



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:01 AM UTC

PDB ID : 2BUB / pdb_00002bub
Title : Crystal Structure Of Human Dipeptidyl Peptidase IV (CD26) in Complex with a Reversed Amide Inhibitor
Authors : Nordhoff, S.; Cerezo-Galvez, S.; Feurer, A.; Hill, O.; Matassa, V.G.; Metz, G.; Rummey, C.; Thiemann, M.; Edwards, P.J.
Deposited on : 2005-06-09
Resolution : 2.66 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

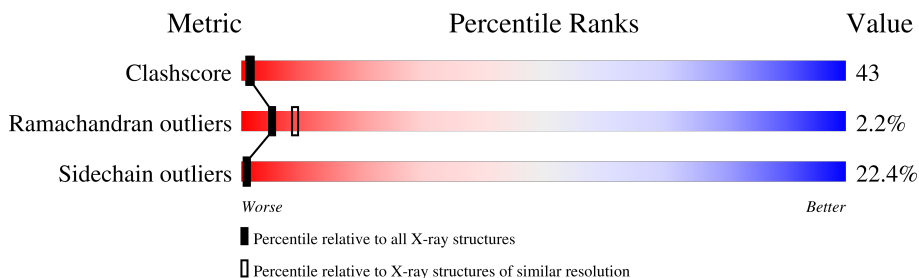
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)

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	728	 40% 46% 13% .
1	B	728	 34% 50% 15% .

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	NAG	A	1769	X	-	-	-
2	NAG	B	1770	X	-	-	-

2 Entry composition [i](#)

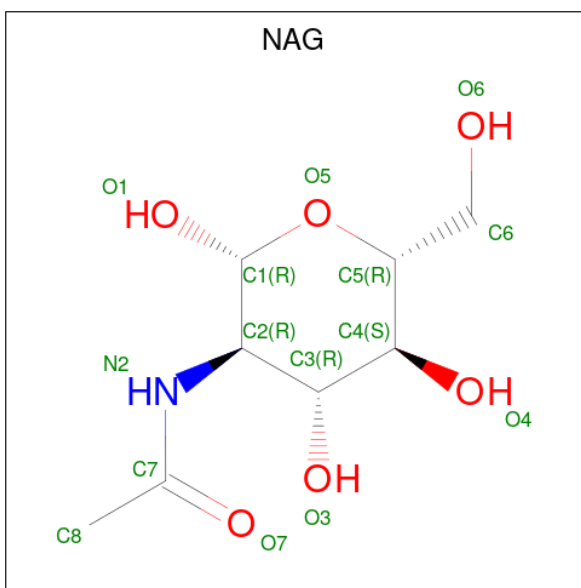
There are 4 unique types of molecules in this entry. The entry contains 12414 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DIPEPTIDYL PEPTIDASE 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	728	Total 5963	C 3827	N 982	O 1128	S 26	0	0	0
1	B	728	Total 5963	C 3827	N 982	O 1128	S 26	0	0	0

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



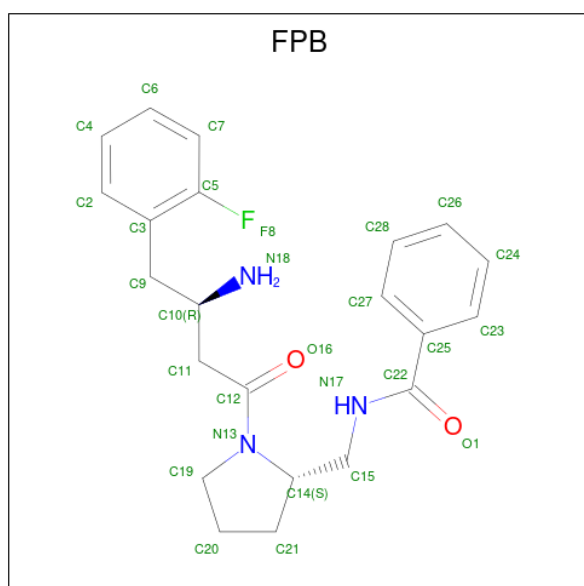
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	A	1	Total 14	C 8	N 1	O 5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is N-((2S)-1-[(3R)-3-AMINO-4-(2-FLUOROPHENYL)BUTANOYL]PYRROLIDIN-2-YL)METHYL)BENZAMIDE (CCD ID: FPB) (formula: C₂₂H₂₆FN₃O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			28	22	1	3	2		
3	B	1	Total	C	F	N	O	0	0
			28	22	1	3	2		

- Molecule 4 is water.

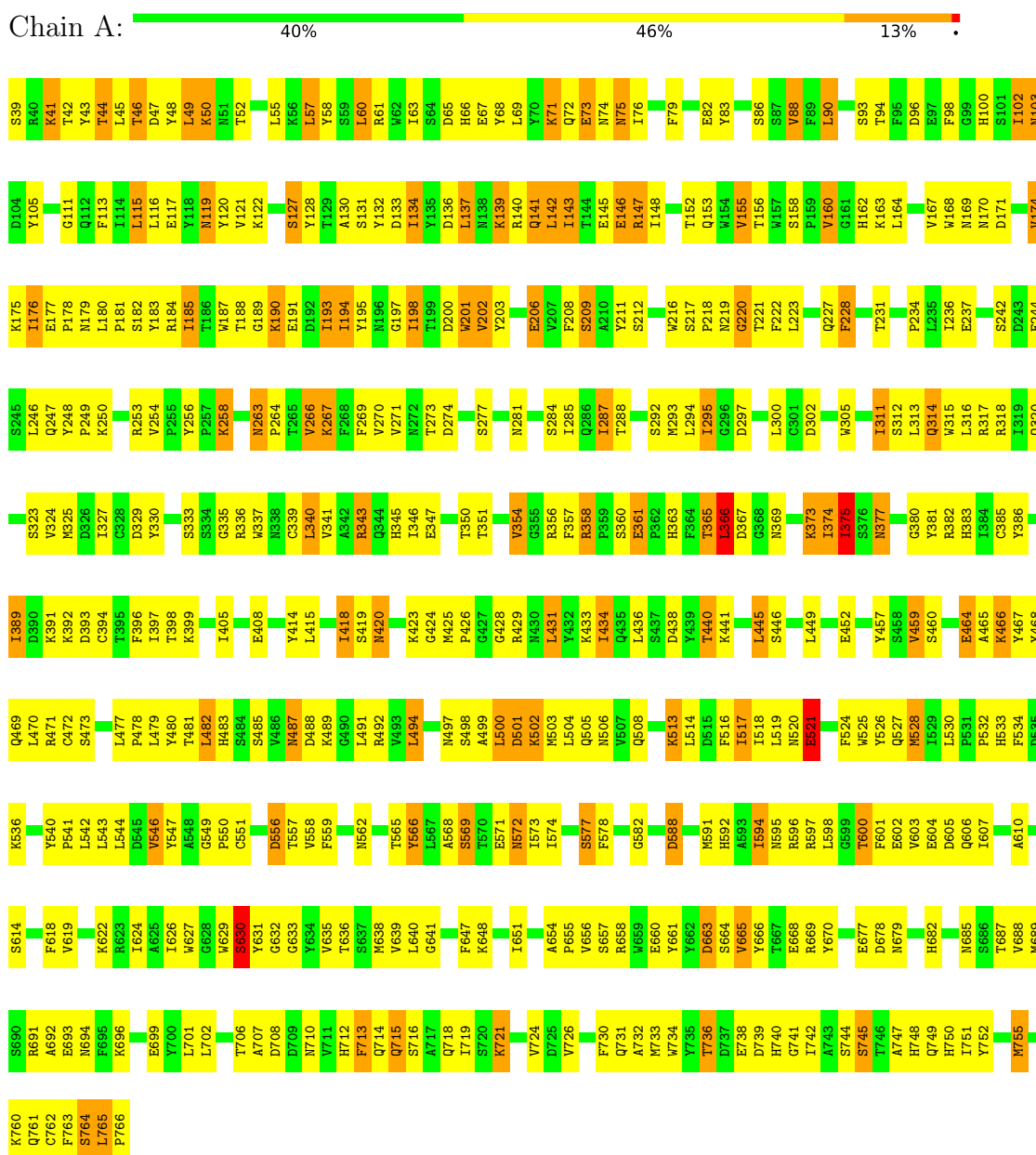
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	161	Total	O	0	0
			161	161		
4	B	159	Total	O	0	0
			159	159		

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: DIPEPTIDYL PEPTIDASE 4



● Molecule 1: DIPEPTIDYL PEPTIDASE 4

Chain B: 

