



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:05 PM UTC

PDB ID : 1CQZ / pdb_00001cqz
Title : CRYSTAL STRUCTURE OF MURINE SOLUBLE EPOXIDE HYDROLASE.
Authors : Argiriadi, M.A.; Morisseau, C.; Hammock, B.D.; Christianson, D.W.
Deposited on : 1999-08-12
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
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
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

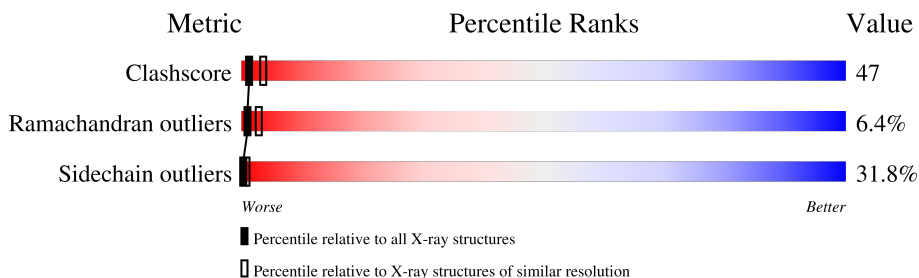
1 Overall quality at a glance

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

There are 2 unique types of molecules in this entry. The entry contains 8218 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 water.

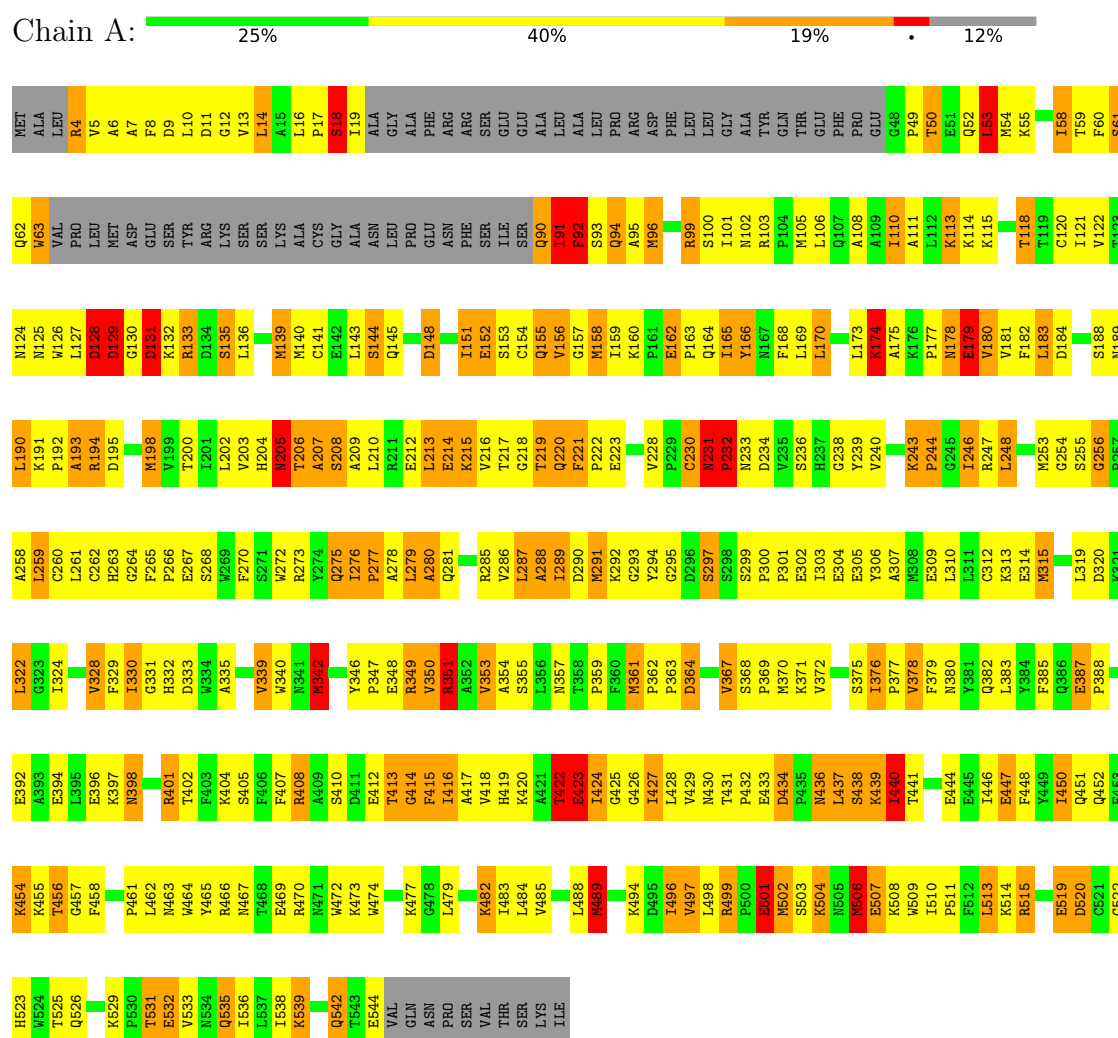
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	18	Total	O	0	0
			18	18		
2	B	22	Total	O	0	0
			22	22		

3 Residue-property plots

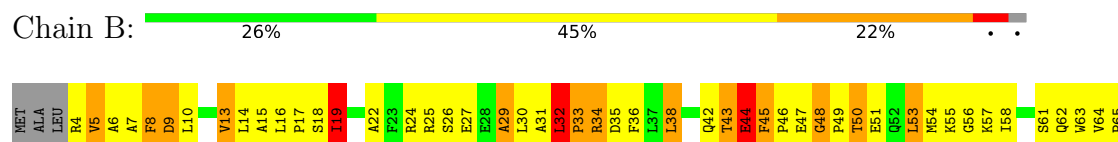
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: EPOXIDE HYDROLASE



K529	P461	K397	F329	G264	V199	D131	L66
P530	L462	N398	I330	P265	T200	K132	M67
T531	N463		G331	P266	I201	R133	D68
E532	V464	R402	H332	E267	L202		E69
V533	V465	T402	D333	G268	V203	M139	S70
H534	R466	F403	N334	W269	H204	M140	Y71
Q535	N467	K404	A335	F270	W205	C141	R72
I536	T468	S405	V339	S271	T206	E142	K73
L537	E469	F406	F406	W272	A207	L143	S74
I538	R470	F407	W340	R273	S208	S144	S75
K539	W471	R408	N341	Y274	A209	Q145	K76
	W472	A409	H342	G275	L210	H146	A77
Q542	K473	S410		I276	R211	F147	C78
T543	W474	D411	Y346	P277	E212	L148	G79
E544		E412	E348	A278	L213	F149	A80
VAL	K477	T413	R349	L279	E214	L150	N81
GLN	G478	G414	R349	A280	K215	I151	L82
ASN	L479	F415	V350	Q281	V216	E152	P83
PRO	G480	I416	R351		T217	S153	E94
SER	R481	A417	A352	R285	G218	C154	N85
VAL	K482	W418	V353	L287	T219		
THR	I483	H419	A354	A288	G220	Q155	S89
L484	R484	K420	S355	I288	F221	M158	Q90
VAL	W485	A421	L356	D289	P222	I159	I91
LYS		T422	N357	D290	E223	K160	F92
	L488	E423	T358	M291	A224	P161	S93
	M489	I424	P359	K292	G225	E162	Q94
		G425	G360	G293		P163	A95
K494		G426	K361	Y294	V228	Q164	N96
D495		I427	P362	G295	P229	I165	
L496		L428	G296	D296	C230	Y166	S100
V497		V429	S297	S297	W231		I101
L498		L430	G298	K298	P232	L169	N102
R499		T431	S299	M299	N233	L170	R103
P500		P432	P300	G299	D234	L171	P104
E501		E433	P301	E301	V235		M105
M502		D434	E302	E302	S236	L173	M05
S503		P435	L303	E304	H237	K176	L06
K504		M436	V372		G238	P177	Q107
N505		L437		E305	Y239		
M506		S438	S375	Y306	V240	N178	T110
E507		K439	I376	A307		E179	A111
K508		L440	P377	M308	K243	V180	L112
W509		T441	F378	E309	P244	F182	K113
I510			F379	L310	G245	L183	K115
P511		E444	N380	L311	I246	L184	G116
F512		E445	V381	C312	R247	D185	F117
L513		I446	Q382	K313	L248	F186	T118
K514		E447	E383	E314		G187	T119
R515		F448	Y384	M315	M253	S188	C120
		Y449	F385		G254	N189	I121
E519		I450	Q386	F318	S255	L190	V122
D520		Q451	R387	L319	G256	K191	T123
C521			P388	D320	P257	P192	N124
G522		K454		R321	A258	A193	N125
H523		K455	E392	L322	L259	R194	W126
W524		T456	A393	G323	C260	D195	L127
T525		G457	K394	I304	L261	M196	D128
		F458	L395		C262	G197	C129
Q526			F396	W298	W252	M198	D130

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)	94.6 (20.00-2.80)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.214 , 0.309	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8218	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.82	3/3981 (0.1%)	1.31	53/5397 (1.0%)
1	B	0.82	2/4413 (0.0%)	1.29	62/5984 (1.0%)
All	All	0.82	5/8394 (0.1%)	1.30	115/11381 (1.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	291	MET	SD-CE	7.16	1.97	1.79
1	B	291	MET	SD-CE	6.44	1.95	1.79
1	B	489	MET	SD-CE	-5.93	1.64	1.79
1	A	489	MET	SD-CE	-5.33	1.66	1.79
1	A	440	ILE	CA-CB	5.12	1.61	1.54

