



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:19 PM UTC

PDB ID : 1FPM / pdb_00001fpm
Title : MONOVALENT CATION BINDING SITES IN N10-FORMYLTETRAHYDROFOLATE SYNTHETASE FROM MOORELLA THERMOACETICA
Authors : Radfar, R.; Leapheart, A.; Brewer, J.M.; Minor, W.; Odom, J.D.
Deposited on : 2000-08-31
Resolution : 3.00 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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

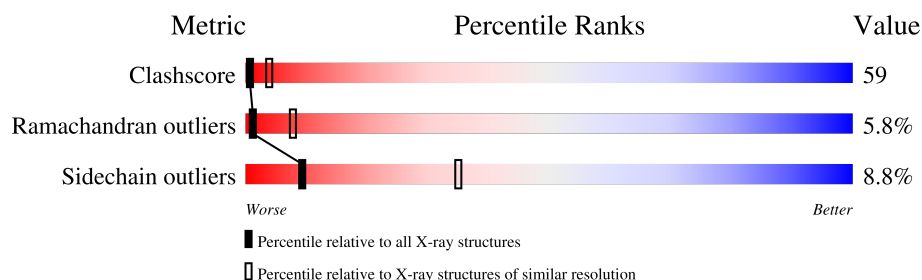
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	557	35% 53% 10% ..
1	B	557	22% 62% 13% ..

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	561	-	-	X	-
2	SO4	A	565	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8585 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 FORMATE--TETRAHYDROFOLATE LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	0
			4133	2617	715	780	21			
1	B	548	Total	C	N	O	S	0	0	0
			4125	2613	714	777	21			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP P21164
A	?	-	VAL	deletion	UNP P21164
B	?	-	GLU	deletion	UNP P21164
B	?	-	VAL	deletion	UNP P21164

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is CESIUM ION (CCD ID: CS) (formula: Cs).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cs 1 1	0	0
3	B	1	Total Cs 1 1	0	0

- Molecule 4 is water.

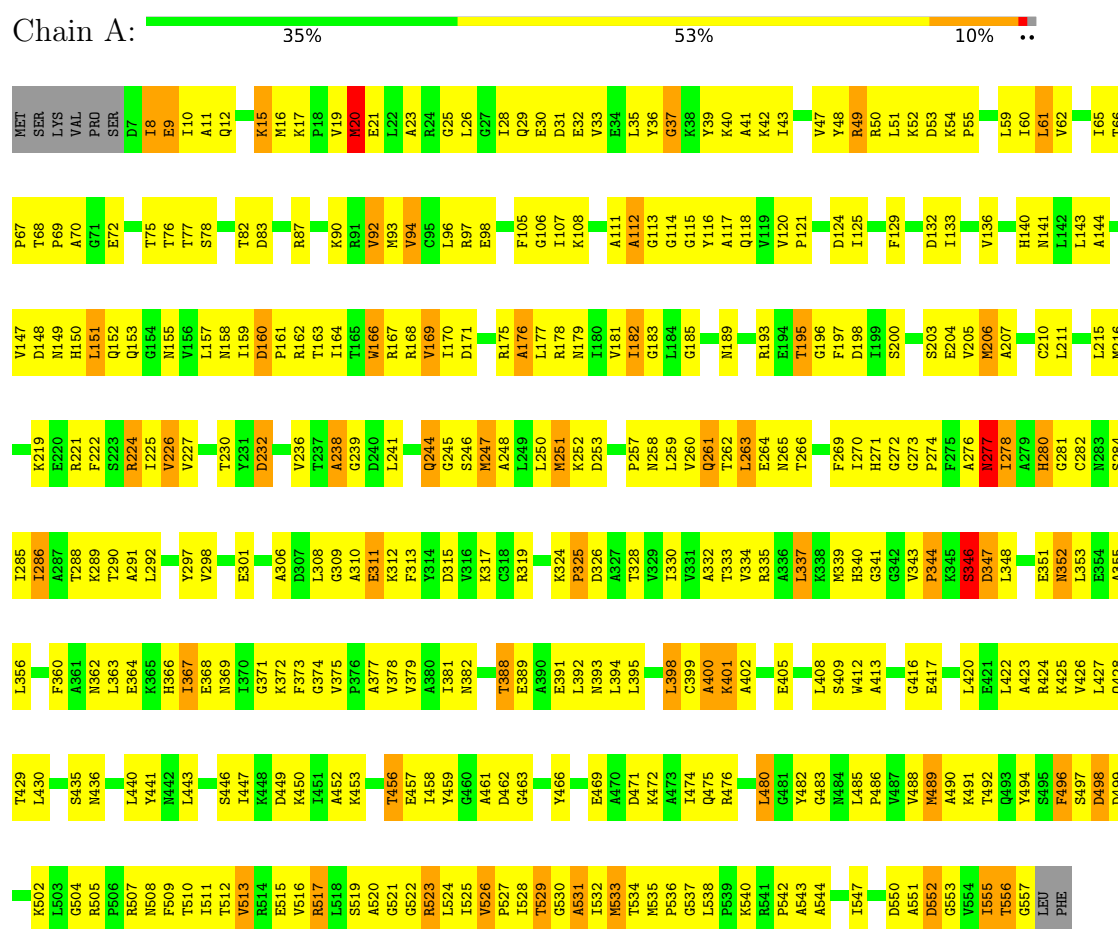
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	200	Total O 200 200	0	0
4	B	70	Total O 70 70	0	0

3 Residue-property plots

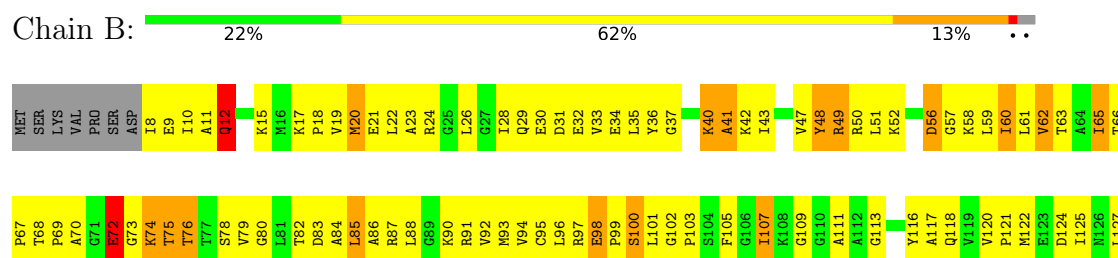
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: FORMATE--TETRAHYDROFOLATE LIGASE



I511	I512	L445	V378	K316	P192	H128
T512	S446	I447	V379	V317	K256	F129
V513	I448	A380	A380	C318	P257	T130
R514	K448	I381	I381	R319	N258	G131
E515	D449	N382	N382	Y320	L259	T195
V516	K450	A383	A383	Y320	V260	G196
R517	K451	F384	F384	G322	Q261	F197
L518	A452	P385	P385	G322	T262	D198
S519	K453	T386	T386	F323	L263	H134
A520	I454	D387	D387	K324	E264	A135
G521	A455	T388	T388	P325	S200	V136
G522	T456	E389	E389	R326	V201	
R523	E457			T328	N265	
L524	I458	L392	L392	V329	F269	H140
T525	Y459	N393	N393	I330	I270	N141
V526	G460	L394	L394	A331	K270	L142
P527	A461	L395	L395	A332	H271	L143
I528	D462	Y396	Y396	T333	A207	A144
T529	G463	E397	E397	V334	C208	M146
		L398	L398	R335	L209	V147
	Y466	C399	C399	F275	C210	D148
I532	A470	A400	A400	A276	L211	N149
M535	D471	K401	K401	M277	A212	H150
L538	K472	A402	A402	I278	S213	L151
P539	A473	G403	G403	M339	D214	Q152
K540	I474	A404	H340	A279	L215	Q153
R541	Q475	E405	G421	H280	M216	G154
	R476		G441	G281	D217	
P542	Y477		G442	C282	L218	M155
A543	E478	L408	V443	N283	K219	V156
		S409	P344	S284	E220	L157
I547	D479	W412		R285	R221	N158
D548	L480	A413	D347	I286	R221	I159
I549	G481	K414	L348	A287	S223	D160
D550	Y482	G415	A349	T288	R224	P161
A551	G483	G416	T350	K289	R225	R162
D552	L484	E417	E351	T290	I225	T163
G553	N485	G418	N352	A291	V226	
V554	P486	L484	L292	L293		I164
		L420	E354	K293	Y229	W166
I555	V487	E421	A355	L294	Y231	R167
T556	V488	L422	L356	A295	D232	R168
G557	M489	A423	R357	D296		V169
LEU	A490	R424	E358	Y297	V236	
PHE	K491	K425	G359	V298	G239	L172
	T492	V426	F360	T300	D240	D174
	Q493		A361	V399	L241	R175
	Q493		N362	E301	E241	A176
	Y494	T429	L363	A302	E242	L177
	S495	L430	G303	G303	A243	R178
	F496		K365	F304	Q244	M179
	S497	R433	H366	G305	G245	I180
	D498	P434	I367	A306	S246	V181
		S435	E368	D367	M247	I182
	L503	N436	N369	L308	A248	
	G504	F437	I370	G309	L249	G185
	R505			A310	M250	G186
	P506	L440	F373	E311	K251	A188
	R507	Y441	G374	K312	C252	K187
M508	I508	N442	V375	F313	D253	N189
F509	T510	D443	P376	Y314	A254	G190
		L444	A377	D315	I255	V191

4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	160.88Å 160.88Å 256.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.00	Depositor
% Data completeness (in resolution range)	84.0 (40.00-3.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.266 , 0.320	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8585	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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: SO4, CS

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	0.65	4/4201 (0.1%)	1.11	26/5690 (0.5%)
1	B	0.53	2/4193 (0.0%)	1.05	24/5679 (0.4%)
All	All	0.59	6/8394 (0.1%)	1.08	50/11369 (0.4%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	MET	SD-CE	-7.82	1.59	1.79
1	A	206	MET	SD-CE	-7.40	1.61	1.79
1	A	489	MET	SD-CE	-7.31	1.61	1.79
1	A	251	MET	SD-CE	-6.65	1.62	1.79
1	B	251	MET	SD-CE	-5.93	1.64	1.79
1	B	535	MET	SD-CE	-5.91	1.64	1.79

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	191	VAL	N-CA-C	9.62	117.07	107.55
1	B	263	LEU	N-CA-C	-9.22	101.13	111.82
1	B	324	LYS	CA-C-N	8.24	130.14	119.84
1	B	324	LYS	C-N-CA	8.24	130.14	119.84
1	A	8	ILE	N-CA-C	-7.78	101.41	110.21
1	B	37	GLY	N-CA-C	-7.61	101.52	112.17
1	B	169	VAL	N-CA-C	7.22	118.16	108.27
1	A	151	LEU	N-CA-C	-7.13	103.20	110.97
1	B	462	ASP	N-CA-C	-7.11	103.87	112.54
1	B	457	GLU	N-CA-C	7.06	118.98	111.28
1	A	20	MET	N-CA-C	-7.06	103.66	111.36
1	B	541	ARG	CA-C-N	6.38	126.29	119.85
1	B	541	ARG	C-N-CA	6.38	126.29	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	ASN	N-CA-C	-6.29	104.81	113.18
1	A	492	THR	N-CA-C	-6.28	100.99	110.28
1	B	41	ALA	N-CA-C	6.16	118.09	107.93
1	B	75	THR	N-CA-C	6.07	117.69	111.14
1	A	367	ILE	N-CA-C	-6.01	103.98	110.23
1	A	280	HIS	N-CA-C	5.95	120.27	113.19
1	A	92	VAL	N-CA-C	5.94	117.64	108.44
1	A	261	GLN	N-CA-C	5.92	118.47	109.95
1	A	496	PHE	N-CA-C	-5.81	106.15	113.18
1	A	346	SER	N-CA-C	5.80	117.28	111.07
1	A	263	LEU	N-CA-C	-5.76	105.14	111.82
1	A	9	GLU	N-CA-C	5.72	117.51	111.28
1	A	408	LEU	N-CA-C	-5.70	104.73	112.26
1	B	451	ILE	N-CA-C	-5.68	104.98	110.72
1	A	15	LYS	N-CA-C	5.66	122.86	110.80
1	A	238	ALA	N-CA-C	-5.62	105.68	112.54
1	A	21	GLU	N-CA-C	-5.60	105.17	111.28
1	A	247	MET	N-CA-C	-5.59	104.20	111.02
1	B	129	PHE	CB-CA-C	-5.58	110.16	116.63
1	A	241	LEU	N-CA-C	-5.56	106.34	113.02
1	A	555	ILE	N-CA-C	5.56	115.89	108.11
1	B	356	LEU	N-CA-C	-5.56	105.32	111.71
1	A	480	LEU	N-CA-C	-5.53	106.51	113.20
1	B	553	GLY	N-CA-C	5.50	119.66	111.18
1	B	217	ASP	N-CA-C	-5.45	104.98	111.03
1	A	206	MET	N-CA-C	-5.26	105.44	111.07
1	B	521	GLY	N-CA-C	-5.25	100.73	113.18
1	B	166	TRP	N-CA-C	5.24	117.21	107.99
1	A	284	SER	N-CA-C	5.22	117.03	110.24
1	A	521	GLY	N-CA-C	-5.21	100.84	113.18
1	A	169	VAL	N-CA-C	5.20	117.53	108.90
1	A	37	GLY	N-CA-C	-5.19	100.97	112.17
1	B	384	PHE	CA-C-N	5.16	126.29	119.84
1	B	384	PHE	C-N-CA	5.16	126.29	119.84
1	B	523	ARG	N-CA-C	5.14	121.75	110.80
1	B	204	GLU	N-CA-C	-5.07	105.88	111.71
1	B	15	LYS	N-CA-C	5.06	121.58	110.80

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	4133	0	4219	411	0
1	B	4125	0	4215	580	1
2	A	35	0	0	10	0
2	B	20	0	0	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	200	0	0	27	0
4	B	70	0	0	14	1
All	All	8585	0	8434	991	1

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 59.