S89	R40	K41	T42	Y43	I114	T44	L45	T46	D47	Y48	L49	K50	M51	L55	K56	L57	L60	R61	M62	H66	E67	Y68	K71	N75	I76	L77	V78	F79	N80	Y83	G84	N86	S86	S87	V88	F89	L90	F91	N92	S93	T94	D96	E97	S101	I102	N103	Y104	Y105	S106	I107	S108	P109						
D110	G111	Q112	F113	I114	L115	L116	Y120	Y121	K122	L123	M124	R125	H126	S127	Y128	Y129	Y132	D133	I134	Y135	D136	L137	N138	K139	R140	Q141	L142	I143	T144	E145	E146	T152	Q153	M154	V155	T156	W157	S158	P159	V160	G161	H162	K163	Y166	V167	M168	N169	I172	Y173	V174	E177	P178	N179					
L180	P181	S182	Y183	R184	L185	T186	W187	T188	K189	G190	L191	I193	N196	G197	I198	T199	D200	W201	V202	Y203	E204	D205	E206	V207	F208	S209	A210	Y211	L214	S217	N218	G219	T221	F222	L223	A224	Y225	A226	Q227	F228	N229	D230	E232	Y233	P234	W305	L236	E237	T307	Q308	E309	R310	I311	S312	D243			
E244	S245	L246	Q247	Y248	P249	K250	R253	T188	V254	K258	M263	P264	T265	V266	K267	F268	F269	V270	V271	N272	T273	S278	V279	T280	N281	A282	T283	S284	L285	Q286	I287	T288	G290	A269	S292	M293	L294	I295	G296	D297	H298	Y299	C301	T301	V303	T304	W305	A306	T307	Q308	E309	R310	I311	S312	C385			
W315	L316	R317	R318	I319	Q320	N321	D393	Y322	S323	M325	D326	I327	C328	D331	S333	K334	G335	R336	C339	L340	V341	A342	R343	Q344	E347	M348	S349	T350	T351	G352	W353	V354	S360	E361	P362	H363	F364	T365	L366	S370	F371	Y372	K373	I374	L375	S376	S377	C378	Y381	R382	C385							
Y386	F387	Q388	I389	S460	F461	K391	K392	D393	C394	I397	T398	K399	G400	T401	W402	E403	O407	L410	T411	S412	D413	Y414	L415	Y416	Y417	I418	S419	M420	E421	Y422	K423	R429	N430	L431	K433	I434	Q435	L436	S437	D438	Y439	T440	K441	V442	T443	C444	L445	S446	C447	N520	E521	E448	L449	M450	R453			
Y457	S458	Y459	L530	F461	S462	K463	E464	A465	K466	Y467	K538	Q469	L470	R471	C472	S473	O474	L479	Y480	T481	L482	H483	S484	S485	V486	M487	D488	K489	R492	A499	L500	M503	L504	Q505	V507	Q508	M509	P510	S511	K512	K513	L514	D515	F516	I517	L518	L519	N520	E521	E522	K523	F524	W525	Y526				
Q527	M528	I529	L530	F531	P532	H533	F534	D535	K536	S537	K538	K539	Y540	P541	L542	S543	O544	P545	V546	F618	V619	D620	N621	K622	L624	A625	T626	V627	G628	M629	S630	F631	G632	G633	Y634	V635	L636	S637	M638	V639	L640	G641	V646	F647	K648	V653	A654	P655	V656	V659	W728	E660	Y661	V662	D663	S664	V665	R596
R597	L598	E599	T600	F601	E602	V603	Q606	L607	E608	A609	A610	R611	Q612	F613	S614	K615	F618	V619	D620	N621	K622	L624	A625	T626	V627	G628	M629	S630	F631	G632	G633	Y634	V635	L636	S637	M638	V639	L640	G641	V646	F647	K648	V653	A654	P655	V656	V659	W728	E660	Y661	V662	D663	S664	V665	R596			
Y666	T667	E668	R669	L673	R674	T675	P676	E677	D678	N679	L680	D681	H682	Y683	R684	N685	S686	M689	S690	R691	A692	F695	K696	Y700	L701	L702	I703	H704	G705	D708	D709	N710	W711	H712	Q715	S716	A717	Q718	I719	S720	L723	V724	Y726	G727	Y728	D729	F730	G731	A732	M733								
T736	D737	E738	D739	H740	G741	L742	A743	S744	T746	A747	H748	Q749	H750	I751	Y752	T753	H754	H755	I759	K760	Q761	G762	F763	S764	P766																																	

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.49Å 66.77Å 425.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.66	Depositor
% Data completeness (in resolution range)	96.6 (20.00-2.66)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.258 , 0.329	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	12414	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

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: FPB, NAG

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	0.77	2/6135 (0.0%)	1.09	20/8344 (0.2%)
1	B	0.75	1/6135 (0.0%)	1.08	17/8344 (0.2%)
All	All	0.76	3/12270 (0.0%)	1.09	37/16688 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	348	MET	SD-CE	6.13	1.94	1.79
1	A	365	THR	CA-CB	5.32	1.61	1.53
1	A	425	MET	SD-CE	5.28	1.92	1.79

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	546	VAL	CB-CA-C	-8.34	99.27	111.19
1	B	407	ILE	N-CA-C	-7.79	96.16	108.86
1	B	459	VAL	N-CA-C	7.55	119.82	108.80
1	A	521	GLU	N-CA-C	-6.97	103.45	113.21
1	A	610	ALA	N-CA-C	-6.67	103.94	111.14
1	B	202	VAL	CB-CA-C	-6.44	103.60	112.04
1	B	472	CYS	N-CA-C	-6.36	102.59	110.41
1	A	139	LYS	N-CA-C	-6.27	101.40	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	96	ASP	N-CA-C	-6.21	105.73	113.55
1	B	683	TYR	N-CA-C	-6.03	104.39	110.97
1	B	466	LYS	N-CA-C	-6.01	104.81	111.36
1	B	299	TYR	N-CA-C	5.95	118.45	109.23
1	A	689	MET	N-CA-C	5.93	118.50	111.33
1	B	460	SER	N-CA-C	5.90	117.76	107.49
1	A	568	ALA	N-CA-C	5.89	117.57	111.03
1	A	220	GLY	N-CA-C	-5.83	107.03	114.37
1	A	274	ASP	N-CA-C	-5.66	106.59	112.93
1	B	254	VAL	N-CA-C	5.66	114.35	107.61
1	B	207	VAL	N-CA-C	5.64	116.78	111.48
1	B	458	SER	N-CA-C	-5.59	101.06	109.95
1	A	141	GLN	N-CA-C	5.53	117.47	109.07
1	A	201	TRP	N-CA-C	5.50	118.20	111.82
1	B	530	LEU	CA-C-N	5.49	123.67	119.66
1	B	530	LEU	C-N-CA	5.49	123.67	119.66
1	A	209	SER	N-CA-C	-5.43	99.22	110.80
1	A	459	VAL	N-CA-C	5.35	116.61	108.80
1	A	588	ASP	N-CA-C	5.34	119.06	112.54
1	B	542	LEU	N-CA-C	5.30	117.25	108.13
1	A	127	SER	N-CA-C	5.30	117.36	110.53
1	A	425	MET	CA-C-N	5.27	124.78	119.19
1	A	425	MET	C-N-CA	5.27	124.78	119.19
1	B	531	PRO	O-C-N	5.17	123.69	121.31
1	A	162	HIS	N-CA-C	5.16	117.06	110.61
1	A	375	ILE	N-CA-C	-5.13	100.50	108.81
1	B	207	VAL	CB-CA-C	-5.11	107.36	111.71
1	A	556	ASP	N-CA-C	5.06	114.83	108.45
1	A	707	ALA	N-CA-C	5.01	119.37	113.16

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	491	LEU	Peptide

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	5963	0	5681	489	0
1	B	5963	0	5681	532	0
2	A	56	0	52	1	0
2	B	56	0	52	2	0
3	A	28	0	26	3	0
3	B	28	0	26	4	0
4	A	161	0	0	29	0
4	B	159	0	0	41	0
All	All	12414	0	11518	1016	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 43.