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	ASN	C-N-CD	-15.19	87.18	120.60
1	A	231	ASN	CA-C-N	13.46	159.29	127.00
1	A	231	ASN	C-N-CA	13.46	159.29	127.00
1	B	215	LYS	N-CA-C	-10.89	99.72	113.23
1	A	436	ASN	N-CA-C	-10.30	96.65	110.55
1	B	436	ASN	N-CA-C	-10.19	96.79	110.55
1	B	9	ASP	N-CA-C	-9.35	98.18	110.53
1	A	434	ASP	CA-C-N	-9.11	110.38	119.76
1	A	434	ASP	C-N-CA	-9.11	110.38	119.76
1	A	53	LEU	N-CA-C	-8.95	101.61	111.36
1	B	387	GLU	CA-C-N	8.94	130.35	119.98
1	B	387	GLU	C-N-CA	8.94	130.35	119.98
1	A	387	GLU	CA-C-N	8.72	130.09	119.98
1	A	387	GLU	C-N-CA	8.72	130.09	119.98
1	B	27	GLU	N-CA-C	-8.67	101.79	111.07
1	B	246	ILE	N-CA-C	8.48	120.49	108.36
1	B	231	ASN	C-N-CD	-8.27	102.40	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	ILE	N-CA-C	7.86	120.42	108.71
1	B	32	LEU	CA-C-N	7.82	129.05	119.98
1	B	32	LEU	C-N-CA	7.82	129.05	119.98
1	B	55	LYS	N-CA-C	-7.77	102.89	113.30
1	B	89	SER	N-CA-C	7.70	119.36	110.97
1	A	120	CYS	N-CA-C	7.63	119.74	108.60
1	A	454	LYS	N-CA-C	-7.51	103.11	111.82
1	A	289	ILE	N-CA-C	7.51	119.91	109.55
1	B	454	LYS	N-CA-C	-7.48	103.14	111.82
1	B	231	ASN	CA-C-N	7.30	144.53	127.00
1	B	231	ASN	C-N-CA	7.30	144.53	127.00
1	A	14	LEU	N-CA-C	-7.24	103.59	113.30
1	A	151	ILE	N-CA-C	7.24	113.95	106.21
1	A	315	MET	N-CA-C	-7.20	103.47	112.90
1	A	351	ARG	N-CA-C	-7.19	103.37	111.07
1	B	231	ASN	N-CA-C	7.18	125.67	109.81
1	B	146	HIS	N-CA-C	7.12	121.97	113.28
1	B	351	ARG	N-CA-C	-7.03	103.55	111.07
1	B	289	ILE	N-CA-C	6.98	119.19	109.55
1	B	315	MET	N-CA-C	-6.97	103.77	112.90
1	B	106	LEU	N-CA-C	-6.91	103.74	111.28
1	A	230	CYS	N-CA-C	-6.91	101.62	110.53
1	A	162	GLU	CA-C-N	6.85	128.40	119.84
1	A	162	GLU	C-N-CA	6.85	128.40	119.84
1	B	420	LYS	N-CA-C	6.58	121.48	113.38
1	B	342	MET	N-CA-C	-6.57	104.04	111.14
1	B	188	SER	N-CA-C	-6.53	104.24	111.82
1	A	342	MET	N-CA-C	-6.50	104.12	111.14
1	A	213	LEU	N-CA-C	-6.47	104.49	112.38
1	B	233	ASN	N-CA-C	-6.45	105.41	113.28
1	B	70	SER	N-CA-C	-6.40	104.73	112.54
1	A	131	ASP	N-CA-C	-6.35	104.59	112.90
1	A	194	ARG	N-CA-C	-6.33	104.48	111.82
1	B	223	GLU	N-CA-C	-6.32	103.69	111.40
1	B	142	GLU	N-CA-C	6.31	118.97	111.71
1	A	286	VAL	N-CA-C	6.24	117.63	109.58
1	B	128	ASP	N-CA-C	6.10	119.10	107.75
1	B	48	GLY	CA-C-N	6.09	127.45	119.84
1	B	48	GLY	C-N-CA	6.09	127.45	119.84
1	A	129	ASP	N-CA-C	-6.05	106.16	112.93
1	A	422	THR	N-CA-C	-6.03	100.18	109.76
1	A	423	GLU	N-CA-C	-5.97	98.08	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	GLN	N-CA-C	5.97	118.47	108.02
1	A	175	ALA	N-CA-C	5.97	116.29	107.88
1	B	164	GLN	N-CA-C	5.94	119.36	111.75
1	B	213	LEU	N-CA-C	-5.91	100.00	109.39
1	A	118	THR	N-CA-C	-5.90	99.67	109.46
1	B	44	GLU	N-CA-C	-5.89	98.25	110.80
1	A	114	LYS	N-CA-C	-5.84	104.10	111.11
1	B	95	ALA	N-CA-C	-5.80	106.05	113.01
1	B	8	PHE	N-CA-C	5.79	118.34	108.90
1	B	286	VAL	N-CA-C	5.79	117.05	109.58
1	A	260	CYS	N-CA-C	5.78	117.72	108.41
1	B	260	CYS	N-CA-C	5.78	117.72	108.41
1	A	425	GLY	N-CA-C	5.75	122.79	114.10
1	B	211	ARG	N-CA-C	-5.69	105.83	112.89
1	A	189	ASN	N-CA-C	-5.67	106.21	113.02
1	B	457	GLY	N-CA-C	-5.64	99.99	112.17
1	A	135	SER	N-CA-C	-5.62	104.16	111.02
1	A	188	SER	N-CA-C	-5.62	105.92	112.89
1	B	176	LYS	CA-C-N	5.57	125.28	119.82
1	B	176	LYS	C-N-CA	5.57	125.28	119.82
1	B	235	VAL	N-CA-C	5.55	117.71	109.17
1	B	189	ASN	N-CA-C	-5.51	106.06	112.89
1	B	114	LYS	N-CA-C	-5.50	104.68	111.33
1	A	457	GLY	N-CA-C	-5.46	100.37	112.17
1	A	221	PHE	N-CA-C	-5.44	103.27	110.40
1	B	145	GLN	N-CA-C	5.43	117.20	111.28
1	B	258	ALA	N-CA-C	5.42	118.30	110.28
1	A	193	ALA	N-CA-C	5.38	117.14	111.28
1	B	101	ILE	N-CA-C	5.35	117.33	109.63
1	B	401	ARG	N-CA-C	-5.34	105.15	110.97
1	A	128	ASP	N-CA-C	5.33	118.00	107.98
1	B	130	GLY	N-CA-C	5.33	118.19	112.33
1	B	280	ALA	N-CA-C	-5.30	105.15	111.03
1	B	307	ALA	N-CA-C	-5.28	102.58	110.23
1	B	19	ILE	N-CA-C	-5.26	104.51	111.09
1	B	33	PRO	N-CA-C	5.26	119.47	110.95
1	A	258	ALA	N-CA-C	5.25	118.06	110.28
1	A	439	LYS	N-CA-C	-5.25	106.55	113.17
1	A	234	ASP	N-CA-C	-5.24	107.18	113.21
1	A	151	ILE	N-CA-CB	-5.20	107.08	112.28
1	B	294	TYR	N-CA-C	5.20	118.21	110.14
1	A	96	MET	N-CA-C	-5.20	104.55	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	PRO	CA-N-CD	-5.20	104.22	111.50
1	A	169	LEU	N-CA-C	-5.17	105.56	111.14
1	A	511	PRO	N-CA-C	-5.16	103.66	111.41
1	A	350	VAL	N-CA-C	5.16	115.00	107.37
1	A	307	ALA	N-CA-C	-5.15	102.76	110.23
1	B	129	ASP	N-CA-C	-5.13	107.18	112.93
1	B	368	SER	CA-C-N	5.11	124.90	119.28
1	B	368	SER	C-N-CA	5.11	124.90	119.28
1	B	511	PRO	N-CA-C	-5.11	103.75	111.41
1	B	14	LEU	N-CA-C	-5.09	107.20	113.41
1	A	280	ALA	N-CA-C	-5.07	105.40	111.03
1	B	255	SER	N-CA-C	5.07	117.16	108.90
1	B	439	LYS	N-CA-C	-5.02	106.85	113.17
1	A	100	SER	N-CA-C	5.00	114.89	108.34

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	358	0
1	B	4299	0	4270	410	0
2	A	18	0	0	4	0
2	B	22	0	0	1	0
All	All	8218	0	8133	750	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 47.