All (991) 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:166:TRP:CZ3	1:B:225:ILE:HD11	1.30	1.59
1:A:166:TRP:CZ3	1:A:225:ILE:HD11	1.42	1.53
1:B:166:TRP:CH2	1:B:225:ILE:HD11	1.58	1.38
1:B:166:TRP:CH2	1:B:225:ILE:CD1	2.11	1.34
1:B:166:TRP:CZ3	1:B:225:ILE:CD1	2.10	1.33
1:A:166:TRP:CE3	1:A:225:ILE:HD11	1.64	1.31
1:A:166:TRP:CZ3	1:A:225:ILE:CD1	2.20	1.23
1:B:43:ILE:HD11	1:B:259:LEU:HD22	1.29	1.15
1:B:222:PHE:O	1:B:225:ILE:HG22	1.49	1.13
1:B:109:GLY:O	4:B:580:HOH:O	1.65	1.12
1:B:195:THR:HG22	1:B:196:GLY:H	1.02	1.12
1:B:376:PRO:HD3	1:B:435:SER:HB3	1.32	1.07
1:B:523:ARG:NE	1:B:523:ARG:H	1.58	1.00
1:B:368:GLU:HG2	1:B:401:LYS:HE2	1.42	0.99
1:B:175:ARG:NH1	2:B:561:SO4:O3	1.95	0.99
1:A:179:ASN:OD1	4:A:757:HOH:O	1.81	0.98
1:B:166:TRP:CH2	1:B:225:ILE:HD13	1.96	0.98
1:A:25:GLY:O	4:A:677:HOH:O	1.82	0.96
1:A:405:GLU:CD	1:A:422:LEU:HA	1.90	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:ILE:HA	1:B:122:MET:HE1	1.48	0.95
1:B:277:ASN:ND2	1:B:278:ILE:H	1.65	0.95
1:B:166:TRP:HH2	1:B:225:ILE:CD1	1.81	0.93
1:B:195:THR:HG22	1:B:196:GLY:N	1.83	0.92
1:B:93:MET:HG2	1:B:267:PRO:HB2	1.52	0.92
1:B:338:LYS:HG2	1:B:343:VAL:HG21	1.51	0.91
1:B:365:LYS:HE3	1:B:369:ASN:HD21	1.34	0.91
1:A:35:LEU:HD22	1:A:37:GLY:O	1.71	0.91
1:A:140:HIS:HD2	1:A:203:SER:OG	1.53	0.91
1:B:20:MET:HE1	1:B:30:GLU:HA	1.50	0.91
1:A:222:PHE:O	1:A:225:ILE:HG22	1.71	0.90
1:A:169:VAL:HG23	1:A:198:ASP:O	1.70	0.90
1:A:557:GLY:O	4:A:582:HOH:O	1.91	0.88
1:B:21:GLU:HA	1:B:24:ARG:HD2	1.54	0.88
1:A:20:MET:HE1	1:A:30:GLU:HA	1.54	0.88
1:A:257:PRO:HD3	1:A:286:ILE:HD11	1.56	0.86
1:B:447:ILE:HD11	1:B:483:GLY:HA2	1.54	0.86
1:B:517:ARG:HH22	1:B:532:ILE:HG13	1.41	0.86
1:B:555:ILE:O	1:B:556:THR:HB	1.74	0.86
1:A:485:LEU:HD13	1:A:523:ARG:HA	1.58	0.85
1:A:9:GLU:HG2	1:A:115:GLY:H	1.42	0.85
1:B:195:THR:CG2	1:B:196:GLY:H	1.85	0.85
1:B:363:LEU:O	1:B:367:ILE:HG12	1.75	0.85
1:B:490:ALA:HB2	1:B:525:ILE:HG22	1.59	0.85
1:B:185:GLY:HA3	1:B:189:ASN:HD22	1.42	0.84
1:B:265:ASN:N	1:B:265:ASN:HD22	1.76	0.83
1:A:47:VAL:HA	1:A:50:ARG:NH1	1.92	0.83
1:B:277:ASN:HD22	1:B:278:ILE:H	1.22	0.83
1:B:172:LEU:O	1:B:535:MET:HE1	1.78	0.83
1:A:277:ASN:HD22	1:A:277:ASN:H	1.26	0.83
1:B:48:TYR:HB2	1:B:290:THR:OG1	1.77	0.83
1:B:394:LEU:O	1:B:398:LEU:HD23	1.78	0.83
1:A:401:LYS:HB2	4:A:748:HOH:O	1.78	0.83
1:B:26:LEU:HD23	1:B:28:ILE:HD11	1.59	0.83
1:A:277:ASN:HD22	1:A:278:ILE:H	1.27	0.82
1:A:169:VAL:HG21	1:A:200:SER:HA	1.61	0.82
1:B:498:ASP:HB3	1:B:528:ILE:HG21	1.61	0.82
1:A:42:LYS:HE3	1:A:258:ASN:OD1	1.80	0.82
1:B:550:ASP:C	1:B:552:ASP:H	1.85	0.82
1:A:326:ASP:HA	1:A:435:SER:OG	1.80	0.81
1:B:36:TYR:HB2	1:B:40:LYS:HZ2	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:ARG:O	1:B:360:PHE:HB3	1.81	0.81
1:A:82:THR:HG21	1:A:94:VAL:HG22	1.62	0.80
1:B:210:CYS:SG	1:B:274:PRO:HD3	2.21	0.80
1:B:33:VAL:HG13	1:B:41:ALA:HB1	1.64	0.80
1:B:337:LEU:HD21	1:B:363:LEU:HB2	1.61	0.80
1:B:166:TRP:HZ3	1:B:225:ILE:HD11	1.00	0.79
1:B:376:PRO:HG3	1:B:433:ARG:HG2	1.64	0.79
1:A:372:LYS:HE2	4:A:728:HOH:O	1.81	0.79
1:A:447:ILE:HD11	1:A:483:GLY:HA2	1.62	0.79
1:B:557:GLY:HA3	4:B:574:HOH:O	1.81	0.79
1:A:17:LYS:H	1:A:261:GLN:NE2	1.81	0.78
1:A:20:MET:HE3	1:A:30:GLU:HG3	1.66	0.78
1:A:66:THR:HB	1:A:340:HIS:NE2	1.99	0.78
1:A:175:ARG:HD3	2:A:563:SO4:O3	1.84	0.78
1:B:335:ARG:NH2	1:B:349:ALA:HA	1.99	0.77
1:B:286:ILE:HA	1:B:289:LYS:HG2	1.66	0.77
1:B:451:ILE:HG12	1:B:489:MET:HE1	1.67	0.77
1:A:417:GLU:HA	1:A:420:LEU:HD23	1.66	0.77
1:A:530:GLY:C	1:A:532:ILE:H	1.92	0.77
1:B:337:LEU:HD23	1:B:360:PHE:HA	1.65	0.77
1:B:215:LEU:HD11	1:B:252:LYS:HA	1.67	0.76
1:B:334:VAL:HG13	1:B:356:LEU:HD21	1.66	0.76
1:A:488:VAL:CG2	1:A:523:ARG:HD3	2.15	0.76
1:B:477:TYR:HE2	1:B:516:VAL:HG12	1.51	0.76
1:B:489:MET:CE	1:B:526:VAL:HG11	2.14	0.76
1:A:210:CYS:SG	1:A:274:PRO:HD3	2.26	0.76
1:B:74:LYS:NZ	1:B:74:LYS:HB2	2.00	0.76
1:A:105:PHE:HB3	1:A:544:ALA:HB2	1.66	0.75
1:B:261:GLN:HB2	1:B:265:ASN:HA	1.69	0.75
1:B:488:VAL:CG2	1:B:523:ARG:HD3	2.17	0.75
1:A:92:VAL:HG23	1:A:297:TYR:O	1.86	0.75
1:A:66:THR:HB	1:A:340:HIS:HE2	1.51	0.75
1:B:516:VAL:HA	1:B:527:PRO:HD2	1.67	0.75
1:A:488:VAL:HG21	1:A:523:ARG:HD3	1.68	0.75
1:A:405:GLU:OE1	1:A:425:LYS:HB2	1.87	0.74
1:B:111:ALA:HB2	1:B:122:MET:SD	2.28	0.74
1:B:47:VAL:HG11	1:B:294:LEU:HD11	1.68	0.74
1:B:136:VAL:HG13	1:B:205:VAL:HG12	1.68	0.74
1:B:488:VAL:HG21	1:B:523:ARG:HD3	1.69	0.74
1:A:96:LEU:O	1:A:270:ILE:HA	1.88	0.74
1:A:498:ASP:HB3	1:A:528:ILE:HG21	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:PRO:O	1:A:523:ARG:HB2	1.86	0.74
1:B:43:ILE:CD1	1:B:259:LEU:HD22	2.15	0.74
1:B:98:GLU:HG2	1:B:99:PRO:HD2	1.70	0.74
1:B:23:ALA:HA	1:B:28:ILE:HD12	1.69	0.73
1:A:333:THR:HG22	1:A:382:ASN:HB3	1.69	0.73
1:B:12:GLN:NE2	1:B:263:LEU:HD13	2.03	0.73
1:B:417:GLU:HA	1:B:420:LEU:HD23	1.71	0.73
1:B:61:LEU:HD12	1:B:300:THR:O	1.88	0.73
1:B:93:MET:HE3	1:B:267:PRO:HB3	1.70	0.73
1:A:446:SER:HB3	1:A:449:ASP:HB2	1.71	0.73
1:B:515:GLU:HB3	1:B:527:PRO:HG2	1.69	0.72
1:A:533:MET:HB2	2:A:561:SO4:O2	1.89	0.72
1:A:488:VAL:HG21	1:A:523:ARG:HH11	1.55	0.72
1:B:83:ASP:OD2	1:B:262:THR:HG21	1.90	0.72
1:B:174:ASP:OD1	1:B:177:LEU:HG	1.88	0.72
1:B:376:PRO:HD3	1:B:435:SER:CB	2.15	0.72
1:B:405:GLU:OE1	1:B:421:GLU:HG2	1.89	0.72
1:A:17:LYS:H	1:A:261:GLN:HE21	1.37	0.71
1:A:169:VAL:CG2	1:A:200:SER:HA	2.20	0.71
1:B:144:ALA:HB1	1:B:168:ARG:HH21	1.54	0.71
1:B:449:ASP:O	1:B:452:ALA:HB3	1.90	0.71
1:A:382:ASN:OD1	2:A:565:SO4:O1	2.08	0.71
1:B:277:ASN:ND2	1:B:278:ILE:N	2.36	0.71
1:B:292:LEU:HD23	1:B:298:VAL:HG21	1.73	0.71
1:A:160:ASP:OD1	1:A:163:THR:HG23	1.89	0.71
1:A:20:MET:HE2	1:A:33:VAL:HB	1.72	0.71
1:B:285:ILE:N	4:B:611:HOH:O	2.22	0.71
1:A:516:VAL:HG22	1:A:526:VAL:HB	1.72	0.71
1:B:169:VAL:HG11	1:B:200:SER:HA	1.72	0.71
1:A:462:ASP:OD2	1:A:508:ASN:HA	1.91	0.70
1:B:136:VAL:HG13	1:B:205:VAL:CG1	2.20	0.70
1:B:169:VAL:CG1	1:B:200:SER:HA	2.21	0.70
1:B:543:ALA:O	1:B:547:ILE:HG13	1.90	0.70
1:A:257:PRO:HD3	1:A:286:ILE:CD1	2.21	0.70
1:B:75:THR:HB	1:B:113:GLY:HA2	1.73	0.70
1:B:173:ASN:HB2	1:B:538:LEU:HD23	1.72	0.70
1:B:472:LYS:HD3	1:B:476:ARG:NH2	2.07	0.70
1:A:82:THR:HG21	1:A:94:VAL:CG2	2.22	0.70
1:A:405:GLU:OE1	1:A:422:LEU:HA	1.92	0.70
1:B:286:ILE:HD12	1:B:287:ALA:N	2.07	0.70
1:A:264:GLU:O	1:A:265:ASN:HB2	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:LYS:HZ2	1:B:40:LYS:HB2	1.57	0.70
1:A:412:TRP:CG	2:A:565:SO4:O4	2.45	0.69
1:B:210:CYS:HA	1:B:284:SER:HA	1.74	0.69
1:A:32:GLU:OE2	1:A:50:ARG:NH1	2.25	0.69
1:A:92:VAL:HB	1:A:297:TYR:HB2	1.74	0.69
1:A:504:GLY:O	4:A:622:HOH:O	2.10	0.69
1:B:85:LEU:HD13	1:B:92:VAL:HG11	1.74	0.69
1:B:265:ASN:HD22	1:B:265:ASN:H	1.40	0.69
1:B:334:VAL:HB	1:B:387:ASP:OD1	1.91	0.69
1:B:353:LEU:N	1:B:353:LEU:HD12	2.07	0.69
1:B:242:GLU:HA	1:B:244:GLN:OE1	1.91	0.69
1:A:148:ASP:OD2	1:A:168:ARG:NH2	2.25	0.69
1:A:286:ILE:HD12	1:A:286:ILE:C	2.18	0.69
1:B:257:PRO:HA	1:B:271:HIS:ND1	2.08	0.69
1:B:40:LYS:NZ	1:B:130:THR:HG22	2.08	0.69
1:B:148:ASP:OD1	4:B:591:HOH:O	2.11	0.69
1:B:517:ARG:HH12	1:B:532:ILE:HD12	1.57	0.69
1:A:262:THR:HG22	1:A:263:LEU:H	1.57	0.68
1:B:9:GLU:HG3	1:B:118:GLN:HE22	1.57	0.68
1:B:550:ASP:C	1:B:552:ASP:N	2.50	0.68
1:A:469:GLU:HG3	4:A:700:HOH:O	1.94	0.68
1:B:262:THR:HG22	1:B:263:LEU:H	1.58	0.68
1:B:306:ALA:O	1:B:310:ALA:HB3	1.93	0.68
1:B:219:LYS:O	1:B:222:PHE:HB2	1.92	0.68
1:A:61:LEU:HD13	1:A:313:PHE:CD2	2.29	0.68
1:A:175:ARG:HG2	1:A:178:ARG:NH2	2.09	0.68
1:A:452:ALA:O	1:A:456:THR:HB	1.94	0.68
1:B:167:ARG:HD3	1:B:198:ASP:OD2	1.94	0.68
1:A:159:ILE:O	1:A:161:PRO:HD3	1.93	0.67
1:B:74:LYS:HB2	1:B:74:LYS:HZ2	1.58	0.67
1:B:271:HIS:ND1	1:B:286:ILE:HD11	2.10	0.67
1:A:363:LEU:O	1:A:367:ILE:HG12	1.94	0.67
1:B:83:ASP:O	1:B:87:ARG:HB2	1.92	0.67
1:B:515:GLU:HB3	1:B:527:PRO:CG	2.24	0.67
1:A:286:ILE:HG23	4:A:627:HOH:O	1.94	0.67
1:B:335:ARG:NH2	1:B:386:THR:HG21	2.10	0.67
1:A:167:ARG:NH2	1:A:178:ARG:O	2.27	0.67
1:A:244:GLN:H	1:A:244:GLN:NE2	1.93	0.67
1:B:166:TRP:HZ3	1:B:225:ILE:CD1	1.79	0.67
1:B:40:LYS:HB2	1:B:40:LYS:NZ	2.10	0.67
1:B:244:GLN:NE2	1:B:244:GLN:H	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:ASP:CB	1:A:528:ILE:HG21	2.25	0.67
1:A:83:ASP:OD1	1:A:262:THR:HG21	1.95	0.67
1:A:532:ILE:HG12	1:A:532:ILE:O	1.95	0.67
1:B:360:PHE:CE2	1:B:364:GLU:HB2	2.30	0.67
1:B:63:THR:HG22	1:B:329:VAL:O	1.95	0.66
1:B:185:GLY:HA3	1:B:189:ASN:ND2	2.10	0.66
1:B:523:ARG:HH11	1:B:525:ILE:HD11	1.60	0.66
1:A:82:THR:HG22	1:A:266:THR:HG21	1.76	0.66
1:A:125:ILE:HG12	1:A:129:PHE:CE1	2.30	0.66
1:B:43:ILE:HD11	1:B:259:LEU:CD2	2.17	0.66
1:B:277:ASN:HD22	1:B:278:ILE:N	1.93	0.66
1:A:20:MET:CE	1:A:30:GLU:HG3	2.26	0.66
