47
1:A:7:ALA:HA	1:A:120:CYS:O	2.15	0.47
1:A:8:PHE:HD1	1:A:147:PHE:HE2	1.58	0.47
1:A:402:THR:O	1:A:406:PHE:HD2	1.97	0.47
1:B:5:VAL:HB	1:B:118:THR:HB	1.95	0.47
1:B:64:VAL:HG11	1:B:89:SER:HB2	1.97	0.47
1:B:198:MET:HE2	1:B:198:MET:HB2	1.74	0.47
1:B:204:HIS:O	1:B:205:ASN:CB	2.62	0.47
1:B:232:PRO:CD	1:B:233:ASN:N	2.55	0.47
1:B:501:GLU:O	1:B:504:LYS:HD3	2.14	0.47
1:A:270:PHE:HB2	1:A:448:PHE:CE2	2.50	0.47
1:A:301:PRO:HA	1:A:459:ARG:HD3	1.96	0.47
1:B:229:PRO:HB2	1:B:231:ASN:ND2	2.25	0.47
1:B:428:LEU:HA	1:B:431:THR:OG1	2.15	0.47
1:B:483:ILE:HD12	1:B:510:ILE:HD11	1.97	0.47
1:A:243:LYS:O	1:A:244:PRO:C	2.58	0.47
1:A:262:CYS:O	1:A:272:TRP:HZ2	1.98	0.47
1:B:256:GLY:N	1:B:285:ARG:HB2	2.30	0.47
1:B:38:LEU:O	1:B:38:LEU:HD23	2.15	0.47
1:B:45:PHE:CG	1:B:45:PHE:O	2.68	0.47
1:B:53:LEU:HD23	1:B:53:LEU:HA	1.67	0.47
1:B:201:ILE:N	1:B:201:ILE:CD1	2.74	0.47
1:B:367:VAL:O	1:B:368:SER:C	2.58	0.47
1:B:524:TRP:O	1:B:528:GLU:HB2	2.15	0.47
1:A:230:CYS:CB	1:A:277:PRO:HG3	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:ARG:HB2	1:B:117:PHE:CE2	2.50	0.46
1:B:24:ARG:O	1:B:26:SER:N	2.48	0.46
1:B:107:GLN:NE2	1:B:107:GLN:CA	2.78	0.46
1:A:512:PHE:N	1:A:512:PHE:CD2	2.82	0.46
1:B:7:ALA:HB2	1:B:120:CYS:SG	2.55	0.46
1:B:207:ALA:O	1:B:210:LEU:N	2.46	0.46
1:A:61:SER:C	1:A:63:TRP:N	2.73	0.46
1:A:182:PHE:HD2	1:A:190:LEU:CD2	2.28	0.46
1:B:243:LYS:O	1:B:244:PRO:C	2.58	0.46
1:A:91:ILE:H	1:A:91:ILE:CD1	2.28	0.46
1:B:21:GLY:C	1:B:25:ARG:HD3	2.40	0.46
1:B:52:GLN:HB3	1:B:58:ILE:HG12	1.98	0.46
1:B:289:ILE:HG22	1:B:290:ASP:N	2.28	0.46
1:B:301:PRO:HA	1:B:459:ARG:HD3	1.96	0.46
1:B:511:PRO:C	1:B:513:LEU:N	2.72	0.46
1:A:511:PRO:C	1:A:513:LEU:N	2.74	0.46
1:B:50:THR:HG22	1:B:63:TRP:HE1	1.79	0.46
1:A:108:ALA:O	1:A:112:LEU:HD12	2.16	0.46
1:A:497:VAL:HG13	2:A:1100:CPU:C12	2.45	0.46
1:A:524:TRP:O	1:A:528:GLU:HB2	2.14	0.46
1:B:5:VAL:HG13	1:B:180:VAL:CB	2.37	0.46
1:B:101:ILE:HG22	1:B:102:ASN:N	2.31	0.46
1:B:312:CYS:O	1:B:315:MET:HB2	2.15	0.46
1:A:158:MET:HE3	1:A:165:ILE:CA	2.42	0.46
1:A:378:VAL:O	1:A:378:VAL:HG13	2.15	0.46
1:B:170:LEU:HD23	1:B:175:ALA:O	2.16	0.46
1:B:428:LEU:HD13	1:B:428:LEU:N	2.31	0.46
1:A:158:MET:HE1	1:A:168:PHE:HB2	1.97	0.46
1:B:22:ALA:HA	1:B:25:ARG:HD3	1.97	0.46
1:A:182:PHE:CE2	1:A:184:ASP:HB2	2.51	0.45
1:B:106:LEU:O	1:B:106:LEU:HD23	2.16	0.45
1:A:312:CYS:O	1:A:315:MET:HB2	2.16	0.45
1:A:535:GLN:HB3	1:A:539:LYS:NZ	2.31	0.45
1:B:49:PRO:O	1:B:52:GLN:HB2	2.17	0.45
1:B:119:THR:HG23	1:B:148:ASP:N	2.29	0.45
1:A:115:LYS:NZ	1:A:219:THR:HG23	2.30	0.45
1:A:193:ALA:CA	1:A:198:MET:HE3	2.46	0.45
1:A:267:GLU:HB3	1:A:271:SER:OG	2.16	0.45
1:B:43:THR:O	1:B:44:GLU:HB2	2.16	0.45
1:B:50:THR:CG2	1:B:63:TRP:NE1	2.72	0.45
1:B:30:LEU:HB3	1:B:32:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:GLY:HA2	1:B:43:THR:HG21	1.98	0.45
1:B:61:SER:O	1:B:65:PRO:HD2	2.16	0.45
1:B:84:GLU:H	1:B:84:GLU:HG3	1.42	0.45
1:A:58:ILE:HG22	1:A:62:GLN:OE1	2.17	0.45
1:B:25:ARG:O	1:B:29:ALA:CB	2.63	0.45
1:B:125:ASN:N	1:B:153:SER:OG	2.50	0.45
1:A:19:ILE:HD12	1:A:126:TRP:HH2	1.82	0.45
1:A:325:PRO:HB3	1:B:138:GLN:HA	1.99	0.45
