



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 09:38 pm BST

PDB ID : 2IU3
Title : Crystal structures of transition state analogue inhibitors of inosine monophosphate cyclohydrolase
Authors : Xu, L.; Chong, Y.; Hwang, I.; D'Onofrio, A.; Amore, K.; Beardsley, G.P.; Li, C.; Olson, A.J.; Boger, D.L.; Wilson, I.A.
Deposited on : 2006-05-27
Resolution : 2.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

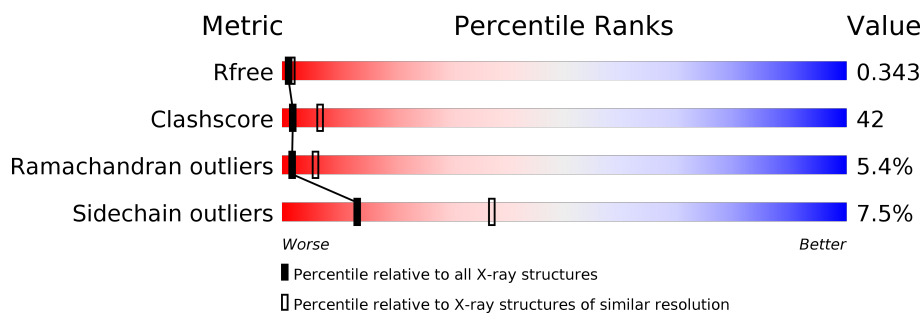
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	593	
1	B	593	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9145 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.

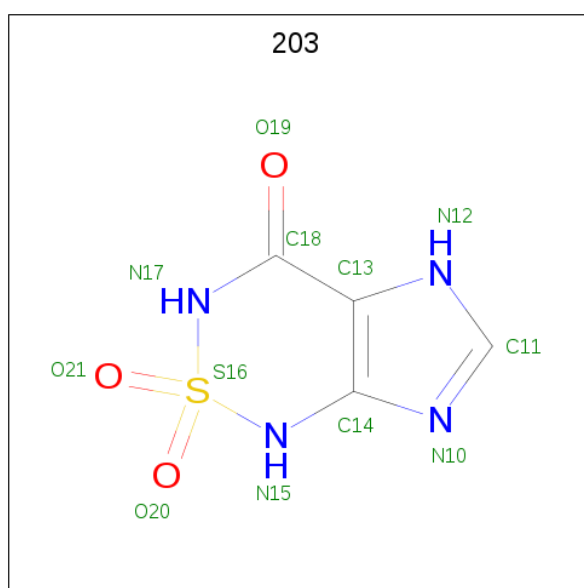
- Molecule 1 is a protein called BIFUNCTIONAL PURINE BIOSYNTHESIS PROTEIN PURH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	590	Total	C	N	O	S	0	1	0
			4523	2852	801	851	19			
1	B	590	Total	C	N	O	S	0	0	0
			4511	2843	800	849	19			

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	K	0	0
			1	1		
2	A	1	Total	K	0	0
			1	1		

- Molecule 3 is 1,5-DIHYDROIMIDAZO[4,5-C][1,2,6]THIADIAZIN-4(3H)-ONE 2,2-DIOXIDE (three-letter code: 203) (formula: C₄H₄N₄O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			12	4	4	3	1		

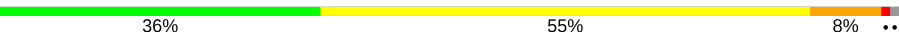
- Molecule 4 is water.

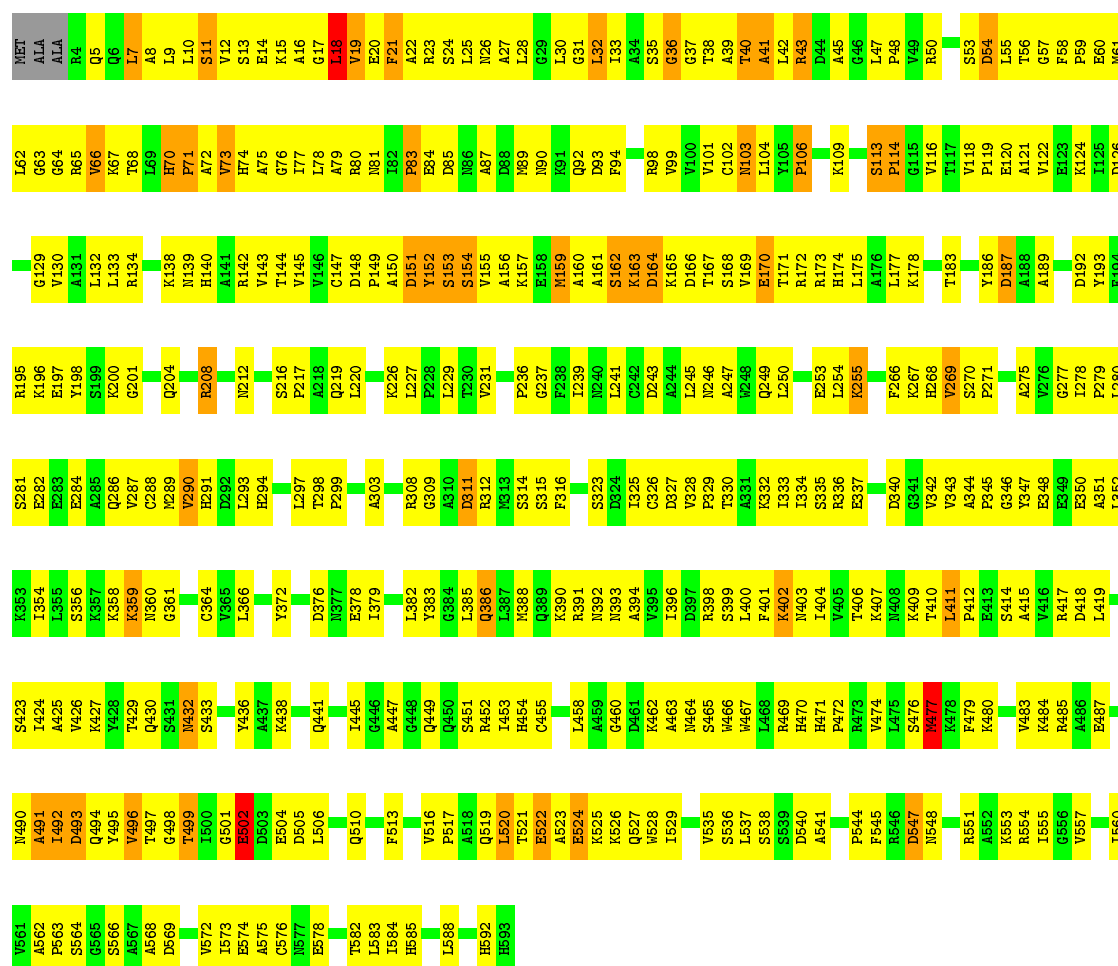
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total	O	0	0
			52	52		
4	B	45	Total	O	0	0
			45	45		

3 Residue-property plots

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

• Molecule 1: BIFUNCTIONAL PURINE BIOSYNTHESIS PROTEIN PURH

Chain A: 



• Molecule 1: BIFUNCTIONAL PURINE BIOSYNTHESIS PROTEIN PURH

Chain B: 



R589	G519	T456	L382	K295	E197	G129	G64
L590	L520	R457	Y383	T296	Y198	G129	G65
F591	E522	A458	G384	L297	S199	A131	R66
H592	A523	G460	L387	P299	V202	L132	K67
H593	K524	D461	K388	S302	S203	L133	T68
	K525	K462	Q389	A303	Q204	R134	
	K526	A463	K390	S307	L205		P71
	Q527	N464	R391	R308	P206	K138	A72
	W528	S465	K392	S307	Q215	N139	H73
		W466	N393	R308	S216	H140	H74
		W467	A394	S307	P217	A141	A75
		L468	V395	D311		R142	G76
		R469	I396	R312	Y221	V143	I77
		H470	D397	M313	T222	T144	L78
		H471	R398	S314			
		P472	S399	F316		G147	R80
		R473	L400	S315	K226	D148	N81
		V474	F401	F316	L227	P149	I82
		L475	K402	I320	P228	A150	P83
		S476	M403	D324	L229	D151	E84
		K477	I404	I325	T230	Y152	D85
		K478	V405	I325	V231	S153	N86
		F479	T406	I325		S154	A87
		K480	K407	V328	G237	V155	D88
			M408			A156	N89
		V483	K409	A331	L241	K157	N90
		K484	T410	K332	C242	E158	K91
		R485	L411	I333		M159	Q92
		A486	P412	I334	L245		
		A487		S335		S162	S95
		V488	V416	V338	L250	K163	L96
		S489	R417		L254	D164	V97
		N490	D418	G341	K255	K165	R98
		A491		V342	Q256	D166	V99
			I424	V343	A257	T167	
		Q494	A425		L258	S168	G102
		Y495	V426			E170	
		V496	K427	G346	K267	T171	Y105
		T497	Y428	Y347	H267	R172	P106
		G498	T429	E348	H268	R173	F107
		T499	Q430	E349	V269	H174	V108
		I500	S431	E350		L175	K109
		G501	M432	A351	Q273	T110	T110
		E502	S433	L352		A176	V111
		D503			G277	L177	S112
		E504	Y436	S356	I278	K178	S113
		D505	A437	K357	P279	T183	P114
		L506	K438	K358	L280	A184	G115
		V507		K359	S281	Q185	V116
		K508	I445	N360	E282	Y186	T117
		W509	Q446	G361	E283		V118
		Q510		G362		A189	P119
		A511	Q449	Y363	Q286	I190	E120
		M512	Q450	L366	V287		A121
		F513	S451	D375		Y193	E123
		E514	R452	D376	H291	F194	K124
			I453		D292	R195	I125
			H454		L293		R126
			C455		H294		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	387.00Å 57.00Å 62.10Å 90.00° 98.90° 90.00°	Depositor
Resolution (Å)	35.20 – 2.90 35.13 – 2.87	Depositor EDS
% Data completeness (in resolution range)	91.5 (35.20-2.90) 90.9 (35.13-2.87)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.85Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.300 0.286 , 0.343	Depositor DCC
R_{free} test set	1210 reflections (3.99%)	wwPDB-VP
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 30.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	9145	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 203, K

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	0.61	0/4608	0.75	1/6249 (0.0%)
1	B	0.59	0/4595	0.75	0/6230
All	All	0.60	0/9203	0.75	1/12479 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	ALA	N-CA-C	-5.98	94.86	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4523	0	4570	434	0
1	B	4511	0	4561	363	4
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	B	12	0	4	1	0
4	A	52	0	0	2	0
4	B	45	0	0	3	0
All	All	9145	0	9135	763	4

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 42.