All (750) 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:122:VAL:HG12	1:B:151:ILE:HG13	1.26	1.17
1:A:348:GLU:HA	1:B:133:ARG:HG3	1.33	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:VAL:HG22	1:A:118:THR:HB	1.33	1.08
1:B:232:PRO:HD2	1:B:233:ASN:H	1.16	1.03
1:A:58:ILE:HG22	1:A:62:GLN:HG3	1.44	1.00
1:B:204:HIS:O	1:B:205:ASN:HB2	1.58	0.99
1:B:19:ILE:HD11	1:B:96:MET:HA	1.41	0.99
1:B:127:LEU:HD12	1:B:127:LEU:H	1.29	0.98
1:B:122:VAL:CG1	1:B:151:ILE:HG13	1.93	0.97
1:B:125:ASN:HD22	1:B:152:GLU:HB3	1.28	0.97
1:B:5:VAL:HG21	1:B:173:LEU:HD21	1.45	0.97
1:A:205:ASN:ND2	1:A:207:ALA:H	1.63	0.96
1:A:193:ALA:O	1:A:198:MET:HG3	1.65	0.96
1:A:484:LEU:HD13	1:B:61:SER:HB2	1.44	0.94
1:B:49:PRO:HD2	1:B:67:MET:HE2	1.48	0.94
1:B:322:LEU:HB3	1:B:324:ILE:HD12	1.50	0.93
1:A:205:ASN:HD22	1:A:207:ALA:H	0.97	0.92
1:A:422:THR:O	1:A:423:GLU:HB2	1.66	0.92
1:B:5:VAL:HG21	1:B:173:LEU:CD2	1.99	0.91
1:B:44:GLU:O	1:B:46:PRO:HD3	1.69	0.91
1:B:259:LEU:HD21	1:B:279:LEU:HD13	1.52	0.91
1:A:158:MET:HG2	1:A:164:GLN:HG3	1.51	0.91
1:B:64:VAL:HB	1:B:65:PRO:HD3	1.52	0.91
1:B:190:LEU:HD22	1:B:200:THR:HB	1.51	0.90
1:A:259:LEU:HD21	1:A:279:LEU:HD13	1.54	0.90
1:B:26:SER:HA	1:B:29:ALA:HB3	1.54	0.89
1:B:127:LEU:HD12	1:B:127:LEU:N	1.88	0.89
1:A:320:ASP:OD1	1:A:349:ARG:NH2	2.06	0.89
1:B:230:CYS:HB3	1:B:277:PRO:HD3	1.55	0.89
1:A:133:ARG:HG3	1:B:348:GLU:HA	1.55	0.88
1:B:320:ASP:OD1	1:B:349:ARG:NH2	2.07	0.88
1:A:322:LEU:HB3	1:A:324:ILE:HD12	1.55	0.88
1:B:291:MET:HE3	1:B:291:MET:HA	1.54	0.88
1:A:339:VAL:HG13	1:A:353:VAL:HG12	1.55	0.87
1:A:291:MET:HE3	1:A:291:MET:HA	1.56	0.87
1:B:339:VAL:HG13	1:B:353:VAL:HG12	1.57	0.87
1:A:369:PRO:O	1:A:372:VAL:HG22	1.74	0.87
1:B:19:ILE:HD11	1:B:96:MET:CA	2.04	0.86
1:B:369:PRO:O	1:B:372:VAL:HG22	1.75	0.86
1:A:158:MET:HB3	1:A:165:ILE:HG12	1.58	0.85
1:B:231:ASN:N	1:B:231:ASN:HD22	1.73	0.84
1:A:263:HIS:CD2	1:A:291:MET:HG2	2.12	0.84
1:B:155:GLN:OE1	1:B:155:GLN:HA	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:GLN:HA	1:A:155:GLN:OE1	1.75	0.83
1:B:263:HIS:CD2	1:B:291:MET:HG2	2.13	0.83
1:A:106:LEU:O	1:A:106:LEU:HD23	1.79	0.83
1:A:378:VAL:HG11	2:A:1015:HOH:O	1.78	0.82
1:B:531:THR:HG23	1:B:532:GLU:OE2	1.79	0.82
1:A:52:GLN:CG	1:A:58:ILE:HD11	2.09	0.82
1:B:232:PRO:CD	1:B:233:ASN:H	1.91	0.82
1:A:193:ALA:HB1	1:A:198:MET:SD	2.20	0.82
1:B:5:VAL:HG23	1:B:118:THR:O	1.80	0.82
1:A:531:THR:HG23	1:A:532:GLU:OE2	1.79	0.81
1:B:62:GLN:O	1:B:65:PRO:HD2	1.79	0.81
1:B:529:LYS:HB3	1:B:532:GLU:CG	2.09	0.81
1:A:484:LEU:HD13	1:B:61:SER:CB	2.11	0.81
1:B:446:ILE:O	1:B:450:ILE:HD12	1.80	0.81
1:A:243:LYS:HG2	1:A:244:PRO:HD2	1.62	0.81
1:A:446:ILE:O	1:A:450:ILE:HD12	1.79	0.81
1:B:515:ARG:HH11	1:B:515:ARG:HG2	1.45	0.81
1:A:166:TYR:O	1:A:170:LEU:HD12	1.80	0.80
1:A:529:LYS:HB3	1:A:532:GLU:HG3	1.62	0.80
1:B:194:ARG:HB2	1:B:200:THR:HG21	1.63	0.80
1:A:535:GLN:O	1:A:539:LYS:HD3	1.82	0.80
1:B:529:LYS:HB3	1:B:532:GLU:HG3	1.61	0.80
1:A:13:VAL:HG22	1:A:203:VAL:HG21	1.64	0.79
1:A:52:GLN:HG2	1:A:58:ILE:HD11	1.65	0.79
1:A:484:LEU:CD1	1:B:61:SER:HB2	2.12	0.79
1:B:535:GLN:O	1:B:539:LYS:HD3	1.83	0.79
1:B:232:PRO:HD2	1:B:233:ASN:N	1.97	0.78
1:A:515:ARG:HG2	1:A:515:ARG:HH11	1.47	0.78
1:A:106:LEU:HD21	1:A:110:ILE:HD11	1.63	0.78
1:A:529:LYS:HB3	1:A:532:GLU:CG	2.12	0.78
1:B:259:LEU:HB2	1:B:328:VAL:HG22	1.66	0.77
1:B:243:LYS:HG2	1:B:244:PRO:HD2	1.64	0.77
1:B:215:LYS:HA	1:B:219:THR:O	1.84	0.77
1:B:183:LEU:HD13	1:B:201:ILE:HB	1.68	0.76
1:A:177:PRO:O	1:A:198:MET:HA	1.86	0.76
1:A:190:LEU:HD22	1:A:200:THR:HB	1.66	0.76
1:B:50:THR:HG23	1:B:63:TRP:HE1	1.50	0.76
1:B:230:CYS:HB3	1:B:277:PRO:CD	2.15	0.75
1:B:231:ASN:N	1:B:231:ASN:ND2	2.34	0.75
1:B:215:LYS:HZ3	1:B:221:PHE:H	1.34	0.75
1:A:108:ALA:O	1:A:111:ALA:HB3	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:TYR:H	1:A:166:TYR:HD1	1.35	0.74
1:B:71:TYR:O	1:B:75:SER:HB3	1.87	0.74
1:A:434:ASP:CG	1:A:434:ASP:O	2.29	0.74
1:B:170:LEU:HD11	1:B:198:MET:HE3	1.68	0.74
1:A:483:ILE:HB	1:A:510:ILE:HG12	1.70	0.74
1:A:259:LEU:HB2	1:A:328:VAL:HG22	1.70	0.73
1:B:300:PRO:HG2	1:B:305:GLU:HG2	1.71	0.73
1:B:127:LEU:H	1:B:127:LEU:CD1	2.02	0.73
1:B:141:CYS:O	1:B:144:SER:HB3	1.89	0.73
1:B:158:MET:CE	1:B:164:GLN:HB2	2.19	0.73
1:B:230:CYS:O	1:B:230:CYS:SG	2.47	0.73
1:B:19:ILE:CD1	1:B:96:MET:HA	2.17	0.73
1:B:330:ILE:HB	1:B:354:ALA:HB3	1.70	0.73
1:B:106:LEU:HD21	1:B:146:HIS:HD2	1.53	0.72
1:A:300:PRO:HG2	1:A:305:GLU:HG2	1.70	0.72
1:B:259:LEU:HD12	1:B:259:LEU:O	1.90	0.72
1:A:60:PHE:O	1:A:63:TRP:HB2	1.90	0.72
1:A:124:ASN:HA	1:A:153:SER:HB3	1.72	0.72
1:B:223:GLU:CD	1:B:223:GLU:H	1.97	0.72
1:B:483:ILE:HB	1:B:510:ILE:HG12	1.70	0.72
1:A:299:SER:CB	1:A:456:THR:HG22	2.19	0.71
1:B:215:LYS:C	1:B:217:THR:H	1.96	0.71
1:A:291:MET:HE1	1:A:315:MET:HE3	1.72	0.71
1:A:330:ILE:HB	1:A:354:ALA:HB3	1.72	0.71
1:B:230:CYS:HB3	1:B:277:PRO:CG	2.20	0.71
1:A:13:VAL:CG2	1:A:203:VAL:HG21	2.20	0.71
1:A:513:LEU:HD22	1:A:514:LYS:O	1.90	0.71
1:B:158:MET:HG2	1:B:164:GLN:HG3	1.72	0.70
1:A:58:ILE:HG22	1:A:62:GLN:CG	2.19	0.70
1:A:61:SER:HB3	1:B:484:LEU:HD13	1.71	0.70
1:B:190:LEU:HD13	1:B:202:LEU:HD12	1.72	0.70
1:A:259:LEU:HD12	1:A:259:LEU:O	1.92	0.70
1:B:75:SER:O	1:B:77:ALA:N	2.25	0.70
1:A:496:ILE:HD12	1:A:496:ILE:H	1.56	0.69
1:B:180:VAL:HG13	1:B:198:MET:HG2	1.73	0.69
1:B:291:MET:HE1	1:B:315:MET:HE3	1.74	0.69
1:A:446:ILE:HG22	1:A:450:ILE:HD11	1.75	0.69
1:B:513:LEU:HD22	1:B:514:LYS:O	1.93	0.69
1:A:328:VAL:HG12	1:A:351:ARG:HB3	1.74	0.69
1:A:53:LEU:HA	1:A:58:ILE:HD12	1.74	0.69
1:A:426:GLY:O	1:A:429:VAL:HG23	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:SER:CB	1:B:456:THR:HG22	2.22	0.68
1:B:75:SER:OG	1:B:76:LYS:N	2.23	0.68
1:A:173:LEU:O	1:A:174:LYS:HB2	1.91	0.68
1:B:211:ARG:O	1:B:215:LYS:HG2	1.93	0.68
1:B:376:ILE:HD12	1:B:379:PHE:CE2	2.28	0.68
1:B:230:CYS:HB3	1:B:277:PRO:HG3	1.74	0.68
1:A:148:ASP:OD1	1:A:148:ASP:N	2.26	0.68
1:B:328:VAL:HG12	1:B:351:ARG:HB3	1.75	0.68
1:A:348:GLU:HA	1:B:133:ARG:CG	2.19	0.67
1:A:106:LEU:CD2	1:A:110:ILE:HD11	2.23	0.67
1:A:210:LEU:O	1:A:214:GLU:HB2	1.94	0.67
1:A:106:LEU:HD23	1:A:106:LEU:C	2.19	0.67
1:A:52:GLN:HG3	1:A:58:ILE:HD11	1.76	0.67
1:B:158:MET:HG2	1:B:164:GLN:CG	2.25	0.67
1:B:194:ARG:HB2	1:B:200:THR:CG2	2.24	0.67
1:A:207:ALA:O	1:A:210:LEU:HB3	1.95	0.66
1:B:112:LEU:O	1:B:117:PHE:HB2	1.94	0.66
1:B:270:PHE:CE1	1:B:273:ARG:HD3	2.30	0.66
1:B:529:LYS:O	1:B:533:VAL:HG23	1.95	0.66
1:A:205:ASN:ND2	1:A:207:ALA:N	2.39	0.66
1:A:248:LEU:HA	1:A:297:SER:HB3	1.77	0.66
1:B:496:ILE:H	1:B:496:ILE:HD12	1.58	0.66
1:B:467:ASN:OD1	1:B:470:ARG:HD2	1.96	0.66
1:B:204:HIS:O	1:B:205:ASN:CB	2.39	0.66
1:B:46:PRO:HG2	1:B:159:ILE:CD1	2.26	0.66
1:B:248:LEU:HA	1:B:297:SER:HB3	1.78	0.65
1:B:446:ILE:HG22	1:B:450:ILE:HD11	1.77	0.65
1:A:58:ILE:HA	1:A:62:GLN:OE1	1.97	0.65
1:A:50:THR:HA	1:A:63:TRP:HZ2	1.61	0.65
1:A:309:GLU:HB2	1:A:474:TRP:CD2	2.32	0.65
1:B:124:ASN:HA	1:B:153:SER:HB3	1.77	0.65
1:A:94:GLN:CD	1:A:94:GLN:H	2.04	0.65
1:A:166:TYR:HD1	1:A:166:TYR:N	1.94	0.65
1:B:106:LEU:HD21	1:B:146:HIS:CD2	2.31	0.65
1:B:158:MET:HE2	1:B:164:GLN:HB2	1.79	0.65
1:B:309:GLU:HB2	1:B:474:TRP:CD2	2.31	0.65
1:A:166:TYR:N	1:A:166:TYR:CD1	2.62	0.64
1:A:398:ASN:C	1:A:398:ASN:OD1	2.39	0.64
1:B:276:ILE:HD11	1:B:288:ALA:CB	2.27	0.64
1:B:259:LEU:HD12	1:B:259:LEU:C	2.23	0.64
1:A:376:ILE:HD12	1:A:379:PHE:CE2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:GLY:HA2	1:B:299:SER:HA	1.78	0.64
1:A:342:MET:HE2	1:A:342:MET:HA	1.80	0.64
1:A:529:LYS:O	1:A:533:VAL:HG23	1.97	0.64
1:B:232:PRO:HD2	1:B:233:ASN:HD22	1.62	0.64
1:B:535:GLN:HG2	1:B:539:LYS:NZ	2.13	0.64
1:A:293:GLY:HA2	1:A:299:SER:HA	1.79	0.64
1:B:159:ILE:O	1:B:162:GLU:HB2	1.97	0.63
1:B:510:ILE:HG22	1:B:513:LEU:HB2	1.80	0.63
1:B:291:MET:HE3	1:B:291:MET:CA	2.23	0.63
1:B:13:VAL:HB	1:B:203:VAL:HG11	1.80	0.63
1:A:177:PRO:O	1:A:198:MET:HB3	1.97	0.63
1:B:342:MET:HE2	1:B:346:TYR:HD2	1.61	0.63
1:B:398:ASN:OD1	1:B:398:ASN:C	2.39	0.63
1:B:75:SER:HB2	1:B:82:LEU:CB	2.29	0.63
1:A:427:ILE:HG12	1:A:427:ILE:O	1.98	0.63
1:B:342:MET:HE2	1:B:342:MET:HA	1.80	0.63
1:A:122:VAL:HG12	1:A:151:ILE:HB	1.79	0.63
1:A:145:GLN:HA	1:A:145:GLN:NE2	2.13	0.63
1:A:446:ILE:HG22	1:A:450:ILE:CD1	2.28	0.63