1:A:182:ILE:CG2	1:A:183:GLY:N	2.58	0.66
1:A:286:ILE:HA	1:A:289:LYS:HG2	1.78	0.66
1:A:68:THR:HB	1:A:69:PRO:HD2	1.78	0.66
1:B:173:ASN:HB2	1:B:538:LEU:CD2	2.25	0.66
1:A:164:ILE:HG21	1:A:193:ARG:HH22	1.60	0.66
1:A:262:THR:HG22	1:A:263:LEU:N	2.09	0.66
1:A:551:ALA:C	4:A:759:HOH:O	2.38	0.65
1:B:276:ALA:HA	1:B:281:GLY:HA3	1.77	0.65
1:A:150:HIS:CE1	1:A:157:LEU:H	2.14	0.65
1:A:185:GLY:HA3	1:A:189:ASN:HD22	1.61	0.65
1:B:488:VAL:HG23	1:B:523:ARG:HG2	1.79	0.65
1:A:423:ALA:C	1:A:427:LEU:HD12	2.22	0.65
1:B:337:LEU:HD21	1:B:363:LEU:CB	2.27	0.65
1:B:491:LYS:HB3	1:B:528:ILE:CG1	2.27	0.65
1:B:265:ASN:N	1:B:265:ASN:ND2	2.42	0.65
1:B:528:ILE:HG22	1:B:529:THR:N	2.12	0.65
1:B:21:GLU:O	1:B:24:ARG:HB2	1.97	0.65
1:B:159:ILE:HD11	1:B:236:VAL:HG11	1.79	0.65
1:B:470:ALA:O	1:B:474:ILE:HG13	1.96	0.65
1:A:177:LEU:HB3	1:A:197:PHE:HB2	1.78	0.64
1:B:120:VAL:HB	1:B:121:PRO:HA	1.77	0.64
1:B:476:ARG:O	1:B:480:LEU:HD22	1.97	0.64
1:A:36:TYR:CE1	1:A:42:LYS:HG3	2.32	0.64
1:A:43:ILE:HD12	1:A:43:ILE:N	2.12	0.64
1:B:143:LEU:HD23	1:B:166:TRP:CE2	2.32	0.64
1:B:513:VAL:HG21	1:B:526:VAL:HG23	1.79	0.64
1:B:369:ASN:OD1	1:B:458:ILE:HA	1.98	0.64
1:A:166:TRP:CE3	1:A:225:ILE:CD1	2.61	0.64
1:B:42:LYS:HD2	1:B:256:LYS:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:GLN:HG2	1:B:245:GLY:H	1.63	0.64
1:B:215:LEU:HG	1:B:255:ILE:HG21	1.78	0.64
1:A:166:TRP:CZ3	1:A:225:ILE:HD12	2.27	0.64
1:B:459:TYR:CZ	1:B:491:LYS:HD3	2.33	0.64
1:B:487:VAL:CG1	1:B:489:MET:HE2	2.28	0.64
1:A:523:ARG:HD2	1:A:523:ARG:C	2.22	0.64
1:B:20:MET:HE1	1:B:30:GLU:CA	2.28	0.64
1:B:498:ASP:CB	1:B:528:ILE:HG21	2.28	0.64
1:A:230:THR:C	1:A:232:ASP:H	2.07	0.63
1:A:405:GLU:OE1	1:A:425:LYS:HD3	1.96	0.63
1:A:490:ALA:HB3	1:A:527:PRO:HA	1.79	0.63
1:B:61:LEU:HD22	1:B:313:PHE:CE2	2.33	0.63
1:B:72:GLU:CD	1:B:73:GLY:H	2.07	0.63
1:A:277:ASN:ND2	1:A:278:ILE:H	1.96	0.63
1:A:136:VAL:HG21	1:A:206:MET:CE	2.29	0.63
1:B:278:ILE:O	1:B:525:ILE:HD12	1.97	0.63
1:A:59:LEU:N	1:A:326:ASP:OD2	2.28	0.63
1:A:175:ARG:O	1:A:178:ARG:HG3	1.98	0.63
1:A:16:MET:HB2	1:A:39:TYR:CE2	2.34	0.63
1:A:166:TRP:CH2	1:A:225:ILE:CD1	2.82	0.63
1:A:488:VAL:HG21	1:A:523:ARG:NH1	2.14	0.63
1:B:334:VAL:HG13	1:B:356:LEU:CD2	2.29	0.63
1:A:136:VAL:HG21	1:A:206:MET:HE2	1.81	0.63
1:A:82:THR:CG2	1:A:94:VAL:HG22	2.28	0.62
1:B:331:VAL:HG12	1:B:332:ALA:H	1.63	0.62
1:B:374:GLY:O	1:B:435:SER:HB2	1.99	0.62
1:A:381:ILE:HD12	1:A:395:LEU:HD21	1.81	0.62
1:A:140:HIS:CD2	1:A:203:SER:OG	2.44	0.62
1:A:239:GLY:HA2	1:A:244:GLN:HE22	1.64	0.62
1:B:258:ASN:O	1:B:269:PHE:HD1	1.81	0.62
1:A:532:ILE:O	1:A:534:THR:HG23	1.99	0.62
1:B:100:SER:HB2	1:B:201:VAL:HG21	1.82	0.62
1:B:350:THR:HG22	1:B:351:GLU:N	2.14	0.62
1:A:153:GLN:HA	1:A:153:GLN:OE1	1.98	0.62
1:B:34:GLU:HB3	1:B:42:LYS:HB2	1.82	0.62
1:B:285:ILE:HD13	1:B:321:ALA:HB2	1.82	0.62
1:B:364:GLU:O	1:B:368:GLU:HG3	1.99	0.62
1:B:555:ILE:O	1:B:555:ILE:HG23	2.00	0.62
1:A:261:GLN:HG3	1:A:265:ASN:HA	1.80	0.62
1:A:277:ASN:HD22	1:A:277:ASN:N	1.89	0.61
1:B:65:ILE:HG23	1:B:332:ALA:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:MET:O	1:B:209:LEU:HB3	2.00	0.61
1:B:59:LEU:HD13	1:B:292:LEU:HD21	1.81	0.61
1:B:116:TYR:HA	1:B:263:LEU:HD12	1.81	0.61
1:A:61:LEU:HD13	1:A:313:PHE:CG	2.35	0.61
1:A:83:ASP:CG	1:A:262:THR:HG21	2.25	0.61
1:A:394:LEU:HG	1:A:398:LEU:HD23	1.81	0.61
1:B:338:LYS:CG	1:B:343:VAL:HG21	2.27	0.61
1:A:425:LYS:O	1:A:429:THR:HG23	2.00	0.61
1:A:405:GLU:OE2	1:A:422:LEU:HD12	2.00	0.61
1:A:523:ARG:HH11	1:A:525:ILE:CD1	2.14	0.61
1:B:161:PRO:O	4:B:605:HOH:O	2.16	0.61
1:B:166:TRP:O	4:B:632:HOH:O	2.16	0.61
1:B:82:THR:HG22	1:B:266:THR:HG21	1.83	0.61
1:B:159:ILE:HG12	1:B:236:VAL:HG21	1.82	0.61
1:A:168:ARG:O	1:A:197:PHE:HA	1.99	0.61
1:A:532:ILE:O	1:A:534:THR:N	2.34	0.61
1:B:150:HIS:HE1	1:B:156:VAL:N	1.98	0.61
1:A:523:ARG:NH1	1:A:525:ILE:HD11	2.15	0.61
1:A:351:GLU:O	1:A:352:ASN:HB2	2.01	0.61
1:B:286:ILE:O	1:B:290:THR:HB	2.00	0.61
1:A:36:TYR:O	1:A:40:LYS:HB2	2.01	0.60
1:A:257:PRO:CD	1:A:286:ILE:HD11	2.30	0.60
1:A:551:ALA:O	4:A:759:HOH:O	2.17	0.60
1:B:62:VAL:HG13	1:B:301:GLU:HB3	1.82	0.60
1:B:353:LEU:HD12	1:B:353:LEU:H	1.66	0.60
1:B:490:ALA:HB3	1:B:527:PRO:HA	1.82	0.60
1:B:523:ARG:H	1:B:523:ARG:CD	2.15	0.60
1:A:76:THR:HG23	1:A:117:ALA:HB3	1.83	0.60
1:A:547:ILE:HD13	1:A:556:THR:O	2.02	0.60
1:B:321:ALA:HB1	1:B:323:PHE:CE2	2.37	0.60
1:A:210:CYS:O	4:A:620:HOH:O	2.16	0.60
1:B:216:MET:HE2	1:B:216:MET:HA	1.84	0.60
1:B:95:CYS:O	1:B:283:ASN:ND2	2.34	0.60
1:B:313:PHE:C	1:B:313:PHE:CD2	2.78	0.60
1:B:292:LEU:HD23	1:B:298:VAL:CG2	2.32	0.59
1:A:87:ARG:HG3	4:A:718:HOH:O	2.02	0.59
1:A:450:LYS:NZ	1:A:485:LEU:O	2.35	0.59
1:A:476:ARG:CD	4:A:610:HOH:O	2.49	0.59
1:B:36:TYR:O	1:B:40:LYS:HE3	2.02	0.59
1:B:86:ALA:C	1:B:88:LEU:H	2.09	0.59
1:B:116:TYR:HB2	1:B:415:GLY:HA2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:HIS:HE1	1:A:157:LEU:H	1.49	0.59
1:A:450:LYS:NZ	1:A:483:GLY:O	2.33	0.59
1:B:69:PRO:HG2	1:B:339:MET:HE1	1.83	0.59
1:B:489:MET:HE2	1:B:526:VAL:HG11	1.85	0.59
1:B:204:GLU:O	1:B:207:ALA:HB3	2.03	0.59
1:B:262:THR:HG22	1:B:263:LEU:N	2.18	0.59
1:A:276:ALA:HB2	1:A:281:GLY:HA3	1.83	0.59
1:A:277:ASN:HD22	1:A:278:ILE:N	1.97	0.59
1:B:344:PRO:HD2	1:B:347:ASP:HB2	1.85	0.59
1:A:116:TYR:CD1	1:A:413:ALA:O	2.56	0.58
1:A:136:VAL:HG22	1:A:251:MET:HE1	1.84	0.58
1:A:476:ARG:HD3	4:A:610:HOH:O	2.01	0.58
1:B:49:ARG:O	1:B:52:LYS:HB2	2.03	0.58
1:A:152:GLN:OE1	1:A:152:GLN:HA	2.04	0.58
1:B:88:LEU:HD21	1:B:420:LEU:CD1	2.34	0.58
1:A:159:ILE:HD11	1:A:236:VAL:HG11	1.84	0.58
1:A:482:TYR:O	1:A:524:LEU:HD11	2.03	0.58
1:A:70:ALA:HB2	1:A:339:MET:SD	2.42	0.58
1:A:422:LEU:O	1:A:426:VAL:HG23	2.04	0.58
1:B:320:TYR:OH	1:B:486:PRO:HG2	2.03	0.58
1:A:19:VAL:HG13	1:A:39:TYR:HA	1.84	0.58
1:B:36:TYR:HB2	1:B:40:LYS:NZ	2.16	0.58
1:A:550:ASP:N	1:A:553:GLY:O	2.36	0.58
1:B:276:ALA:HA	1:B:281:GLY:CA	2.34	0.58
1:A:277:ASN:ND2	1:A:277:ASN:N	2.51	0.58
1:A:116:TYR:CZ	2:A:566:SO4:O1	2.57	0.57
1:B:116:TYR:HA	1:B:263:LEU:CD1	2.34	0.57
1:A:360:PHE:CD2	1:A:398:LEU:HD12	2.39	0.57
1:A:486:PRO:HD2	1:A:523:ARG:HB3	1.86	0.57
1:A:544:ALA:HA	1:A:547:ILE:HG13	1.86	0.57
1:B:22:LEU:HD11	1:B:261:GLN:CD	2.28	0.57
1:B:133:ILE:O	1:B:136:VAL:N	2.37	0.57
1:A:182:ILE:HG23	1:A:183:GLY:H	1.69	0.57
1:A:424:ARG:O	1:A:428:GLN:HB2	2.04	0.57
1:A:540:LYS:O	1:A:542:PRO:HD3	2.03	0.57
1:A:447:ILE:HD13	1:A:524:LEU:HD13	1.86	0.57
1:A:472:LYS:O	1:A:476:ARG:HG3	2.04	0.57
1:B:271:HIS:CE1	1:B:286:ILE:HD11	2.39	0.57
1:A:253:ASP:HB2	4:A:753:HOH:O	2.03	0.57
1:A:498:ASP:OD2	1:A:511:ILE:HA	2.05	0.57
1:B:167:ARG:NH2	1:B:196:GLY:HA3	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:ARG:HA	1:B:195:THR:CG2	2.34	0.57
1:B:166:TRP:CZ3	1:B:225:ILE:CG1	2.86	0.57
1:A:277:ASN:H	1:A:277:ASN:ND2	2.00	0.57
1:B:523:ARG:NE	1:B:523:ARG:N	2.41	0.57
1:A:169:VAL:HG22	1:A:170:ILE:N	2.20	0.57
1:A:347:ASP:OD2	1:A:347:ASP:N	2.36	0.57
1:A:544:ALA:HA	1:A:547:ILE:CG1	2.35	0.57
1:B:288:THR:HG23	1:B:298:VAL:HG11	1.86	0.57
1:A:164:ILE:HG21	1:A:193:ARG:NH2	2.18	0.57
1:B:365:LYS:CE	1:B:369:ASN:HD21	2.12	0.57
1:B:408:LEU:HD13	1:B:414:LYS:CE	2.35	0.57
1:A:311:GLU:HG3	1:A:312:LYS:HG3	1.87	0.57
1:A:423:ALA:O	1:A:427:LEU:HD12	2.04	0.57
1:B:353:LEU:HB3	1:B:394:LEU:HD22	1.87	0.57
1:B:405:GLU:HB2	1:B:422:LEU:HD13	1.85	0.57
1:A:120:VAL:HB	1:A:121:PRO:HA	1.86	0.56
1:B:485:LEU:HD22	1:B:522:GLY:O	2.05	0.56
1:B:513:VAL:CG2	1:B:526:VAL:HG23	2.34	0.56
1:B:548:ASP:O	1:B:555:ILE:HG22	2.04	0.56
1:A:167:ARG:NH2	1:A:196:GLY:HA3	2.20	0.56
1:B:91:ARG:HB3	1:B:296:ASP:CG	2.31	0.56
1:A:466:TYR:CD2	1:A:513:VAL:HG22	2.41	0.56
1:A:523:ARG:NH1	1:A:525:ILE:CD1	2.68	0.56
1:A:533:MET:HG3	1:A:533:MET:O	2.05	0.56
1:B:331:VAL:HG12	1:B:332:ALA:N	2.20	0.56
1:A:306:ALA:O	1:A:310:ALA:HB3	2.05	0.56
1:B:136:VAL:HG22	1:B:251:MET:HE1	1.86	0.56
1:A:225:ILE:CG2	1:A:238:ALA:CB	2.84	0.56
1:B:40:LYS:HZ3	1:B:130:THR:HG22	1.69	0.56
1:B:132:ASP:OD2	1:B:254:ALA:HA	2.05	0.56
1:B:426:VAL:O	1:B:430:LEU:HB3	2.04	0.56
1:A:141:ASN:HB3	4:A:598:HOH:O	2.06	0.56
1:B:43:ILE:O	1:B:257:PRO:HD2	2.06	0.56
1:B:331:VAL:HA	1:B:380:ALA:HB3	1.87	0.56
1:A:9:GLU:CG	1:A:115:GLY:H	2.17	0.56
1:B:517:ARG:HH22	1:B:532:ILE:CG1	2.16	0.56
1:A:219:LYS:HG3	1:A:248:ALA:HB2	1.89	0.55
1:A:225:ILE:CG2	1:A:238:ALA:HB2	2.36	0.55
1:B:331:VAL:O	1:B:332:ALA:HB2	2.05	0.55
1:B:40:LYS:NZ	1:B:40:LYS:CB	2.69	0.55
1:B:91:ARG:HG2	1:B:295:ALA:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:LEU:C	1:B:400:ALA:H	2.15	0.55
1:A:8:ILE:CG1	1:A:11:ALA:HB2	2.36	0.55
1:A:540:LYS:C	1:A:542:PRO:HD3	2.31	0.55
1:B:83:ASP:HB3	1:B:264:GLU:OE2	2.07	0.55
1:B:455:ALA:HB1	1:B:461:ALA:HB3	1.89	0.55