All (763) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:GLN:HE21	1:A:516:VAL:HG21	1.19	1.04
1:B:485:ARG:HG2	1:B:485:ARG:HH11	1.22	1.04
1:A:379:ILE:HG12	1:A:388:MET:HG3	1.34	1.04
1:A:510:GLN:NE2	1:A:516:VAL:HG21	1.76	1.00
1:B:479:PHE:HA	1:B:513:PHE:HA	1.46	0.97
1:A:502:GLU:HA	1:A:506:LEU:HB2	1.45	0.97
1:A:9:LEU:HD23	1:A:33:ILE:HB	1.45	0.95
1:B:407:LYS:O	1:B:409:LYS:HG3	1.67	0.93
1:A:520:LEU:H	1:A:520:LEU:HD12	1.33	0.92
1:B:80:ARG:HB2	1:B:82:ILE:HG12	1.51	0.92
1:B:408:ASN:HD21	1:B:577:ASN:HA	1.32	0.91
1:A:65:ARG:HD3	1:B:78:LEU:HD22	1.52	0.91
1:B:484:LYS:HB2	1:B:487:GLU:HG3	1.53	0.91
1:A:545:PHE:HB2	1:A:547:ASP:OD1	1.70	0.90
1:A:212:ASN:OD1	1:B:589:ARG:HD2	1.72	0.90
1:B:61:MET:H	1:B:61:MET:HE2	1.36	0.89
1:A:106:PRO:HD2	1:A:109:LYS:HE2	1.54	0.89
1:B:468:LEU:HD23	1:B:528:TRP:CD1	2.09	0.88
1:B:356:SER:O	1:B:361:GLY:HA2	1.74	0.87
1:B:406:THR:HG22	1:B:573:ILE:HG23	1.56	0.86
1:B:9:LEU:HD13	1:B:10:LEU:N	1.90	0.85
1:A:26:ASN:HB2	1:A:32:LEU:HD21	1.55	0.84
1:A:254:LEU:HD23	1:A:424:ILE:HD12	1.60	0.84
1:B:26:ASN:HB2	1:B:32:LEU:HD11	1.58	0.84
1:A:118:VAL:O	1:A:122:VAL:HG23	1.78	0.84
1:A:148:ASP:OD1	1:A:150:ALA:HB3	1.78	0.83
1:B:129:GLY:HA2	1:B:132:LEU:HD12	1.57	0.83
1:B:12:VAL:HG12	1:B:102:CYS:HA	1.60	0.82
1:B:22:ALA:HA	1:B:25:LEU:HD21	1.60	0.82
1:B:121:ALA:O	1:B:124:LYS:HB2	1.78	0.82
1:B:283:GLU:HG3	4:B:2018:HOH:O	1.80	0.81
1:B:485:ARG:HH11	1:B:485:ARG:CG	1.93	0.81
1:B:535:VAL:HB	1:B:557:VAL:HA	1.61	0.80
1:B:43:ARG:HG3	1:B:49:VAL:CG1	2.12	0.80
1:A:270:SER:OG	1:A:430:GLN:HG2	1.82	0.80
1:B:156:ALA:HB3	1:B:157:LYS:HE3	1.61	0.79
1:B:171:THR:O	1:B:175:LEU:HD23	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:PRO:O	1:A:568:ALA:HB3	1.83	0.78
1:B:74:HIS:HA	1:B:77:ILE:HD12	1.64	0.78
1:A:535:VAL:HB	1:A:557:VAL:HA	1.65	0.77
1:A:208:ARG:CZ	1:A:237:GLY:HA2	2.15	0.77
1:A:163:LYS:HG2	1:A:164:ASP:OD1	1.85	0.76
1:B:474:VAL:HA	1:B:477:MET:HG3	1.67	0.76
1:B:566:SER:HB3	1:B:569:ASP:OD1	1.84	0.76
1:A:56:THR:HG22	1:A:72:ALA:HB3	1.68	0.76
1:A:583:LEU:HD12	1:A:584:ILE:N	2.01	0.76
1:B:470:HIS:O	1:B:475:LEU:HD11	1.86	0.76
1:B:464:ASN:ND2	1:B:555:ILE:HD13	2.01	0.76
1:A:28:LEU:HG	1:A:165:LYS:HE2	1.68	0.75
1:A:174:HIS:HD2	1:A:175:LEU:HD22	1.51	0.75
1:A:410:THR:O	1:A:582:THR:HG21	1.86	0.74
1:A:522:GLU:C	1:A:524:GLU:H	1.88	0.74
1:B:83:PRO:HA	1:B:86:ASN:HD22	1.52	0.74
1:A:464:ASN:ND2	1:A:555:ILE:HD13	2.02	0.74
1:B:7:LEU:HA	1:B:31:GLY:H	1.53	0.74
1:A:25:LEU:O	1:A:30:LEU:HD12	1.88	0.74
1:A:50:ARG:HD2	1:A:54:ASP:OD2	1.87	0.74
1:A:537:LEU:C	1:A:537:LEU:HD23	2.08	0.73
1:B:167:THR:O	1:B:172:ARG:NH1	2.21	0.73
1:B:118:VAL:O	1:B:122:VAL:HG23	1.88	0.73
1:B:56:THR:OG1	1:B:58:PHE:HB2	1.87	0.73
1:A:200:LYS:HD3	1:A:200:LYS:C	2.07	0.73
1:A:289:MET:HG3	1:A:312:ARG:CZ	2.17	0.73
1:A:378:GLU:HG3	1:A:391:ARG:HB3	1.71	0.73
1:A:172:ARG:HG3	1:A:172:ARG:HH11	1.53	0.73
1:B:520:LEU:HB2	1:B:525:LYS:HE2	1.70	0.73
1:B:503:ASP:O	1:B:507:VAL:HG23	1.89	0.73
1:A:522:GLU:C	1:A:526:LYS:HE2	2.09	0.72
1:B:22:ALA:HA	1:B:25:LEU:CD2	2.19	0.72
1:A:471:HIS:ND1	1:A:472:PRO:HD2	2.05	0.72
1:A:520:LEU:HD13	1:A:525:LYS:HE2	1.70	0.72
1:A:241:LEU:O	1:A:245:LEU:HD23	1.88	0.71
1:B:537:LEU:HD23	1:B:537:LEU:C	2.10	0.71
1:B:408:ASN:ND2	1:B:577:ASN:HA	2.05	0.71
1:B:410:THR:O	1:B:582:THR:HG21	1.89	0.71
1:B:280:LEU:HD11	1:B:302:SER:HB2	1.71	0.71
1:B:410:THR:HG22	1:B:412:PRO:HD3	1.73	0.71
1:B:545:PHE:HB2	1:B:547:ASP:OD1	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:ASP:O	1:B:573:ILE:HG13	1.91	0.70
1:A:37:GLY:O	1:A:40:THR:HB	1.92	0.70
1:B:496:VAL:HG23	1:B:497:THR:H	1.56	0.70
1:B:80:ARG:HD2	1:B:82:ILE:CD1	2.22	0.70
1:A:458:LEU:HD21	1:A:462:LYS:HE3	1.73	0.70
1:A:547:ASP:OD1	1:A:547:ASP:N	2.24	0.70
1:A:38:THR:O	1:A:42:LEU:HG	1.92	0.70
1:A:70:HIS:CD2	1:A:72:ALA:H	2.10	0.70
1:A:61:MET:SD	1:B:92:GLN:HG3	2.31	0.70
1:A:106:PRO:HG2	1:A:109:LYS:HZ1	1.56	0.69
1:B:521:THR:HG23	1:B:524:GLU:OE1	1.92	0.69
1:A:169:VAL:O	1:A:173:ARG:HG3	1.91	0.69
1:A:432:ASN:HD21	1:A:449:GLN:HB2	1.56	0.69
1:B:468:LEU:HD23	1:B:528:TRP:HD1	1.57	0.69
1:B:485:ARG:NH1	1:B:485:ARG:HG2	2.03	0.69
1:B:583:LEU:HD12	1:B:584:ILE:N	2.08	0.69
1:A:418:ASP:OD2	1:A:438:LYS:HA	1.92	0.69
1:B:43:ARG:HG3	1:B:49:VAL:HG11	1.75	0.69
1:A:104:LEU:O	1:A:106:PRO:HD3	1.93	0.68
1:B:250:LEU:HD11	1:B:425:ALA:HA	1.76	0.68
1:A:9:LEU:CD2	1:A:33:ILE:HB	2.23	0.68
1:B:418:ASP:OD2	1:B:438:LYS:HA	1.94	0.68
1:B:472:PRO:HA	1:B:475:LEU:HD12	1.74	0.68
1:A:80:ARG:HG3	1:B:65:ARG:HH12	1.58	0.68
1:A:37:GLY:HA2	1:A:40:THR:HB	1.76	0.68
1:A:502:GLU:H	1:A:505:ASP:HB2	1.59	0.68
1:B:496:VAL:HG23	1:B:497:THR:N	2.09	0.68
1:A:289:MET:HG3	1:A:312:ARG:NH2	2.07	0.68
1:B:113:SER:OG	1:B:114:PRO:HD2	1.93	0.68
1:B:10:LEU:HB2	1:B:34:ALA:HB2	1.74	0.68
1:A:378:GLU:CG	1:A:391:ARG:HB3	2.23	0.67
1:A:153:SER:O	1:A:157:LYS:HG3	1.95	0.67
1:A:208:ARG:NH2	1:A:237:GLY:HA2	2.10	0.67
1:B:87:ALA:HA	1:B:90:ASN:OD1	1.95	0.67
1:B:280:LEU:N	1:B:280:LEU:HD12	2.09	0.67
1:A:200:LYS:HD3	1:A:201:GLY:N	2.09	0.67
1:A:521:THR:OG1	1:A:524:GLU:HB2	1.95	0.67
1:A:522:GLU:OE2	1:A:522:GLU:HA	1.94	0.67
1:A:53:SER:O	1:A:57:GLY:N	2.28	0.67
1:A:298:THR:HB	1:A:299:PRO:HD2	1.75	0.66
1:A:522:GLU:C	1:A:524:GLU:N	2.49	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:LEU:HD12	1:A:584:ILE:H	1.60	0.66
1:A:495:TYR:CE1	1:A:519:GLN:HA	2.31	0.66
1:A:129:GLY:HA2	1:A:132:LEU:HD12	1.76	0.66
1:B:335:SER:HA	1:B:358:LYS:HD2	1.78	0.66
1:A:282:GLU:HA	1:A:294:HIS:CE1	2.30	0.66
1:A:335:SER:HA	1:A:358:LYS:HD2	1.78	0.66
1:B:495:TYR:HD1	1:B:500:ILE:HD11	1.61	0.66
1:B:157:LYS:N	1:B:157:LYS:HE3	2.10	0.65
1:B:453:ILE:HD11	1:B:457:ARG:NH2	2.12	0.65
1:B:7:LEU:HA	1:B:31:GLY:N	2.11	0.65
1:A:76:GLY:O	1:A:142:ARG:NH2	2.27	0.65
1:A:493:ASP:O	1:A:496:VAL:HG22	1.97	0.65
1:A:74:HIS:HA	1:A:77:ILE:HD12	1.77	0.65
1:A:333:ILE:O	1:A:337:GLU:HG2	1.96	0.65
1:A:376:ASP:HB3	1:A:390:LYS:HD3	1.79	0.65
1:A:106:PRO:HB2	1:A:109:LYS:HZ3	1.61	0.65
1:A:426:VAL:CG1	1:A:540:ASP:HB3	2.27	0.65
1:A:61:MET:HG3	1:A:62:LEU:H	1.62	0.65
1:A:55:LEU:HD22	1:A:72:ALA:HB1	1.79	0.65
1:A:148:ASP:HB3	1:A:178:LYS:HE3	1.79	0.65
1:A:277:GLY:N	1:A:303:ALA:HB2	2.11	0.65
1:B:51:ASP:O	1:B:54:ASP:HB2	1.96	0.65
1:A:198:TYR:CE1	1:B:173:ARG:HD3	2.32	0.65
1:A:280:LEU:HB3	1:A:284:GLU:HB3	1.78	0.64
1:B:299:PRO:O	1:B:303:ALA:N	2.29	0.64
1:A:106:PRO:HG2	1:A:109:LYS:NZ	2.12	0.64
1:A:28:LEU:HA	1:A:165:LYS:NZ	2.13	0.64
1:A:40:THR:HG22	1:A:41:ALA:N	2.12	0.64
1:B:85:ASP:O	1:B:89:MET:HG2	1.97	0.64
1:A:452:ARG:NH2	1:A:541:ALA:HB3	2.13	0.64
1:A:154:SER:HA	1:A:157:LYS:HD2	1.78	0.64