1:A:467:ASN:OD1	1:A:470:ARG:HD2	1.98	0.63
1:A:158:MET:CG	1:A:164:GLN:HG3	2.26	0.63
1:A:342:MET:HE2	1:A:346:TYR:HD2	1.64	0.62
1:B:124:ASN:HA	1:B:153:SER:CB	2.29	0.62
1:B:38:LEU:HD13	1:B:42:GLN:HB3	1.81	0.62
1:A:291:MET:HE3	1:A:291:MET:CA	2.26	0.62
1:B:25:ARG:HH11	1:B:25:ARG:HG2	1.65	0.62
1:A:276:ILE:HD11	1:A:288:ALA:CB	2.30	0.62
1:B:139:MET:O	1:B:143:LEU:HD12	1.99	0.61
1:B:426:GLY:HA3	1:B:429:VAL:CG2	2.29	0.61
1:B:8:PHE:O	1:B:121:ILE:HG23	2.00	0.61
1:B:489:MET:HG2	1:B:506:MET:HE1	1.82	0.61
1:A:394:GLU:OE2	1:A:428:LEU:HB2	2.00	0.61
1:B:9:ASP:O	1:B:13:VAL:HG22	2.01	0.61
1:A:159:ILE:C	1:A:165:ILE:HD11	2.25	0.61
1:A:270:PHE:CE1	1:A:273:ARG:HD3	2.35	0.61
1:B:264:GLY:HA3	1:B:333:ASP:HB3	1.83	0.61
1:B:259:LEU:HD21	1:B:279:LEU:CD1	2.29	0.61
1:B:394:GLU:OE2	1:B:428:LEU:HB2	2.01	0.61
1:A:535:GLN:HG2	1:A:539:LYS:NZ	2.15	0.61
1:A:359:PRO:HA	1:A:489:MET:CE	2.30	0.60
1:A:416:ILE:CG2	1:A:427:ILE:HD11	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:VAL:HA	2:A:1015:HOH:O	2.00	0.60
1:B:232:PRO:HD2	1:B:233:ASN:ND2	2.16	0.60
1:A:378:VAL:HG21	2:A:1015:HOH:O	2.00	0.60
1:B:75:SER:C	1:B:77:ALA:N	2.56	0.60
1:A:264:GLY:HA3	1:A:333:ASP:HB3	1.83	0.60
1:B:146:HIS:N	1:B:146:HIS:ND1	2.50	0.60
1:B:16:LEU:HD13	1:B:206:THR:HG22	1.83	0.60
1:A:329:PHE:HB3	1:A:339:VAL:HG22	1.84	0.60
1:A:159:ILE:O	1:A:165:ILE:HD11	2.02	0.60
1:A:180:VAL:HG13	1:A:198:MET:HB3	1.83	0.60
1:A:259:LEU:HD12	1:A:259:LEU:C	2.26	0.60
1:B:268:SER:HB2	2:B:1004:HOH:O	2.02	0.59
1:A:322:LEU:HD22	1:A:324:ILE:HD11	1.84	0.59
1:B:187:GLY:HA2	1:B:202:LEU:HD11	1.83	0.59
1:B:446:ILE:HG22	1:B:450:ILE:CD1	2.31	0.59
1:B:529:LYS:HB3	1:B:532:GLU:HG2	1.83	0.59
1:A:489:MET:HG2	1:A:506:MET:HE1	1.85	0.59
1:B:322:LEU:HD22	1:B:324:ILE:HD11	1.83	0.59
1:A:304:GLU:H	1:A:304:GLU:CD	2.10	0.59
1:B:424:ILE:N	1:B:424:ILE:HD13	2.17	0.59
1:B:342:MET:CE	1:B:346:TYR:HD2	2.15	0.59
1:B:74:SER:O	1:B:75:SER:O	2.21	0.59
1:B:215:LYS:C	1:B:217:THR:N	2.59	0.59
1:B:230:CYS:CB	1:B:277:PRO:HG3	2.33	0.59
1:B:359:PRO:HA	1:B:489:MET:CE	2.33	0.59
1:B:447:GLU:HA	1:B:450:ILE:HD13	1.84	0.59
1:A:92:PHE:CD1	1:A:92:PHE:C	2.80	0.58
1:B:270:PHE:HB2	1:B:448:PHE:CE2	2.38	0.58
1:B:329:PHE:HB3	1:B:339:VAL:HG22	1.85	0.58
1:A:5:VAL:CG1	1:A:6:ALA:N	2.67	0.58
1:A:510:ILE:HG22	1:A:513:LEU:HB2	1.84	0.58
1:A:474:TRP:O	1:A:477:LYS:HG3	2.04	0.58
1:B:538:ILE:O	1:B:542:GLN:HG2	2.04	0.58
1:B:125:ASN:ND2	1:B:152:GLU:HB3	2.10	0.58
1:A:270:PHE:HB2	1:A:448:PHE:CE2	2.39	0.58
1:A:310:LEU:O	1:A:314:GLU:HG3	2.03	0.58
1:B:304:GLU:CD	1:B:304:GLU:H	2.12	0.58
1:A:7:ALA:O	1:A:183:LEU:HD23	2.04	0.58
1:A:496:ILE:HD12	1:A:496:ILE:N	2.18	0.58
1:B:426:GLY:C	1:B:429:VAL:HG23	2.28	0.58
1:A:159:ILE:O	1:A:159:ILE:HD12	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:LYS:O	1:A:408:ARG:HD2	2.04	0.58
1:A:303:ILE:HD13	1:A:463:ASN:CG	2.29	0.57
1:B:424:ILE:H	1:B:424:ILE:CD1	2.17	0.57
1:A:496:ILE:H	1:A:496:ILE:CD1	2.17	0.57
1:A:177:PRO:O	1:A:198:MET:CA	2.52	0.57
1:B:160:LYS:HA	1:B:165:ILE:HD11	1.86	0.57
1:A:342:MET:CE	1:A:346:TYR:HD2	2.17	0.57
1:A:431:THR:HG23	1:A:432:PRO:HD2	1.86	0.57
1:A:538:ILE:O	1:A:542:GLN:HG2	2.03	0.57
1:B:203:VAL:HG12	1:B:203:VAL:O	2.04	0.57
1:B:187:GLY:HA2	1:B:190:LEU:HB2	1.86	0.57
1:B:215:LYS:NZ	1:B:221:PHE:H	1.99	0.57
1:B:404:LYS:O	1:B:408:ARG:HD2	2.05	0.57
1:A:447:GLU:HA	1:A:450:ILE:HD13	1.86	0.57
1:B:75:SER:HB2	1:B:82:LEU:HB2	1.86	0.57
1:B:122:VAL:HG21	1:B:182:PHE:CE2	2.40	0.57
1:A:312:CYS:HB3	1:A:342:MET:HE3	1.86	0.57
1:B:36:PHE:HZ	1:B:75:SER:HA	1.69	0.57
1:B:232:PRO:O	1:B:235:VAL:HG22	2.04	0.57
1:B:26:SER:HA	1:B:29:ALA:CB	2.29	0.56
1:A:16:LEU:HA	1:A:17:PRO:C	2.31	0.56
1:B:22:ALA:HA	1:B:25:ARG:HD3	1.86	0.56
1:A:61:SER:HB2	1:A:129:ASP:OD1	2.06	0.56
1:B:427:ILE:HG13	1:B:428:LEU:HD13	1.87	0.56
1:A:312:CYS:CB	1:A:342:MET:HE3	2.35	0.56
1:B:158:MET:HE3	1:B:164:GLN:HB2	1.86	0.56
1:B:36:PHE:HE2	1:B:82:LEU:HD13	1.71	0.56
1:A:294:TYR:CZ	1:A:461:PRO:HB3	2.41	0.56
1:B:193:ALA:O	1:B:198:MET:HB2	2.06	0.56
1:B:346:TYR:O	1:B:350:VAL:HG23	2.06	0.56
1:A:4:ARG:HG3	1:A:179:GLU:HB3	1.88	0.56
1:A:206:THR:O	1:A:207:ALA:CB	2.54	0.56
1:B:158:MET:HE2	1:B:164:GLN:C	2.30	0.56
1:B:312:CYS:HB3	1:B:342:MET:HE3	1.87	0.56
1:A:17:PRO:O	1:A:18:SER:O	2.24	0.56
1:B:474:TRP:O	1:B:477:LYS:HG3	2.05	0.56
1:A:529:LYS:HB3	1:A:532:GLU:HG2	1.87	0.55
1:B:161:PRO:O	1:B:162:GLU:C	2.49	0.55
1:B:178:ASN:N	1:B:178:ASN:ND2	2.53	0.55
1:B:180:VAL:O	1:B:199:VAL:HG23	2.06	0.55
1:A:8:PHE:O	1:A:121:ILE:HA	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:LYS:O	1:B:77:ALA:HB3	2.05	0.55
1:B:532:GLU:O	1:B:536:ILE:HG13	2.07	0.55
1:A:532:GLU:O	1:A:536:ILE:HG13	2.06	0.55
1:B:440:ILE:HG22	1:B:441:THR:HG23	1.88	0.55
1:A:231:ASN:N	1:A:231:ASN:HD22	2.04	0.55
1:B:180:VAL:HG11	1:B:198:MET:CE	2.36	0.55
1:A:52:GLN:HE21	1:A:58:ILE:HG12	1.71	0.55
1:B:434:ASP:H	1:B:435:PRO:HD3	1.71	0.55
1:A:262:CYS:HB2	1:A:335:ALA:HB1	1.89	0.55
1:B:128:ASP:O	1:B:133:ARG:HD3	2.07	0.55
1:B:496:ILE:H	1:B:496:ILE:CD1	2.19	0.55
1:B:496:ILE:HD12	1:B:496:ILE:N	2.21	0.55
1:A:346:TYR:O	1:A:350:VAL:HG23	2.07	0.55
1:A:156:VAL:HG11	1:A:168:PHE:HE2	1.72	0.55
1:B:303:ILE:HD13	1:B:463:ASN:CG	2.31	0.55
1:A:231:ASN:N	1:A:231:ASN:ND2	2.53	0.54
1:A:463:ASN:HA	1:A:466:ARG:HG3	1.88	0.54
1:A:215:LYS:HB2	1:A:219:THR:O	2.06	0.54
1:A:497:VAL:O	1:A:498:LEU:HB2	2.07	0.54
1:B:159:ILE:O	1:B:165:ILE:HD11	2.07	0.54
1:A:299:SER:HB2	1:A:456:THR:HG22	1.89	0.54
1:B:5:VAL:HG21	1:B:173:LEU:HD23	1.86	0.54
1:B:180:VAL:HG11	1:B:198:MET:HE3	1.90	0.54
1:B:310:LEU:O	1:B:314:GLU:HG3	2.07	0.54
1:B:434:ASP:O	1:B:435:PRO:C	2.51	0.54
1:B:497:VAL:O	1:B:498:LEU:HB2	2.08	0.54
1:A:264:GLY:O	1:A:267:GLU:HG3	2.06	0.54
1:B:202:LEU:HD23	1:B:204:HIS:CD2	2.42	0.54
1:A:428:LEU:O	1:A:431:THR:HB	2.07	0.54
1:A:256:GLY:N	1:A:285:ARG:HB2	2.23	0.54
1:B:292:LYS:NZ	1:B:305:GLU:HG3	2.23	0.54
1:A:159:ILE:O	1:A:162:GLU:HB2	2.07	0.54
1:B:434:ASP:N	1:B:435:PRO:HD3	2.22	0.54
1:A:416:ILE:HG21	1:A:427:ILE:HD11	1.89	0.54
1:B:53:LEU:HD22	1:B:126:TRP:HB2	1.90	0.54
1:B:367:VAL:O	1:B:368:SER:C	2.51	0.54
1:B:205:ASN:HB3	1:B:207:ALA:H	1.73	0.54
1:B:256:GLY:N	1:B:285:ARG:HB2	2.23	0.54
1:B:421:ALA:HA	1:B:424:ILE:HD11	1.90	0.54
1:A:166:TYR:O	1:A:170:LEU:CD1	2.54	0.54
1:A:182:PHE:HD1	1:A:183:LEU:H	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:GLU:HB2	1:B:474:TRP:CE2	2.43	0.54
1:A:131:ASP:N	1:A:131:ASP:OD1	2.42	0.53
1:A:205:ASN:OD1	1:A:209:ALA:N	2.40	0.53
1:A:287:LEU:O	1:A:289:ILE:HG13	2.08	0.53
1:B:312:CYS:CB	1:B:342:MET:HE3	2.37	0.53
1:B:380:ASN:HB3	1:B:418:VAL:O	2.09	0.53
1:B:498:LEU:HD12	1:B:523:HIS:CE1	2.43	0.53
1:A:62:GLN:OE1	1:B:481:ARG:HA	2.08	0.53
1:A:194:ARG:HB2	1:A:200:THR:HG21	1.90	0.53
1:B:47:GLU:HG2	1:B:48:GLY:H	1.71	0.53
1:B:82:LEU:O	1:B:83:PRO:C	2.52	0.53
1:B:463:ASN:HA	1:B:466:ARG:HG3	1.91	0.53
1:A:230:CYS:HB3	1:A:277:PRO:HG3	1.89	0.53
1:B:223:GLU:CD	1:B:223:GLU:N	2.66	0.53
1:B:395:LEU:HD21	1:B:427:ILE:HD11	1.90	0.53
1:B:107:GLN:HG3	1:B:225:PRO:HG2	1.91	0.53
1:B:424:ILE:N	1:B:424:ILE:CD1	2.70	0.53
1:A:125:ASN:HD22	1:A:152:GLU:HB2	1.73	0.53
1:B:299:SER:HB2	1:B:456:THR:HG22	1.90	0.53
1:A:292:LYS:NZ	1:A:305:GLU:HG3	2.24	0.53
1:A:416:ILE:HG23	1:A:427:ILE:HG12	1.91	0.53
1:A:503:SER:O	1:A:506:MET:HB2	2.09	0.53
1:B:206:THR:O	1:B:207:ALA:HB2	2.09	0.53
1:A:10:LEU:CD2	1:A:140:MET:HE1	2.39	0.53
1:A:255:SER:O	1:A:256:GLY:O	2.28	0.53
1:A:501:GLU:O	1:A:504:LYS:HG2	2.09	0.53
1:A:9:ASP:OD1	1:A:160:LYS:NZ	2.37	0.52
1:B:255:SER:O	1:B:256:GLY:O	2.27	0.52
1:B:535:GLN:HG2	1:B:539:LYS:HZ2	1.72	0.52
1:A:5:VAL:HG12	1:A:6:ALA:N	2.24	0.52
1:A:5:VAL:CG2	1:A:118:THR:HB	2.24	0.52
1:A:182:PHE:CD1	1:A:183:LEU:N	2.76	0.52
1:A:192:PRO:O	1:A:195:ASP:HB2	2.10	0.52
1:A:259:LEU:HD21	1:A:279:LEU:CD1	2.32	0.52
1:B:515:ARG:HG2	1:B:515:ARG:NH1	2.21	0.52
1:A:50:THR:OG1	1:A:63:TRP:CZ2	2.59	0.52
1:A:265:PHE:CD1	1:A:265:PHE:C	2.87	0.52
1:A:275:GLN:O	1:A:279:LEU:HB2	2.10	0.52
1:A:407:PHE:C	1:A:408:ARG:HG2	2.34	0.52
1:A:440:ILE:HG22	1:A:441:THR:HG23	1.91	0.52
1:B:141:CYS:O	1:B:144:SER:CB	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:LEU:CD1	1:B:201:ILE:HB	2.37	0.52
1:A:212:GLU:C	1:A:214:GLU:N	2.67	0.52