1:B:125:ASN:O	1:B:154:CYS:HB3	2.16	0.45
1:B:364:ASP:HA	1:B:365:PRO:HD3	1.76	0.45
1:B:538:ILE:O	1:B:539:LYS:C	2.59	0.45
1:A:491:THR:OG1	1:A:517:HIS:HD2	2.00	0.45
1:B:26:SER:CA	1:B:29:ALA:HB3	2.46	0.45
1:A:238:GLY:HA3	1:A:250:PHE:CE1	2.51	0.45
1:A:401:ARG:O	1:A:402:THR:C	2.60	0.45
1:A:484:LEU:HD12	1:B:129:ASP:OD1	2.16	0.45
1:A:507:GLU:H	1:A:507:GLU:HG2	1.41	0.45
1:B:112:LEU:HD23	1:B:117:PHE:CE1	2.51	0.45
1:A:430:ASN:HD22	1:A:430:ASN:N	1.87	0.45
1:A:367:VAL:O	1:A:368:SER:C	2.59	0.45
1:A:8:PHE:HB2	1:A:14:LEU:HD11	1.99	0.44
1:A:52:GLN:HA	1:A:55:LYS:HB2	1.99	0.44
1:A:215:LYS:HA	1:A:219:THR:O	2.17	0.44
1:A:275:GLN:NE2	1:A:526:GLN:HB3	2.32	0.44
1:A:381:TYR:HB2	1:A:427:ILE:HD12	1.99	0.44
1:B:275:GLN:NE2	1:B:526:GLN:HB3	2.32	0.44
1:A:9:ASP:OD2	1:A:160:LYS:NZ	2.44	0.44
1:A:17:PRO:O	1:A:18:SER:C	2.59	0.44
1:A:139:MET:HG2	1:A:143:LEU:HD12	1.98	0.44
1:A:183:LEU:CD1	1:A:201:ILE:HB	2.46	0.44
1:B:334:TRP:O	1:B:337:VAL:HB	2.17	0.44
1:A:127:LEU:HD12	1:A:127:LEU:N	2.32	0.44
1:A:155:GLN:OE1	1:A:155:GLN:CA	2.51	0.44
1:A:322:LEU:HD12	1:B:236:SER:HB2	1.99	0.44
1:A:380:ASN:CB	1:A:419:HIS:O	2.65	0.44
1:B:71:TYR:HE1	1:B:88:ILE:HD13	1.83	0.44
1:B:216:VAL:HG12	1:B:217:THR:OG1	2.17	0.44
1:B:75:SER:C	1:B:77:ALA:N	2.76	0.44
1:A:97:ALA:C	1:A:99:ARG:H	2.25	0.44
1:A:133:ARG:CG	1:B:348:GLU:HA	2.42	0.44
1:A:165:ILE:HG13	1:A:165:ILE:H	1.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:MET:HB2	1:B:159:ILE:HG21	1.99	0.44
1:A:125:ASN:O	1:A:126:TRP:HB3	2.16	0.44
1:B:30:LEU:HD11	1:B:83:PRO:CG	2.48	0.44
1:B:144:SER:OG	1:B:145:GLN:NE2	2.44	0.44
1:B:162:GLU:O	1:B:165:ILE:CD1	2.66	0.44
1:B:206:THR:O	1:B:207:ALA:CB	2.66	0.44
1:B:230:CYS:HB3	1:B:277:PRO:HG3	2.00	0.44
1:B:262:CYS:O	1:B:272:TRP:HZ2	2.00	0.44
1:A:346:TYR:O	1:A:350:VAL:HG23	2.17	0.44
1:A:381:TYR:CB	1:A:427:ILE:HD12	2.48	0.44
1:B:76:LYS:HE2	1:B:76:LYS:O	2.17	0.44
1:B:121:ILE:HB	1:B:150:LEU:HD12	2.00	0.44
1:B:154:CYS:O	1:B:154:CYS:SG	2.76	0.44
1:B:190:LEU:HD11	1:B:202:LEU:HA	2.00	0.44
1:B:420:LYS:O	1:B:421:ALA:C	2.59	0.44
1:B:512:PHE:CD2	1:B:512:PHE:N	2.84	0.44
1:A:420:LYS:O	1:A:424:ILE:HG12	2.17	0.44
1:B:68:ASP:O	1:B:71:TYR:HB2	2.18	0.44
1:B:210:LEU:O	1:B:214:GLU:CB	2.66	0.44
1:A:122:VAL:HG13	1:A:182:PHE:HE1	1.82	0.44
1:A:394:GLU:OE1	1:A:427:ILE:HG22	2.17	0.44
1:B:5:VAL:CG1	1:B:180:VAL:HB	2.41	0.44
1:B:107:GLN:CA	1:B:107:GLN:HE21	2.30	0.44
1:A:5:VAL:HG23	1:A:6:ALA:N	2.32	0.43
1:A:16:LEU:HB3	1:A:17:PRO:HA	1.99	0.43
1:A:334:TRP:O	1:A:337:VAL:HB	2.18	0.43
1:B:19:ILE:HD13	1:B:19:ILE:HA	1.89	0.43
1:B:300:PRO:HG2	1:B:305:GLU:CG	2.26	0.43
1:A:158:MET:HB3	1:A:164:GLN:HG3	2.00	0.43
1:B:183:LEU:HD13	1:B:201:ILE:HB	2.00	0.43
1:A:60:PHE:O	1:A:62:GLN:N	2.50	0.43
1:A:209:ALA:HA	1:A:212:GLU:HB2	2.01	0.43
1:B:215:LYS:O	1:B:219:THR:O	2.37	0.43
1:B:466:ARG:H	1:B:466:ARG:HG2	1.49	0.43
1:A:113:LYS:HE2	1:A:113:LYS:HB3	1.86	0.43
1:A:329:PHE:O	1:A:353:VAL:HA	2.18	0.43
1:A:365:PRO:HG3	1:A:479:LEU:HD13	2.00	0.43
1:B:50:THR:HG22	1:B:63:TRP:NE1	2.33	0.43
1:A:17:PRO:C	1:A:18:SER:O	2.61	0.43
1:A:192:PRO:C	1:A:195:ASP:HB2	2.43	0.43