1:A:401:PHE:HB3	1:A:584:ILE:HD13	1.80	0.64
1:A:171:THR:O	1:A:175:LEU:HD23	1.97	0.64
1:A:61:MET:HB2	1:B:88:ASP:HB3	1.80	0.63
1:B:130:VAL:HG13	1:B:183:THR:HG22	1.78	0.63
1:B:25:LEU:HA	1:B:28:LEU:HD12	1.79	0.63
1:A:451:SER:HB3	1:A:454:HIS:HB2	1.79	0.63
1:B:282:GLU:HA	1:B:294:HIS:HE1	1.62	0.63
1:B:9:LEU:C	1:B:10:LEU:HD12	2.18	0.63
1:B:205:LEU:HD12	1:B:206:PRO:HD2	1.80	0.63
1:B:151:ASP:O	1:B:152:TYR:C	2.35	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:PHE:HB3	1:B:564:SER:O	1.99	0.63
1:A:7:LEU:N	1:A:7:LEU:HD12	2.14	0.62
1:A:92:GLN:HG3	1:B:61:MET:SD	2.39	0.62
1:B:82:ILE:HG13	1:B:85:ASP:HB2	1.81	0.62
1:A:163:LYS:HG2	1:A:164:ASP:N	2.14	0.62
1:A:480:LYS:O	1:A:483:VAL:HG23	2.00	0.62
1:A:143:VAL:O	1:A:172:ARG:HD2	1.99	0.62
1:A:159:MET:HE2	1:A:166:ASP:HA	1.80	0.62
1:A:163:LYS:HG2	1:A:164:ASP:H	1.63	0.62
1:B:282:GLU:HA	1:B:294:HIS:CE1	2.35	0.62
1:A:85:ASP:O	1:A:89:MET:HG2	1.99	0.62
1:B:320:ILE:O	1:B:342:VAL:HA	2.00	0.62
1:A:196:LYS:HG2	1:A:204:GLN:NE2	2.15	0.61
1:A:220:LEU:HD13	1:B:387:LEU:HD12	1.82	0.61
1:B:254:LEU:HD23	1:B:424:ILE:HD12	1.81	0.61
1:B:471:HIS:ND1	1:B:472:PRO:HD2	2.15	0.61
1:A:399:SER:O	1:A:402:LYS:HG3	2.00	0.61
1:A:37:GLY:CA	1:A:40:THR:HB	2.31	0.61
1:A:15:LYS:O	1:A:18:LEU:HB3	1.99	0.61
1:A:208:ARG:H	1:A:208:ARG:HD3	1.66	0.61
1:B:9:LEU:HD13	1:B:10:LEU:H	1.60	0.61
1:B:480:LYS:O	1:B:483:VAL:HG12	2.00	0.61
1:A:163:LYS:HZ2	1:A:163:LYS:H	1.48	0.61
1:B:186:TYR:O	1:B:189:ALA:HB3	2.01	0.61
1:A:359:LYS:C	1:A:361:GLY:H	2.03	0.61
1:A:37:GLY:C	1:A:40:THR:HB	2.22	0.61
1:A:37:GLY:HA2	1:A:40:THR:CB	2.31	0.61
1:B:521:THR:O	1:B:525:LYS:HG3	2.01	0.61
1:A:208:ARG:NH1	1:A:237:GLY:HA2	2.15	0.60
1:A:61:MET:HG3	1:A:62:LEU:N	2.16	0.60
1:A:19:VAL:HG12	1:A:20:GLU:N	2.17	0.60
1:B:514:GLU:OE2	1:B:514:GLU:HA	2.01	0.60
1:B:547:ASP:OD1	1:B:547:ASP:N	2.35	0.60
1:B:108:VAL:HG23	1:B:109:LYS:N	2.16	0.60
1:B:446:GLY:HA2	1:B:458:LEU:HD22	1.83	0.60
1:B:126:ASP:OD1	1:B:130:VAL:HG23	2.01	0.60
1:B:7:LEU:HD13	1:B:33:ILE:HD12	1.83	0.60
1:B:108:VAL:HG23	1:B:109:LYS:H	1.67	0.59
1:B:460:GLY:O	1:B:463:ALA:HB3	2.00	0.59
1:A:152:TYR:O	1:A:155:VAL:HB	2.02	0.59
1:A:7:LEU:HD23	1:A:33:ILE:CG1	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:ASN:O	1:B:494:GLN:HG2	2.01	0.59
1:B:105:TYR:CE1	1:B:109:LYS:HD3	2.37	0.59
1:A:325:ILE:HG23	1:A:346:GLY:C	2.22	0.59
1:B:7:LEU:CD1	1:B:33:ILE:HD12	2.33	0.59
1:B:384:GLY:N	4:B:2026:HOH:O	2.33	0.59
1:A:399:SER:HB3	4:A:2030:HOH:O	2.02	0.59
1:A:98:ARG:O	1:A:98:ARG:HG2	2.01	0.59
1:A:520:LEU:HD13	1:A:525:LYS:CE	2.32	0.59
1:A:159:MET:CE	1:A:166:ASP:HA	2.33	0.59
1:A:410:THR:O	1:A:411:LEU:HB2	2.02	0.59
1:B:108:VAL:O	1:B:111:VAL:HG22	2.03	0.59
1:A:394:ALA:CB	1:A:588:LEU:HD11	2.32	0.59
1:A:458:LEU:HD23	1:A:458:LEU:C	2.23	0.58
1:B:164:ASP:OD1	1:B:165:LYS:N	2.36	0.58
1:A:172:ARG:HG3	1:A:172:ARG:NH1	2.16	0.58
1:A:151:ASP:O	1:A:152:TYR:C	2.40	0.58
1:A:154:SER:HA	1:A:157:LYS:CD	2.33	0.58
1:A:398:ARG:HB2	1:A:398:ARG:NH1	2.18	0.58
1:B:37:GLY:HA2	1:B:40:THR:HB	1.85	0.58
1:B:26:ASN:HB2	1:B:32:LEU:HD21	1.85	0.58
1:A:506:LEU:O	1:A:510:GLN:HG3	2.04	0.58
1:B:159:MET:HA	1:B:162:SER:OG	2.04	0.58
1:B:376:ASP:HB3	1:B:390:LYS:NZ	2.19	0.58
1:A:382:LEU:HD21	1:B:242:CYS:HA	1.85	0.58
1:B:458:LEU:HD21	1:B:462:LYS:HE3	1.86	0.58
1:A:65:ARG:CD	1:B:78:LEU:HD22	2.29	0.58
1:A:396:ILE:HG23	1:A:400:LEU:HD23	1.85	0.58
1:B:156:ALA:HB3	1:B:157:LYS:CE	2.31	0.58
1:A:495:TYR:HD1	1:A:519:GLN:HE21	1.51	0.57
1:A:139:ASN:HB3	1:A:143:VAL:HG23	1.86	0.57
1:A:10:LEU:CD1	1:A:42:LEU:HD11	2.34	0.57
1:A:171:THR:O	1:A:174:HIS:HB3	2.05	0.57
1:B:64:GLY:HA2	1:B:66:VAL:O	2.05	0.57
1:A:198:TYR:CD1	1:B:173:ARG:HD3	2.40	0.57
1:A:75:ALA:O	1:A:79:ALA:HB2	2.05	0.57
1:A:7:LEU:HD23	1:A:33:ILE:HD11	1.85	0.57
1:B:164:ASP:O	1:B:165:LYS:HG2	2.05	0.57
1:B:229:LEU:C	1:B:229:LEU:HD23	2.25	0.57
1:B:480:LYS:HA	1:B:514:GLU:CD	2.24	0.57
1:B:7:LEU:HD23	1:B:7:LEU:N	2.19	0.57
1:A:87:ALA:HA	1:A:90:ASN:OD1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:SER:HB2	1:B:402:LYS:NZ	2.19	0.57
1:A:36:GLY:C	1:A:38:THR:N	2.57	0.57
1:A:398:ARG:HB2	1:A:398:ARG:HH11	1.69	0.57
1:B:25:LEU:HA	1:B:28:LEU:CD1	2.35	0.57
1:A:277:GLY:HA3	1:A:299:PRO:O	2.05	0.57
1:A:7:LEU:HD23	1:A:33:ILE:HG13	1.87	0.57
1:B:231:VAL:HG22	1:B:366:LEU:CD2	2.34	0.57
1:B:453:ILE:HD11	1:B:457:ARG:CZ	2.35	0.57
1:B:80:ARG:HD2	1:B:82:ILE:HD11	1.86	0.57
1:A:328:VAL:HG12	1:A:332:LYS:HE3	1.87	0.56
1:B:10:LEU:HD12	1:B:10:LEU:N	2.20	0.56
1:A:36:GLY:C	1:A:38:THR:H	2.06	0.56
1:A:502:GLU:HA	1:A:506:LEU:CB	2.28	0.56
1:A:386:GLN:HG3	1:B:221:TYR:CZ	2.40	0.56
1:A:35:SER:O	1:A:39:ALA:HB3	2.05	0.56
1:A:495:TYR:HE1	1:A:519:GLN:HA	1.68	0.56
1:B:278:ILE:HG22	1:B:279:PRO:O	2.04	0.56
1:B:547:ASP:HA	1:B:550:ASP:OD2	2.04	0.56
1:B:483:VAL:O	1:B:484:LYS:O	2.23	0.56
1:B:506:LEU:O	1:B:510:GLN:HG3	2.05	0.56
1:A:378:GLU:CD	1:A:391:ARG:HB3	2.26	0.56
1:A:163:LYS:NZ	1:A:163:LYS:H	2.04	0.56
1:A:58:PHE:CD2	1:A:59:PRO:HD2	2.41	0.56
1:A:70:HIS:HD2	1:A:72:ALA:N	2.04	0.56
1:B:500:ILE:HG23	1:B:509:TRP:CG	2.41	0.56
1:A:522:GLU:OE2	1:A:522:GLU:CA	2.53	0.55
1:B:71:PRO:O	1:B:75:ALA:N	2.35	0.55
1:A:35:SER:O	1:A:36:GLY:O	2.23	0.55
1:B:570:GLU:O	1:B:574:GLU:HG2	2.06	0.55
1:A:491:ALA:O	1:A:492:ILE:C	2.45	0.55
1:B:61:MET:H	1:B:61:MET:CE	2.13	0.55
1:A:28:LEU:HA	1:A:165:LYS:HZ1	1.69	0.55
1:A:287:VAL:HG11	1:A:470:HIS:CE1	2.42	0.55
1:B:283:GLU:O	1:B:286:GLN:N	2.39	0.55
1:A:126:ASP:OD1	1:A:130:VAL:HG23	2.07	0.55
1:B:113:SER:O	1:B:116:VAL:HG12	2.06	0.55
1:A:106:PRO:CD	1:A:109:LYS:HE2	2.32	0.55
1:A:432:ASN:HD22	1:A:432:ASN:C	2.11	0.55
1:A:564:SER:HB3	1:A:585:HIS:ND1	2.22	0.55
1:B:216:SER:OG	1:B:217:PRO:HA	2.07	0.55
1:B:31:GLY:O	1:B:33:ILE:HG13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:VAL:HG22	1:A:144:THR:HB	1.88	0.55
1:A:151:ASP:O	1:A:155:VAL:HG23	2.07	0.55
1:B:432:ASN:HB2	1:B:452:ARG:NH2	2.22	0.55
1:A:12:VAL:HB	1:A:103:ASN:OD1	2.06	0.54
1:A:74:HIS:O	1:A:78:LEU:HB2	2.06	0.54
1:B:148:ASP:O	1:B:151:ASP:HB2	2.07	0.54
1:B:202:VAL:HG12	1:B:226:LYS:HG2	1.89	0.54
1:B:308:ARG:NH2	1:B:316:PHE:HA	2.22	0.54
1:B:426:VAL:CG1	1:B:540:ASP:HB3	2.37	0.54
1:A:130:VAL:HG13	1:A:183:THR:HG22	1.89	0.54
1:A:70:HIS:C	1:A:70:HIS:CD2	2.80	0.54
1:A:70:HIS:CD2	1:A:72:ALA:N	2.74	0.54
1:B:399:SER:O	1:B:402:LYS:HE2	2.07	0.54
1:A:464:ASN:HD22	1:A:555:ILE:HD13	1.72	0.54
1:A:220:LEU:HD13	1:B:387:LEU:CD1	2.38	0.54
1:A:376:ASP:O	1:A:391:ARG:HG2	2.08	0.54
1:B:64:GLY:C	1:B:66:VAL:N	2.57	0.54
1:A:174:HIS:CD2	1:A:175:LEU:HD22	2.37	0.54
1:A:386:GLN:HG3	1:B:221:TYR:CE1	2.42	0.54