1:A:380:ASN:HB3	1:A:418:VAL:O	2.09	0.52
1:B:49:PRO:HG2	1:B:67:MET:HG2	1.91	0.52
1:A:422:THR:O	1:A:423:GLU:CB	2.47	0.52
1:A:498:LEU:HD12	1:A:523:HIS:CE1	2.44	0.52
1:A:141:CYS:O	1:A:144:SER:HB3	2.09	0.52
1:B:6:ALA:O	1:B:119:THR:HA	2.10	0.52
1:B:222:PRO:HG2	1:B:225:PRO:HG3	1.90	0.52
1:B:187:GLY:CA	1:B:202:LEU:HD11	2.40	0.52
1:A:10:LEU:C	1:A:12:GLY:N	2.65	0.52
1:B:16:LEU:HB3	1:B:17:PRO:HA	1.91	0.52
1:B:434:ASP:N	1:B:435:PRO:CD	2.72	0.52
1:A:293:GLY:O	1:A:456:THR:HG21	2.10	0.51
1:B:501:GLU:O	1:B:504:LYS:HG2	2.10	0.51
1:B:92:PHE:CD1	1:B:92:PHE:C	2.87	0.51
1:A:212:GLU:HA	1:A:215:LYS:HD2	1.92	0.51
1:B:75:SER:C	1:B:77:ALA:H	2.18	0.51
1:B:294:TYR:CZ	1:B:461:PRO:HB3	2.45	0.51
1:A:9:ASP:CG	1:A:10:LEU:H	2.18	0.51
1:A:91:ILE:HD13	1:A:91:ILE:H	1.75	0.51
1:A:469:GLU:HA	1:A:469:GLU:OE1	2.10	0.51
1:B:498:LEU:HD12	1:B:523:HIS:HE1	1.76	0.51
1:A:190:LEU:CD2	1:A:200:THR:HB	2.39	0.51
1:A:380:ASN:ND2	1:A:422:THR:OG1	2.43	0.51
1:A:49:PRO:O	1:A:52:GLN:HG2	2.11	0.51
1:A:173:LEU:O	1:A:174:LYS:CB	2.59	0.51
1:A:309:GLU:HB2	1:A:474:TRP:CE2	2.46	0.51
1:A:367:VAL:O	1:A:368:SER:C	2.54	0.51
1:B:102:ASN:ND2	1:B:105:MET:HG3	2.26	0.51
1:A:515:ARG:HH11	1:A:515:ARG:CG	2.23	0.51
1:B:535:GLN:CB	1:B:539:LYS:HZ2	2.23	0.51
1:B:45:PHE:CG	1:B:45:PHE:O	2.63	0.51
1:B:162:GLU:O	1:B:165:ILE:CD1	2.59	0.51
1:B:407:PHE:C	1:B:408:ARG:HG2	2.35	0.51
1:A:101:ILE:HG22	1:A:102:ASN:N	2.25	0.51
1:A:497:VAL:HG22	1:A:498:LEU:HG	1.93	0.51
1:B:56:GLY:HA2	1:B:127:LEU:HD11	1.92	0.51
1:B:262:CYS:HB2	1:B:335:ALA:HB1	1.93	0.51
1:A:10:LEU:HD12	1:A:14:LEU:HB2	1.92	0.50
1:A:156:VAL:HG11	1:A:168:PHE:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:PRO:O	1:B:231:ASN:ND2	2.44	0.50
1:A:178:ASN:O	1:A:180:VAL:N	2.42	0.50
1:A:499:ARG:O	1:A:502:MET:HG3	2.12	0.50
1:B:149:PHE:CD2	1:B:173:LEU:HD12	2.46	0.50
1:B:276:ILE:HD11	1:B:288:ALA:HB2	1.93	0.50
1:A:498:LEU:HD12	1:A:523:HIS:HE1	1.76	0.50
1:A:535:GLN:HG2	1:A:539:LYS:HZ2	1.75	0.50
1:A:159:ILE:C	1:A:165:ILE:CD1	2.85	0.50
1:B:499:ARG:O	1:B:502:MET:HG3	2.11	0.50
1:A:16:LEU:HD23	1:A:18:SER:N	2.27	0.50
1:A:52:GLN:HE21	1:A:58:ILE:CG1	2.24	0.50
1:A:392:GLU:HG3	1:A:462:LEU:HD12	1.93	0.50
1:A:515:ARG:HG2	1:A:515:ARG:NH1	2.23	0.50
1:B:121:ILE:O	1:B:151:ILE:HG12	2.12	0.50
1:B:158:MET:HB2	1:B:165:ILE:HG23	1.94	0.50
1:B:264:GLY:O	1:B:267:GLU:HG3	2.11	0.50
1:B:265:PHE:CD1	1:B:265:PHE:C	2.90	0.50
1:B:291:MET:HA	1:B:291:MET:CE	2.35	0.50
1:B:101:ILE:HG22	1:B:102:ASN:N	2.26	0.50
1:B:275:GLN:O	1:B:279:LEU:HB2	2.10	0.50
1:A:289:ILE:HG22	1:A:290:ASP:N	2.27	0.50
1:B:289:ILE:HG22	1:B:290:ASP:N	2.27	0.50
1:B:428:LEU:HA	1:B:431:THR:OG1	2.12	0.50
1:B:54:MET:HA	1:B:125:ASN:O	2.12	0.49
1:B:178:ASN:C	1:B:180:VAL:H	2.19	0.49
1:B:426:GLY:CA	1:B:429:VAL:CG2	2.89	0.49
1:B:469:GLU:OE1	1:B:469:GLU:HA	2.11	0.49
1:A:125:ASN:HD22	1:A:152:GLU:CB	2.25	0.49
1:A:128:ASP:O	1:A:133:ARG:HD3	2.11	0.49
1:A:193:ALA:CB	1:A:198:MET:SD	2.96	0.49
1:A:153:SER:HB2	1:A:158:MET:O	2.12	0.49
1:A:291:MET:HA	1:A:291:MET:CE	2.36	0.49
1:B:216:VAL:O	1:B:216:VAL:CG1	2.60	0.49
1:A:165:ILE:O	1:A:168:PHE:HB3	2.12	0.49
1:B:33:PRO:O	1:B:34:ARG:C	2.55	0.49
1:B:177:PRO:O	1:B:198:MET:HA	2.11	0.49
1:B:216:VAL:O	1:B:216:VAL:HG13	2.11	0.49
1:A:243:LYS:O	1:A:244:PRO:C	2.55	0.49
1:A:93:SER:O	1:A:96:MET:HB3	2.13	0.49
1:B:30:LEU:O	1:B:31:ALA:HB3	2.13	0.49
1:B:144:SER:OG	1:B:145:GLN:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:LYS:O	1:B:244:PRO:C	2.55	0.49
1:B:287:LEU:O	1:B:289:ILE:HG13	2.13	0.49
1:A:439:LYS:HG2	1:A:440:ILE:HD13	1.94	0.49
1:A:424:ILE:O	1:A:424:ILE:HG13	2.13	0.49
1:A:535:GLN:CB	1:A:539:LYS:HZ2	2.25	0.49
1:A:263:HIS:NE2	1:A:291:MET:HG2	2.28	0.48
1:B:270:PHE:CZ	1:B:273:ARG:HD3	2.47	0.48
1:A:10:LEU:HD22	1:A:140:MET:HE1	1.96	0.48
1:B:4:ARG:HE	1:B:179:GLU:HA	1.78	0.48
1:B:309:GLU:HB2	1:B:474:TRP:CG	2.48	0.48
1:B:340:TRP:CZ2	1:B:355:SER:HB2	2.49	0.48
1:A:319:LEU:HB3	1:A:324:ILE:O	2.14	0.48
1:B:75:SER:O	1:B:76:LYS:C	2.55	0.48
1:B:73:LYS:O	1:B:74:SER:C	2.56	0.48
1:A:162:GLU:O	1:A:165:ILE:HD12	2.14	0.48
1:B:4:ARG:HB3	1:B:4:ARG:CZ	2.42	0.48
1:B:458:PHE:C	1:B:461:PRO:HD2	2.38	0.48
1:B:118:THR:HA	1:B:148:ASP:OD2	2.13	0.48
1:B:150:LEU:HG	1:B:152:GLU:HG2	1.96	0.48
1:B:342:MET:CE	1:B:346:TYR:CD2	2.95	0.48
1:B:497:VAL:HG22	1:B:498:LEU:HG	1.96	0.48
1:A:90:GLN:O	1:A:92:PHE:N	2.45	0.48
1:A:106:LEU:CD2	1:A:106:LEU:C	2.86	0.48
1:A:276:ILE:HD11	1:A:288:ALA:HB2	1.96	0.48
1:B:64:VAL:CB	1:B:65:PRO:HD3	2.32	0.48
1:B:17:PRO:O	1:B:18:SER:C	2.55	0.48
1:A:330:ILE:O	1:A:330:ILE:HG13	2.11	0.48
1:A:375:SER:OG	1:A:376:ILE:N	2.47	0.48
1:B:103:ARG:O	1:B:107:GLN:HB2	2.14	0.48
1:B:151:ILE:HG12	1:B:151:ILE:H	1.34	0.48
1:B:462:LEU:C	1:B:464:TRP:H	2.22	0.48
1:A:182:PHE:C	1:A:183:LEU:HD22	2.39	0.48
1:A:270:PHE:CZ	1:A:273:ARG:HD3	2.49	0.48
1:A:54:MET:SD	1:A:124:ASN:HB3	2.55	0.47
1:B:93:SER:OG	1:B:132:LYS:NZ	2.47	0.47
1:B:503:SER:O	1:B:506:MET:HB2	2.13	0.47
1:A:92:PHE:N	1:A:94:GLN:OE1	2.47	0.47
1:B:7:ALA:HB2	1:B:120:CYS:SG	2.54	0.47
1:B:300:PRO:CG	1:B:305:GLU:HG2	2.42	0.47
1:A:122:VAL:O	1:A:122:VAL:HG23	2.14	0.47
1:A:179:GLU:H	1:A:179:GLU:HG3	1.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:PHE:HE1	1:B:184:ASP:HB2	1.78	0.47
1:B:439:LYS:HG2	1:B:440:ILE:HD13	1.95	0.47
1:A:53:LEU:HD23	1:A:58:ILE:O	2.13	0.47
1:A:92:PHE:O	1:A:95:ALA:HB3	2.14	0.47
1:A:124:ASN:HA	1:A:153:SER:CB	2.43	0.47
1:B:232:PRO:CD	1:B:233:ASN:N	2.59	0.47
1:A:254:GLY:H	1:B:323:GLY:HA3	1.79	0.47
1:B:160:LYS:HG2	1:B:165:ILE:HD13	1.95	0.47
1:B:222:PRO:HG2	1:B:225:PRO:HB3	1.97	0.47
1:B:230:CYS:C	1:B:231:ASN:ND2	2.72	0.47
1:B:319:LEU:HB3	1:B:324:ILE:O	2.14	0.47
1:A:380:ASN:OD1	1:A:422:THR:N	2.45	0.47
1:B:36:PHE:CE2	1:B:82:LEU:HD13	2.50	0.47
1:B:364:ASP:OD1	1:B:364:ASP:N	2.48	0.47
1:A:101:ILE:CG2	1:A:102:ASN:N	2.78	0.47
1:A:177:PRO:O	1:A:198:MET:CB	2.62	0.47
1:A:180:VAL:CG1	1:A:198:MET:HE2	2.45	0.47
1:B:58:ILE:HD12	1:B:63:TRP:HB2	1.96	0.47
1:A:10:LEU:O	1:A:12:GLY:N	2.47	0.47
1:A:309:GLU:HB2	1:A:474:TRP:CG	2.50	0.47
1:B:64:VAL:HB	1:B:65:PRO:CD	2.36	0.47
1:A:340:TRP:CZ2	1:A:355:SER:HB2	2.50	0.47
1:B:270:PHE:CD2	1:B:448:PHE:CD2	3.03	0.47
1:B:413:THR:HB	1:B:414:GLY:H	1.51	0.47
1:B:10:LEU:HD11	1:B:15:ALA:HB2	1.97	0.47
1:B:462:LEU:C	1:B:464:TRP:N	2.73	0.47
1:A:62:GLN:HE22	1:B:482:LYS:N	2.13	0.46
1:A:165:ILE:H	1:A:165:ILE:HG13	1.49	0.46
1:A:359:PRO:HA	1:A:489:MET:HE3	1.96	0.46
1:A:328:VAL:O	1:A:328:VAL:CG2	2.63	0.46
1:A:342:MET:CE	1:A:346:TYR:CD2	2.98	0.46
1:A:364:ASP:N	1:A:364:ASP:OD1	2.47	0.46
1:B:107:GLN:HA	1:B:107:GLN:NE2	2.29	0.46
1:B:124:ASN:HA	1:B:153:SER:OG	2.14	0.46
1:A:507:GLU:H	1:A:507:GLU:HG2	1.36	0.46
1:B:106:LEU:HD23	1:B:106:LEU:O	2.16	0.46
1:B:145:GLN:HB2	1:B:146:HIS:CE1	2.51	0.46
1:B:446:ILE:C	1:B:450:ILE:HD12	2.41	0.46
1:A:106:LEU:O	1:A:110:ILE:HG13	2.15	0.46
1:A:165:ILE:HD12	1:A:166:TYR:HE1	1.80	0.46
1:A:413:THR:HB	1:A:414:GLY:H	1.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:PHE:C	1:A:461:PRO:HD2	2.40	0.46
1:B:13:VAL:CB	1:B:203:VAL:HG11	2.44	0.46
1:B:401:ARG:O	1:B:402:THR:C	2.58	0.46
1:A:469:GLU:O	1:A:472:TRP:HB3	2.15	0.46
1:A:416:ILE:HG23	1:A:427:ILE:HD11	1.97	0.46
1:B:206:THR:O	1:B:207:ALA:CB	2.64	0.46
1:A:54:MET:O	1:A:154:CYS:HA	2.16	0.46
1:B:178:ASN:ND2	1:B:178:ASN:H	2.12	0.46
1:B:359:PRO:HG2	1:B:361:MET:HG2	1.98	0.46
1:B:149:PHE:HD2	1:B:173:LEU:CD1	2.29	0.46
1:B:293:GLY:O	1:B:456:THR:HG21	2.16	0.46
1:B:434:ASP:H	1:B:435:PRO:CD	2.29	0.46
1:A:347:PRO:O	1:B:133:ARG:HD2	2.15	0.46
1:B:36:PHE:CZ	1:B:75:SER:HA	2.51	0.46
1:B:160:LYS:HA	1:B:165:ILE:CD1	2.46	0.46
1:A:126:TRP:NE1	1:A:128:ASP:OD1	2.32	0.45
1:B:49:PRO:CD	1:B:67:MET:HE2	2.33	0.45
1:A:94:GLN:CD	1:A:94:GLN:N	2.74	0.45
1:B:46:PRO:O	1:B:51:GLU:OE1	2.33	0.45
2:A:1028:HOH:O	1:B:285:ARG:HD2	2.17	0.45
1:B:100:SER:HA	1:B:139:MET:HE1	1.99	0.45
1:A:127:LEU:HD12	1:A:127:LEU:N	2.31	0.45
1:B:121:ILE:HB	1:B:150:LEU:HD12	1.98	0.45
1:A:401:ARG:O	1:A:402:THR:C	2.57	0.45
1:B:75:SER:HB2	1:B:82:LEU:HB3	1.98	0.45
1:A:205:ASN:ND2	1:A:207:ALA:C	2.75	0.45
1:A:312:CYS:SG	1:A:342:MET:HE3	2.56	0.45
1:A:416:ILE:HG23	1:A:427:ILE:CD1	2.47	0.45
1:A:462:LEU:C	1:A:464:TRP:H	2.25	0.45