All (1016) 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:136:ASP:OD2	1:B:139:LYS:HD2	1.35	1.26
1:A:75:ASN:N	1:A:75:ASN:HD22	1.27	1.23
1:B:594:ILE:CD1	1:B:601:PHE:HB2	1.67	1.23
1:B:600:THR:CG2	1:B:601:PHE:H	1.54	1.20
1:A:682:HIS:ND1	1:A:685:ASN:HB3	1.57	1.19
1:A:597:ARG:O	1:A:600:THR:HG23	1.01	1.19
1:A:316:LEU:CD2	1:A:320:GLN:HG2	1.72	1.18
1:A:597:ARG:HB3	1:A:600:THR:HG21	1.26	1.18
1:A:316:LEU:HD21	1:A:320:GLN:CG	1.76	1.16
1:A:597:ARG:O	1:A:600:THR:CG2	1.92	1.16
1:A:340:LEU:N	1:A:340:LEU:CD1	2.09	1.14
1:B:429:ARG:HH11	1:B:429:ARG:CG	1.59	1.14
1:B:177:GLU:HB2	1:B:180:LEU:HD22	1.24	1.14
1:B:614:SER:HA	1:B:619:VAL:CG2	1.78	1.13
1:B:429:ARG:HH11	1:B:429:ARG:HG2	0.97	1.10
1:B:306:ALA:HB3	1:B:310:ARG:HG2	1.23	1.09
1:A:327:ILE:HD13	1:A:389:ILE:HD12	1.29	1.08
1:A:302:ASP:HB3	1:A:314:GLN:HG3	1.36	1.06
1:B:560:ARG:HG3	1:B:560:ARG:HH11	1.20	1.06
1:B:600:THR:HG23	1:B:601:PHE:H	0.93	1.06
1:A:340:LEU:HD13	1:A:340:LEU:H	1.18	1.06
1:A:751:ILE:HG12	1:A:755:MET:CE	1.86	1.06
1:B:600:THR:HG23	1:B:601:PHE:N	1.61	1.06
1:B:361:GLU:OE2	4:B:2072:HOH:O	1.72	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:507:VAL:CG1	1:B:509:MET:HG2	1.86	1.05
1:A:297:ASP:HB3	4:A:2066:HOH:O	1.57	1.05
1:B:306:ALA:CB	1:B:310:ARG:HG2	1.88	1.04
1:B:236:ILE:CD1	1:B:236:ILE:O	2.04	1.03
1:A:601:PHE:HD1	1:A:604:GLU:OE1	1.41	1.03
1:B:43:TYR:CD2	1:B:565:THR:HG22	1.93	1.03
1:A:343:ARG:HG3	1:A:343:ARG:HH11	1.23	1.02
1:A:340:LEU:N	1:A:340:LEU:HD12	1.73	1.02
1:A:751:ILE:HG12	1:A:755:MET:HE1	1.39	1.02
1:B:596:ARG:O	1:B:597:ARG:HG3	1.58	1.02
1:A:316:LEU:HD21	1:A:320:GLN:HG2	1.02	1.01
1:B:614:SER:HA	1:B:619:VAL:HG21	1.40	1.00
1:A:327:ILE:HD13	1:A:389:ILE:CD1	1.91	0.99
1:B:594:ILE:HD11	1:B:601:PHE:HB2	1.41	0.99
1:B:738:GLU:OE2	1:B:744:SER:HB3	1.61	0.99
1:B:308:GLN:HA	1:B:308:GLN:OE1	1.63	0.99
1:A:75:ASN:N	1:A:75:ASN:ND2	2.03	0.99
1:B:429:ARG:HG2	1:B:429:ARG:NH1	1.72	0.99
1:B:84:GLY:N	1:B:492:ARG:NH2	2.11	0.98
1:B:747:ALA:O	1:B:751:ILE:HG22	1.64	0.97
1:B:83:TYR:C	1:B:492:ARG:NH2	2.23	0.97
1:B:720:SER:HA	1:B:723:LEU:HD12	1.47	0.96
1:B:332:GLU:HG2	1:B:333:SER:N	1.78	0.96
1:A:724:VAL:HG22	1:B:750:HIS:ND1	1.81	0.96
1:B:278:SER:HB3	4:B:2061:HOH:O	1.64	0.96
1:A:499:ALA:O	1:A:502:LYS:HE2	1.66	0.96
1:B:144:THR:HG23	1:B:144:THR:O	1.65	0.96
1:B:486:VAL:HG12	1:B:487:ASN:N	1.81	0.96
1:B:236:ILE:O	1:B:236:ILE:HD12	1.67	0.95
1:A:514:LEU:HD12	1:A:557:THR:HG22	1.49	0.94
1:A:142:LEU:HD12	1:A:142:LEU:H	1.32	0.94
1:A:682:HIS:ND1	1:A:685:ASN:CB	2.31	0.94
1:B:312:SER:HB2	1:B:325:MET:HE3	1.48	0.94
1:B:373:LYS:HD3	1:B:375:ILE:HD11	1.47	0.94
1:B:453:ARG:HD3	1:B:479:LEU:CD1	1.98	0.94
1:B:163:LYS:CE	1:B:273:THR:HG21	1.97	0.93
1:A:682:HIS:CE1	1:A:685:ASN:HB3	2.04	0.93
1:B:377:ASN:HD21	1:B:381:TYR:H	1.13	0.93
1:B:630:SER:HG	1:B:740:HIS:HE2	1.16	0.92
1:B:562:ASN:O	1:B:565:THR:HB	1.69	0.92
1:B:341:VAL:O	1:B:344:GLN:HG3	1.71	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:LYS:HD3	1:B:193:ILE:HD12	1.51	0.91
1:B:236:ILE:O	1:B:236:ILE:HD13	1.69	0.90
1:B:746:THR:HA	1:B:749:GLN:HE21	1.38	0.89
1:B:177:GLU:CB	1:B:180:LEU:HD22	2.03	0.89
1:A:528:MET:HE1	1:A:618:PHE:HE1	1.34	0.88
1:A:626:ILE:HG12	1:A:636:THR:HG23	1.52	0.88
1:B:507:VAL:HG12	1:B:509:MET:HG2	1.56	0.88
1:A:565:THR:HG22	1:A:565:THR:O	1.74	0.87
1:B:512:LYS:HD3	4:B:2117:HOH:O	1.71	0.87
1:A:318:ARG:HD2	4:A:2066:HOH:O	1.75	0.87
1:A:340:LEU:CD1	1:A:340:LEU:H	1.78	0.86
1:B:320:GLN:NE2	1:B:669:ARG:HB2	1.90	0.86
1:A:651:ILE:HD13	1:A:755:MET:HG2	1.57	0.85
1:A:734:TRP:CD1	1:A:736:THR:HG22	2.12	0.85
1:A:726:VAL:O	1:A:726:VAL:HG22	1.77	0.85
1:B:466:LYS:HD2	4:B:2099:HOH:O	1.77	0.85
1:A:75:ASN:HD22	1:A:75:ASN:H	1.18	0.84
1:B:109:PRO:HD2	1:B:161:GLY:O	1.77	0.84
1:A:327:ILE:CD1	1:A:389:ILE:CD1	2.56	0.84
1:B:156:THR:HG21	4:B:2019:HOH:O	1.77	0.84
1:B:267:LYS:HB2	1:B:269:PHE:CE2	2.12	0.84
1:A:519:LEU:HD12	1:A:524:PHE:CD2	2.12	0.84
1:A:738:GLU:HG3	1:A:742:ILE:HG23	1.58	0.84
1:B:163:LYS:HE2	1:B:273:THR:HG21	1.58	0.83
1:A:360:SER:HB2	4:A:2078:HOH:O	1.78	0.83
1:B:594:ILE:HD12	1:B:601:PHE:HB2	1.57	0.83
1:B:453:ARG:NE	1:B:479:LEU:HD12	1.93	0.83
1:A:60:LEU:CD1	1:A:469:GLN:OE1	2.26	0.82
1:A:415:LEU:HD22	1:A:434:ILE:HD11	1.60	0.82
1:A:597:ARG:HB3	1:A:600:THR:CG2	2.07	0.82
1:B:453:ARG:CD	1:B:479:LEU:HD12	2.09	0.82
1:B:560:ARG:HG3	1:B:560:ARG:NH1	1.93	0.82
1:B:453:ARG:HD3	1:B:479:LEU:HD12	1.61	0.82
1:B:236:ILE:CD1	1:B:236:ILE:C	2.51	0.82
1:B:136:ASP:OD2	1:B:139:LYS:CD	2.24	0.81
1:A:145:GLU:HG2	4:A:2032:HOH:O	1.79	0.81
1:B:377:ASN:ND2	1:B:381:TYR:H	1.79	0.81
1:A:136:ASP:O	1:A:139:LYS:O	1.99	0.81
1:A:601:PHE:CD1	1:A:604:GLU:OE1	2.32	0.81
1:A:343:ARG:HD2	1:A:389:ILE:HG23	1.62	0.81
1:B:62:TRP:CE3	1:B:462:SER:HB3	2.16	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:ASP:OD1	1:A:558:VAL:HG23	1.79	0.80
1:A:193:ILE:O	1:A:194:ILE:HD13	1.81	0.80