1:A:186:TYR:O	1:A:189:ALA:HB3	2.08	0.54
1:A:383:TYR:HA	1:B:391:ARG:NH2	2.23	0.54
1:B:406:THR:HB	1:B:577:ASN:OD1	2.08	0.54
1:A:460:GLY:O	1:A:463:ALA:HB3	2.06	0.54
1:A:254:LEU:CD2	1:A:424:ILE:HD12	2.37	0.54
1:A:492:ILE:O	1:A:493:ASP:C	2.47	0.54
1:B:172:ARG:HG3	1:B:172:ARG:HH11	1.71	0.54
1:B:411:LEU:HD11	1:B:416:VAL:HG22	1.89	0.54
1:A:32:LEU:HD12	1:A:48:PRO:O	2.08	0.53
1:A:61:MET:SD	1:B:92:GLN:CG	2.95	0.53
1:B:190:ILE:O	1:B:193:TYR:HB3	2.08	0.53
1:A:216:SER:OG	1:A:217:PRO:HA	2.09	0.53
1:B:359:LYS:HE2	1:B:363:TYR:HD1	1.73	0.53
1:A:113:SER:HB2	1:A:114:PRO:CD	2.39	0.53
1:A:330:THR:HG22	1:A:334:ILE:CD1	2.38	0.53
1:A:40:THR:HA	1:A:43:ARG:CZ	2.37	0.53
1:A:220:LEU:CD1	1:B:387:LEU:HD12	2.37	0.53
1:A:569:ASP:O	1:A:573:ILE:HG13	2.08	0.53
1:B:273:GLY:HA3	1:B:307:SER:O	2.08	0.53
1:B:102:CYS:O	1:B:147:CYS:HA	2.09	0.53
1:B:484:LYS:CB	1:B:487:GLU:HG3	2.34	0.53
1:B:83:PRO:HA	1:B:86:ASN:ND2	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ALA:O	1:A:157:LYS:C	2.47	0.53
1:A:396:ILE:HG23	1:A:400:LEU:CD2	2.39	0.53
1:A:326:CYS:O	1:A:348:GLU:HG3	2.09	0.53
1:A:328:VAL:N	1:A:329:PRO:HD2	2.23	0.52
1:B:552:ALA:O	1:B:555:ILE:HG22	2.09	0.52
1:B:467:TRP:O	1:B:470:HIS:HB2	2.10	0.52
1:A:169:VAL:HG12	1:A:170:GLU:OE1	2.09	0.52
1:A:328:VAL:CG1	1:A:332:LYS:HE3	2.40	0.52
1:A:290:VAL:HA	1:A:336:ARG:HH22	1.73	0.52
1:A:490:ASN:O	1:A:493:ASP:HB3	2.09	0.52
1:A:396:ILE:HG21	1:A:423:SER:HB2	1.91	0.52
1:A:474:VAL:O	1:A:477:MET:HB2	2.10	0.52
1:B:465:SER:O	1:B:469:ARG:HG3	2.09	0.52
1:A:18:LEU:O	1:A:19:VAL:C	2.47	0.52
1:A:7:LEU:HD23	1:A:33:ILE:CD1	2.40	0.52
1:B:151:ASP:O	1:B:155:VAL:HG23	2.10	0.52
1:A:12:VAL:HG12	1:A:101:VAL:HG12	1.92	0.52
1:A:290:VAL:HA	1:A:336:ARG:NH2	2.25	0.52
1:A:348:GLU:O	1:A:351:ALA:HB3	2.09	0.52
1:B:458:LEU:C	1:B:458:LEU:HD23	2.30	0.52
1:B:490:ASN:O	1:B:491:ALA:C	2.48	0.52
1:B:537:LEU:HD23	1:B:538:SER:N	2.25	0.52
1:A:65:ARG:HD3	1:B:78:LEU:HB3	1.90	0.52
1:A:537:LEU:HD23	1:A:538:SER:N	2.25	0.52
1:B:376:ASP:HB3	1:B:390:LYS:HZ3	1.74	0.52
1:A:103:ASN:HD22	1:A:104:LEU:N	2.08	0.51
1:A:16:ALA:C	1:A:18:LEU:H	2.13	0.51
1:A:63:GLY:O	1:B:80:ARG:NH2	2.43	0.51
1:A:65:ARG:HD3	1:B:78:LEU:CD2	2.34	0.51
1:B:589:ARG:HG2	1:B:590:LEU:N	2.25	0.51
1:A:516:VAL:HG23	1:A:517:PRO:HD2	1.92	0.51
1:B:10:LEU:HD22	1:B:42:LEU:HD11	1.93	0.51
1:B:433:SER:HA	1:B:455:CYS:SG	2.50	0.51
1:B:589:ARG:HD3	1:B:591:PHE:CG	2.46	0.51
1:A:28:LEU:HA	1:A:165:LYS:CE	2.40	0.51
1:A:576:CYS:SG	1:A:583:LEU:HD22	2.51	0.51
1:A:309:GLY:O	1:A:469:ARG:NH2	2.42	0.51
1:A:445:ILE:HG23	1:A:445:ILE:O	2.11	0.51
1:B:58:PHE:O	1:B:60:GLU:N	2.41	0.51
1:A:325:ILE:HG23	1:A:346:GLY:O	2.11	0.51
1:B:408:ASN:HD21	1:B:577:ASN:CA	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ASN:HB3	1:A:143:VAL:CG2	2.40	0.51
1:A:14:GLU:HA	1:A:14:GLU:OE2	2.11	0.51
1:A:414:SER:O	1:A:417:ARG:HB3	2.11	0.51
1:B:157:LYS:H	1:B:157:LYS:HE3	1.74	0.51
1:B:26:ASN:HB2	1:B:32:LEU:CD1	2.37	0.51
1:B:24:SER:O	1:B:28:LEU:HG	2.11	0.51
1:A:102:CYS:O	1:A:147:CYS:HA	2.11	0.50
1:A:116:VAL:HG23	1:A:120:GLU:OE2	2.10	0.50
1:A:193:TYR:O	1:A:197:GLU:HG2	2.11	0.50
1:A:510:GLN:HA	1:A:513:PHE:HD1	1.76	0.50
1:A:71:PRO:O	1:A:75:ALA:CB	2.59	0.50
1:B:331:ALA:O	1:B:332:LYS:C	2.49	0.50
1:A:537:LEU:C	1:A:537:LEU:CD2	2.78	0.50
1:A:84:GLU:OE1	1:A:84:GLU:N	2.38	0.50
1:A:28:LEU:HA	1:A:165:LYS:HE2	1.93	0.50
1:B:412:PRO:O	1:B:416:VAL:HG23	2.11	0.50
1:A:12:VAL:CG1	1:A:101:VAL:HG12	2.41	0.50
1:A:344:ALA:HB1	1:A:345:PRO:HD2	1.94	0.50
1:B:451:SER:HB3	1:B:454:HIS:HB2	1.92	0.50
1:B:522:GLU:O	1:B:526:LYS:HG3	2.12	0.50
1:A:376:ASP:HB3	1:A:390:LYS:CD	2.42	0.50
1:A:449:GLN:HB2	1:A:455:CYS:HB2	1.92	0.50
1:A:458:LEU:CD2	1:A:462:LYS:HE3	2.39	0.50
1:B:18:LEU:C	1:B:18:LEU:HD12	2.32	0.50
1:B:341:GLY:HA2	1:B:363:TYR:CZ	2.47	0.50
1:B:400:LEU:O	1:B:400:LEU:HG	2.11	0.50
1:B:432:ASN:HB2	1:B:452:ARG:HH22	1.76	0.50
1:B:506:LEU:HD12	1:B:506:LEU:O	2.11	0.50
1:B:82:ILE:HD11	1:B:85:ASP:CG	2.32	0.50
1:A:19:VAL:O	1:A:22:ALA:HB3	2.12	0.50
1:A:520:LEU:N	1:A:520:LEU:HD12	2.12	0.50
1:A:458:LEU:HD23	1:A:458:LEU:O	2.11	0.50
1:A:525:LYS:O	1:A:529:ILE:HG13	2.12	0.50
1:A:562:ALA:O	1:A:585:HIS:HA	2.11	0.50
1:B:537:LEU:CD2	1:B:537:LEU:C	2.80	0.50
1:A:453:ILE:HG23	1:A:454:HIS:N	2.27	0.50
1:A:523:ALA:O	1:A:527:GLN:HB2	2.12	0.49
1:B:325:ILE:HA	1:B:346:GLY:O	2.11	0.49
1:B:76:GLY:HA2	1:B:89:MET:HE1	1.92	0.49
1:A:168:SER:OG	1:A:171:THR:OG1	2.10	0.49
1:A:342:VAL:HG22	1:A:343:VAL:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ASP:OD1	1:B:150:ALA:HB3	2.11	0.49
1:B:18:LEU:HG	1:B:19:VAL:N	2.26	0.49
1:B:426:VAL:HG13	1:B:540:ASP:HB3	1.93	0.49
1:A:116:VAL:HG23	1:A:120:GLU:CD	2.32	0.49
1:A:255:LYS:HG3	1:A:323:SER:HB2	1.92	0.49
1:B:172:ARG:HG3	1:B:172:ARG:NH1	2.27	0.49
1:B:523:ALA:C	1:B:525:LYS:N	2.65	0.49
1:A:426:VAL:HG13	1:A:540:ASP:HB3	1.94	0.49
1:B:7:LEU:HD13	1:B:33:ILE:CD1	2.42	0.49
1:A:522:GLU:O	1:A:526:LYS:HE2	2.11	0.49
1:B:572:VAL:O	1:B:575:ALA:N	2.43	0.49
1:A:520:LEU:HA	1:A:524:GLU:OE1	2.13	0.49
1:B:107:PHE:O	1:B:110:THR:HB	2.13	0.49
1:A:391:ARG:NH1	1:A:393:ASN:OD1	2.46	0.49
1:B:331:ALA:O	1:B:334:ILE:N	2.46	0.49
1:B:348:GLU:O	1:B:351:ALA:HB3	2.12	0.49
1:A:496:VAL:HG23	1:A:497:THR:HG23	1.94	0.49
1:A:566:SER:C	1:A:568:ALA:H	2.16	0.49
1:A:537:LEU:HD22	1:A:560:ILE:HG23	1.93	0.49
1:A:145:VAL:O	1:A:175:LEU:HD12	2.13	0.48
1:B:250:LEU:HD12	1:B:428:TYR:HB2	1.95	0.48
1:B:431:SER:HB2	1:B:592:HIS:H	1.78	0.48
1:B:496:VAL:O	1:B:498:GLY:N	2.46	0.48
1:B:496:VAL:CG2	1:B:497:THR:H	2.25	0.48
1:A:103:ASN:C	1:A:104:LEU:HG	2.33	0.48
1:A:161:ALA:HB3	4:A:2006:HOH:O	2.13	0.48
1:B:255:LYS:HE2	1:B:324:ASP:OD2	2.13	0.48
1:B:71:PRO:O	1:B:72:ALA:C	2.49	0.48
1:A:293:LEU:O	1:A:297:LEU:HG	2.14	0.48
1:B:375:ASP:OD2	1:B:375:ASP:N	2.44	0.48
1:B:58:PHE:HD2	1:B:61:MET:CE	2.26	0.48
1:A:25:LEU:C	1:A:27:ALA:N	2.66	0.48
1:A:226:LYS:HG2	1:A:227:LEU:N	2.29	0.48
1:A:350:GLU:O	1:A:354:ILE:HG13	2.13	0.48
1:A:275:ALA:HB2	1:A:441:GLN:HB2	1.96	0.48
1:A:471:HIS:CE1	1:A:472:PRO:HD2	2.47	0.48
1:A:485:ARG:CZ	1:A:485:ARG:HB2	2.43	0.48
1:B:496:VAL:C	1:B:498:GLY:N	2.67	0.48
1:A:269:VAL:HG12	1:A:269:VAL:O	2.14	0.48
1:A:544:PRO:HA	1:A:566:SER:OG	2.14	0.48
1:A:71:PRO:O	1:A:75:ALA:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:ALA:O	1:B:25:LEU:HD23	2.13	0.48
1:B:296:THR:O	1:B:297:LEU:HD23	2.14	0.48
1:B:464:ASN:ND2	1:B:555:ILE:CD1	2.76	0.48
1:B:473:ARG:HD3	1:B:518:ALA:O	2.14	0.48
1:A:21:PHE:CZ	1:A:155:VAL:HB	2.49	0.48
1:A:471:HIS:ND1	1:A:472:PRO:CD	2.75	0.48
1:A:311:ASP:OD2	1:A:314:SER:CB	2.62	0.47
1:A:392:ASN:OD1	1:A:427:LYS:HE3	2.14	0.47