1:A:276:ILE:HD11	1:A:288:ALA:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:GLY:CA	1:A:429:VAL:HG23	2.49	0.43
1:B:41:TYR:HB3	1:B:42:GLN:H	1.63	0.43
1:B:119:THR:CG2	1:B:147:PHE:HA	2.46	0.43
1:A:8:PHE:HB2	1:A:14:LEU:CD1	2.49	0.43
1:A:210:LEU:C	1:A:212:GLU:N	2.76	0.43
1:A:222:PRO:HG2	1:A:225:PRO:HB3	1.99	0.43
1:A:230:CYS:HB3	1:A:277:PRO:HD3	2.01	0.43
1:A:303:ILE:C	1:A:305:GLU:N	2.72	0.43
1:B:5:VAL:CG2	1:B:6:ALA:N	2.81	0.43
1:B:105:MET:O	1:B:108:ALA:HB3	2.19	0.43
1:B:263:HIS:HD2	1:B:291:MET:HG2	1.74	0.43
1:B:276:ILE:CB	1:B:277:PRO:HD3	2.49	0.43
1:A:126:TRP:CD1	1:A:126:TRP:C	2.97	0.43
1:A:272:TRP:O	1:A:273:ARG:C	2.62	0.43
1:B:278:ALA:HA	1:B:281:GLN:NE2	2.34	0.43
1:B:303:ILE:C	1:B:305:GLU:N	2.73	0.43
1:B:373:ILE:HG22	1:B:383:LEU:HD11	2.00	0.43
1:A:207:ALA:HA	1:A:210:LEU:HB3	2.00	0.43
1:A:481:ARG:HG2	1:B:57:LYS:O	2.19	0.43
1:B:222:PRO:CB	1:B:225:PRO:HG3	2.47	0.43
1:B:358:THR:HG22	1:B:359:PRO:O	2.19	0.43
1:B:134:ASP:O	1:B:135:SER:C	2.62	0.43
1:B:265:PHE:HA	1:B:266:PRO:HA	1.87	0.43
1:A:253:MET:HE3	1:A:253:MET:HB2	1.78	0.42
1:A:373:ILE:HG22	1:A:383:LEU:HD11	2.00	0.42
1:B:222:PRO:HA	1:B:223:GLU:OE2	2.19	0.42
1:B:229:PRO:C	1:B:231:ASN:ND2	2.75	0.42
1:B:458:PHE:O	1:B:459:ARG:C	2.60	0.42
1:A:127:LEU:HD12	1:A:127:LEU:H	1.84	0.42
1:A:220:GLN:HE21	1:A:220:GLN:HB2	1.58	0.42
1:B:6:ALA:HA	1:B:181:VAL:HG13	2.01	0.42
1:A:50:THR:HA	1:A:63:TRP:HZ2	1.83	0.42
1:A:60:PHE:O	1:A:63:TRP:HB2	2.20	0.42
1:A:111:ALA:O	1:A:114:LYS:N	2.53	0.42
1:A:483:ILE:HD12	1:A:510:ILE:HD11	2.01	0.42
1:B:33:PRO:HG3	1:B:80:ALA:HB2	2.01	0.42
1:A:54:MET:HE3	1:A:124:ASN:HB3	2.00	0.42
1:A:90:GLN:CG	1:A:91:ILE:N	2.82	0.42
1:A:205:ASN:O	1:A:207:ALA:N	2.52	0.42
1:A:360:PHE:HB2	1:A:506:MET:HE3	2.00	0.42
1:B:30:LEU:HD11	1:B:83:PRO:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LEU:N	1:A:226:LEU:CD2	2.82	0.42
1:A:490:VAL:HA	1:A:516:GLY:O	2.20	0.42
1:B:8:PHE:HD1	1:B:120:CYS:O	2.03	0.42
1:B:119:THR:HG22	1:B:148:ASP:OD1	2.20	0.42
1:B:122:VAL:HG22	1:B:160:LYS:HE2	2.01	0.42
1:B:187:GLY:HA2	1:B:190:LEU:HB2	2.01	0.42
1:A:152:GLU:O	1:A:153:SER:C	2.62	0.42
1:A:157:GLY:C	1:A:158:MET:CG	2.92	0.42
1:A:181:VAL:O	1:A:181:VAL:HG22	2.19	0.42
1:B:36:PHE:CE2	1:B:82:LEU:HD13	2.54	0.42
1:B:64:VAL:CB	1:B:65:PRO:CD	2.88	0.42
1:B:401:ARG:O	1:B:402:THR:C	2.63	0.42
1:A:232:PRO:HD2	1:A:233:ASN:N	2.11	0.42
1:B:24:ARG:C	1:B:26:SER:N	2.77	0.42
1:B:63:TRP:CE2	1:B:67:MET:HG3	2.55	0.42
1:B:281:GLN:C	1:B:283:GLY:N	2.77	0.42
1:B:61:SER:HG	1:B:129:ASP:CG	2.28	0.42
1:B:112:LEU:HA	1:B:115:LYS:HB3	2.02	0.42
1:A:205:ASN:C	1:A:207:ALA:N	2.70	0.42
1:B:25:ARG:HH11	1:B:25:ARG:HG2	1.84	0.42
1:B:180:VAL:HG22	1:B:198:MET:HG2	2.01	0.42
1:B:187:GLY:O	1:B:190:LEU:HB2	2.19	0.42
1:B:214:GLU:HG3	1:B:221:PHE:CE1	2.54	0.42
1:B:265:PHE:CD2	1:B:265:PHE:C	2.98	0.42
1:B:511:PRO:O	1:B:513:LEU:N	2.52	0.42
1:A:8:PHE:O	1:A:121:ILE:HA	2.20	0.42
1:A:276:ILE:CB	1:A:277:PRO:HD3	2.50	0.42
1:B:350:VAL:HG13	1:B:352:ALA:O	2.20	0.42
1:B:369:PRO:O	1:B:373:ILE:CD1	2.68	0.42
1:A:92:PHE:O	1:A:95:ALA:HB3	2.20	0.41
1:A:277:PRO:O	1:A:280:ALA:N	2.53	0.41
1:A:422:THR:O	1:A:423:GLU:CB	2.56	0.41