1:B:677:GLU:CD	1:B:677:GLU:H	1.86	0.80
1:B:364:PHE:CE2	1:B:371:PHE:HD1	2.00	0.80
1:B:466:LYS:O	1:B:485:SER:HB2	1.82	0.80
1:B:470:LEU:HD12	1:B:483:HIS:CE1	2.18	0.79
1:A:142:LEU:H	1:A:142:LEU:CD1	1.94	0.79
1:A:712:HIS:O	1:A:714:GLN:N	2.15	0.79
1:A:482:LEU:HB2	1:A:494:LEU:HD21	1.65	0.79
1:A:500:LEU:HA	1:A:503:MET:HE3	1.64	0.79
1:A:528:MET:HE1	1:A:618:PHE:CE1	2.17	0.79
1:A:571:GLU:OE1	1:A:765:LEU:CD1	2.30	0.79
1:B:361:GLU:CD	4:B:2072:HOH:O	2.18	0.79
1:A:130:ALA:HB3	1:A:132:TYR:CE2	2.17	0.79
1:B:317:ARG:HG3	1:B:322:TYR:HB3	1.63	0.79
1:A:651:ILE:HD13	1:A:755:MET:CG	2.13	0.78
1:A:721:LYS:HG3	4:B:2152:HOH:O	1.82	0.78
1:B:595:ASN:O	1:B:597:ARG:NE	2.17	0.78
1:A:664:SER:HB2	1:A:668:GLU:OE2	1.84	0.78
1:A:603:VAL:HG13	1:A:639:VAL:CG2	2.13	0.78
1:A:271:VAL:CG2	1:A:284:SER:OG	2.33	0.77
1:A:603:VAL:HG13	1:A:639:VAL:HG23	1.65	0.77
1:B:163:LYS:HE3	1:B:273:THR:HG21	1.63	0.77
1:B:459:VAL:HG22	1:B:460:SER:H	1.50	0.77
1:A:158:SER:HB3	1:A:163:LYS:HB2	1.67	0.77
1:A:163:LYS:HZ3	1:A:273:THR:HG22	1.50	0.76
1:A:415:LEU:HB3	1:A:434:ILE:CD1	2.15	0.76
1:A:751:ILE:HG12	1:A:755:MET:HE2	1.67	0.76
1:B:567:LEU:O	1:B:573:ILE:HB	1.84	0.76
1:A:208:PHE:O	1:A:209:SER:C	2.28	0.76
1:B:474:GLY:HA3	1:B:558:VAL:HA	1.67	0.76
1:B:600:THR:CG2	1:B:601:PHE:N	2.26	0.76
1:A:43:TYR:CD2	1:A:565:THR:HG22	2.20	0.76
1:B:84:GLY:CA	1:B:492:ARG:NH2	2.48	0.76
1:A:316:LEU:HD23	1:A:317:ARG:O	1.86	0.76
1:A:142:LEU:HD12	1:A:142:LEU:N	2.01	0.75
1:B:420:ASN:HD22	1:B:420:ASN:H	1.34	0.75
1:A:489:LYS:HD3	4:A:2105:HOH:O	1.85	0.75
1:B:392:LYS:HD3	1:B:393:ASP:CG	2.12	0.75
1:B:83:TYR:C	1:B:492:ARG:HH21	1.93	0.75
1:B:429:ARG:CG	1:B:429:ARG:NH1	2.33	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASN:ND2	1:A:75:ASN:H	1.77	0.75
1:A:514:LEU:HD12	1:A:557:THR:CG2	2.17	0.75
1:A:60:LEU:HD11	1:A:469:GLN:OE1	1.85	0.74
1:A:164:LEU:HB2	1:A:175:LYS:HB3	1.69	0.74
1:B:486:VAL:CG1	1:B:487:ASN:N	2.49	0.74
1:A:177:GLU:HB2	1:A:180:LEU:HG	1.67	0.74
1:A:98:PHE:CE2	1:A:100:HIS:HB2	2.22	0.74
1:B:144:THR:O	1:B:144:THR:CG2	2.34	0.74
1:B:614:SER:CA	1:B:619:VAL:HG21	2.17	0.74
1:A:74:ASN:C	1:A:75:ASN:HD22	1.94	0.74
1:A:571:GLU:OE1	1:A:765:LEU:HD12	1.87	0.74
1:B:236:ILE:HD13	1:B:236:ILE:C	2.11	0.74
1:B:289:ALA:HB2	1:B:315:TRP:CH2	2.22	0.74
1:B:614:SER:HA	1:B:619:VAL:HG23	1.67	0.74
1:A:382:ARG:HH21	1:A:591:MET:CE	2.01	0.74
1:B:163:LYS:HE3	1:B:273:THR:CG2	2.16	0.74
1:B:486:VAL:HG12	1:B:487:ASN:H	1.49	0.74
1:A:519:LEU:HD12	1:A:524:PHE:CE2	2.23	0.74
1:A:682:HIS:HB2	4:A:2135:HOH:O	1.87	0.74
3:B:1771:FPB:C24	4:B:2131:HOH:O	2.34	0.74
1:A:119:ASN:HD22	1:A:131:SER:CB	2.01	0.73
1:B:614:SER:CA	1:B:619:VAL:CG2	2.64	0.73
1:A:90:LEU:HD11	1:A:94:THR:CB	2.18	0.73
1:A:565:THR:O	1:A:565:THR:CG2	2.35	0.73
1:B:373:LYS:HB3	1:B:375:ILE:CD1	2.19	0.73
1:B:603:VAL:HG13	1:B:639:VAL:HG23	1.71	0.72
1:B:402:TRP:CD1	1:B:421:GLU:HG3	2.23	0.72
1:A:45:LEU:HB2	1:A:566:TYR:CE1	2.23	0.72
1:B:310:ARG:HD3	1:B:327:ILE:CG2	2.19	0.72
1:B:371:PHE:HE2	1:B:387:PHE:CD1	2.08	0.72
1:A:446:SER:HA	1:A:449:LEU:HD12	1.69	0.72
1:B:43:TYR:CD2	1:B:565:THR:CG2	2.71	0.72
1:A:312:SER:OG	1:A:325:MET:HE3	1.88	0.72
1:A:739:ASP:HB2	4:A:2152:HOH:O	1.88	0.72
1:A:295:ILE:HG23	4:A:2070:HOH:O	1.89	0.72
1:A:459:VAL:HG22	1:A:460:SER:N	2.05	0.72
1:A:600:THR:OG1	1:A:601:PHE:N	2.21	0.72
1:A:597:ARG:C	1:A:600:THR:HG23	2.09	0.71
1:B:371:PHE:CE2	1:B:387:PHE:CD1	2.77	0.71
1:A:316:LEU:HD21	1:A:320:GLN:CB	2.20	0.71
1:A:167:VAL:HG11	1:A:198:ILE:HG12	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:ASN:OD1	1:B:227:GLN:HG3	1.90	0.71
1:B:163:LYS:CE	1:B:273:THR:CG2	2.68	0.71
1:A:571:GLU:OE1	1:A:760:LYS:HD3	1.90	0.71
1:A:542:LEU:HD12	1:A:619:VAL:HG22	1.72	0.71
1:A:377:ASN:HD21	1:A:381:TYR:H	1.37	0.71
1:A:184:ARG:HD3	1:A:187:TRP:CE2	2.26	0.71
1:A:206:GLU:OE1	1:A:206:GLU:HA	1.91	0.70
1:B:364:PHE:CD2	1:B:371:PHE:HB3	2.25	0.70
1:A:115:LEU:CD2	1:A:132:TYR:HD1	2.04	0.70
1:A:237:GLU:HG3	1:A:253:ARG:HG2	1.72	0.70
1:A:82:GLU:HG3	1:A:82:GLU:O	1.91	0.70
1:A:145:GLU:C	1:A:146:GLU:HG2	2.17	0.70
1:A:200:ASP:OD1	1:A:200:ASP:C	2.34	0.70
1:B:289:ALA:HB2	1:B:315:TRP:CZ3	2.26	0.70
1:A:228:PHE:N	1:A:228:PHE:CD2	2.58	0.70
1:A:297:ASP:CB	4:A:2066:HOH:O	2.26	0.70
1:A:343:ARG:HG3	1:A:343:ARG:NH1	1.97	0.70
1:A:377:ASN:ND2	1:A:381:TYR:H	1.89	0.70
1:A:502:LYS:HE3	1:A:503:MET:HG3	1.74	0.70
1:A:446:SER:HB2	1:A:457:TYR:CE2	2.27	0.69
1:B:306:ALA:HB3	1:B:310:ARG:CG	2.12	0.69
1:B:507:VAL:CG1	1:B:509:MET:CG	2.68	0.69
1:B:386:TYR:HB2	1:B:397:ILE:HD11	1.75	0.69
1:B:621:ASN:HA	1:B:624:ILE:HD11	1.73	0.69
1:A:508:GLN:O	1:A:569:SER:HB2	1.93	0.69
1:B:94:THR:O	1:B:95:PHE:HB2	1.92	0.69
1:B:397:ILE:N	1:B:397:ILE:HD12	2.08	0.69
1:B:613:PHE:O	1:B:619:VAL:HG21	1.93	0.69
1:B:507:VAL:HG11	1:B:509:MET:SD	2.33	0.68
1:A:327:ILE:CD1	1:A:343:ARG:HB3	2.24	0.68
1:A:692:ALA:CB	1:A:726:VAL:HG11	2.24	0.68
1:A:365:THR:HB	4:A:2081:HOH:O	1.93	0.68