1:B:485:ARG:NH1	1:B:485:ARG:CG	2.63	0.47
1:A:113:SER:CB	1:A:114:PRO:CD	2.92	0.47
1:A:26:ASN:HB2	1:A:32:LEU:HD11	1.96	0.47
1:A:73:VAL:HG12	1:A:74:HIS:N	2.29	0.47
1:B:523:ALA:C	1:B:525:LYS:H	2.18	0.47
1:B:431:SER:OG	1:B:432:ASN:HA	2.13	0.47
1:B:67:LYS:NZ	3:B:1595:203:H12	2.13	0.47
1:A:42:LEU:HD22	1:A:47:LEU:HD12	1.96	0.47
1:A:429:THR:HG22	1:A:433:SER:OG	2.15	0.47
1:A:36:GLY:O	1:A:39:ALA:N	2.47	0.47
1:B:496:VAL:CG2	1:B:497:THR:N	2.78	0.47
1:A:58:PHE:CG	1:A:59:PRO:HD2	2.49	0.47
1:A:106:PRO:CB	1:A:109:LYS:HZ3	2.27	0.47
1:A:118:VAL:N	1:A:119:PRO:HD2	2.29	0.47
1:A:25:LEU:C	1:A:27:ALA:H	2.18	0.47
1:A:231:VAL:HG22	1:A:366:LEU:CD2	2.45	0.47
1:B:130:VAL:O	1:B:134:ARG:HG3	2.15	0.47
1:B:483:VAL:O	1:B:484:LYS:C	2.53	0.47
1:B:495:TYR:HA	1:B:500:ILE:HD11	1.97	0.47
1:B:99:VAL:HG22	1:B:144:THR:HB	1.95	0.47
1:A:467:TRP:O	1:A:470:HIS:HB2	2.15	0.47
1:A:70:HIS:CD2	1:A:71:PRO:HG2	2.50	0.47
1:B:193:TYR:O	1:B:197:GLU:HG2	2.15	0.47
1:A:372:TYR:OH	1:B:384:GLY:HA3	2.15	0.47
1:B:53:SER:HG	1:B:60:GLU:CD	2.18	0.47
1:A:148:ASP:O	1:A:151:ASP:HB2	2.14	0.47
1:A:522:GLU:O	1:A:524:GLU:N	2.48	0.47
1:B:466:TRP:O	1:B:469:ARG:HB2	2.15	0.47
1:A:25:LEU:O	1:A:28:LEU:HB2	2.14	0.46
1:B:483:VAL:O	1:B:483:VAL:HG22	2.16	0.46
1:B:64:GLY:C	1:B:66:VAL:H	2.18	0.46
1:B:6:GLN:OE1	1:B:98:ARG:NH2	2.47	0.46
1:A:495:TYR:CD1	1:A:519:GLN:NE2	2.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:ALA:O	1:B:466:TRP:HB3	2.15	0.46
1:B:59:PRO:O	1:B:60:GLU:C	2.53	0.46
1:A:22:ALA:HB1	1:A:47:LEU:HD13	1.96	0.46
1:A:246:ASN:HD21	1:A:592:HIS:CE1	2.32	0.46
1:B:20:GLU:OE2	1:B:20:GLU:HA	2.16	0.46
1:B:280:LEU:H	1:B:280:LEU:HD12	1.79	0.46
1:A:330:THR:CG2	1:A:334:ILE:HD11	2.45	0.46
1:A:73:VAL:O	1:A:77:ILE:HG13	2.15	0.46
1:B:139:ASN:OD1	1:B:143:VAL:HG23	2.16	0.46
1:B:476:SER:O	1:B:478:LYS:HD2	2.15	0.46
1:B:572:VAL:O	1:B:575:ALA:HB3	2.15	0.46
1:A:330:THR:HG22	1:A:334:ILE:HD11	1.96	0.46
1:A:477:MET:CE	1:A:492:ILE:HG12	2.46	0.46
1:A:59:PRO:O	1:A:60:GLU:C	2.53	0.46
1:A:36:GLY:O	1:A:38:THR:N	2.49	0.46
1:A:70:HIS:O	1:A:73:VAL:HB	2.16	0.46
1:B:342:VAL:HG22	1:B:343:VAL:N	2.31	0.46
1:A:278:ILE:O	1:A:279:PRO:C	2.54	0.46
1:A:18:LEU:HD12	1:A:18:LEU:C	2.36	0.46
1:A:286:GLN:C	1:A:288:CYS:N	2.68	0.46
1:B:231:VAL:HG22	1:B:366:LEU:HD21	1.98	0.46
1:B:494:GLN:HA	1:B:497:THR:HB	1.97	0.46
1:A:50:ARG:HD2	1:A:54:ASP:CG	2.35	0.46
1:A:56:THR:O	1:A:57:GLY:C	2.54	0.46
1:B:352:LEU:HD12	1:B:352:LEU:O	2.16	0.46
1:A:429:THR:CG2	1:A:433:SER:OG	2.64	0.46
1:A:492:ILE:O	1:A:495:TYR:HB3	2.16	0.46
1:B:396:ILE:O	1:B:397:ASP:HB3	2.16	0.46
1:A:106:PRO:CG	1:A:109:LYS:NZ	2.79	0.45
1:A:298:THR:HG23	1:A:329:PRO:HG3	1.97	0.45
1:A:359:LYS:HE3	1:A:359:LYS:HB3	1.85	0.45
1:A:523:ALA:HA	1:A:526:LYS:CE	2.46	0.45
1:B:397:ASP:C	1:B:397:ASP:OD1	2.55	0.45
1:A:359:LYS:C	1:A:361:GLY:N	2.68	0.45
1:A:476:SER:O	1:A:477:MET:C	2.53	0.45
1:B:406:THR:CG2	1:B:583:LEU:HB3	2.47	0.45
1:B:438:LYS:HE2	1:B:533:THR:O	2.17	0.45
1:B:575:ALA:O	1:B:579:LEU:HG	2.16	0.45
1:B:589:ARG:HG2	1:B:590:LEU:H	1.82	0.45
1:A:25:LEU:O	1:A:28:LEU:N	2.44	0.45
1:A:38:THR:O	1:A:42:LEU:CG	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:ILE:O	1:A:495:TYR:N	2.49	0.45
1:A:390:LYS:O	1:B:215:GLN:HG2	2.17	0.45
1:B:44:ASP:C	1:B:46:GLY:N	2.70	0.45
1:A:102:CYS:O	1:A:147:CYS:CB	2.65	0.45
1:A:287:VAL:O	1:A:287:VAL:HG12	2.17	0.45
1:A:464:ASN:O	1:A:465:SER:C	2.54	0.45
1:A:551:ARG:O	1:A:554:ARG:HB2	2.16	0.45
1:B:134:ARG:CZ	1:B:134:ARG:HB3	2.46	0.45
1:B:152:TYR:O	1:B:155:VAL:HB	2.16	0.45
1:B:158:GLU:CD	1:B:168:SER:H	2.20	0.45
1:A:92:GLN:O	1:A:93:ASP:HB3	2.17	0.45
1:B:5:GLN:O	1:B:5:GLN:HG3	2.16	0.45
1:A:208:ARG:CD	1:A:208:ARG:H	2.29	0.45
1:A:502:GLU:N	1:A:505:ASP:HB2	2.29	0.45
1:A:208:ARG:NH2	1:A:237:GLY:CA	2.79	0.45
1:A:563:PRO:HG3	1:A:588:LEU:O	2.17	0.45
1:B:14:GLU:HA	1:B:14:GLU:OE1	2.16	0.45
1:B:398:ARG:O	1:B:401:PHE:HD2	1.99	0.45
1:B:509:TRP:HH2	1:B:517:PRO:HG2	1.81	0.45
1:A:229:LEU:HD23	1:A:229:LEU:C	2.37	0.45
1:A:311:ASP:OD2	1:A:314:SER:HB2	2.17	0.45
1:A:494:GLN:O	1:A:498:GLY:N	2.50	0.45
1:B:118:VAL:N	1:B:119:PRO:HD2	2.32	0.45
1:B:496:VAL:C	1:B:498:GLY:H	2.20	0.45
1:A:64:GLY:C	1:A:65:ARG:HG3	2.37	0.44
1:B:497:THR:O	1:B:497:THR:HG22	2.17	0.44
1:B:49:VAL:O	1:B:49:VAL:HG13	2.17	0.44
1:B:429:THR:O	1:B:592:HIS:HB3	2.16	0.44
1:A:26:ASN:HB2	1:A:32:LEU:CD2	2.37	0.44
1:A:37:GLY:HA2	1:A:40:THR:OG1	2.17	0.44
1:A:64:GLY:O	1:A:65:ARG:HG3	2.16	0.44
1:B:44:ASP:C	1:B:46:GLY:H	2.20	0.44
1:A:429:THR:HG22	1:A:430:GLN:N	2.32	0.44
1:A:501:GLY:O	1:A:502:GLU:HB3	2.18	0.44
1:A:246:ASN:ND2	1:A:592:HIS:NE2	2.62	0.44
1:A:7:LEU:CD1	1:A:7:LEU:N	2.78	0.44
1:B:477:MET:C	1:B:478:LYS:HD2	2.37	0.44
1:A:103:ASN:O	1:A:104:LEU:HD23	2.17	0.44
1:A:98:ARG:HD3	1:A:166:ASP:OD2	2.17	0.44
1:A:239:ILE:HG22	1:A:243:ASP:OD2	2.17	0.44
1:B:495:TYR:CD1	1:B:500:ILE:HD11	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:ARG:O	1:B:549:VAL:N	2.50	0.44
1:B:82:ILE:HD11	1:B:85:ASP:OD1	2.17	0.44
1:A:187:ASP:HB3	1:B:184:ALA:HB2	1.99	0.44
1:A:80:ARG:HB2	1:A:80:ARG:HE	1.45	0.44
1:A:103:ASN:O	1:A:104:LEU:HG	2.17	0.44
1:A:237:GLY:O	1:A:241:LEU:HG	2.18	0.44
1:B:22:ALA:CA	1:B:25:LEU:CD2	2.92	0.44
1:A:102:CYS:HB3	1:A:133:LEU:HD21	2.00	0.44
1:A:250:LEU:HD11	1:A:425:ALA:HA	1.98	0.44
1:A:407:LYS:O	1:A:409:LYS:HD3	2.17	0.44
1:A:436:TYR:CE2	1:A:555:ILE:HG21	2.53	0.44
1:B:156:ALA:CB	1:B:157:LYS:HE3	2.41	0.44
1:B:257:ALA:O	1:B:258:LEU:HD23	2.18	0.44
1:B:471:HIS:ND1	1:B:472:PRO:CD	2.81	0.44
1:B:169:VAL:O	1:B:173:ARG:HG3	2.17	0.44
1:B:89:MET:HE1	1:B:96:LEU:HD23	1.99	0.44
1:A:10:LEU:HD13	1:A:42:LEU:HD11	2.00	0.44
1:A:286:GLN:C	1:A:288:CYS:H	2.21	0.44
1:B:164:ASP:OD2	1:B:166:ASP:HB3	2.17	0.44
1:B:467:TRP:CE3	1:B:467:TRP:HA	2.53	0.44
1:B:7:LEU:HD21	1:B:95:SER:HB3	2.00	0.44
1:B:71:PRO:O	1:B:75:ALA:CB	2.66	0.43
1:A:245:LEU:HD22	1:A:245:LEU:N	2.33	0.43
1:A:385:LEU:HD22	1:B:227:LEU:CD2	2.48	0.43
1:A:490:ASN:O	1:A:491:ALA:C	2.56	0.43
1:A:432:ASN:HD21	1:A:455:CYS:HB2	1.83	0.43
1:A:148:ASP:OD1	1:A:150:ALA:CB	2.59	0.43
1:A:163:LYS:N	1:A:163:LYS:NZ	2.66	0.43
1:A:281:SER:OG	1:A:284:GLU:HB2	2.19	0.43
1:B:473:ARG:HD2	1:B:520:LEU:HD21	2.01	0.43
1:A:192:ASP:HA	1:A:195:ARG:NH2	2.33	0.43
1:A:308:ARG:HG3	1:A:315:SER:HB3	2.01	0.43
1:B:311:ASP:OD1	1:B:314:SER:HB2	2.17	0.43
1:B:509:TRP:HE3	1:B:510:GLN:HG2	1.83	0.43
1:A:352:LEU:O	1:A:352:LEU:HD12	2.18	0.43
1:A:451:SER:HB3	1:A:454:HIS:CG	2.54	0.43
1:A:89:MET:HE3	1:A:94:PHE:HB2	2.01	0.43
1:B:164:ASP:C	1:B:165:LYS:HG2	2.38	0.43
1:B:21:PHE:O	1:B:25:LEU:HD23	2.17	0.43