1:B:76:LYS:HB2	1:B:81:ASN:HD22	1.81	0.45
1:B:149:PHE:HD2	1:B:173:LEU:HD12	1.82	0.45
1:B:392:GLU:HG3	1:B:462:LEU:HD12	1.96	0.45
1:A:145:GLN:NE2	1:A:145:GLN:CA	2.80	0.45
1:A:362:PRO:HG3	1:A:509:TRP:CE2	2.52	0.45
1:B:113:LYS:O	1:B:116:GLY:N	2.49	0.45
1:B:535:GLN:CG	1:B:539:LYS:HZ2	2.30	0.45
1:A:396:GLU:OE2	1:A:458:PHE:N	2.47	0.45
1:B:61:SER:OG	1:B:129:ASP:OD1	2.35	0.45
1:B:362:PRO:HG3	1:B:509:TRP:CE2	2.52	0.45
1:A:153:SER:OG	1:A:154:CYS:N	2.49	0.45
1:B:77:ALA:O	1:B:78:CYS:CB	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:VAL:CG1	1:B:198:MET:HG2	2.45	0.45
1:B:50:THR:OG1	1:B:67:MET:HE3	2.17	0.45
1:B:306:TYR:CD1	1:B:306:TYR:N	2.84	0.45
1:A:434:ASP:O	1:A:434:ASP:OD1	2.35	0.44
1:B:158:MET:HE2	1:B:164:GLN:O	2.17	0.44
1:B:261:LEU:HB3	1:B:272:TRP:CE2	2.53	0.44
1:B:263:HIS:NE2	1:B:291:MET:HG2	2.31	0.44
1:B:333:ASP:OD2	1:B:523:HIS:NE2	2.41	0.44
1:B:26:SER:CA	1:B:29:ALA:HB3	2.38	0.44
1:A:270:PHE:CD2	1:A:448:PHE:CD2	3.04	0.44
1:A:405:SER:OG	1:A:431:THR:HG21	2.17	0.44
1:A:416:ILE:HG23	1:A:427:ILE:CG1	2.46	0.44
1:A:446:ILE:C	1:A:450:ILE:HD12	2.42	0.44
1:B:19:ILE:HD11	1:B:96:MET:CB	2.47	0.44
1:B:32:LEU:HA	1:B:33:PRO:HD3	1.79	0.44
1:B:158:MET:CG	1:B:164:GLN:HG3	2.45	0.44
1:A:261:LEU:HB3	1:A:272:TRP:CE2	2.53	0.44
1:A:306:TYR:CD1	1:A:306:TYR:N	2.85	0.44
1:A:482:LYS:HG3	1:B:62:GLN:HE21	1.82	0.44
1:B:329:PHE:O	1:B:353:VAL:HA	2.18	0.44
1:B:469:GLU:O	1:B:472:TRP:HB3	2.17	0.44
1:A:53:LEU:HA	1:A:58:ILE:CD1	2.43	0.44
1:A:162:GLU:O	1:A:165:ILE:CD1	2.65	0.44
1:A:238:GLY:C	1:A:239:TYR:CD1	2.96	0.44
1:A:359:PRO:HG2	1:A:361:MET:HG2	1.99	0.44
1:B:8:PHE:CD1	1:B:8:PHE:N	2.85	0.44
1:B:196:MET:HE3	1:B:196:MET:HB2	1.87	0.44
1:B:359:PRO:HA	1:B:489:MET:HE3	1.99	0.44
1:B:375:SER:OG	1:B:376:ILE:N	2.50	0.44
1:A:54:MET:O	1:A:154:CYS:CA	2.66	0.44
1:B:158:MET:HG2	1:B:164:GLN:HG2	2.00	0.44
1:A:101:ILE:HG21	1:A:106:LEU:HD12	2.00	0.44
1:B:238:GLY:C	1:B:239:TYR:CD1	2.96	0.44
1:B:331:GLY:N	1:B:339:VAL:HG21	2.33	0.44
1:B:363:PRO:HD2	1:B:479:LEU:HD21	1.99	0.44
1:A:136:LEU:HD23	1:B:348:GLU:HG2	2.00	0.44
1:B:119:THR:O	1:B:120:CYS:HB3	2.17	0.44
1:B:122:VAL:HG12	1:B:151:ILE:CG1	2.19	0.44
1:B:278:ALA:HA	1:B:281:GLN:HE21	1.83	0.44
1:B:410:SER:HB3	1:B:522:GLY:N	2.33	0.44
1:A:5:VAL:HG11	1:A:173:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:LEU:C	1:A:464:TRP:N	2.76	0.43
1:B:5:VAL:HG11	1:B:173:LEU:HD23	1.99	0.43
1:B:268:SER:OG	1:B:269:TRP:N	2.51	0.43
1:B:126:TRP:CD1	1:B:126:TRP:C	2.94	0.43
1:B:153:SER:OG	1:B:154:CYS:N	2.50	0.43
1:A:52:GLN:HG3	1:A:58:ILE:CD1	2.47	0.43
1:A:385:PHE:HD2	1:A:465:TYR:CD2	2.36	0.43
1:A:489:MET:CG	1:A:506:MET:HE1	2.49	0.43
1:B:43:THR:HB	1:B:44:GLU:H	1.50	0.43
1:B:74:SER:O	1:B:78:CYS:HB2	2.17	0.43
1:B:253:MET:HG2	1:B:280:ALA:CB	2.47	0.43
1:B:396:GLU:OE2	1:B:458:PHE:N	2.49	0.43
1:B:402:THR:O	1:B:406:PHE:HD1	2.02	0.43
1:A:194:ARG:HB2	1:A:200:THR:CG2	2.48	0.43
1:A:205:ASN:HD22	1:A:207:ALA:N	1.82	0.43
1:B:291:MET:CA	1:B:291:MET:CE	2.95	0.43
1:A:359:PRO:HA	1:A:489:MET:HE2	1.99	0.43
1:B:507:GLU:H	1:B:507:GLU:HG2	1.36	0.43
1:A:105:MET:HE3	1:A:105:MET:O	2.18	0.43
1:A:413:THR:O	1:A:415:PHE:N	2.51	0.43
1:B:33:PRO:HD3	1:B:80:ALA:CB	2.48	0.43
1:A:59:THR:H	1:A:62:GLN:CD	2.26	0.43
1:A:184:ASP:HB3	1:A:190:LEU:CD1	2.48	0.43
1:B:91:ILE:HG12	1:B:92:PHE:N	2.34	0.43
1:B:125:ASN:N	1:B:153:SER:OG	2.51	0.43
1:A:281:GLN:HE21	1:A:281:GLN:HB2	1.59	0.43
1:A:380:ASN:CB	1:A:419:HIS:O	2.66	0.43
1:A:482:LYS:HG3	1:B:62:GLN:NE2	2.34	0.43
1:B:125:ASN:HD22	1:B:152:GLU:CB	2.13	0.43
1:B:215:LYS:HZ3	1:B:221:PHE:N	2.11	0.43
1:A:53:LEU:HD22	1:A:126:TRP:HB2	2.01	0.43
1:A:133:ARG:NH1	1:B:350:VAL:O	2.52	0.43
1:A:331:GLY:N	1:A:339:VAL:HG21	2.33	0.43
1:A:410:SER:HB3	1:A:522:GLY:N	2.34	0.43
1:B:158:MET:CB	1:B:165:ILE:HG23	2.49	0.43
1:B:253:MET:HG2	1:B:280:ALA:HB2	2.01	0.43
1:B:328:VAL:O	1:B:328:VAL:CG2	2.65	0.43
1:B:357:ASN:OD1	1:B:357:ASN:N	2.51	0.43
1:A:300:PRO:CG	1:A:305:GLU:HG2	2.41	0.42
1:B:162:GLU:O	1:B:165:ILE:HD11	2.18	0.42
1:B:228:VAL:O	1:B:277:PRO:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ASN:OD1	1:A:357:ASN:N	2.52	0.42
1:B:103:ARG:HB2	1:B:104:PRO:CD	2.49	0.42
1:B:432:PRO:HB2	1:B:434:ASP:OD1	2.20	0.42
1:B:537:LEU:HD23	1:B:537:LEU:HA	1.85	0.42
1:A:378:VAL:O	1:A:378:VAL:HG13	2.17	0.42
1:A:387:GLU:HA	1:A:388:PRO:HD3	1.75	0.42
1:B:413:THR:O	1:B:415:PHE:N	2.52	0.42
1:B:414:GLY:O	1:B:415:PHE:O	2.37	0.42
1:A:13:VAL:HG21	1:A:203:VAL:HG21	2.01	0.42
1:A:212:GLU:O	1:A:215:LYS:N	2.50	0.42
1:A:8:PHE:CE2	1:A:105:MET:HE1	2.55	0.42
1:A:162:GLU:HB3	1:A:164:GLN:HE21	1.84	0.42
1:A:262:CYS:O	1:A:272:TRP:HZ2	2.03	0.42
1:A:417:ALA:HB2	1:A:430:ASN:OD1	2.20	0.42
1:A:144:SER:OG	1:A:145:GLN:N	2.53	0.42
1:A:332:HIS:ND1	1:A:333:ASP:HB2	2.35	0.42
1:B:253:MET:HE3	1:B:253:MET:HB2	1.87	0.42
1:A:212:GLU:C	1:A:214:GLU:H	2.27	0.42
1:A:278:ALA:HA	1:A:281:GLN:HE21	1.85	0.42
1:A:437:LEU:O	1:A:438:SER:C	2.63	0.42
1:A:9:ASP:CG	1:A:10:LEU:N	2.78	0.42
1:A:113:LYS:HB3	1:A:113:LYS:HE2	1.69	0.42
1:A:232:PRO:HD2	1:A:233:ASN:N	2.34	0.42
1:A:243:LYS:NZ	1:A:246:ILE:HD13	2.35	0.42
1:B:385:PHE:HD2	1:B:465:TYR:CD2	2.38	0.42
1:A:363:PRO:HD2	1:A:479:LEU:HD21	2.01	0.42
1:A:497:VAL:CG2	1:A:498:LEU:N	2.83	0.42
1:A:529:LYS:O	1:A:532:GLU:HG2	2.20	0.42
1:A:535:GLN:CG	1:A:539:LYS:HZ2	2.33	0.42
1:B:178:ASN:O	1:B:180:VAL:N	2.53	0.42
1:B:330:ILE:O	1:B:330:ILE:HG13	2.12	0.42
1:A:126:TRP:CD1	1:A:126:TRP:C	2.98	0.41
1:B:302:GLU:CD	1:B:302:GLU:H	2.28	0.41
1:B:387:GLU:HA	1:B:388:PRO:HD3	1.75	0.41
1:A:253:MET:HG2	1:A:280:ALA:CB	2.51	0.41
1:B:165:ILE:H	1:B:165:ILE:HG13	1.34	0.41
1:B:211:ARG:C	1:B:214:GLU:HB2	2.45	0.41
1:B:276:ILE:HG22	1:B:277:PRO:N	2.35	0.41
1:B:420:LYS:O	1:B:421:ALA:C	2.61	0.41
1:B:440:ILE:HD12	1:B:440:ILE:HA	1.79	0.41
1:A:350:VAL:O	1:B:133:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:ASP:OD1	1:B:131:ASP:N	2.52	0.41
1:B:318:PHE:O	1:B:322:LEU:HB2	2.19	0.41
1:A:376:ILE:HG22	1:A:378:VAL:HG12	2.03	0.41
1:A:433:GLU:HA	1:A:433:GLU:OE1	2.20	0.41
1:A:484:LEU:HD12	1:B:129:ASP:OD2	2.19	0.41
1:B:34:ARG:O	1:B:35:ASP:HB2	2.19	0.41
1:A:91:ILE:H	1:A:91:ILE:CD1	2.33	0.41
1:B:33:PRO:HD3	1:B:80:ALA:HB3	2.02	0.41
1:A:50:THR:C	1:A:52:GLN:N	2.78	0.41
1:A:54:MET:HB2	1:A:159:ILE:HG21	2.01	0.41
1:A:162:GLU:HA	1:A:163:PRO:HD2	1.69	0.41
1:A:339:VAL:HG13	1:A:353:VAL:CG1	2.39	0.41
1:A:364:ASP:HB2	1:A:367:VAL:HG23	2.02	0.41
1:B:359:PRO:HA	1:B:489:MET:HE2	2.02	0.41
1:A:105:MET:HE3	1:A:105:MET:CA	2.50	0.41
1:B:515:ARG:NH1	1:B:515:ARG:CG	2.83	0.41
1:A:133:ARG:CG	1:B:348:GLU:HA	2.38	0.41
1:B:22:ALA:CB	1:B:95:ALA:HB2	2.51	0.41
1:B:61:SER:O	1:B:65:PRO:HD3	2.20	0.41
1:A:139:MET:O	1:A:143:LEU:HD12	2.21	0.41
1:A:205:ASN:ND2	1:A:207:ALA:CA	2.84	0.41
1:A:230:CYS:O	1:A:231:ASN:HB3	2.20	0.41
1:A:291:MET:O	1:A:292:LYS:C	2.63	0.41
1:A:302:GLU:H	1:A:302:GLU:CD	2.29	0.41
1:A:448:PHE:O	1:A:452:GLN:HG2	2.21	0.41
1:A:519:GLU:O	1:A:520:ASP:C	2.62	0.41
1:B:5:VAL:HB	1:B:118:THR:HB	2.01	0.41
1:B:67:MET:O	1:B:68:ASP:C	2.64	0.41
1:B:125:ASN:HB3	1:B:154:CYS:SG	2.61	0.41
1:B:177:PRO:O	1:B:197:GLY:O	2.39	0.41
1:B:230:CYS:O	1:B:231:ASN:CB	2.63	0.41
1:B:342:MET:HE1	1:B:346:TYR:CD2	2.56	0.41
1:B:417:ALA:HB3	1:B:427:ILE:HA	2.02	0.41
1:B:184:ASP:OD1	1:B:185:ASP:N	2.53	0.41
1:B:526:GLN:H	1:B:526:GLN:HG3	1.62	0.41
1:B:529:LYS:O	1:B:532:GLU:HG2	2.21	0.41
1:A:376:ILE:HA	1:A:377:PRO:HD2	1.96	0.40
1:B:82:LEU:O	1:B:83:PRO:O	2.38	0.40
1:A:4:ARG:HH11	1:A:4:ARG:CG	2.34	0.40
1:A:17:PRO:HD2	1:A:99:ARG:HA	2.03	0.40
1:A:53:LEU:HD21	1:A:59:THR:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:TYR:O	1:B:169:LEU:HB3	2.21	0.40
1:B:376:ILE:HG22	1:B:378:VAL:HG12	2.02	0.40
1:B:420:LYS:O	1:B:422:THR:N	2.55	0.40
1:A:59:THR:H	1:A:62:GLN:HG2	1.86	0.40
1:A:414:GLY:O	1:A:415:PHE:O	2.39	0.40
1:A:8:PHE:HB2	1:A:14:LEU:HD11	2.04	0.40
1:A:332:HIS:CE1	1:A:333:ASP:HB2	2.56	0.40
1:A:398:ASN:OD1	1:A:398:ASN:O	2.39	0.40
1:B:462:LEU:O	1:B:464:TRP:N	2.54	0.40
1:B:489:MET:CG	1:B:506:MET:HE1	2.48	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%)	390 (81%)	59 (12%)	32 (7%)	1	3
1	B	539/554 (97%)	438 (81%)	68 (13%)	33 (6%)	1	3
All	All	1020/1108 (92%)	828 (81%)	127 (12%)	65 (6%)	1	3