1:A:760:LYS:HE3	4:A:2155:HOH:O	1.91	0.68
1:B:103:ASN:HD22	1:B:120:TYR:HB2	1.57	0.68
1:A:60:LEU:HD13	1:A:469:GLN:OE1	1.93	0.68
1:A:68:TYR:CE1	1:A:79:PHE:CD1	2.82	0.68
1:A:44:THR:HB	1:A:47:ASP:OD2	1.93	0.67
1:B:663:ASP:OD1	1:B:663:ASP:O	2.12	0.67
1:A:44:THR:O	1:A:47:ASP:HB2	1.94	0.67
1:A:500:LEU:HD22	1:A:504:LEU:HG	1.77	0.67
1:A:360:SER:OG	1:A:373:LYS:HG3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:HIS:HA	1:A:685:ASN:HB2	1.77	0.67
1:B:512:LYS:CD	4:B:2117:HOH:O	2.37	0.67
1:A:68:TYR:CE1	1:A:79:PHE:HB2	2.30	0.67
1:A:651:ILE:CD1	1:A:755:MET:HG2	2.25	0.67
1:A:732:ALA:HB3	1:B:733:MET:HG2	1.77	0.67
1:A:415:LEU:O	1:A:434:ILE:HG13	1.95	0.66
1:A:119:ASN:ND2	1:A:131:SER:HB2	2.09	0.66
1:B:538:LYS:HG2	4:B:2113:HOH:O	1.95	0.66
1:A:44:THR:HG22	1:A:47:ASP:H	1.59	0.66
1:A:751:ILE:O	1:A:755:MET:HE2	1.95	0.66
1:A:763:PHE:O	1:A:765:LEU:N	2.28	0.66
1:B:382:ARG:HG2	1:B:382:ARG:HH11	1.61	0.66
1:A:692:ALA:HB1	1:A:726:VAL:CG1	2.26	0.66
1:B:177:GLU:C	4:B:2038:HOH:O	2.38	0.66
1:B:178:PRO:N	4:B:2038:HOH:O	2.27	0.66
1:B:746:THR:HA	1:B:749:GLN:NE2	2.09	0.66
1:A:236:ILE:HG12	1:A:712:HIS:CE1	2.31	0.66
1:A:65:ASP:HB2	1:A:466:LYS:HG3	1.78	0.66
1:B:453:ARG:CD	1:B:479:LEU:CD1	2.70	0.66
1:A:726:VAL:O	1:A:726:VAL:CG2	2.44	0.65
1:A:656:VAL:HG12	1:A:657:SER:H	1.62	0.65
1:A:626:ILE:HB	1:A:647:PHE:CE2	2.31	0.65
1:B:402:TRP:CE3	1:B:402:TRP:O	2.50	0.65
1:A:656:VAL:HG13	1:A:715:GLN:HE22	1.61	0.65
1:B:293:MET:HG3	1:B:315:TRP:CB	2.26	0.65
1:B:311:ILE:HD12	1:B:328:CYS:HB2	1.79	0.65
1:B:534:PHE:HZ	1:B:618:PHE:CD1	2.14	0.65
1:B:371:PHE:CE2	1:B:387:PHE:HB2	2.31	0.65
1:A:168:TRP:CD2	1:A:169:ASN:OD1	2.50	0.65
1:B:267:LYS:HB2	1:B:269:PHE:HE2	1.59	0.65
1:B:373:LYS:HD3	1:B:375:ILE:CD1	2.24	0.65
1:B:206:GLU:CD	1:B:666:TYR:HB2	2.22	0.64
1:A:712:HIS:O	1:A:713:PHE:C	2.39	0.64
1:B:45:LEU:HG	1:B:49:LEU:CD2	2.28	0.64
1:B:364:PHE:CE2	1:B:371:PHE:CD1	2.84	0.64
1:B:690:SER:HA	4:B:2139:HOH:O	1.98	0.64
1:A:132:TYR:CE1	1:A:155:VAL:HG21	2.32	0.64
1:A:46:THR:HG22	1:A:50:LYS:HG2	1.80	0.64
1:A:459:VAL:CG2	1:A:460:SER:N	2.61	0.64
1:A:656:VAL:HG12	1:A:657:SER:N	2.13	0.64
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:VAL:HA	1:B:344:GLN:NE2	2.13	0.63
1:B:305:TRP:CD2	1:B:311:ILE:HG23	2.33	0.63
1:A:258:LYS:NZ	1:A:712:HIS:ND1	2.45	0.63
1:A:327:ILE:HD12	1:A:343:ARG:O	1.98	0.63
1:A:693:GLU:CD	1:A:726:VAL:HG21	2.23	0.63
1:B:153:GLN:HB2	1:B:167:VAL:HG12	1.79	0.63
1:B:663:ASP:OD1	1:B:663:ASP:C	2.40	0.63
1:B:219:ASN:HB2	1:B:308:GLN:OE1	1.97	0.63
1:A:237:GLU:CG	1:A:253:ARG:HG2	2.28	0.63
1:B:504:LEU:HD13	1:B:509:MET:HE2	1.79	0.63
1:B:676:PRO:HD3	1:B:680:LEU:HD12	1.80	0.63
1:A:466:LYS:HB2	1:A:467:TYR:CD2	2.34	0.63
1:B:125:ARG:HA	4:B:2025:HOH:O	1.98	0.63
1:B:295:ILE:HD13	1:B:295:ILE:O	1.98	0.63
1:A:377:ASN:C	1:A:377:ASN:HD22	2.07	0.63
1:A:594:ILE:HG23	1:A:598:LEU:HD23	1.81	0.62
1:A:571:GLU:O	1:A:572:ASN:C	2.42	0.62
1:A:603:VAL:CG1	1:A:639:VAL:HG22	2.30	0.62
1:B:43:TYR:CE2	1:B:565:THR:CG2	2.82	0.62
1:B:83:TYR:C	1:B:492:ARG:HH22	2.04	0.62
1:A:60:LEU:CD1	1:A:469:GLN:CD	2.73	0.62
1:A:115:LEU:HD21	1:A:132:TYR:HD1	1.64	0.62
1:A:693:GLU:HG2	1:A:726:VAL:HG21	1.82	0.62
1:A:591:MET:O	1:A:591:MET:HG2	1.98	0.62
1:A:340:LEU:N	1:A:340:LEU:HD13	1.84	0.62
1:B:109:PRO:HG2	1:B:158:SER:O	1.99	0.62
1:B:308:GLN:OE1	1:B:308:GLN:CA	2.44	0.62
1:B:512:LYS:HE3	1:B:527:GLN:OE1	1.99	0.62
1:B:302:ASP:OD1	1:B:303:VAL:N	2.33	0.62
1:B:624:ILE:HG22	1:B:647:PHE:CD2	2.35	0.62
1:A:201:TRP:O	1:A:201:TRP:CE3	2.53	0.61
1:B:518:ILE:O	1:B:519:LEU:HD12	1.99	0.61
1:A:365:THR:O	1:A:366:LEU:C	2.42	0.61
1:B:105:TYR:HB2	1:B:114:ILE:HD11	1.82	0.61
1:B:629:TRP:O	1:B:630:SER:C	2.43	0.61
1:B:125:ARG:HG2	1:B:126:HIS:CE1	2.36	0.61
1:B:520:ASN:O	1:B:521:GLU:CB	2.48	0.61
1:B:94:THR:O	1:B:95:PHE:CB	2.49	0.61
1:B:500:LEU:HD22	1:B:500:LEU:O	2.00	0.61
1:A:513:LYS:O	1:A:527:GLN:HA	2.00	0.61
1:B:742:ILE:O	1:B:742:ILE:HG22	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.36	0.61
1:B:306:ALA:C	1:B:307:THR:CG2	2.74	0.61
1:A:68:TYR:HE1	1:A:79:PHE:CD1	2.18	0.60
1:A:271:VAL:HG22	1:A:284:SER:HA	1.83	0.60
1:A:499:ALA:O	1:A:500:LEU:C	2.42	0.60
1:A:639:VAL:O	1:A:639:VAL:HG12	1.99	0.60
1:B:624:ILE:HG22	1:B:647:PHE:HD2	1.66	0.60
1:A:382:ARG:HH21	1:A:591:MET:HE2	1.66	0.60
1:B:184:ARG:HD3	1:B:187:TRP:CD2	2.35	0.60
1:B:320:GLN:HE22	1:B:669:ARG:HB2	1.64	0.60
1:A:163:LYS:NZ	1:A:273:THR:HG22	2.16	0.60
1:B:278:SER:CB	4:B:2061:HOH:O	2.36	0.60
1:A:692:ALA:HB3	1:A:726:VAL:HG11	1.83	0.60
1:B:214:LEU:HD12	1:B:225:TYR:HB3	1.82	0.60
1:B:633:GLY:HA3	1:B:655:PRO:HB3	1.82	0.60
1:B:634:TYR:HB2	1:B:656:VAL:O	2.02	0.60
1:B:62:TRP:CZ3	1:B:462:SER:HB3	2.36	0.60
1:A:431:LEU:O	1:A:445:LEU:HB2	2.02	0.60
1:B:595:ASN:HB3	1:B:597:ARG:HH21	1.66	0.60
1:A:217:SER:O	1:A:220:GLY:N	2.34	0.60
1:B:71:LYS:O	1:B:71:LYS:HG2	2.01	0.60
1:A:217:SER:HB3	1:A:222:PHE:H	1.67	0.60