1:B:490:VAL:HA	1:B:516:GLY:O	2.20	0.41
1:A:137:ALA:HB1	1:B:325:PRO:O	2.20	0.41
1:A:180:VAL:HG22	1:A:198:MET:HG2	2.02	0.41
1:A:265:PHE:CD2	1:A:265:PHE:C	2.98	0.41
1:A:380:ASN:OD1	1:A:422:THR:N	2.48	0.41
1:B:54:MET:O	1:B:153:SER:C	2.63	0.41
1:B:122:VAL:HG22	1:B:122:VAL:O	2.20	0.41
1:B:207:ALA:O	1:B:209:ALA:N	2.53	0.41
1:A:10:LEU:HA	1:A:10:LEU:HD12	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:ARG:O	1:A:500:PRO:C	2.63	0.41
1:B:122:VAL:CA	1:B:151:ILE:HG13	2.50	0.41
1:B:230:CYS:O	1:B:230:CYS:SG	2.77	0.41
1:B:303:ILE:HG21	1:B:466:ARG:HB2	2.03	0.41
1:B:346:TYR:O	1:B:350:VAL:HG23	2.19	0.41
1:B:380:ASN:HB3	1:B:418:VAL:O	2.20	0.41
1:B:481:ARG:HH11	1:B:481:ARG:HD2	1.70	0.41
1:A:358:THR:HG22	1:A:359:PRO:O	2.19	0.41
1:A:380:ASN:HB3	1:A:418:VAL:O	2.20	0.41
1:B:167:ASN:O	1:B:171:ASP:OD2	2.39	0.41
1:B:263:HIS:HE1	1:B:294:TYR:CD2	2.38	0.41
1:A:303:ILE:HG21	1:A:466:ARG:HB2	2.03	0.41
1:B:54:MET:HA	1:B:125:ASN:O	2.21	0.41
1:B:67:MET:O	1:B:68:ASP:C	2.63	0.41
1:B:378:VAL:O	1:B:378:VAL:HG13	2.20	0.41
1:A:228:VAL:HA	1:A:229:PRO:HD3	1.79	0.41
1:A:280:ALA:HA	1:A:284:PHE:O	2.20	0.41
1:B:56:GLY:HA2	1:B:127:LEU:HD11	2.03	0.41
1:B:206:THR:O	1:B:207:ALA:HB3	2.20	0.41
1:B:277:PRO:O	1:B:278:ALA:C	2.64	0.41
1:B:106:LEU:C	1:B:106:LEU:CD2	2.94	0.41
1:B:126:TRP:CD1	1:B:126:TRP:C	2.97	0.41
1:B:199:VAL:HG12	1:B:201:ILE:HD11	2.03	0.41
1:B:281:GLN:HE21	1:B:281:GLN:HB2	1.62	0.41
1:A:110:ILE:HD13	1:A:228:VAL:HG12	2.03	0.41
1:A:484:LEU:CD1	1:B:61:SER:OG	2.69	0.41
1:B:71:TYR:CE1	1:B:88:ILE:HD13	2.55	0.41
1:B:396:GLU:OE1	1:B:458:PHE:N	2.54	0.41
1:A:198:MET:HB2	1:A:198:MET:HE3	1.76	0.41
1:B:20:ALA:HA	1:B:23:PHE:HB2	2.03	0.41
1:A:170:LEU:HD21	1:A:177:PRO:HA	2.03	0.40
1:A:191:LYS:CB	1:A:192:PRO:CD	2.99	0.40
1:A:191:LYS:HB2	1:A:192:PRO:HD3	2.03	0.40
1:A:289:ILE:CG2	1:A:290:ASP:N	2.84	0.40
1:B:11:ASP:OD2	1:B:19:ILE:HG12	2.22	0.40
1:B:30:LEU:HD23	1:B:30:LEU:HA	1.77	0.40
1:B:73:LYS:O	1:B:77:ALA:HB3	2.20	0.40
1:B:380:ASN:CB	1:B:419:HIS:O	2.69	0.40
1:A:58:ILE:HG22	1:A:62:GLN:CB	2.47	0.40
1:A:278:ALA:O	1:A:282:ALA:N	2.53	0.40
1:A:324:ILE:HA	1:A:325:PRO:HD3	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:MET:HB2	1:B:159:ILE:HG22	2.03	0.40
1:B:280:ALA:HA	1:B:284:PHE:O	2.20	0.40
1:B:408:ARG:HA	1:B:438:SER:OG	2.21	0.40
1:A:4:ARG:HH11	1:A:4:ARG:HB2	1.86	0.40
1:A:438:SER:C	1:A:440:ILE:H	2.27	0.40
1:B:291:MET:HE1	1:B:338:MET:HE1	2.03	0.40
1:B:303:ILE:CG2	1:B:466:ARG:HB2	2.52	0.40
1:B:499:ARG:O	1:B:500:PRO:C	2.62	0.40
1:A:278:ALA:HA	1:A:281:GLN:NE2	2.36	0.40
1:A:334:TRP:CE3	2:A:1100:CPU:H4	2.55	0.40
1:A:493:GLU:HG2	1:A:494:LYS:HG2	2.03	0.40
1:A:496:ILE:CD1	1:A:496:ILE:N	2.70	0.40
1:B:277:PRO:O	1:B:280:ALA:N	2.54	0.40
1:B:360:PHE:HB2	1:B:506:MET:HE3	2.01	0.40
1:A:303:ILE:CG2	1:A:466:ARG:HB2	2.52	0.40
1:A:511:PRO:O	1:A:513:LEU:N	2.55	0.40
1:A:519:GLU:O	1:A:520:ASP:C	2.64	0.40
1:B:272:TRP:O	1:B:273:ARG:C	2.63	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	481/554 (87%)	392 (82%)	59 (12%)	30 (6%)	1	3
1	B	539/554 (97%)	431 (80%)	77 (14%)	31 (6%)	1	4
All	All	1020/1108 (92%)	823 (81%)	136 (13%)	61 (6%)	1	3