1:B:328:VAL:HG21	1:B:350:GLU:OE1	2.18	0.43
1:A:219:GLN:NE2	1:B:388:MET:CE	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:GLU:OE1	1:A:197:GLU:HA	2.19	0.43
1:A:298:THR:OG1	1:A:327:ASP:OD2	2.24	0.43
1:A:463:ALA:O	1:A:466:TRP:HB3	2.19	0.43
1:A:382:LEU:CD2	1:B:242:CYS:HA	2.48	0.43
1:B:286:GLN:HG2	1:B:291:HIS:HB2	2.00	0.43
1:B:30:LEU:HD21	1:B:98:ARG:HD2	2.01	0.43
1:B:347:TYR:OH	1:B:366:LEU:O	2.28	0.43
1:A:268:HIS:NE2	1:B:432:ASN:HB3	2.33	0.43
1:B:502:GLU:H	1:B:502:GLU:HG2	1.45	0.43
1:A:27:ALA:C	1:A:28:LEU:HD12	2.38	0.43
1:A:429:THR:CG2	1:A:447:ALA:HB2	2.49	0.43
1:A:484:LYS:HB2	1:A:487:GLU:HG3	2.01	0.43
1:B:174:HIS:O	1:B:178:LYS:HG3	2.18	0.43
1:B:17:GLY:O	1:B:18:LEU:C	2.57	0.43
1:A:330:THR:O	1:A:334:ILE:HG13	2.19	0.43
1:B:445:ILE:HG23	1:B:445:ILE:O	2.18	0.43
1:B:478:LYS:N	1:B:478:LYS:CD	2.82	0.43
1:B:520:LEU:O	1:B:525:LYS:HE3	2.19	0.43
1:A:130:VAL:O	1:A:134:ARG:HG3	2.19	0.43
1:A:81:ASN:O	1:A:81:ASN:CG	2.56	0.43
1:A:89:MET:HE3	1:A:94:PHE:CB	2.49	0.43
1:A:385:LEU:HD21	1:B:228:PRO:HD2	2.01	0.43
1:B:474:VAL:CA	1:B:477:MET:HG3	2.45	0.43
1:A:162:SER:O	1:A:165:LYS:N	2.51	0.42
1:A:245:LEU:O	1:A:249:GLN:HG3	2.18	0.42
1:A:419:LEU:HD23	1:A:536:SER:HB3	2.01	0.42
1:B:118:VAL:HB	1:B:119:PRO:CD	2.49	0.42
1:B:195:ARG:HB3	1:B:204:GLN:HB2	2.01	0.42
1:B:121:ALA:C	1:B:124:LYS:HB2	2.39	0.42
1:B:18:LEU:O	1:B:19:VAL:C	2.56	0.42
1:B:281:SER:HB2	4:B:2018:HOH:O	2.19	0.42
1:B:504:GLU:O	1:B:507:VAL:HB	2.19	0.42
1:A:247:ALA:HB2	1:A:266:PHE:CD1	2.54	0.42
1:A:249:GLN:O	1:A:253:GLU:HG3	2.19	0.42
1:A:398:ARG:CB	1:A:398:ARG:NH1	2.83	0.42
1:A:40:THR:HA	1:A:43:ARG:NH2	2.34	0.42
1:A:89:MET:O	1:A:93:ASP:N	2.52	0.42
1:B:237:GLY:O	1:B:241:LEU:HG	2.19	0.42
1:B:269:VAL:O	1:B:269:VAL:HG12	2.18	0.42
1:B:399:SER:O	1:B:402:LYS:HG2	2.18	0.42
1:A:15:LYS:O	1:A:18:LEU:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:GLU:O	1:A:23:ARG:HB3	2.20	0.42
1:B:140:HIS:O	1:B:141:ALA:C	2.58	0.42
1:A:196:LYS:HD3	1:A:219:GLN:NE2	2.34	0.42
1:A:200:LYS:CD	1:A:200:LYS:C	2.85	0.42
1:A:404:ILE:HG12	1:A:584:ILE:HG12	2.02	0.42
1:A:572:VAL:O	1:A:575:ALA:HB3	2.19	0.42
1:B:58:PHE:CD2	1:B:59:PRO:HD2	2.55	0.42
1:A:59:PRO:HG3	1:B:92:GLN:OE1	2.20	0.42
1:A:523:ALA:HA	1:A:526:LYS:HE3	2.00	0.42
1:A:555:ILE:O	1:A:555:ILE:HG13	2.19	0.42
1:A:65:ARG:NH2	1:B:138:LYS:HE2	2.33	0.42
1:B:222:THR:O	1:B:222:THR:HG23	2.18	0.42
1:B:33:ILE:HD13	1:B:55:LEU:HG	2.01	0.42
1:B:98:ARG:O	1:B:98:ARG:HG2	2.20	0.42
1:A:467:TRP:CD1	1:A:529:ILE:HA	2.54	0.42
1:A:553:LYS:O	1:A:554:ARG:C	2.57	0.42
1:B:286:GLN:HG2	1:B:291:HIS:CG	2.55	0.42
1:A:452:ARG:HG3	1:A:548:ASN:OD1	2.19	0.42
1:B:267:LYS:O	1:B:268:HIS:HB2	2.20	0.42
1:A:18:LEU:O	1:A:21:PHE:N	2.51	0.42
1:A:280:LEU:HD12	1:A:280:LEU:N	2.35	0.42
1:A:282:GLU:HG3	1:A:291:HIS:CE1	2.54	0.42
1:A:379:ILE:CG1	1:A:388:MET:HG3	2.25	0.42
1:A:470:HIS:O	1:A:471:HIS:C	2.57	0.42
1:B:287:VAL:HG11	1:B:470:HIS:CE1	2.55	0.42
1:A:419:LEU:HA	1:A:419:LEU:HD23	1.87	0.42
1:B:107:PHE:O	1:B:108:VAL:C	2.58	0.42
1:B:25:LEU:HD23	1:B:25:LEU:H	1.85	0.42
1:A:330:THR:HG22	1:A:334:ILE:HD12	2.02	0.41
1:A:412:PRO:C	1:A:414:SER:N	2.72	0.41
1:B:97:VAL:O	1:B:142:ARG:NH1	2.53	0.41
1:B:196:LYS:HG2	1:B:204:GLN:NE2	2.34	0.41
1:B:71:PRO:O	1:B:75:ALA:HB2	2.20	0.41
1:B:80:ARG:HD2	1:B:82:ILE:HD13	2.01	0.41
1:A:467:TRP:NE1	1:A:528:TRP:O	2.48	0.41
1:A:574:GLU:O	1:A:578:GLU:HG2	2.20	0.41
1:B:108:VAL:CG2	1:B:109:LYS:N	2.83	0.41
1:A:386:GLN:HG2	1:B:221:TYR:O	2.20	0.41
1:B:464:ASN:HD22	1:B:555:ILE:CD1	2.33	0.41
1:B:532:LEU:HA	1:B:532:LEU:HD12	1.74	0.41
1:B:553:LYS:O	1:B:555:ILE:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:TYR:CE2	1:B:555:ILE:HG21	2.55	0.41
1:B:81:ASN:O	1:B:81:ASN:CG	2.58	0.41
1:B:89:MET:CE	1:B:96:LEU:HD23	2.50	0.41
1:A:138:LYS:C	1:A:140:HIS:H	2.23	0.41
1:A:149:PRO:C	1:A:151:ASP:N	2.73	0.41
1:A:356:SER:O	1:A:361:GLY:HA2	2.20	0.41
1:B:313:MET:C	1:B:315:SER:N	2.74	0.41
1:B:393:ASN:O	1:B:394:ALA:C	2.58	0.41
1:B:539:SER:HB2	1:B:543:PHE:CZ	2.55	0.41
1:A:520:LEU:H	1:A:520:LEU:CD1	2.13	0.41
1:B:153:SER:HA	1:B:157:LYS:HZ1	1.84	0.41
1:B:553:LYS:C	1:B:555:ILE:H	2.22	0.41
1:B:537:LEU:HD22	1:B:560:ILE:HG23	2.02	0.41
1:A:267:LYS:HG2	1:B:450:GLN:HB3	2.02	0.41
1:A:493:ASP:O	1:A:494:GLN:C	2.59	0.41
1:A:566:SER:C	1:A:568:ALA:N	2.73	0.41
1:A:87:ALA:O	1:A:90:ASN:HB2	2.20	0.41
1:A:412:PRO:HD2	1:A:415:ALA:HB2	2.02	0.41
1:A:7:LEU:HB3	1:A:8:ALA:H	1.57	0.41
1:B:108:VAL:CG2	1:B:109:LYS:H	2.33	0.41
1:B:250:LEU:HG	1:B:424:ILE:HG22	2.03	0.41
1:B:449:GLN:NE2	1:B:449:GLN:HA	2.35	0.41
1:B:453:ILE:HG13	1:B:453:ILE:O	2.20	0.41
1:B:480:LYS:N	1:B:512:MET:O	2.46	0.41
1:A:236:PRO:HB3	1:A:364:CYS:SG	2.61	0.41
1:A:378:GLU:HG3	1:A:391:ARG:CB	2.47	0.41
1:A:495:TYR:C	1:A:497:THR:H	2.23	0.41
1:B:22:ALA:O	1:B:23:ARG:C	2.59	0.41
1:A:212:ASN:OD1	1:B:591:PHE:HB2	2.21	0.41
1:A:418:ASP:OD1	1:A:418:ASP:N	2.54	0.41
1:B:590:LEU:HD23	1:B:590:LEU:HA	1.91	0.41
1:B:6:GLN:O	1:B:30:LEU:HD23	2.21	0.41
1:A:13:SER:HB3	1:A:103:ASN:ND2	2.36	0.41
1:B:566:SER:C	1:B:568:ALA:N	2.72	0.41
1:A:467:TRP:CE3	1:A:467:TRP:HA	2.55	0.41
1:B:241:LEU:O	1:B:245:LEU:HG	2.20	0.41
1:B:280:LEU:CD1	1:B:280:LEU:N	2.80	0.41
1:B:26:ASN:CA	1:B:32:LEU:HD21	2.50	0.41
1:B:331:ALA:O	1:B:333:ILE:N	2.53	0.41
1:B:575:ALA:O	1:B:578:GLU:HG2	2.21	0.41
1:A:121:ALA:O	1:A:124:LYS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:TYR:CD1	1:A:347:TYR:N	2.88	0.41
1:B:406:THR:HG23	1:B:583:LEU:HB3	2.02	0.41
1:A:16:ALA:O	1:A:18:LEU:N	2.54	0.40
1:A:271:PRO:HD2	1:A:429:THR:HA	2.03	0.40
1:A:10:LEU:HD12	1:A:42:LEU:HD11	2.02	0.40
1:A:494:GLN:HA	1:A:499:THR:OG1	2.21	0.40
1:B:360:ASN:HA	1:B:360:ASN:HD22	1.70	0.40
1:B:575:ALA:HA	1:B:578:GLU:HG2	2.03	0.40
1:A:254:LEU:HD23	1:A:254:LEU:HA	1.87	0.40
1:A:65:ARG:HB3	1:A:66:VAL:H	1.68	0.40
1:B:164:ASP:O	1:B:165:LYS:CG	2.68	0.40
1:B:35:SER:N	1:B:39:ALA:HB2	2.37	0.40
1:A:7:LEU:CD2	1:A:33:ILE:HD11	2.49	0.40
1:A:523:ALA:N	1:A:526:LYS:HE2	2.34	0.40
1:A:39:ALA:O	1:A:40:THR:C	2.59	0.40
1:B:464:ASN:HD21	1:B:555:ILE:HD13	1.79	0.40
1:A:103:ASN:O	1:A:104:LEU:CD2	2.70	0.40
1:A:144:THR:HG21	1:A:167:THR:HG21	2.04	0.40
1:A:219:GLN:HE21	1:B:388:MET:CE	2.34	0.40
1:A:229:LEU:HD23	1:A:229:LEU:O	2.21	0.40
1:A:7:LEU:HA	1:A:31:GLY:H	1.85	0.40
1:A:464:ASN:HD22	1:A:555:ILE:CD1	2.32	0.40
1:A:520:LEU:CD1	1:A:525:LYS:HE2	2.47	0.40
1:A:71:PRO:O	1:A:75:ALA:N	2.46	0.40
1:A:55:LEU:CD2	1:A:72:ALA:HB1	2.49	0.40
1:B:446:GLY:CA	1:B:458:LEU:HD22	2.52	0.40
1:B:473:ARG:NH1	1:B:524:GLU:OE2	2.53	0.40
1:B:546:ARG:HA	1:B:549:VAL:HG23	2.03	0.40
1:B:583:LEU:HD12	1:B:584:ILE:H	1.81	0.40