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	SER
1	A	208	SER
1	A	232	PRO
1	A	256	GLY
1	A	415	PHE
1	A	423	GLU
1	B	44	GLU
1	B	75	SER

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Mol	Chain	Res	Type
1	B	76	LYS
1	B	78	CYS
1	B	205	ASN
1	B	207	ALA
1	B	208	SER
1	B	232	PRO
1	B	256	GLY
1	B	415	PHE
1	B	421	ALA
1	A	174	LYS
1	A	205	ASN
1	A	207	ALA
1	A	414	GLY
1	A	501	GLU
1	A	520	ASP
1	B	73	LYS
1	B	179	GLU
1	B	414	GLY
1	B	501	GLU
1	B	520	ASP
1	A	130	GLY
1	A	244	PRO
1	A	295	GLY
1	B	29	ALA
1	B	83	PRO
1	B	206	THR
1	B	244	PRO
1	A	92	PHE
1	A	179	GLU
1	A	367	VAL
1	A	438	SER
1	A	506	MET
1	B	74	SER
1	B	214	GLU
1	B	295	GLY
1	B	434	ASP
1	B	438	SER
1	B	506	MET
1	A	11	ASP
1	A	91	ILE
1	B	111	ALA
1	B	203	VAL

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Mol	Chain	Res	Type
1	B	367	VAL
1	A	222	PRO
1	A	266	PRO
1	A	277	PRO
1	A	288	ALA
1	A	496	ILE
1	B	266	PRO
1	B	277	PRO
1	A	218	GLY
1	A	301	PRO
1	B	496	ILE
1	B	301	PRO
1	A	231	ASN
1	A	157	GLY
1	A	180	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	424/480 (88%)	290 (68%)	134 (32%)	0	1
1	B	468/480 (98%)	318 (68%)	150 (32%)	0	1
All	All	892/960 (93%)	608 (68%)	284 (32%)	0	1