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	207	ALA
1	A	231	ASN
1	A	244	PRO
1	A	256	GLY
1	A	415	PHE
1	A	423	GLU
1	B	41	TYR
1	B	75	SER
1	B	78	CYS
1	B	207	ALA
1	B	208	SER
1	B	222	PRO
1	B	232	PRO
1	B	244	PRO
1	B	256	GLY
1	B	415	PHE
1	B	421	ALA
1	A	18	SER
1	A	98	ALA
1	A	158	MET
1	A	466	ARG
1	A	520	ASP
1	B	25	ARG
1	B	44	GLU
1	B	80	ALA
1	B	205	ASN
1	B	386	GLN
1	B	466	ARG
1	B	520	ASP
1	A	154	CYS
1	A	288	ALA
1	A	402	THR
1	B	63	TRP
1	A	126	TRP
1	A	210	LEU
1	A	232	PRO
1	A	386	GLN
1	A	496	ILE
1	B	288	ALA
1	B	402	THR
1	B	434	ASP
1	A	125	ASN

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Mol	Chain	Res	Type
1	A	206	THR
1	A	230	CYS
1	A	277	PRO
1	B	34	ARG
1	B	203	VAL
1	B	219	THR
1	B	277	PRO
1	B	432	PRO
1	B	496	ILE
1	A	187	GLY
1	A	295	GLY
1	B	295	GLY
1	A	229	PRO
1	A	12	GLY
1	B	216	VAL
1	A	91	ILE
1	A	266	PRO
1	B	266	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	424/480 (88%)	309 (73%)	115 (27%)	0	1
1	B	468/480 (98%)	328 (70%)	140 (30%)	0	1
All	All	892/960 (93%)	637 (71%)	255 (29%)	0	1