1:A:267:LYS:HB2	4:A:2055:HOH:O	2.01	0.60
1:A:597:ARG:CB	1:A:600:THR:HG21	2.18	0.60
1:B:203:TYR:OH	1:B:299:TYR:HB3	2.02	0.60
1:B:45:LEU:HG	1:B:49:LEU:HD22	1.84	0.60
1:B:341:VAL:HA	1:B:344:GLN:CD	2.27	0.60
1:A:61:ARG:NH1	1:A:105:TYR:CE1	2.70	0.59
1:A:374:ILE:C	1:A:375:ILE:HD13	2.27	0.59
1:B:206:GLU:OE2	1:B:663:ASP:OD2	2.19	0.59
1:B:472:CYS:HB3	1:B:479:LEU:HB2	1.84	0.59
1:B:629:TRP:HD1	1:B:630:SER:H	1.50	0.59
1:B:708:ASP:O	4:B:2143:HOH:O	2.17	0.59
1:A:201:TRP:CE3	1:A:201:TRP:C	2.80	0.59
1:A:477:LEU:HD22	1:A:500:LEU:HD13	1.84	0.59
1:A:588:ASP:O	1:A:592:HIS:HB2	2.02	0.59
1:B:470:LEU:HD12	1:B:483:HIS:NE2	2.17	0.59
1:B:103:ASN:HD22	1:B:120:TYR:CB	2.16	0.59
1:B:143:ILE:HD12	1:B:145:GLU:O	2.02	0.59
1:A:358:ARG:NH1	4:A:2077:HOH:O	2.21	0.59
1:A:466:LYS:HE3	1:A:466:LYS:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:MET:HG3	1:B:315:TRP:HB2	1.83	0.59
1:B:310:ARG:HD3	1:B:327:ILE:HG23	1.84	0.59
1:B:680:LEU:CD2	1:B:684:ARG:HD2	2.32	0.59
1:B:347:GLU:HB3	1:B:354:VAL:HG11	1.85	0.59
1:B:141:GLN:HB2	4:B:2030:HOH:O	2.01	0.59
1:B:748:HIS:O	1:B:751:ILE:HG23	2.03	0.59
1:A:117:GLU:HG3	1:A:132:TYR:CE1	2.37	0.59
1:A:744:SER:HB3	4:A:2150:HOH:O	2.03	0.59
1:A:167:VAL:HA	1:A:171:ASP:O	2.03	0.58
1:A:248:TYR:HD1	4:A:2063:HOH:O	1.85	0.58
1:B:242:SER:HB3	1:B:246:LEU:HD12	1.84	0.58
1:A:119:ASN:ND2	1:A:131:SER:CB	2.64	0.58
1:B:227:GLN:O	1:B:266:VAL:HA	2.03	0.58
1:B:377:ASN:ND2	1:B:381:TYR:N	2.50	0.58
1:B:629:TRP:O	1:B:632:GLY:N	2.36	0.58
1:A:498:SER:O	1:A:501:ASP:HB3	2.02	0.58
1:B:599:GLY:HA3	1:B:634:TYR:OH	2.03	0.58
1:A:327:ILE:HD13	1:A:343:ARG:HB3	1.85	0.58
1:B:46:THR:HG22	1:B:50:LYS:HD3	1.85	0.58
1:B:543:LEU:CD2	1:B:627:TRP:HD1	2.16	0.58
1:B:84:GLY:N	1:B:492:ARG:HH22	2.00	0.58
1:B:237:GLU:OE2	1:B:253:ARG:HD3	2.03	0.58
1:B:320:GLN:OE1	1:B:669:ARG:HD3	2.03	0.58
1:B:596:ARG:C	1:B:597:ARG:HG3	2.28	0.58
1:A:44:THR:HG22	1:A:47:ASP:N	2.18	0.58
1:A:120:TYR:O	1:A:120:TYR:CD1	2.56	0.58
1:B:431:LEU:HD12	1:B:432:TYR:H	1.68	0.58
1:A:327:ILE:CD1	1:A:389:ILE:HD11	2.34	0.57
1:B:66:HIS:C	1:B:67:GLU:HG3	2.28	0.57
1:B:102:ILE:HG22	1:B:102:ILE:O	2.03	0.57
1:B:507:VAL:HG11	1:B:509:MET:HG2	1.82	0.57
1:A:90:LEU:HD11	1:A:94:THR:OG1	2.04	0.57
1:B:463:LYS:C	1:B:465:ALA:H	2.11	0.57
1:A:102:ILE:HD12	1:A:102:ILE:H	1.69	0.57
1:B:306:ALA:O	1:B:307:THR:HG22	2.04	0.57
1:B:526:TYR:HB2	1:B:577:SER:O	2.03	0.57
1:B:595:ASN:HB3	1:B:597:ARG:NH2	2.19	0.57
1:A:508:GLN:NE2	1:A:533:HIS:HE1	2.02	0.57
1:A:528:MET:HE3	1:A:574:ILE:HG21	1.85	0.57
1:B:200:ASP:OD1	1:B:203:TYR:HB2	2.04	0.57
1:A:382:ARG:NH2	1:A:591:MET:HE1	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1769:NAG:O4	4:B:2159:HOH:O	2.16	0.57
1:A:358:ARG:HD2	4:A:2072:HOH:O	2.05	0.56
1:B:744:SER:OG	1:B:747:ALA:CB	2.52	0.56
1:B:386:TYR:O	1:B:394:CYS:HB2	2.05	0.56
1:B:598:LEU:O	1:B:682:HIS:HE1	1.88	0.56
1:B:621:ASN:O	1:B:624:ILE:CD1	2.52	0.56
1:A:228:PHE:H	1:A:228:PHE:HD2	1.53	0.56
1:A:571:GLU:OE1	1:A:765:LEU:HD13	2.05	0.56
1:B:93:SER:O	1:B:94:THR:C	2.49	0.56
1:B:620:ASP:C	1:B:622:LYS:H	2.13	0.56
1:B:726:VAL:HG22	1:B:726:VAL:O	2.05	0.56
1:A:68:TYR:CE1	1:A:79:PHE:CG	2.93	0.56
1:A:127:SER:HB3	1:A:211:TYR:CG	2.41	0.56
1:B:341:VAL:O	1:B:342:ALA:C	2.47	0.56
1:B:60:LEU:HB2	1:B:68:TYR:CD1	2.41	0.56
1:B:388:GLN:HB3	1:B:391:LYS:HG3	1.88	0.56
1:B:453:ARG:HD3	1:B:479:LEU:HD11	1.84	0.56
1:A:603:VAL:CG1	1:A:639:VAL:CG2	2.84	0.56
1:A:68:TYR:CD1	1:A:68:TYR:C	2.84	0.56
1:A:733:MET:HE1	1:B:730:PHE:O	2.06	0.56
1:B:318:ARG:HE	1:B:668:GLU:CD	2.14	0.56
1:B:410:LEU:HD23	4:B:2075:HOH:O	2.05	0.56
1:A:518:ILE:HG22	1:A:521:GLU:HA	1.88	0.56
1:A:734:TRP:HD1	1:A:736:THR:HG22	1.68	0.56
1:B:166:TYR:CZ	1:B:173:TYR:HB2	2.41	0.56
1:B:641:GLY:O	1:B:691:ARG:HB3	2.05	0.56
1:A:88:VAL:HG23	1:A:88:VAL:O	2.04	0.55
1:A:445:LEU:HD13	1:A:468:TYR:OH	2.06	0.55
1:B:543:LEU:HD21	1:B:627:TRP:HD1	1.71	0.55
1:B:556:ASP:OD1	1:B:558:VAL:HG13	2.06	0.55
1:B:610:ALA:O	1:B:613:PHE:HB2	2.06	0.55
1:B:621:ASN:O	1:B:624:ILE:HD12	2.06	0.55
1:A:120:TYR:CD1	1:A:120:TYR:C	2.83	0.55
1:A:130:ALA:HB3	1:A:132:TYR:HE2	1.67	0.55
1:A:145:GLU:C	1:A:146:GLU:CG	2.78	0.55
1:B:568:ALA:HA	1:B:573:ILE:H	1.69	0.55
1:A:60:LEU:HD11	1:A:469:GLN:CD	2.30	0.55
1:A:127:SER:HB3	1:A:211:TYR:CD1	2.41	0.55
1:A:208:PHE:O	1:A:209:SER:O	2.23	0.55
1:B:519:LEU:O	1:B:520:ASN:C	2.48	0.55
1:B:371:PHE:C	1:B:371:PHE:CD2	2.85	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:VAL:HB	1:A:665:VAL:HG21	1.87	0.55
1:A:445:LEU:CD1	1:A:468:TYR:OH	2.54	0.55
1:A:751:ILE:O	1:A:755:MET:CE	2.54	0.55
1:B:587:GLY:O	4:B:2127:HOH:O	2.17	0.55
1:B:50:LYS:O	1:B:51:ASN:CB	2.54	0.55
1:B:281:ASN:ND2	4:B:2062:HOH:O	2.40	0.55
1:B:371:PHE:CE2	1:B:387:PHE:CG	2.95	0.55
1:A:751:ILE:HG23	1:A:752:TYR:H	1.71	0.55
1:B:677:GLU:CD	1:B:677:GLU:N	2.63	0.55
1:A:88:VAL:O	1:A:88:VAL:CG2	2.54	0.55
1:A:716:SER:O	1:A:719:ILE:HB	2.06	0.55