All (284) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	18	SER
1	A	19	ILE
1	A	50	THR
1	A	53	LEU
1	A	55	LYS
1	A	58	ILE
1	A	61	SER

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Mol	Chain	Res	Type
1	A	63	TRP
1	A	90	GLN
1	A	91	ILE
1	A	92	PHE
1	A	94	GLN
1	A	99	ARG
1	A	103	ARG
1	A	110	ILE
1	A	113	LYS
1	A	115	LYS
1	A	128	ASP
1	A	129	ASP
1	A	131	ASP
1	A	132	LYS
1	A	133	ARG
1	A	135	SER
1	A	139	MET
1	A	144	SER
1	A	148	ASP
1	A	152	GLU
1	A	155	GLN
1	A	156	VAL
1	A	158	MET
1	A	165	ILE
1	A	166	TYR
1	A	170	LEU
1	A	174	LYS
1	A	178	ASN
1	A	179	GLU
1	A	181	VAL
1	A	183	LEU
1	A	190	LEU
1	A	191	LYS
1	A	198	MET
1	A	202	LEU
1	A	204	HIS
1	A	205	ASN
1	A	206	THR
1	A	208	SER
1	A	213	LEU
1	A	214	GLU
1	A	215	LYS

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Mol	Chain	Res	Type
1	A	216	VAL
1	A	217	THR
1	A	219	THR
1	A	220	GLN
1	A	221	PHE
1	A	223	GLU
1	A	228	VAL
1	A	231	ASN
1	A	236	SER
1	A	240	VAL
1	A	243	LYS
1	A	247	ARG
1	A	248	LEU
1	A	259	LEU
1	A	268	SER
1	A	275	GLN
1	A	276	ILE
1	A	279	LEU
1	A	287	LEU
1	A	297	SER
1	A	313	LYS
1	A	322	LEU
1	A	328	VAL
1	A	330	ILE
1	A	339	VAL
1	A	342	MET
1	A	349	ARG
1	A	351	ARG
1	A	353	VAL
1	A	361	MET
1	A	364	ASP
1	A	370	MET
1	A	371	LYS
1	A	376	ILE
1	A	378	VAL
1	A	382	GLN
1	A	383	LEU
1	A	397	LYS
1	A	398	ASN
1	A	401	ARG
1	A	408	ARG
1	A	412	GLU

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Mol	Chain	Res	Type
1	A	413	THR
1	A	416	ILE
1	A	420	LYS
1	A	422	THR
1	A	423	GLU
1	A	424	ILE
1	A	427	ILE
1	A	436	ASN
1	A	437	LEU
1	A	440	ILE
1	A	444	GLU
1	A	447	GLU
1	A	450	ILE
1	A	451	GLN
1	A	454	LYS
1	A	455	LYS
1	A	456	THR
1	A	473	LYS
1	A	482	LYS
1	A	485	VAL
1	A	488	LEU
1	A	489	MET
1	A	494	LYS
1	A	497	VAL
1	A	499	ARG
1	A	501	GLU
1	A	502	MET
1	A	504	LYS
1	A	506	MET
1	A	507	GLU
1	A	508	LYS
1	A	513	LEU
1	A	515	ARG
1	A	519	GLU
1	A	525	THR
1	A	526	GLN
1	A	531	THR
1	A	532	GLU
1	A	535	GLN
1	A	539	LYS
1	A	542	GLN
1	A	544	GLU

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Mol	Chain	Res	Type
1	B	5	VAL
1	B	13	VAL
1	B	19	ILE
1	B	24	ARG
1	B	32	LEU
1	B	34	ARG
1	B	38	LEU
1	B	43	THR
1	B	45	PHE
1	B	50	THR
1	B	53	LEU
1	B	57	LYS
1	B	66	LEU
1	B	67	MET
1	B	69	GLU
1	B	72	ARG
1	B	73	LYS
1	B	74	SER
1	B	84	GLU
1	B	85	ASN
1	B	91	ILE
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	115	LYS
1	B	122	VAL
1	B	127	LEU
1	B	128	ASP
1	B	131	ASP
1	B	132	LYS
1	B	133	ARG
1	B	140	MET
1	B	146	HIS
1	B	148	ASP
1	B	151	ILE
1	B	152	GLU
1	B	154	CYS
1	B	155	GLN
1	B	158	MET

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Mol	Chain	Res	Type
1	B	159	ILE
1	B	164	GLN
1	B	165	ILE
1	B	173	LEU
1	B	178	ASN
1	B	179	GLU
1	B	181	VAL
1	B	190	LEU
1	B	191	LYS
1	B	199	VAL
1	B	200	THR
1	B	202	LEU
1	B	204	HIS
1	B	205	ASN
1	B	206	THR
1	B	208	SER
1	B	210	LEU
1	B	212	GLU
1	B	213	LEU
1	B	214	GLU
1	B	215	LYS
1	B	216	VAL
1	B	217	THR
1	B	219	THR
1	B	223	GLU
1	B	228	VAL
1	B	230	CYS
1	B	231	ASN
1	B	236	SER
1	B	240	VAL
1	B	243	LYS
1	B	247	ARG
1	B	248	LEU
1	B	259	LEU
1	B	268	SER
1	B	275	GLN
1	B	276	ILE
1	B	279	LEU
1	B	287	LEU
1	B	297	SER
1	B	308	MET
1	B	309	GLU

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Mol	Chain	Res	Type
1	B	313	LYS
1	B	322	LEU
1	B	328	VAL
1	B	330	ILE
1	B	339	VAL
1	B	342	MET
1	B	349	ARG
1	B	351	ARG
1	B	353	VAL
1	B	361	MET
1	B	364	ASP
1	B	370	MET
1	B	371	LYS
1	B	376	ILE
1	B	378	VAL
1	B	382	GLN
1	B	383	LEU
1	B	397	LYS
1	B	398	ASN
1	B	401	ARG
1	B	408	ARG
1	B	412	GLU
1	B	413	THR
1	B	416	ILE
1	B	420	LYS
1	B	422	THR
1	B	423	GLU
1	B	424	ILE
1	B	427	ILE
1	B	428	LEU
1	B	431	THR
1	B	436	ASN
1	B	437	LEU
1	B	440	ILE
1	B	444	GLU
1	B	447	GLU
1	B	450	ILE
1	B	451	GLN
1	B	454	LYS
1	B	455	LYS
1	B	456	THR
1	B	473	LYS

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Mol	Chain	Res	Type
1	B	482	LYS
1	B	485	VAL
1	B	488	LEU
1	B	489	MET
1	B	494	LYS
1	B	497	VAL
1	B	499	ARG
1	B	501	GLU
1	B	502	MET
1	B	504	LYS
1	B	506	MET
1	B	507	GLU
1	B	508	LYS
1	B	513	LEU
1	B	515	ARG
1	B	519	GLU
1	B	525	THR
1	B	526	GLN
1	B	531	THR
1	B	532	GLU
1	B	535	GLN
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 (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	125	ASN
1	A	145	GLN
1	A	164	GLN
1	A	220	GLN
1	A	231	ASN
1	A	281	GLN
1	A	451	GLN
1	B	81	ASN
1	B	85	ASN
1	B	125	ASN
1	B	145	GLN
1	B	146	HIS
1	B	178	ASN

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Mol	Chain	Res	Type
1	B	204	HIS
1	B	231	ASN
1	B	233	ASN
1	B	281	GLN
1	B	430	ASN
1	B	451	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.