1:A:167:ARG:HH21	1:A:196:GLY:HA3	1.72	0.55
1:A:195:THR:HG21	4:A:596:HOH:O	2.06	0.55
1:B:70:ALA:HB2	1:B:339:MET:SD	2.47	0.55
1:B:182:ILE:O	1:B:192:PRO:HA	2.07	0.55
1:A:41:ALA:O	1:A:258:ASN:HA	2.07	0.55
1:A:529:THR:C	1:A:531:ALA:H	2.14	0.55
1:B:94:VAL:HG12	1:B:95:CYS:N	2.21	0.55
1:B:339:MET:HA	1:B:343:VAL:HB	1.89	0.55
1:B:446:SER:O	1:B:450:LYS:HG3	2.07	0.55
1:A:143:LEU:HD23	1:A:166:TRP:CE2	2.43	0.54
1:A:353:LEU:H	1:A:353:LEU:CD1	2.19	0.54
1:B:42:LYS:HZ1	1:B:254:ALA:HA	1.72	0.54
1:B:88:LEU:HD21	1:B:420:LEU:HD11	1.90	0.54
1:B:212:ALA:O	1:B:286:ILE:HG23	2.06	0.54
1:B:318:CYS:SG	1:B:323:PHE:HB2	2.47	0.54
1:B:335:ARG:HD3	1:B:348:LEU:HB3	1.89	0.54
1:B:516:VAL:HG12	1:B:516:VAL:O	2.07	0.54
1:A:158:ASN:O	1:A:230:THR:HA	2.07	0.54
1:B:149:ASN:O	1:B:153:GLN:HG2	2.08	0.54
1:B:150:HIS:CE1	1:B:157:LEU:H	2.26	0.54
1:B:523:ARG:NH1	1:B:525:ILE:HD11	2.21	0.54
1:B:84:ALA:HB2	1:B:416:GLY:O	2.07	0.54
1:B:152:GLN:OE1	1:B:190:GLY:HA2	2.08	0.54
1:A:36:TYR:HE1	1:A:42:LYS:HG3	1.72	0.54
1:A:92:VAL:HG23	1:A:297:TYR:C	2.33	0.54
1:B:61:LEU:HD13	1:B:313:PHE:CE1	2.43	0.54
1:B:509:PHE:HD1	1:B:510:THR:N	2.05	0.54
1:A:143:LEU:CD2	1:A:225:ILE:HD13	2.38	0.54
1:B:220:GLU:OE2	1:B:224:ARG:NH1	2.40	0.54
1:B:277:ASN:HB3	1:B:304:PHE:CE2	2.42	0.54
1:B:326:ASP:O	1:B:376:PRO:HD2	2.08	0.54
1:B:354:GLU:O	1:B:357:ARG:HB3	2.08	0.54
1:A:412:TRP:CD2	2:A:565:SO4:O4	2.60	0.54
1:B:219:LYS:HE3	4:B:621:HOH:O	2.05	0.54
1:B:451:ILE:HD12	1:B:466:TYR:OH	2.08	0.54
1:A:49:ARG:CZ	4:A:692:HOH:O	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ILE:HA	1:A:129:PHE:CD1	2.42	0.54
1:A:301:GLU:OE1	4:A:714:HOH:O	2.18	0.54
1:A:341:GLY:HA3	1:A:355:ALA:O	2.07	0.54
1:B:370:ILE:HG21	1:B:377:ALA:HB2	1.90	0.54
1:B:133:ILE:O	1:B:134:HIS:C	2.51	0.54
1:B:405:GLU:HB2	1:B:422:LEU:CD1	2.38	0.54
1:B:75:THR:HA	1:B:301:GLU:OE2	2.08	0.53
1:B:244:GLN:H	1:B:244:GLN:CD	2.17	0.53
1:B:488:VAL:HG23	1:B:523:ARG:HD3	1.91	0.53
1:B:519:SER:C	1:B:521:GLY:H	2.16	0.53
1:A:488:VAL:HG23	1:A:523:ARG:HD3	1.88	0.53
1:B:50:ARG:HG3	1:B:51:LEU:N	2.23	0.53
1:B:121:PRO:HG2	1:B:124:ASP:HB2	1.89	0.53
1:B:339:MET:C	1:B:341:GLY:H	2.16	0.53
1:B:459:TYR:HA	1:B:496:PHE:HB3	1.90	0.53
1:B:8:ILE:HG13	1:B:11:ALA:HB2	1.90	0.53
1:B:375:VAL:HA	1:B:435:SER:CB	2.39	0.53
1:A:47:VAL:HA	1:A:50:ARG:HH12	1.72	0.53
1:A:529:THR:OG1	1:A:530:GLY:N	2.39	0.53
1:B:167:ARG:NH1	1:B:198:ASP:OD1	2.42	0.53
1:B:49:ARG:HD3	1:B:49:ARG:C	2.33	0.53
1:B:417:GLU:C	1:B:419:GLY:H	2.17	0.53
1:B:420:LEU:O	1:B:421:GLU:C	2.52	0.53
1:A:65:ILE:O	1:A:66:THR:C	2.52	0.53
1:B:141:ASN:O	1:B:144:ALA:HB3	2.09	0.53
1:B:339:MET:HE3	1:B:348:LEU:HD11	1.90	0.53
1:A:497:SER:C	1:A:499:ASP:H	2.17	0.53
1:B:23:ALA:CA	1:B:28:ILE:HD12	2.36	0.53
1:A:459:TYR:N	1:A:459:TYR:CD1	2.75	0.53
1:B:408:LEU:HD13	1:B:414:LYS:HE3	1.91	0.53
1:A:167:ARG:NH1	1:A:198:ASP:OD1	2.42	0.52
1:A:169:VAL:CG2	1:A:170:ILE:N	2.71	0.52
1:B:335:ARG:HH21	1:B:349:ALA:HA	1.71	0.52
1:B:515:GLU:HG2	1:B:516:VAL:H	1.74	0.52
1:A:466:TYR:HD2	1:A:513:VAL:HG22	1.74	0.52
1:A:515:GLU:HB3	1:A:527:PRO:HG2	1.92	0.52
1:B:80:GLY:N	1:B:117:ALA:HB1	2.25	0.52
1:A:31:ASP:OD2	1:A:32:GLU:HG3	2.10	0.52
1:B:51:LEU:O	1:B:293:LYS:HG2	2.09	0.52
1:B:325:PRO:HD2	1:B:437:PHE:CD2	2.44	0.52
1:A:49:ARG:NE	4:A:692:HOH:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:VAL:HG11	1:A:405:GLU:OE2	2.09	0.52
1:A:533:MET:HE1	1:A:536:PRO:HA	1.92	0.52
1:B:143:LEU:HD23	1:B:166:TRP:CZ2	2.45	0.52
1:B:441:TYR:CE2	1:B:454:ILE:HD11	2.44	0.52
1:A:111:ALA:O	1:A:113:GLY:N	2.43	0.52
1:A:440:LEU:HD22	1:A:458:ILE:HD11	1.91	0.52
1:B:36:TYR:CE2	1:B:130:THR:HB	2.45	0.52
1:B:315:ASP:O	1:B:319:ARG:HD2	2.10	0.52
1:B:58:LYS:HA	1:B:326:ASP:OD2	2.09	0.52
1:B:487:VAL:HG11	1:B:489:MET:HE2	1.91	0.52
1:B:363:LEU:HD23	1:B:395:LEU:HD11	1.92	0.52
1:B:472:LYS:O	1:B:476:ARG:HG3	2.10	0.52
1:A:66:THR:HB	1:A:340:HIS:CE1	2.45	0.51
1:B:379:VAL:HB	1:B:404:ALA:HA	1.91	0.51
1:B:399:CYS:O	1:B:401:LYS:N	2.43	0.51
1:A:198:ASP:C	1:A:535:MET:HE2	2.35	0.51
1:B:79:VAL:HB	1:B:117:ALA:O	2.10	0.51
1:B:210:CYS:CA	1:B:284:SER:HA	2.40	0.51
1:A:83:ASP:OD2	1:A:262:THR:HG21	2.10	0.51
1:A:175:ARG:HG2	1:A:178:ARG:CZ	2.40	0.51
1:A:533:MET:CE	1:A:536:PRO:HA	2.41	0.51
1:B:9:GLU:OE2	1:B:111:ALA:HB3	2.11	0.51
1:B:150:HIS:CE1	1:B:156:VAL:N	2.78	0.51
1:B:277:ASN:HD22	1:B:277:ASN:N	2.09	0.51
1:B:285:ILE:O	1:B:287:ALA:N	2.43	0.51
1:A:181:VAL:HG13	1:A:193:ARG:O	2.09	0.51
1:A:230:THR:C	1:A:232:ASP:N	2.66	0.51
1:A:319:ARG:NH2	1:A:441:TYR:O	2.42	0.51
1:A:550:ASP:C	1:A:552:ASP:H	2.17	0.51
1:B:75:THR:O	1:B:76:THR:C	2.53	0.51
1:B:275:PHE:HD2	1:B:277:ASN:HD21	1.57	0.51
1:B:550:ASP:O	1:B:552:ASP:N	2.43	0.51
1:A:66:THR:CB	1:A:362:ASN:HD21	2.22	0.51
1:A:118:GLN:HG3	1:A:263:LEU:HD21	1.91	0.51
1:A:389:GLU:HB3	1:A:393:ASN:ND2	2.25	0.51
1:A:550:ASP:C	1:A:552:ASP:N	2.69	0.51
1:B:10:ILE:CA	1:B:122:MET:HE1	2.32	0.51
1:B:75:THR:CB	1:B:113:GLY:HA2	2.41	0.51
1:A:459:TYR:HB3	1:A:496:PHE:O	2.10	0.51
1:B:303:GLY:HA2	2:B:560:SO4:O1	2.11	0.51
1:B:420:LEU:O	1:B:423:ALA:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:ARG:HD2	1:B:528:ILE:O	2.10	0.51
1:A:175:ARG:NH1	1:A:537:GLY:HA3	2.26	0.51
1:A:515:GLU:O	1:A:527:PRO:HD2	2.11	0.51
1:B:221:ARG:HG2	1:B:221:ARG:HH21	1.76	0.51
1:B:323:PHE:N	1:B:323:PHE:CD2	2.77	0.51
1:B:497:SER:HA	1:B:511:ILE:HD11	1.93	0.51
1:B:58:LYS:HG2	1:B:297:TYR:HD1	1.77	0.50
1:B:75:THR:HG23	1:B:301:GLU:OE1	2.11	0.50
1:A:459:TYR:OH	4:A:741:HOH:O	2.13	0.50
1:B:257:PRO:HD3	1:B:286:ILE:HD13	1.93	0.50
1:B:275:PHE:O	1:B:279:ALA:HB3	2.11	0.50
1:B:329:VAL:HG12	1:B:330:ILE:N	2.27	0.50
1:B:448:LYS:HD3	1:B:466:TYR:CZ	2.46	0.50
1:B:150:HIS:HE1	1:B:157:LEU:H	1.57	0.50
1:A:440:LEU:HD11	1:A:457:GLU:OE1	2.11	0.50
1:A:512:THR:O	1:A:528:ILE:HG23	2.11	0.50
1:B:60:ILE:HD12	1:B:299:VAL:HG22	1.92	0.50
1:B:50:ARG:C	1:B:52:LYS:H	2.18	0.50
1:B:229:TYR:CD1	1:B:229:TYR:N	2.79	0.50
1:B:277:ASN:N	1:B:304:PHE:HE2	2.10	0.50
1:B:443:LEU:HG	1:B:484:ASN:O	2.12	0.50
1:B:487:VAL:HG12	1:B:489:MET:HE2	1.93	0.50
1:B:159:ILE:HA	1:B:230:THR:HA	1.93	0.50
1:B:451:ILE:HG12	1:B:489:MET:CE	2.38	0.50
1:B:556:THR:O	1:B:556:THR:CG2	2.60	0.50
1:B:42:LYS:NZ	1:B:254:ALA:HA	2.26	0.50
1:B:350:THR:CG2	1:B:351:GLU:N	2.75	0.50
1:A:16:MET:HE3	1:A:39:TYR:CD2	2.47	0.50
1:A:17:LYS:N	1:A:261:GLN:NE2	2.55	0.49
1:A:42:LYS:NZ	1:A:132:ASP:OD2	2.44	0.49
1:A:520:ALA:C	1:A:522:GLY:H	2.21	0.49
1:B:152:GLN:NE2	1:B:187:LYS:O	2.38	0.49
1:A:530:GLY:C	1:A:532:ILE:N	2.61	0.49
1:A:530:GLY:O	1:A:532:ILE:N	2.45	0.49
1:B:472:LYS:HD3	1:B:476:ARG:HH21	1.74	0.49
1:B:486:PRO:HD2	1:B:523:ARG:HB3	1.94	0.49
1:A:36:TYR:O	1:A:40:LYS:NZ	2.40	0.49
1:A:143:LEU:O	1:A:147:VAL:HG23	2.12	0.49
1:A:150:HIS:NE2	1:A:157:LEU:HD12	2.27	0.49
1:A:343:VAL:HG23	1:A:355:ALA:CB	2.42	0.49
1:B:12:GLN:NE2	1:B:263:LEU:CD1	2.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ILE:HD12	1:B:269:PHE:CE1	2.47	0.49
1:B:335:ARG:HB3	1:B:348:LEU:HD22	1.93	0.49
1:A:72:GLU:HA	1:A:333:THR:HG23	1.94	0.49
1:B:327:ALA:HB2	1:B:430:LEU:HD13	1.94	0.49
1:A:112:ALA:O	1:A:118:GLN:HA	2.12	0.49
1:A:120:VAL:O	1:A:260:VAL:HB	2.11	0.49
1:A:353:LEU:HD12	1:A:353:LEU:N	2.26	0.49
1:B:150:HIS:HE2	1:B:157:LEU:HG	1.78	0.49
1:B:389:GLU:O	1:B:393:ASN:ND2	2.45	0.49
1:A:461:ALA:HB2	1:A:509:PHE:CE1	2.48	0.49
1:B:285:ILE:O	1:B:286:ILE:C	2.55	0.49
1:B:125:ILE:HG12	1:B:129:PHE:CE1	2.46	0.49
1:B:258:ASN:O	1:B:269:PHE:CD1	2.64	0.49
1:B:377:ALA:O	1:B:378:VAL:HG23	2.12	0.49
1:B:429:THR:O	1:B:433:ARG:HB3	2.13	0.49
1:A:340:HIS:ND1	1:A:504:GLY:N	2.53	0.49
1:B:47:VAL:CG1	1:B:294:LEU:HD21	2.43	0.49
1:B:288:THR:O	1:B:292:LEU:HG	2.13	0.49
1:B:494:TYR:O	1:B:495:SER:HB2	2.13	0.49
1:A:147:VAL:HG11	1:A:164:ILE:HD13	1.93	0.49
1:A:344:PRO:O	1:A:348:LEU:HG	2.13	0.49
1:A:401:LYS:CB	4:A:748:HOH:O	2.48	0.49
1:B:61:LEU:O	1:B:328:THR:HA	2.13	0.49
1:B:276:ALA:CA	1:B:281:GLY:HA3	2.42	0.49
1:B:277:ASN:ND2	1:B:278:ILE:HD13	2.28	0.49
1:B:477:TYR:CE2	1:B:516:VAL:HG12	2.40	0.49
1:A:140:HIS:HE1	1:A:167:ARG:O	1.96	0.48
1:A:277:ASN:ND2	1:A:278:ILE:N	2.60	0.48
1:B:63:THR:O	1:B:331:VAL:HG23	2.13	0.48
1:B:220:GLU:O	1:B:223:SER:OG	2.30	0.48
1:A:133:ILE:HG21	1:A:171:ASP:OD1	2.13	0.48
1:A:426:VAL:O	1:A:430:LEU:HB2	2.12	0.48
1:B:8:ILE:HG13	1:B:11:ALA:CB	2.43	0.48
1:B:36:TYR:CB	1:B:40:LYS:NZ	2.76	0.48
1:B:193:ARG:NH2	1:B:195:THR:OG1	2.45	0.48
1:B:225:ILE:HG23	1:B:225:ILE:O	2.13	0.48
1:A:149:ASN:OD1	1:A:153:GLN:HG2	2.13	0.48
1:B:65:ILE:HB	1:B:66:THR:H	1.44	0.48
1:B:157:LEU:O	1:B:230:THR:CG2	2.61	0.48
1:B:417:GLU:O	1:B:419:GLY:N	2.46	0.48