All (4) 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:47:LEU:O	1:B:47:LEU:O[2_656]	1.94	0.26
1:B:46:GLY:O	1:B:48:PRO:C[2_656]	2.02	0.18
1:B:46:GLY:CA	1:B:49:VAL:O[2_656]	2.07	0.13
1:B:46:GLY:O	1:B:48:PRO:CA[2_656]	2.11	0.09

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	589/593 (99%)	464 (79%)	90 (15%)	35 (6%)	1	5
1	B	588/593 (99%)	484 (82%)	75 (13%)	29 (5%)	2	8
All	All	1177/1186 (99%)	948 (80%)	165 (14%)	64 (5%)	2	6

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	18	LEU
1	A	19	VAL
1	A	40	THR
1	A	66	VAL
1	A	83	PRO
1	A	114	PRO
1	A	152	TYR
1	A	403	ASN
1	B	18	LEU
1	B	114	PRO
1	B	152	TYR
1	B	164	ASP
1	B	477	MET
1	B	484	LYS
1	B	503	ASP
1	A	36	GLY
1	A	67	LYS
1	A	269	VAL
1	A	402	LYS
1	A	477	MET
1	A	479	PHE
1	A	492	ILE
1	A	502	GLU
1	B	19	VAL

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Mol	Chain	Res	Type
1	B	60	GLU
1	B	67	LYS
1	B	73	VAL
1	B	269	VAL
1	B	489	SER
1	B	554	ARG
1	A	41	ALA
1	A	162	SER
1	A	491	ALA
1	A	499	THR
1	B	27	ALA
1	B	316	PHE
1	A	5	GLN
1	A	17	GLY
1	A	160	ALA
1	A	311	ASP
1	A	316	PHE
1	A	493	ASP
1	B	59	PRO
1	B	394	ALA
1	B	476	SER
1	A	73	VAL
1	A	153	SER
1	A	411	LEU
1	B	153	SER
1	B	277	GLY
1	B	332	LYS
1	B	404	ILE
1	B	497	THR
1	A	113	SER
1	B	71	PRO
1	B	315	SER
1	B	526	LYS
1	B	567	ALA
1	A	496	VAL
1	B	488	VAL
1	A	290	VAL
1	A	71	PRO
1	A	106	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	485/485 (100%)	450 (93%)	35 (7%)	14	39
1	B	484/485 (100%)	446 (92%)	38 (8%)	12	34
All	All	969/970 (100%)	896 (92%)	73 (8%)	13	37