All (255) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	5	VAL
1	A	13	VAL
1	A	18	SER
1	A	19	ILE

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Mol	Chain	Res	Type
1	A	53	LEU
1	A	55	LYS
1	A	57	LYS
1	A	58	ILE
1	A	61	SER
1	A	90	GLN
1	A	91	ILE
1	A	92	PHE
1	A	93	SER
1	A	94	GLN
1	A	99	ARG
1	A	102	ASN
1	A	103	ARG
1	A	119	THR
1	A	122	VAL
1	A	125	ASN
1	A	128	ASP
1	A	129	ASP
1	A	131	ASP
1	A	136	LEU
1	A	152	GLU
1	A	154	CYS
1	A	155	GLN
1	A	158	MET
1	A	160	LYS
1	A	164	GLN
1	A	165	ILE
1	A	169	LEU
1	A	170	LEU
1	A	173	LEU
1	A	174	LYS
1	A	180	VAL
1	A	181	VAL
1	A	196	MET
1	A	198	MET
1	A	200	THR
1	A	202	LEU
1	A	204	HIS
1	A	208	SER
1	A	213	LEU
1	A	214	GLU
1	A	216	VAL

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Mol	Chain	Res	Type
1	A	220	GLN
1	A	221	PHE
1	A	223	GLU
1	A	226	LEU
1	A	230	CYS
1	A	231	ASN
1	A	247	ARG
1	A	248	LEU
1	A	268	SER
1	A	275	GLN
1	A	290	ASP
1	A	297	SER
1	A	299	SER
1	A	310	LEU
1	A	313	LYS
1	A	315	MET
1	A	322	LEU
1	A	339	VAL
1	A	349	ARG
1	A	351	ARG
1	A	353	VAL
1	A	361	MET
1	A	366	ASP
1	A	368	SER
1	A	370	MET
1	A	371	LYS
1	A	372	VAL
1	A	376	ILE
1	A	378	VAL
1	A	383	LEU
1	A	398	ASN
1	A	404	LYS
1	A	408	ARG
1	A	412	GLU
1	A	413	THR
1	A	420	LYS
1	A	422	THR
1	A	423	GLU
1	A	427	ILE
1	A	430	ASN
1	A	437	LEU
1	A	439	LYS

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Mol	Chain	Res	Type
1	A	440	ILE
1	A	447	GLU
1	A	451	GLN
1	A	466	ARG
1	A	468	THR
1	A	470	ARG
1	A	475	SER
1	A	485	VAL
1	A	488	LEU
1	A	494	LYS
1	A	496	ILE
1	A	497	VAL
1	A	501	GLU
1	A	502	MET
1	A	504	LYS
1	A	505	ASN
1	A	507	GLU
1	A	512	PHE
1	A	513	LEU
1	A	519	GLU
1	A	526	GLN
1	A	531	THR
1	A	532	GLU
1	A	539	LYS
1	A	542	GLN
1	A	544	GLU
1	B	4	ARG
1	B	5	VAL
1	B	8	PHE
1	B	10	LEU
1	B	13	VAL
1	B	16	LEU
1	B	19	ILE
1	B	23	PHE
1	B	24	ARG
1	B	25	ARG
1	B	30	LEU
1	B	35	ASP
1	B	41	TYR
1	B	42	GLN
1	B	43	THR
1	B	47	GLU

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Mol	Chain	Res	Type
1	B	53	LEU
1	B	57	LYS
1	B	61	SER
1	B	67	MET
1	B	69	GLU
1	B	70	SER
1	B	72	ARG
1	B	73	LYS
1	B	74	SER
1	B	76	LYS
1	B	78	CYS
1	B	84	GLU
1	B	85	ASN
1	B	91	ILE
1	B	94	GLN
1	B	99	ARG
1	B	100	SER
1	B	101	ILE
1	B	103	ARG
1	B	105	MET
1	B	106	LEU
1	B	107	GLN
1	B	110	ILE
1	B	118	THR
1	B	121	ILE
1	B	122	VAL
1	B	125	ASN
1	B	127	LEU
1	B	131	ASP
1	B	133	ARG
1	B	135	SER
1	B	136	LEU
1	B	151	ILE
1	B	154	CYS
1	B	155	GLN
1	B	158	MET
1	B	159	ILE
1	B	160	LYS
1	B	164	GLN
1	B	165	ILE
1	B	169	LEU
1	B	170	LEU

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Mol	Chain	Res	Type
1	B	174	LYS
1	B	180	VAL
1	B	181	VAL
1	B	183	LEU
1	B	194	ARG
1	B	198	MET
1	B	200	THR
1	B	201	ILE
1	B	202	LEU
1	B	206	THR
1	B	208	SER
1	B	210	LEU
1	B	213	LEU
1	B	216	VAL
1	B	217	THR
1	B	219	THR
1	B	223	GLU
1	B	228	VAL
1	B	233	ASN
1	B	247	ARG
1	B	248	LEU
1	B	268	SER
1	B	275	GLN
1	B	290	ASP
1	B	297	SER
1	B	299	SER
1	B	310	LEU
1	B	313	LYS
1	B	315	MET
1	B	322	LEU
1	B	339	VAL
1	B	349	ARG
1	B	351	ARG
1	B	353	VAL
1	B	361	MET
1	B	366	ASP
1	B	368	SER
1	B	370	MET
1	B	371	LYS
1	B	372	VAL
1	B	376	ILE
1	B	378	VAL