1:B:481:GLY:C	1:B:483:GLY:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:ALA:O	1:A:547:ILE:HG12	2.14	0.48
1:B:304:PHE:CE1	1:B:493:GLN:NE2	2.81	0.48
1:A:182:ILE:HG23	1:A:183:GLY:N	2.26	0.48
1:B:94:VAL:HG12	1:B:95:CYS:H	1.79	0.48
1:B:164:ILE:HD12	1:B:193:ARG:NE	2.28	0.48
1:B:393:ASN:HB3	4:B:597:HOH:O	2.14	0.48
1:B:493:GLN:CD	1:B:494:TYR:CE1	2.92	0.48
1:B:440:LEU:CD2	1:B:458:ILE:HD11	2.43	0.48
1:B:492:THR:HG23	1:B:492:THR:O	2.14	0.48
1:A:35:LEU:HD23	1:A:40:LYS:O	2.13	0.48
1:A:92:VAL:HG22	1:A:93:MET:N	2.27	0.48
1:B:35:LEU:HD23	1:B:41:ALA:HB2	1.95	0.48
1:B:276:ALA:HB2	1:B:303:GLY:HA3	1.95	0.48
1:B:388:THR:O	1:B:392:LEU:HG	2.13	0.48
1:A:204:GLU:O	1:A:207:ALA:HB3	2.14	0.48
1:A:211:LEU:HA	1:A:285:ILE:HD12	1.96	0.48
1:A:446:SER:HB3	1:A:449:ASP:CB	2.41	0.48
1:B:150:HIS:O	1:B:151:LEU:C	2.56	0.48
1:B:286:ILE:HD12	1:B:286:ILE:C	2.37	0.48
1:B:461:ALA:HA	1:B:509:PHE:CE1	2.48	0.48
1:A:136:VAL:HG13	1:A:205:VAL:HG12	1.95	0.48
1:A:221:ARG:HA	1:A:224:ARG:HG3	1.94	0.48
1:A:400:ALA:O	1:A:401:LYS:HB2	2.12	0.48
1:B:555:ILE:O	1:B:556:THR:CB	2.55	0.48
1:A:106:GLY:CA	1:A:538:LEU:HD22	2.44	0.48
1:A:332:ALA:O	1:A:381:ILE:HA	2.13	0.48
1:B:414:LYS:O	1:B:417:GLU:HB3	2.14	0.48
1:A:288:THR:O	1:A:291:ALA:N	2.47	0.47
1:A:463:GLY:O	1:A:510:THR:HG23	2.14	0.47
1:A:533:MET:CB	2:A:561:SO4:O2	2.61	0.47
1:B:241:LEU:O	1:B:242:GLU:HB2	2.14	0.47
1:B:313:PHE:CE2	1:B:318:CYS:SG	3.06	0.47
1:B:351:GLU:OE2	1:B:353:LEU:HD11	2.14	0.47
1:B:247:MET:HA	1:B:250:LEU:HD23	1.96	0.47
1:A:312:LYS:NZ	1:A:489:MET:O	2.47	0.47
1:A:399:CYS:O	1:A:401:LYS:N	2.47	0.47
1:B:144:ALA:HB1	1:B:168:ARG:NH2	2.28	0.47
1:B:358:GLU:O	1:B:359:GLY:C	2.57	0.47
1:B:466:TYR:HA	1:B:513:VAL:HG13	1.97	0.47
1:A:360:PHE:CE2	1:A:364:GLU:HB2	2.50	0.47
1:B:175:ARG:HG2	1:B:178:ARG:CZ	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ILE:O	1:A:108:LYS:HB2	2.13	0.47
1:B:169:VAL:HG12	1:B:200:SER:OG	2.15	0.47
1:A:61:LEU:HD13	1:A:313:PHE:CE2	2.50	0.47
1:A:225:ILE:HG23	1:A:238:ALA:HB2	1.96	0.47
1:A:288:THR:HG22	1:A:292:LEU:HD12	1.95	0.47
1:B:450:LYS:O	1:B:454:ILE:HG13	2.14	0.47
1:A:87:ARG:NH1	1:A:264:GLU:OE1	2.48	0.47
1:A:140:HIS:CE1	1:A:166:TRP:CZ2	3.02	0.47
1:B:42:LYS:NZ	1:B:132:ASP:OD2	2.38	0.47
1:B:83:ASP:O	4:B:612:HOH:O	2.21	0.47
1:B:304:PHE:CD1	1:B:493:GLN:HG3	2.50	0.47
1:B:408:LEU:O	1:B:408:LEU:CD2	2.63	0.47
1:B:459:TYR:HE2	1:B:489:MET:HG3	1.80	0.47
1:A:75:THR:O	1:A:76:THR:C	2.58	0.47
1:A:533:MET:HA	2:A:561:SO4:O2	2.15	0.47
1:B:207:ALA:O	1:B:208:CYS:C	2.57	0.47
1:B:304:PHE:HE1	1:B:493:GLN:HE21	1.60	0.47
1:B:523:ARG:H	1:B:523:ARG:HE	1.51	0.47
1:A:9:GLU:OE1	1:A:114:GLY:HA3	2.14	0.47
1:A:32:GLU:OE1	1:A:47:VAL:HG22	2.15	0.47
1:B:215:LEU:HD21	1:B:255:ILE:HB	1.97	0.47
1:B:303:GLY:O	1:B:309:GLY:HA3	2.14	0.47
1:B:384:PHE:CD1	1:B:385:PRO:HD2	2.50	0.47
1:B:507:ARG:C	1:B:509:PHE:H	2.23	0.47
1:A:20:MET:HE2	1:A:33:VAL:CB	2.44	0.47
1:A:54:LYS:HB3	1:A:55:PRO:HD2	1.97	0.47
1:A:405:GLU:CD	1:A:425:LYS:HB2	2.40	0.47
1:A:459:TYR:O	1:A:509:PHE:HZ	1.98	0.47
1:B:357:ARG:O	1:B:358:GLU:C	2.58	0.47
1:A:43:ILE:N	1:A:43:ILE:CD1	2.78	0.46
1:B:42:LYS:HE2	1:B:258:ASN:OD1	2.15	0.46
1:B:353:LEU:N	1:B:353:LEU:CD1	2.77	0.46
1:B:375:VAL:HA	1:B:435:SER:HB2	1.97	0.46
1:A:20:MET:HE1	1:A:30:GLU:CA	2.38	0.46
1:B:86:ALA:C	1:B:88:LEU:N	2.72	0.46
1:B:140:HIS:HE1	1:B:167:ARG:O	1.97	0.46
1:B:402:ALA:O	1:B:403:GLY:C	2.58	0.46
1:B:491:LYS:HB3	1:B:528:ILE:HG13	1.95	0.46
1:A:20:MET:CE	1:A:33:VAL:HB	2.43	0.46
1:A:259:LEU:O	1:A:260:VAL:HG13	2.15	0.46
1:B:338:LYS:O	1:B:341:GLY:N	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:LEU:HD23	1:A:166:TRP:CZ2	2.50	0.46
1:A:144:ALA:HB1	1:A:168:ARG:HE	1.81	0.46
1:A:417:GLU:O	1:A:420:LEU:HD23	2.15	0.46
1:A:489:MET:HE2	1:A:526:VAL:HG13	1.98	0.46
1:B:36:TYR:CB	1:B:40:LYS:HZ2	2.24	0.46
1:B:86:ALA:HA	1:B:90:LYS:HB2	1.96	0.46
1:B:333:THR:HB	1:B:382:ASN:HB3	1.97	0.46
1:B:515:GLU:O	1:B:516:VAL:HG23	2.15	0.46
1:A:97:ARG:HB3	1:A:273:GLY:HA3	1.98	0.46
1:A:150:HIS:CE1	1:A:157:LEU:HB2	2.51	0.46
1:A:308:LEU:O	1:A:309:GLY:C	2.58	0.46
1:B:12:GLN:HE22	1:B:263:LEU:HD13	1.76	0.46
1:B:31:ASP:OD2	1:B:32:GLU:HG3	2.16	0.46
1:B:335:ARG:HH21	1:B:386:THR:HG21	1.80	0.46
1:B:357:ARG:O	1:B:360:PHE:CB	2.61	0.46
1:B:489:MET:HE1	1:B:526:VAL:HG11	1.95	0.46
1:A:526:VAL:HG22	1:A:526:VAL:O	2.15	0.46
1:B:323:PHE:O	1:B:324:LYS:HG3	2.15	0.46
1:B:417:GLU:C	1:B:419:GLY:N	2.71	0.46
1:B:515:GLU:O	1:B:527:PRO:HD2	2.14	0.46
1:A:374:GLY:HA3	1:A:436:ASN:O	2.16	0.46
1:A:394:LEU:O	1:A:398:LEU:HB2	2.16	0.46
1:A:476:ARG:HD2	4:A:610:HOH:O	2.11	0.46
1:B:323:PHE:N	1:B:323:PHE:HD2	2.14	0.46
1:B:440:LEU:HD22	1:B:458:ILE:HD11	1.96	0.46
1:A:39:TYR:O	1:A:40:LYS:HG3	2.16	0.46
1:A:346:SER:HB3	4:A:732:HOH:O	2.16	0.46
1:B:40:LYS:HZ1	1:B:130:THR:HG22	1.80	0.46
1:A:10:ILE:C	1:A:12:GLN:H	2.23	0.46
1:A:90:LYS:HD2	1:A:297:TYR:CE2	2.51	0.46
1:A:155:ASN:CG	1:A:155:ASN:O	2.59	0.46
1:B:144:ALA:CB	1:B:168:ARG:HE	2.29	0.46
1:B:146:MET:SD	1:B:243:ALA:HB2	2.55	0.46
1:B:83:ASP:HB3	1:B:416:GLY:CA	2.45	0.46
1:B:393:ASN:O	1:B:397:GLU:HG2	2.16	0.46
1:B:51:LEU:HD12	1:B:294:LEU:HD23	1.97	0.45
1:B:66:THR:O	1:B:68:THR:HG23	2.15	0.45
1:B:239:GLY:HA2	1:B:244:GLN:NE2	2.30	0.45
1:B:314:TYR:OH	1:B:328:THR:HG21	2.16	0.45
1:A:51:LEU:O	1:A:53:ASP:N	2.49	0.45
1:A:337:LEU:HD12	1:A:337:LEU:HA	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:PHE:CE2	1:B:440:LEU:HB2	2.51	0.45
1:A:315:ASP:O	1:A:319:ARG:HD2	2.15	0.45
1:A:353:LEU:H	1:A:353:LEU:HD12	1.82	0.45
1:B:66:THR:HB	1:B:362:ASN:HD21	1.81	0.45
1:B:69:PRO:HG2	1:B:339:MET:CE	2.46	0.45
1:B:75:THR:CG2	1:B:113:GLY:HA2	2.46	0.45
1:B:116:TYR:HB2	1:B:415:GLY:CA	2.45	0.45
1:B:339:MET:C	1:B:341:GLY:N	2.75	0.45
1:A:215:LEU:HD11	1:A:252:LYS:HA	1.98	0.45
1:A:505:ARG:HG2	1:A:507:ARG:NH2	2.31	0.45
1:B:280:HIS:HA	1:B:312:LYS:HD3	1.97	0.45
1:B:447:ILE:HD12	1:B:478:GLU:HG3	1.98	0.45
1:B:61:LEU:HD22	1:B:313:PHE:CZ	2.52	0.45
1:B:95:CYS:HB3	1:B:283:ASN:ND2	2.32	0.45
1:B:408:LEU:O	1:B:408:LEU:HD23	2.17	0.45
1:B:463:GLY:O	1:B:510:THR:HG23	2.15	0.45
1:B:505:ARG:HG2	1:B:505:ARG:O	2.16	0.45
1:A:105:PHE:CD1	1:A:105:PHE:N	2.84	0.45
1:A:245:GLY:O	1:A:248:ALA:HB3	2.17	0.45
1:A:311:GLU:HG3	1:A:312:LYS:N	2.32	0.45
1:A:353:LEU:CD1	1:A:353:LEU:N	2.79	0.45
1:B:40:LYS:HD3	1:B:124:ASP:OD2	2.17	0.45
1:B:96:LEU:C	1:B:97:ARG:HG3	2.41	0.45
1:B:150:HIS:NE2	1:B:157:LEU:HG	2.32	0.45
1:B:127:LEU:HB3	1:B:128:HIS:H	1.55	0.45
1:B:312:LYS:HE2	1:B:488:VAL:HG13	1.99	0.45
1:B:509:PHE:CD1	1:B:510:THR:N	2.84	0.45
1:B:540:LYS:C	1:B:542:PRO:HD3	2.42	0.45
1:A:227:VAL:HG22	1:A:236:VAL:O	2.16	0.45
1:B:22:LEU:HD11	1:B:261:GLN:NE2	2.32	0.45
1:B:125:ILE:HA	1:B:129:PHE:CD1	2.52	0.45
1:B:175:ARG:O	1:B:178:ARG:HG3	2.17	0.45
1:B:541:ARG:N	1:B:542:PRO:HD3	2.32	0.45
1:B:18:PRO:O	1:B:22:LEU:HG	2.16	0.45
1:B:74:LYS:NZ	1:B:74:LYS:CB	2.76	0.45
1:B:93:MET:HB3	1:B:94:VAL:H	1.55	0.45
1:A:182:ILE:HG22	1:A:183:GLY:N	2.31	0.44
1:B:8:ILE:CG1	1:B:11:ALA:HB2	2.47	0.44
1:B:10:ILE:HG23	1:B:11:ALA:N	2.32	0.44
1:B:160:ASP:HB3	1:B:163:THR:HG23	1.97	0.44
1:B:167:ARG:HH11	1:B:198:ASP:CG	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ILE:CG2	1:A:238:ALA:HB3	2.46	0.44
1:A:343:VAL:HG23	1:A:355:ALA:HB1	1.99	0.44
1:A:476:ARG:HH11	1:A:476:ARG:HG2	1.81	0.44
1:B:174:ASP:OD1	1:B:177:LEU:CG	2.63	0.44
1:B:287:ALA:O	1:B:291:ALA:HB2	2.17	0.44
1:B:405:GLU:HG3	1:B:425:LYS:HB2	1.98	0.44
1:B:437:PHE:CD1	1:B:437:PHE:C	2.95	0.44
1:B:8:ILE:HB	1:B:10:ILE:HG22	2.00	0.44
1:B:12:GLN:HE21	1:B:263:LEU:HD13	1.79	0.44
1:B:166:TRP:HZ3	1:B:225:ILE:CG1	2.27	0.44
1:A:140:HIS:CE1	1:A:166:TRP:CE2	3.04	0.44
1:A:523:ARG:HH11	1:A:525:ILE:HD11	1.79	0.44
1:B:136:VAL:CG2	1:B:251:MET:HE1	2.47	0.44
1:B:215:LEU:CG	1:B:255:ILE:HG21	2.47	0.44
1:B:329:VAL:HG12	1:B:330:ILE:H	1.82	0.44
1:A:77:THR:O	1:A:78:SER:C	2.60	0.44
1:A:140:HIS:HD2	1:A:203:SER:HG	1.60	0.44
1:A:216:MET:N	1:A:216:MET:HE2	2.32	0.44
1:A:334:VAL:HG21	1:A:392:LEU:HD23	2.00	0.44
1:A:446:SER:CB	1:A:449:ASP:HB2	2.45	0.44
1:B:100:SER:O	1:B:103:PRO:HD2	2.17	0.44
1:B:157:LEU:O	1:B:230:THR:HG21	2.17	0.44
1:B:276:ALA:O	1:B:279:ALA:O	2.36	0.44
1:B:277:ASN:HB3	1:B:304:PHE:HE2	1.82	0.44
1:A:10:ILE:C	1:A:12:GLN:N	2.75	0.44
1:B:24:ARG:C	1:B:26:LEU:H	2.24	0.44
1:B:68:THR:C	1:B:70:ALA:H	2.26	0.44
1:B:160:ASP:OD1	1:B:162:ARG:HB2	2.18	0.44
1:B:245:GLY:O	1:B:248:ALA:HB3	2.18	0.44
1:B:274:PRO:HG2	1:B:281:GLY:HA2	2.00	0.44
1:B:288:THR:HA	1:B:291:ALA:HB3	2.00	0.44
1:B:339:MET:CG	1:B:348:LEU:HD21	2.47	0.44
1:B:515:GLU:HB3	1:B:527:PRO:HG3	1.99	0.44
1:A:82:THR:CG2	1:A:266:THR:HG21	2.45	0.44
1:A:93:MET:HE1	1:A:269:PHE:CE2	2.53	0.44
1:A:363:LEU:HD11	1:A:379:VAL:HG22	2.00	0.44