1:B:586:GLN:C	4:B:2127:HOH:O	2.50	0.55
1:A:66:HIS:C	1:A:67:GLU:HG3	2.31	0.55
1:A:614:SER:HB3	1:A:624:ILE:CD1	2.36	0.55
1:A:712:HIS:C	1:A:714:GLN:N	2.63	0.55
1:B:177:GLU:CG	1:B:180:LEU:HD22	2.37	0.55
1:B:529:ILE:N	1:B:529:ILE:HD12	2.21	0.55
1:A:43:TYR:CD2	1:A:565:THR:CG2	2.89	0.54
1:B:594:ILE:HD11	1:B:601:PHE:CB	2.27	0.54
1:B:417:TYR:CE1	1:B:434:ILE:HD11	2.41	0.54
1:B:719:ILE:O	1:B:723:LEU:HG	2.06	0.54
1:A:45:LEU:HD13	1:A:566:TYR:CE2	2.42	0.54
1:B:127:SER:HB3	1:B:211:TYR:CG	2.42	0.54
1:B:236:ILE:HG21	1:B:712:HIS:CE1	2.42	0.54
1:A:195:TYR:O	1:A:227:GLN:HA	2.07	0.54
1:A:365:THR:O	1:A:367:ASP:N	2.40	0.54
1:A:542:LEU:HD23	1:A:543:LEU:N	2.22	0.54
1:B:414:TYR:HB3	1:B:416:TYR:CE1	2.43	0.54
1:B:681:ASP:O	1:B:685:ASN:HB2	2.07	0.54
1:A:293:MET:HE1	1:A:323:SER:HA	1.90	0.54
1:A:373:LYS:HD3	1:A:375:ILE:HD11	1.90	0.54
1:A:542:LEU:HD12	1:A:619:VAL:CG2	2.37	0.54
1:A:658:ARG:HD2	1:A:687:THR:HG21	1.88	0.54
1:B:353:TRP:N	1:B:353:TRP:CE3	2.75	0.54
1:B:567:LEU:O	1:B:571:GLU:HB2	2.08	0.54
1:A:65:ASP:HB2	1:A:466:LYS:CG	2.38	0.54
1:A:320:GLN:O	1:A:354:VAL:HG23	2.07	0.54
1:A:415:LEU:HB3	1:A:434:ILE:HG13	1.90	0.54
1:A:692:ALA:CB	1:A:726:VAL:CG1	2.85	0.54
1:B:543:LEU:HB3	1:B:575:VAL:HG13	1.89	0.54
1:A:90:LEU:CD1	1:A:94:THR:OG1	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:ASN:C	1:B:562:ASN:HD22	2.15	0.54
1:A:374:ILE:O	1:A:375:ILE:CD1	2.55	0.54
1:B:524:PHE:HB3	1:B:578:PHE:CE1	2.43	0.54
1:B:560:ARG:NH1	1:B:560:ARG:CG	2.63	0.54
1:A:386:TYR:O	1:A:394:CYS:HB2	2.07	0.54
1:B:120:TYR:CE2	1:B:128:TYR:CG	2.96	0.54
1:B:222:PHE:HA	1:B:271:VAL:O	2.08	0.54
1:A:206:GLU:OE2	1:A:663:ASP:OD2	2.26	0.53
1:A:693:GLU:CG	1:A:726:VAL:HG21	2.38	0.53
1:B:596:ARG:NH2	1:B:678:ASP:OD1	2.40	0.53
1:A:464:GLU:O	1:A:465:ALA:HB3	2.08	0.53
1:B:459:VAL:HG22	1:B:460:SER:N	2.19	0.53
1:B:710:ASN:C	1:B:710:ASN:ND2	2.64	0.53
1:B:76:ILE:C	1:B:77:LEU:HD23	2.33	0.53
1:B:219:ASN:HB2	1:B:308:GLN:CD	2.32	0.53
1:B:462:SER:O	1:B:463:LYS:C	2.52	0.53
1:B:529:ILE:HD12	1:B:529:ILE:H	1.71	0.53
1:B:613:PHE:O	1:B:619:VAL:CG2	2.56	0.53
1:B:710:ASN:C	1:B:710:ASN:HD22	2.15	0.53
1:B:541:PRO:HG2	1:B:573:ILE:HG12	1.89	0.53
1:A:209:SER:HB2	4:A:2050:HOH:O	2.08	0.53
1:A:382:ARG:NH2	1:A:591:MET:CE	2.70	0.53
1:A:734:TRP:NE1	1:A:736:THR:HG22	2.23	0.53
1:B:397:ILE:N	1:B:397:ILE:CD1	2.72	0.53
1:B:551:CYS:HA	1:B:584:GLY:N	2.24	0.53
1:A:415:LEU:HB3	1:A:434:ILE:HD12	1.87	0.53
1:A:466:LYS:HE3	1:A:466:LYS:CA	2.39	0.53
1:B:107:ILE:O	1:B:108:SER:C	2.48	0.53
1:A:424:GLY:O	1:A:426:PRO:HD3	2.09	0.53
1:A:528:MET:CE	1:A:618:PHE:HE1	2.14	0.53
1:B:295:ILE:HD13	1:B:295:ILE:C	2.34	0.53
1:B:629:TRP:CD1	1:B:630:SER:H	2.25	0.53
3:B:1771:FPB:H24	4:B:2131:HOH:O	2.02	0.53
1:A:158:SER:OG	1:A:160:VAL:O	2.25	0.53
1:B:414:TYR:CD1	1:B:433:LYS:HG2	2.43	0.53
1:B:483:HIS:ND1	1:B:483:HIS:N	2.56	0.53
1:B:614:SER:O	1:B:619:VAL:HG22	2.10	0.53
1:A:514:LEU:CD1	1:A:557:THR:CG2	2.85	0.52
1:A:693:GLU:OE1	1:A:696:LYS:CE	2.57	0.52
1:A:339:CYS:C	1:A:340:LEU:HD12	2.34	0.52
1:A:374:ILE:O	1:A:375:ILE:HD12	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:TYR:HB2	1:B:114:ILE:CD1	2.38	0.52
1:A:184:ARG:HD3	1:A:187:TRP:CZ2	2.43	0.52
1:A:710:ASN:HD22	1:A:710:ASN:C	2.17	0.52
1:B:489:LYS:HB3	4:B:2102:HOH:O	2.08	0.52
1:A:185:ILE:HD13	1:A:185:ILE:N	2.24	0.52
1:B:75:ASN:HD21	2:B:1770:NAG:H62	1.74	0.52
1:B:159:PRO:O	1:B:160:VAL:HG13	2.10	0.52
1:A:601:PHE:HA	1:A:604:GLU:HB2	1.90	0.52
1:B:243:ASP:HA	4:B:2053:HOH:O	2.08	0.52
1:B:312:SER:CB	1:B:325:MET:HE3	2.32	0.52
1:A:327:ILE:HD12	1:A:343:ARG:HB3	1.91	0.52
1:A:654:ALA:N	1:A:655:PRO:HD3	2.25	0.52
1:A:748:HIS:O	1:A:751:ILE:HG22	2.09	0.52
1:B:438:ASP:OD1	1:B:440:THR:OG1	2.25	0.52
1:A:60:LEU:HA	1:A:69:LEU:O	2.09	0.52
1:A:478:PRO:HB2	1:A:497:ASN:ND2	2.25	0.52
1:A:530:LEU:HD22	1:A:534:PHE:CE1	2.45	0.52
1:B:75:ASN:OD1	1:B:92:ASN:HB3	2.09	0.52
1:B:115:LEU:HD13	1:B:132:TYR:CD1	2.45	0.52
1:A:184:ARG:C	1:A:185:ILE:HD13	2.35	0.52
1:A:751:ILE:HG23	1:A:752:TYR:N	2.25	0.52
1:B:71:LYS:O	1:B:71:LYS:CG	2.57	0.52
1:B:623:ARG:HH12	1:B:765:LEU:HD21	1.72	0.52
1:A:219:ASN:HB3	1:A:221:THR:H	1.75	0.52
1:A:517:ILE:HD11	1:A:578:PHE:HE1	1.75	0.52
1:B:382:ARG:HG2	1:B:382:ARG:NH1	2.24	0.52
1:A:373:LYS:HG2	1:A:375:ILE:HD13	1.92	0.51
1:B:341:VAL:C	1:B:343:ARG:N	2.66	0.51
1:B:108:SER:OG	1:B:113:PHE:HB2	2.10	0.51
1:B:620:ASP:O	1:B:622:LYS:N	2.43	0.51
1:A:666:TYR:O	1:A:670:TYR:CD2	2.63	0.51
1:B:720:SER:HB2	4:B:2147:HOH:O	2.09	0.51
1:A:174:VAL:HG12	1:A:175:LYS:H	1.75	0.51
1:A:492:ARG:HD2	4:A:2012:HOH:O	2.10	0.51
1:A:526:TYR:C	1:A:526:TYR:CD2	2.88	0.51
1:A:591:MET:HE3	1:A:592:HIS:HE1	1.75	0.51
1:B:587:GLY:N	4:B:2127:HOH:O	2.43	0.51
1:A:472:CYS:O	1:A:478:PRO:HA	2.10	0.51
1:A:591:MET:HE3	1:A:592:HIS:CE1	2.46	0.51
1:B:77:LEU:HD22	1:B:88:VAL:HA	1.92	0.51
1:B:543:LEU:HD23	1:B:544:LEU:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ILE:C	1:A:194:ILE:HD13	2.36	0.51