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Mol	Chain	Res	Type
1	B	383	LEU
1	B	398	ASN
1	B	404	LYS
1	B	408	ARG
1	B	412	GLU
1	B	413	THR
1	B	422	THR
1	B	424	ILE
1	B	427	ILE
1	B	428	LEU
1	B	429	VAL
1	B	431	THR
1	B	437	LEU
1	B	439	LYS
1	B	440	ILE
1	B	447	GLU
1	B	451	GLN
1	B	466	ARG
1	B	468	THR
1	B	470	ARG
1	B	475	SER
1	B	485	VAL
1	B	488	LEU
1	B	494	LYS
1	B	496	ILE
1	B	497	VAL
1	B	501	GLU
1	B	502	MET
1	B	504	LYS
1	B	505	ASN
1	B	507	GLU
1	B	512	PHE
1	B	513	LEU
1	B	519	GLU
1	B	526	GLN
1	B	531	THR
1	B	532	GLU
1	B	539	LYS
1	B	542	GLN
1	B	544	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	102	ASN
1	A	107	GLN
1	A	125	ASN
1	A	146	HIS
1	A	164	GLN
1	A	205	ASN
1	A	220	GLN
1	A	275	GLN
1	A	281	GLN
1	A	332	HIS
1	A	341	ASN
1	A	430	ASN
1	A	451	GLN
1	A	517	HIS
1	B	81	ASN
1	B	90	GLN
1	B	102	ASN
1	B	107	GLN
1	B	146	HIS
1	B	204	HIS
1	B	231	ASN
1	B	233	ASN
1	B	275	GLN
1	B	281	GLN
1	B	332	HIS
1	B	341	ASN
1	B	517	HIS

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

2 ligands are modelled in this entry.

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	$\# Z > 2$
2	CPU	A	1100	-	20,20,20	1.89	10 (50%)	24,24,24	1.95	4 (16%)
2	CPU	B	1200	-	20,20,20	2.04	12 (60%)	24,24,24	1.99	6 (25%)

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
2	CPU	A	1100	-	-	5/11/19/19	0/2/2/2
2	CPU	B	1200	-	-	3/11/19/19	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1200	CPU	C1-C6	3.91	1.46	1.38
2	A	1100	CPU	C1-C6	3.39	1.45	1.38
2	A	1100	CPU	C4-C5	3.20	1.44	1.38
2	B	1200	CPU	C4-C3	2.98	1.44	1.38
2	B	1200	CPU	C12-C11	2.57	1.57	1.52
2	B	1200	CPU	C4-C5	2.54	1.43	1.38
2	A	1100	CPU	C16-C11	2.53	1.57	1.52
2	A	1100	CPU	C12-C11	2.45	1.57	1.52
2	A	1100	CPU	C15-C16	2.38	1.59	1.53
2	B	1200	CPU	C13-C12	2.38	1.59	1.53
2	B	1200	CPU	C16-C11	2.37	1.57	1.52
2	A	1100	CPU	C13-C12	2.36	1.59	1.53
2	B	1200	CPU	C15-C14	2.32	1.60	1.51
2	B	1200	CPU	C3-C2	2.23	1.43	1.38
2	A	1100	CPU	C2-C1	2.22	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1100	CPU	C4-C3	2.21	1.43	1.38
2	A	1100	CPU	C14-C13	2.19	1.59	1.51
2	B	1200	CPU	C5-C6	2.14	1.43	1.38
2	B	1200	CPU	C15-C16	2.14	1.58	1.53
2	A	1100	CPU	C15-C14	2.11	1.59	1.51
2	B	1200	CPU	C14-C13	2.01	1.59	1.51
2	B	1200	CPU	C2-C1	2.00	1.42	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1100	CPU	C9-C8-C7	-6.75	100.41	113.10
2	B	1200	CPU	C9-C8-C7	-5.90	102.02	113.10
2	B	1200	CPU	O1-C10-N1	-4.03	115.55	122.47
2	A	1100	CPU	O1-C10-N1	-3.73	116.06	122.47
2	B	1200	CPU	C11-N2-C10	3.03	129.44	122.92
2	A	1100	CPU	C8-C7-C6	2.81	124.15	113.67
2	B	1200	CPU	C13-C12-C11	2.49	115.56	111.09
2	A	1100	CPU	N1-C10-N2	2.33	121.64	115.82
2	B	1200	CPU	C8-C7-C6	2.19	121.85	113.67
2	B	1200	CPU	N1-C10-N2	2.10	121.07	115.82

There are no chirality outliers.

All (8) torsion outliers are listed below:

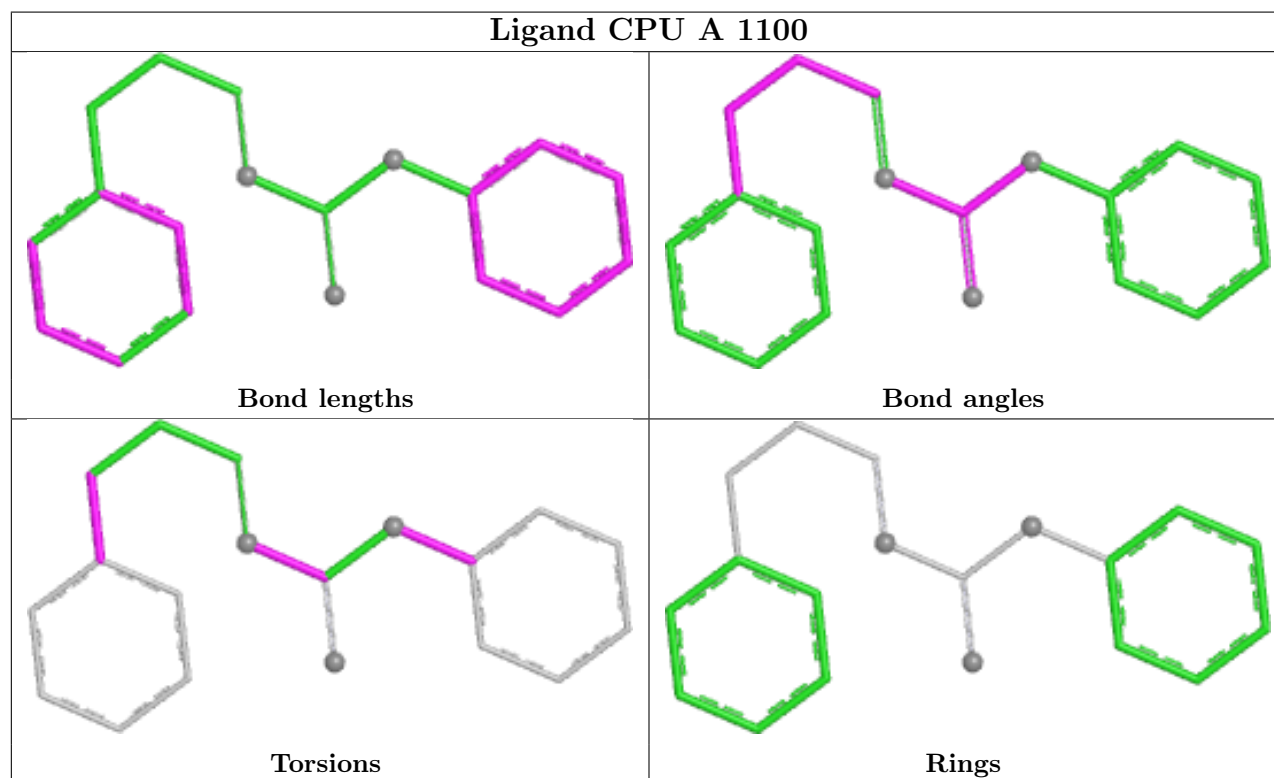
Mol	Chain	Res	Type	Atoms
2	B	1200	CPU	C16-C11-N2-C10
2	A	1100	CPU	C16-C11-N2-C10
2	A	1100	CPU	O1-C10-N1-C9
2	B	1200	CPU	O1-C10-N1-C9
2	A	1100	CPU	N2-C10-N1-C9
2	B	1200	CPU	N2-C10-N1-C9
2	A	1100	CPU	C5-C6-C7-C8
2	A	1100	CPU	C1-C6-C7-C8

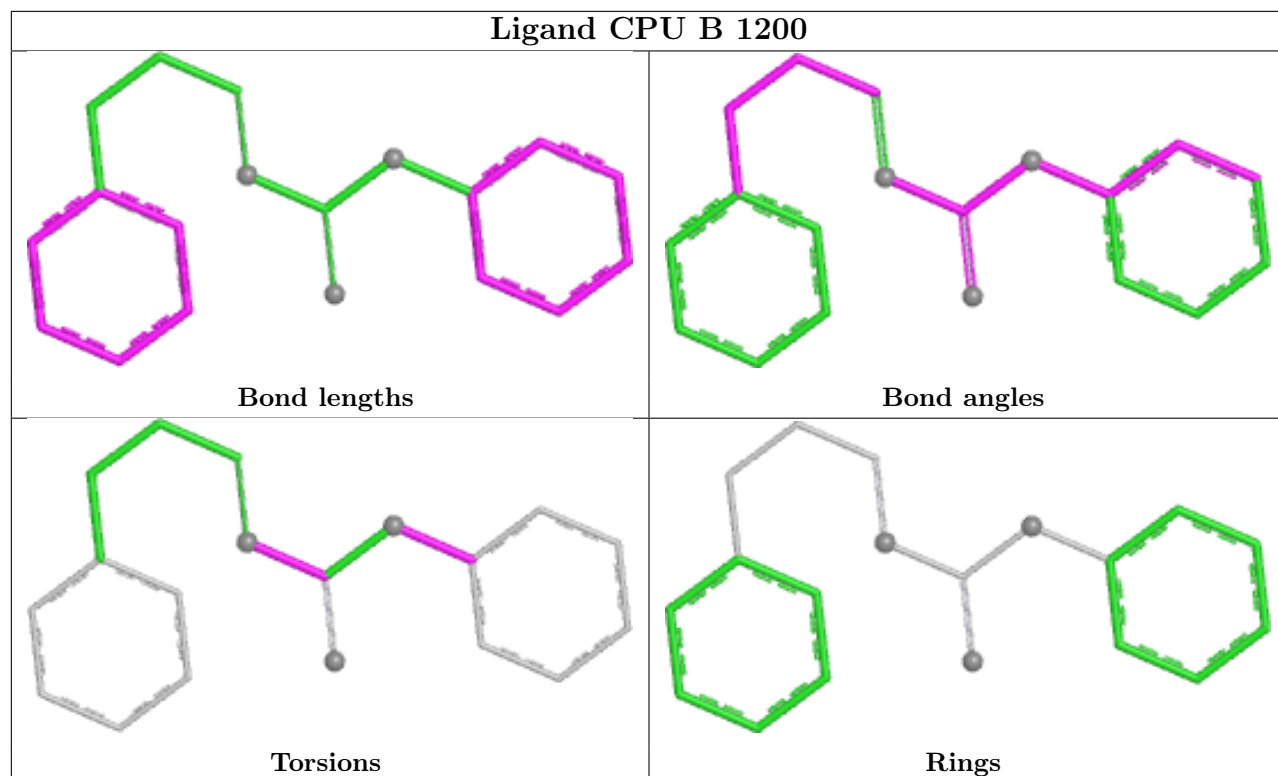
There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1100	CPU	5	0
2	B	1200	CPU	5	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.