1:B:202:ALA:HB2	1:B:275:PHE:CE1	2.52	0.44
1:B:210:CYS:HA	1:B:284:SER:CA	2.47	0.44
1:B:522:GLY:HA3	1:B:523:ARG:HH21	1.83	0.44
1:B:285:ILE:O	1:B:288:THR:N	2.51	0.44
1:B:367:ILE:O	1:B:370:ILE:HB	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:LEU:HD12	1:B:424:ARG:HH12	1.82	0.44
1:A:90:LYS:HB3	1:A:297:TYR:CD2	2.53	0.44
1:A:143:LEU:HD21	1:A:225:ILE:HD13	1.99	0.44
1:A:369:ASN:O	1:A:372:LYS:N	2.48	0.44
1:B:12:GLN:HE21	1:B:263:LEU:CD1	2.31	0.44
1:B:97:ARG:HB3	1:B:273:GLY:HA2	2.00	0.44
1:B:178:ARG:HD3	1:B:535:MET:O	2.17	0.44
1:B:205:VAL:O	1:B:206:MET:C	2.61	0.44
1:B:220:GLU:C	1:B:222:PHE:N	2.76	0.44
1:A:136:VAL:HG21	1:A:206:MET:HE1	2.00	0.43
1:A:175:ARG:O	1:A:177:LEU:N	2.51	0.43
1:A:556:THR:O	1:A:556:THR:HG22	2.18	0.43
1:B:65:ILE:CG2	1:B:332:ALA:HB2	2.48	0.43
1:B:488:VAL:HG23	1:B:523:ARG:CG	2.47	0.43
1:A:36:TYR:HB3	1:A:40:LYS:HZ3	1.83	0.43
1:A:160:ASP:OD2	1:A:162:ARG:NH2	2.43	0.43
1:A:311:GLU:HG2	4:A:741:HOH:O	2.17	0.43
1:B:29:GLN:HB2	1:B:31:ASP:OD2	2.18	0.43
1:B:523:ARG:HB2	1:B:524:LEU:H	1.41	0.43
1:A:262:THR:CG2	1:A:263:LEU:N	2.79	0.43
1:A:555:ILE:O	1:A:556:THR:CB	2.67	0.43
1:B:9:GLU:HG3	1:B:118:GLN:NE2	2.29	0.43
1:B:42:LYS:HE2	1:B:130:THR:OG1	2.18	0.43
1:B:353:LEU:H	1:B:353:LEU:CD1	2.32	0.43
1:B:409:SER:O	1:B:412:TRP:C	2.62	0.43
1:A:246:SER:O	1:A:250:LEU:HD23	2.17	0.43
1:B:99:PRO:HD2	1:B:125:ILE:HG22	2.01	0.43
1:B:366:HIS:O	1:B:367:ILE:C	2.61	0.43
1:B:466:TYR:N	1:B:466:TYR:CD1	2.87	0.43
1:A:97:ARG:HG2	1:A:273:GLY:HA2	1.99	0.43
1:A:226:VAL:HG23	4:A:760:HOH:O	2.18	0.43
1:A:447:ILE:HA	1:A:450:LYS:HD2	2.01	0.43
1:B:221:ARG:HG2	1:B:221:ARG:NH2	2.34	0.43
1:B:257:PRO:CA	1:B:271:HIS:ND1	2.81	0.43
1:B:277:ASN:HD22	1:B:277:ASN:H	1.65	0.43
1:B:320:TYR:N	1:B:320:TYR:CD2	2.86	0.43
1:A:16:MET:HB2	1:A:39:TYR:CD2	2.54	0.43
1:A:48:TYR:O	1:A:51:LEU:N	2.34	0.43
1:A:381:ILE:HD12	1:A:395:LEU:CD2	2.47	0.43
1:B:32:GLU:O	1:B:33:VAL:HG23	2.19	0.43
1:B:286:ILE:CA	1:B:289:LYS:HG2	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:GLY:C	1:B:417:GLU:N	2.76	0.43
1:A:87:ARG:HD2	1:A:416:GLY:HA3	2.00	0.43
1:A:499:ASP:CG	1:A:502:LYS:HG3	2.43	0.43
1:B:285:ILE:HG22	1:B:286:ILE:N	2.33	0.43
1:B:332:ALA:HB1	1:B:337:LEU:HD11	2.01	0.43
1:B:384:PHE:CG	1:B:385:PRO:HD2	2.54	0.43
1:A:453:LYS:HA	4:A:658:HOH:O	2.18	0.43
1:A:23:ALA:HB1	1:A:28:ILE:HB	2.00	0.43
1:A:246:SER:O	1:A:250:LEU:CD2	2.67	0.43
1:A:412:TRP:CB	2:A:565:SO4:O4	2.67	0.42
1:A:474:ILE:O	1:A:475:GLN:C	2.61	0.42
1:B:10:ILE:C	1:B:12:GLN:N	2.75	0.42
1:B:215:LEU:HD23	1:B:215:LEU:HA	1.88	0.42
1:B:280:HIS:CD2	1:B:282:CYS:SG	3.12	0.42
1:A:8:ILE:HG13	1:A:11:ALA:HB2	2.01	0.42
1:A:388:THR:HG23	1:A:391:GLU:OE1	2.19	0.42
1:B:83:ASP:CG	1:B:262:THR:HG21	2.44	0.42
1:B:111:ALA:HA	1:B:122:MET:HG3	2.00	0.42
1:B:440:LEU:HG	1:B:440:LEU:O	2.18	0.42
1:A:366:HIS:O	1:A:367:ILE:C	2.61	0.42
1:B:212:ALA:O	1:B:286:ILE:CG2	2.66	0.42
1:B:232:ASP:HB2	4:B:610:HOH:O	2.20	0.42
1:B:333:THR:O	1:B:337:LEU:HD13	2.19	0.42
1:B:488:VAL:HG23	1:B:523:ARG:CD	2.49	0.42
1:B:491:LYS:HB3	1:B:528:ILE:HG12	2.00	0.42
1:A:286:ILE:CD1	1:A:286:ILE:C	2.86	0.42
1:B:164:ILE:HD12	1:B:193:ARG:CD	2.49	0.42
1:B:332:ALA:O	1:B:381:ILE:HA	2.20	0.42
1:B:335:ARG:HA	1:B:338:LYS:HE3	2.01	0.42
1:B:337:LEU:O	1:B:359:GLY:HA3	2.19	0.42
1:B:442:ASN:OD1	1:B:443:LEU:N	2.51	0.42
1:B:455:ALA:HA	1:B:459:TYR:HD2	1.85	0.42
1:B:473:ALA:O	1:B:474:ILE:C	2.61	0.42
1:A:151:LEU:HA	1:A:155:ASN:HB2	2.01	0.42
1:A:371:GLY:C	1:A:373:PHE:H	2.27	0.42
1:B:51:LEU:O	1:B:293:LYS:CG	2.67	0.42
1:B:61:LEU:HD22	1:B:313:PHE:CD2	2.53	0.42
1:A:278:ILE:O	1:A:278:ILE:HG23	2.19	0.42
1:B:35:LEU:HD23	1:B:41:ALA:CB	2.49	0.42
1:B:83:ASP:HB3	1:B:416:GLY:HA3	2.02	0.42
1:B:99:PRO:O	1:B:100:SER:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:MET:HG2	1:B:348:LEU:HD21	2.02	0.42
1:B:555:ILE:O	1:B:555:ILE:CG2	2.67	0.42
1:A:278:ILE:HD12	1:A:278:ILE:HA	1.79	0.42
1:B:47:VAL:HG13	1:B:294:LEU:HD21	2.01	0.42
1:B:150:HIS:O	1:B:153:GLN:N	2.48	0.42
1:B:199:ILE:CD1	4:B:609:HOH:O	2.67	0.42
1:A:60:ILE:HD13	1:A:426:VAL:HG11	2.01	0.42
1:A:105:PHE:O	1:A:544:ALA:N	2.52	0.42
1:A:244:GLN:O	1:A:248:ALA:HB2	2.18	0.42
1:A:75:THR:HA	1:A:301:GLU:OE2	2.20	0.42
1:B:517:ARG:NH2	1:B:532:ILE:HG13	2.22	0.42
1:A:324:LYS:O	1:A:325:PRO:C	2.63	0.42
1:A:297:TYR:HE1	1:A:430:LEU:HD23	1.85	0.41
1:A:343:VAL:HA	1:A:344:PRO:HD3	1.94	0.41
1:A:367:ILE:HG21	1:A:401:LYS:HD3	2.02	0.41
1:B:97:ARG:NH1	1:B:281:GLY:O	2.53	0.41
1:B:459:TYR:OH	1:B:489:MET:CB	2.68	0.41
1:A:280:HIS:CD2	1:A:282:CYS:HB2	2.55	0.41
1:A:440:LEU:O	1:A:453:LYS:HE2	2.20	0.41
1:B:19:VAL:HA	1:B:22:LEU:HG	2.02	0.41
1:B:101:LEU:HG	1:B:105:PHE:HE1	1.85	0.41
1:B:286:ILE:CD1	1:B:287:ALA:N	2.81	0.41
1:B:490:ALA:HB2	1:B:525:ILE:CG2	2.42	0.41
1:B:492:THR:HG21	1:B:498:ASP:O	2.20	0.41
1:A:48:TYR:HB2	1:A:290:THR:OG1	2.19	0.41
1:A:204:GLU:OE1	1:A:519:SER:HB3	2.20	0.41
1:B:66:THR:CB	1:B:362:ASN:HD21	2.33	0.41
1:B:532:ILE:HD11	4:B:603:HOH:O	2.21	0.41
1:A:29:GLN:HB2	1:A:32:GLU:HG3	2.02	0.41
1:A:92:VAL:CG2	1:A:93:MET:N	2.83	0.41
1:A:175:ARG:O	1:A:176:ALA:C	2.64	0.41
1:A:292:LEU:HG	1:A:298:VAL:HG21	2.02	0.41
1:A:369:ASN:O	1:A:372:LYS:HB2	2.20	0.41
1:A:377:ALA:O	1:A:402:ALA:HB1	2.21	0.41
1:A:471:ASP:O	1:A:472:LYS:C	2.62	0.41
1:B:408:LEU:HD13	1:B:414:LYS:NZ	2.35	0.41
1:B:448:LYS:HD3	1:B:466:TYR:CE2	2.54	0.41
1:B:554:VAL:HG12	1:B:555:ILE:N	2.34	0.41
1:A:246:SER:O	1:A:247:MET:C	2.62	0.41
1:B:190:GLY:O	1:B:192:PRO:HD3	2.19	0.41
1:B:193:ARG:NE	4:B:605:HOH:O	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:GLU:C	1:B:222:PHE:H	2.27	0.41
1:B:334:VAL:HB	1:B:387:ASP:CG	2.45	0.41
1:A:225:ILE:HG22	1:A:238:ALA:HB3	2.02	0.41
1:A:335:ARG:HH11	1:A:335:ARG:CB	2.34	0.41
1:A:488:VAL:HB	1:A:525:ILE:HD12	2.02	0.41
1:A:519:SER:O	1:A:523:ARG:N	2.54	0.41
1:B:56:ASP:HB3	1:B:57:GLY:H	1.71	0.41
1:B:144:ALA:HB1	1:B:168:ARG:HE	1.84	0.41
1:B:324:LYS:O	1:B:326:ASP:N	2.53	0.41
1:B:352:ASN:O	1:B:356:LEU:HB2	2.21	0.41
1:B:32:GLU:CD	1:B:50:ARG:HH12	2.29	0.41
1:B:293:LYS:C	1:B:295:ALA:H	2.28	0.41
1:B:370:ILE:CG2	1:B:377:ALA:HB2	2.50	0.41
1:B:426:VAL:O	1:B:430:LEU:CB	2.69	0.41
1:B:509:PHE:CD1	1:B:509:PHE:C	2.98	0.41
1:B:515:GLU:C	1:B:527:PRO:HG2	2.45	0.41
1:A:515:GLU:OE2	1:A:517:ARG:HD3	2.21	0.41
1:A:547:ILE:CD1	1:A:556:THR:O	2.68	0.41
1:B:62:VAL:HG21	1:B:78:SER:OG	2.20	0.41
1:B:66:THR:HA	1:B:67:PRO:HD2	1.93	0.41
1:B:124:ASP:O	1:B:129:PHE:CA	2.69	0.41
1:B:292:LEU:O	1:B:293:LYS:C	2.64	0.41
1:B:311:GLU:OE1	1:B:315:ASP:OD1	2.39	0.41
1:B:363:LEU:CD2	1:B:395:LEU:HD11	2.50	0.41
1:B:477:TYR:CZ	1:B:518:LEU:HB2	2.56	0.41
1:A:170:ILE:HD12	1:A:170:ILE:HA	1.90	0.41
1:A:247:MET:O	1:A:248:ALA:C	2.64	0.41
1:A:398:LEU:C	1:A:400:ALA:H	2.29	0.41
1:A:422:LEU:O	1:A:423:ALA:C	2.63	0.41
1:A:507:ARG:O	1:A:508:ASN:C	2.64	0.41
1:A:529:THR:C	1:A:531:ALA:N	2.78	0.41
1:A:533:MET:CA	2:A:561:SO4:O2	2.67	0.41
1:A:542:PRO:C	1:A:544:ALA:N	2.76	0.41
1:B:62:VAL:HG11	1:B:78:SER:CB	2.51	0.41
1:B:65:ILE:HG21	1:B:337:LEU:HD11	2.03	0.41
1:B:308:LEU:O	1:B:312:LYS:HG3	2.20	0.41
1:B:367:ILE:HG21	1:B:401:LYS:HD3	2.02	0.41
1:B:490:ALA:HB3	1:B:527:PRO:CA	2.49	0.41
1:A:67:PRO:O	1:A:494:TYR:HD2	2.03	0.41
1:A:106:GLY:HA3	1:A:538:LEU:HD22	2.03	0.41
1:A:360:PHE:CE2	1:A:398:LEU:HD12	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:PHE:CD2	1:B:291:ALA:HB2	2.57	0.41
1:B:523:ARG:HH11	1:B:525:ILE:CD1	2.30	0.41
1:A:159:ILE:O	1:A:161:PRO:CD	2.67	0.40
1:A:368:GLU:CG	1:A:401:LYS:HE2	2.51	0.40
1:A:389:GLU:HB3	1:A:393:ASN:HD21	1.85	0.40
1:A:491:LYS:HZ2	1:A:496:PHE:C	2.29	0.40
1:B:466:TYR:CG	1:B:513:VAL:CG1	3.04	0.40
1:A:149:ASN:O	1:A:153:GLN:HG2	2.21	0.40
1:A:517:ARG:HH12	1:A:532:ILE:HG13	1.86	0.40
1:B:17:LYS:O	1:B:261:GLN:NE2	2.51	0.40
1:B:65:ILE:CD1	1:B:332:ALA:HA	2.51	0.40
1:B:245:GLY:O	1:B:246:SER:C	2.63	0.40
1:B:327:ALA:O	1:B:328:THR:OG1	2.36	0.40
1:B:393:ASN:CB	4:B:597:HOH:O	2.70	0.40
1:A:159:ILE:HG12	1:A:236:VAL:HG21	2.04	0.40
1:B:107:ILE:HD12	1:B:107:ILE:O	2.21	0.40
1:B:142:LEU:O	1:B:143:LEU:C	2.65	0.40
1:B:350:THR:CG2	1:B:351:GLU:H	2.34	0.40
1:A:271:HIS:CD2	1:A:272:GLY:H	2.40	0.40
1:B:214:ASP:O	1:B:215:LEU:C	2.64	0.40
1:B:319:ARG:HH21	1:B:443:LEU:HB2	1.86	0.40
1:B:446:SER:O	1:B:447:ILE:C	2.63	0.40
1:B:539:PRO:O	1:B:542:PRO:HG3	2.22	0.40
1:A:33:VAL:HG13	1:A:41:ALA:HB1	2.02	0.40
1:A:124:ASP:OD1	1:A:124:ASP:N	2.55	0.40
1:A:311:GLU:OE1	1:A:315:ASP:OD1	2.39	0.40
1:A:497:SER:C	1:A:499:ASP:N	2.80	0.40
1:B:92:VAL:HG23	1:B:297:TYR:C	2.46	0.40
1:B:203:SER:OG	1:B:205:VAL:HB	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:LYS:NZ	4:B:572:HOH:O[4_555]	2.02	0.18