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	11	SER
1	A	18	LEU
1	A	21	PHE
1	A	24	SER
1	A	32	LEU
1	A	43	ARG
1	A	54	ASP
1	A	68	THR
1	A	70	HIS
1	A	83	PRO
1	A	103	ASN
1	A	151	ASP
1	A	154	SER
1	A	159	MET
1	A	163	LYS
1	A	164	ASP
1	A	170	GLU
1	A	177	LEU
1	A	187	ASP
1	A	208	ARG
1	A	255	LYS
1	A	340	ASP
1	A	359	LYS
1	A	360	ASN
1	A	386	GLN
1	A	406	THR

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Mol	Chain	Res	Type
1	A	432	ASN
1	A	477	MET
1	A	502	GLU
1	A	504	GLU
1	A	520	LEU
1	A	522	GLU
1	A	524	GLU
1	A	547	ASP
1	B	5	GLN
1	B	7	LEU
1	B	9	LEU
1	B	11	SER
1	B	19	VAL
1	B	54	ASP
1	B	56	THR
1	B	60	GLU
1	B	61	MET
1	B	68	THR
1	B	114	PRO
1	B	154	SER
1	B	157	LYS
1	B	167	THR
1	B	170	GLU
1	B	177	LEU
1	B	199	SER
1	B	280	LEU
1	B	282	GLU
1	B	292	ASP
1	B	293	LEU
1	B	294	HIS
1	B	296	THR
1	B	314	SER
1	B	338	VAL
1	B	349	GLU
1	B	375	ASP
1	B	382	LEU
1	B	391	ARG
1	B	399	SER
1	B	408	ASN
1	B	478	LYS
1	B	483	VAL
1	B	485	ARG

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Mol	Chain	Res	Type
1	B	499	THR
1	B	502	GLU
1	B	506	LEU
1	B	517	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	70	HIS
1	A	81	ASN
1	A	86	ASN
1	A	174	HIS
1	A	185	GLN
1	A	286	GLN
1	A	291	HIS
1	A	294	HIS
1	A	386	GLN
1	A	403	ASN
1	A	432	ASN
1	A	450	GLN
1	A	464	ASN
1	A	510	GLN
1	A	519	GLN
1	B	5	GLN
1	B	70	HIS
1	B	86	ASN
1	B	185	GLN
1	B	360	ASN
1	B	393	ASN
1	B	403	ASN
1	B	408	ASN
1	B	454	HIS
1	B	464	ASN
1	B	494	GLN
1	B	510	GLN
1	B	527	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z > 2$
3	203	B	1595	-	6,13,13	7.86	4 (66%)	5,20,20	8.02	5 (100%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	203	B	1595	-	-	-	0/1/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1595	203	O20-S16	15.37	1.65	1.43
3	B	1595	203	O21-S16	9.84	1.57	1.43
3	B	1595	203	C14-N15	4.30	1.42	1.37
3	B	1595	203	C13-C18	4.06	1.55	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1595	203	O21-S16-O20	-16.63	97.97	118.85
3	B	1595	203	C11-N12-C13	-4.78	93.89	102.99
3	B	1595	203	O19-C18-C13	-3.27	117.98	124.37
3	B	1595	203	O19-C18-N17	2.75	124.53	120.82
3	B	1595	203	C13-C18-N17	2.03	117.49	113.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1595	203	1	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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.