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	547/557 (98%)	445 (81%)	84 (15%)	18 (3%)	3	17
1	B	546/557 (98%)	392 (72%)	109 (20%)	45 (8%)	0	3
All	All	1093/1114 (98%)	837 (77%)	193 (18%)	63 (6%)	1	8

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	52	LYS
1	A	352	ASN
1	A	556	THR
1	B	65	ILE
1	B	286	ILE
1	B	325	PRO
1	B	400	ALA
1	B	445	LEU
1	A	166	TRP
1	A	176	ALA
1	A	317	LYS
1	A	401	LYS
1	A	531	ALA
1	A	533	MET
1	B	56	ASP
1	B	72	GLU
1	B	187	LYS
1	B	294	LEU
1	B	332	ALA
1	B	388	THR
1	B	401	LYS
1	B	412	TRP
1	B	509	PHE
1	B	556	THR

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Mol	Chain	Res	Type
1	A	49	ARG
1	A	400	ALA
1	B	244	GLN
1	B	317	LYS
1	B	456	THR
1	B	495	SER
1	B	520	ALA
1	A	112	ALA
1	A	498	ASP
1	B	48	TYR
1	B	76	THR
1	B	100	SER
1	B	102	GLY
1	B	176	ALA
1	B	273	GLY
1	B	328	THR
1	B	399	CYS
1	B	403	GLY
1	B	418	GLY
1	B	551	ALA
1	B	554	VAL
1	A	26	LEU
1	B	12	GLN
1	B	49	ARG
1	B	285	ILE
1	B	319	ARG
1	B	334	VAL
1	B	367	ILE
1	A	160	ASP
1	B	376	PRO
1	A	344	PRO
1	B	154	GLY
1	B	385	PRO
1	B	486	PRO
1	B	516	VAL
1	A	325	PRO
1	B	60	ILE
1	B	528	ILE

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	432/440 (98%)	398 (92%)	34 (8%)	11	39
1	B	431/440 (98%)	389 (90%)	42 (10%)	8	30
All	All	863/880 (98%)	787 (91%)	76 (9%)	9	35

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	MET
1	A	61	LEU
1	A	62	VAL
1	A	94	VAL
1	A	98	GLU
1	A	182	ILE
1	A	195	THR
1	A	224	ARG
1	A	226	VAL
1	A	232	ASP
1	A	244	GLN
1	A	277	ASN
1	A	278	ILE
1	A	286	ILE
1	A	311	GLU
1	A	328	THR
1	A	330	ILE
1	A	337	LEU
1	A	346	SER
1	A	347	ASP
1	A	356	LEU
1	A	375	VAL
1	A	388	THR
1	A	398	LEU
1	A	409	SER
1	A	443	LEU
1	A	456	THR

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Mol	Chain	Res	Type
1	A	480	LEU
1	A	513	VAL
1	A	517	ARG
1	A	523	ARG
1	A	526	VAL
1	A	529	THR
1	A	552	ASP
1	B	12	GLN
1	B	20	MET
1	B	40	LYS
1	B	62	VAL
1	B	72	GLU
1	B	74	LYS
1	B	85	LEU
1	B	98	GLU
1	B	107	ILE
1	B	148	ASP
1	B	168	ARG
1	B	180	ILE
1	B	193	ARG
1	B	199	ILE
1	B	222	PHE
1	B	226	VAL
1	B	229	TYR
1	B	244	GLN
1	B	265	ASN
1	B	266	THR
1	B	270	ILE
1	B	275	PHE
1	B	277	ASN
1	B	290	THR
1	B	311	GLU
1	B	313	PHE
1	B	325	PRO
1	B	333	THR
1	B	375	VAL
1	B	396	TYR
1	B	466	TYR
1	B	480	LEU
1	B	503	LEU
1	B	513	VAL
1	B	523	ARG

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Mol	Chain	Res	Type
1	B	525	ILE
1	B	526	VAL
1	B	529	THR
1	B	535	MET
1	B	538	LEU
1	B	549	ILE
1	B	556	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	140	HIS
1	A	150	HIS
1	A	189	ASN
1	A	244	GLN
1	A	277	ASN
1	A	362	ASN
1	A	366	HIS
1	A	382	ASN
1	A	393	ASN
1	A	465	ASN
1	B	29	GLN
1	B	118	GLN
1	B	140	HIS
1	B	150	HIS
1	B	153	GLN
1	B	189	ASN
1	B	244	GLN
1	B	265	ASN
1	B	277	ASN
1	B	280	HIS
1	B	362	ASN
1	B	382	ASN
1	B	484	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	566	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	562	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	B	561	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	563	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	560	-	4,4,4	0.68	0	6,6,6	0.49	0
2	SO4	B	562	-	4,4,4	0.68	0	6,6,6	0.49	0
2	SO4	A	564	-	4,4,4	0.68	0	6,6,6	0.49	0
2	SO4	A	565	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	B	563	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	B	560	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	561	-	4,4,4	0.68	0	6,6,6	0.49	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	566	SO4	1	0
2	B	561	SO4	1	0
2	A	563	SO4	1	0
2	A	565	SO4	4	0
2	B	560	SO4	1	0
2	A	561	SO4	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.