1:A:550:PRO:HA	1:A:582:GLY:O	2.11	0.51
1:B:507:VAL:HG11	1:B:509:MET:CG	2.39	0.51
1:A:115:LEU:HD21	1:A:132:TYR:CD1	2.43	0.51
1:B:124:TRP:HB3	4:B:2027:HOH:O	2.11	0.51
1:B:172:ILE:HG22	1:B:185:ILE:HG13	1.92	0.51
1:A:528:MET:HE2	1:A:530:LEU:HD21	1.92	0.51
1:A:45:LEU:HB2	1:A:566:TYR:CZ	2.45	0.51
1:A:292:SER:HB2	1:A:317:ARG:HH21	1.75	0.51
1:A:626:ILE:HG22	1:A:647:PHE:CD2	2.45	0.51
1:B:417:TYR:HE1	1:B:434:ILE:CG1	2.23	0.51
1:B:438:ASP:OD1	1:B:438:ASP:C	2.52	0.51
1:B:512:LYS:CE	1:B:527:GLN:OE1	2.59	0.51
1:A:415:LEU:HB3	1:A:434:ILE:CG1	2.40	0.50
1:A:420:ASN:OD1	1:A:426:PRO:HA	2.11	0.50
1:B:159:PRO:HG2	1:B:217:SER:O	2.11	0.50
1:A:656:VAL:HG13	1:A:715:GLN:NE2	2.25	0.50
1:A:730:PHE:C	1:A:730:PHE:CD2	2.89	0.50
1:A:369:ASN:O	1:A:389:ILE:HB	2.11	0.50
1:A:377:ASN:ND2	1:A:377:ASN:C	2.63	0.50
1:A:489:LYS:HB2	4:A:2105:HOH:O	2.11	0.50
1:A:594:ILE:CD1	1:A:601:PHE:HB2	2.42	0.50
1:B:542:LEU:HD12	1:B:574:ILE:CG2	2.41	0.50
1:A:90:LEU:HD11	1:A:94:THR:HB	1.92	0.50
1:B:77:LEU:HD23	1:B:77:LEU:N	2.27	0.50
1:B:307:THR:O	1:B:308:GLN:C	2.54	0.50
1:A:508:GLN:NE2	1:A:533:HIS:CE1	2.79	0.50
1:B:295:ILE:C	1:B:295:ILE:CD1	2.85	0.50
1:B:341:VAL:O	1:B:343:ARG:N	2.44	0.50
1:B:499:ALA:O	1:B:503:MET:HE3	2.12	0.50
1:B:512:LYS:HE2	1:B:556:ASP:O	2.11	0.50
1:A:68:TYR:CE1	1:A:79:PHE:CB	2.95	0.50
1:A:664:SER:O	1:A:668:GLU:HB2	2.11	0.50
1:B:84:GLY:HA2	1:B:492:ARG:CZ	2.42	0.50
1:B:736:THR:O	1:B:737:ASP:HB2	2.11	0.50
1:A:145:GLU:O	1:A:146:GLU:CB	2.60	0.50
1:A:176:ILE:HG22	1:A:177:GLU:HG2	1.93	0.50
1:B:78:VAL:HG23	1:B:89:PHE:HB2	1.93	0.50
1:A:120:TYR:O	1:A:120:TYR:HD1	1.95	0.50
1:A:377:ASN:ND2	1:A:380:GLY:N	2.59	0.50
1:A:83:TYR:HB3	4:A:2017:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:THR:CG2	1:B:570:THR:OG1	2.60	0.50
1:B:115:LEU:HD13	1:B:132:TYR:HD1	1.77	0.50
1:A:459:VAL:HG23	1:A:469:GLN:O	2.11	0.49
1:B:373:LYS:CD	1:B:375:ILE:HD11	2.32	0.49
1:B:414:TYR:CE1	1:B:435:GLN:HG2	2.47	0.49
1:B:433:LYS:HB2	1:B:445:LEU:HD21	1.94	0.49
1:A:751:ILE:C	1:A:755:MET:CE	2.85	0.49
1:B:364:PHE:CZ	1:B:371:PHE:CD1	2.99	0.49
1:B:458:SER:HB3	1:B:471:ARG:HG2	1.94	0.49
1:B:461:PHE:CE1	1:B:468:TYR:HB3	2.46	0.49
1:A:373:LYS:HG2	1:A:375:ILE:CD1	2.43	0.49
1:A:516:PHE:HA	1:A:525:TRP:HA	1.94	0.49
1:A:556:ASP:OD1	1:A:558:VAL:CG2	2.57	0.49
1:B:296:GLY:O	1:B:298:HIS:HD2	1.95	0.49
1:B:410:LEU:CD2	4:B:2075:HOH:O	2.60	0.49
1:B:516:PHE:HB2	1:B:524:PHE:O	2.13	0.49
1:B:746:THR:O	1:B:747:ALA:C	2.56	0.49
3:B:1771:FPB:O16	3:B:1771:FPB:H9C2	2.13	0.49
1:A:76:ILE:HG22	1:A:76:ILE:O	2.10	0.49
1:A:82:GLU:O	1:A:82:GLU:CG	2.59	0.49
1:B:155:VAL:HG13	1:B:166:TYR:HB3	1.93	0.49
1:A:266:VAL:HG22	1:A:267:LYS:N	2.28	0.49
1:A:497:ASN:O	1:A:498:SER:C	2.55	0.49
1:B:267:LYS:HD2	1:B:286:GLN:HE22	1.77	0.49
1:B:295:ILE:HG23	1:B:296:GLY:N	2.26	0.49
1:B:593:ALA:O	1:B:601:PHE:CD2	2.65	0.49
1:B:621:ASN:C	1:B:621:ASN:HD22	2.20	0.49
1:A:763:PHE:O	1:A:764:SER:C	2.56	0.49
1:B:178:PRO:CD	4:B:2038:HOH:O	2.60	0.49
1:B:541:PRO:HB2	1:B:763:PHE:CD2	2.47	0.49
1:A:203:TYR:CD2	1:A:228:PHE:HE1	2.30	0.49
1:B:433:LYS:HB2	1:B:445:LEU:HD11	1.94	0.49
1:A:216:TRP:O	1:A:305:TRP:CD1	2.66	0.49
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.47	0.49
1:B:112:GLN:HG2	1:B:138:ASN:HD21	1.77	0.49
1:B:208:PHE:O	1:B:209:SER:C	2.56	0.49
1:B:285:ILE:HD12	1:B:285:ILE:N	2.27	0.49
1:A:638:MET:C	1:A:640:LEU:H	2.20	0.49
1:B:595:ASN:O	1:B:597:ARG:NH2	2.45	0.49
1:A:297:ASP:HB2	1:A:318:ARG:HB2	1.95	0.48
1:A:408:GLU:HG3	1:A:418:ILE:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:MET:C	1:A:295:ILE:H	2.20	0.48
1:B:163:LYS:HE3	1:B:273:THR:HG22	1.94	0.48
1:B:563:TRP:O	1:B:564:ALA:C	2.55	0.48
1:A:293:MET:HG3	1:A:315:TRP:HB2	1.96	0.48
1:A:311:ILE:HD11	1:A:337:TRP:CZ3	2.47	0.48
1:B:120:TYR:HE2	1:B:128:TYR:CD2	2.31	0.48
1:B:371:PHE:CE2	1:B:387:PHE:CB	2.96	0.48
1:B:593:ALA:O	1:B:601:PHE:HD2	1.96	0.48
1:A:98:PHE:CD2	1:A:100:HIS:HB2	2.48	0.48
1:B:50:LYS:O	1:B:51:ASN:HB3	2.14	0.48
1:B:84:GLY:CA	1:B:492:ARG:CZ	2.91	0.48
1:A:115:LEU:HD22	1:A:132:TYR:HD1	1.78	0.48
1:A:183:TYR:HE2	1:A:277:SER:C	2.21	0.48
1:A:184:ARG:HD3	1:A:187:TRP:CD2	2.48	0.48
1:A:269:PHE:HA	1:A:285:ILE:O	2.13	0.48
1:A:517:ILE:HD11	1:A:578:PHE:CE1	2.48	0.48
1:A:111:GLY:O	1:A:137:LEU:CD1	2.62	0.48
1:A:113:PHE:CE2	1:A:178:PRO:HG2	2.48	0.48
1:A:596:ARG:NH2	1:A:678:ASP:OD1	2.47	0.48
1:B:320:GLN:CD	1:B:669:ARG:HB2	2.36	0.48
1:B:748:HIS:O	1:B:751:ILE:CG2	2.61	0.48
1:A:72:GLN:O	1:A:73:GLU:C	2.56	0.48
1:A:739:ASP:C	1:A:739:ASP:OD1	2.56	0.48
1:A:244:GLU:HA	1:B:661:TYR:OH	2.13	0.48
1:A:330:TYR:CE1	1:A:335:GLY:HA2	2.49	0.48
1:A:518:ILE:CG2	1:A:521:GLU:HA	2.43	0.48
1:B:463:LYS:O	1:B:465:ALA:N	2.47	0.48
1:A:549:GLY:O	1:A:550:PRO:C	2.56	0.48
1:B:45:LEU:HG	1:B:49:LEU:HD21	1.96	0.48
1:B:429:ARG:HH11	1:B:429:ARG:HG3	1.67	0.48
1:A:105:TYR:CD1	1:A:105:TYR:C	2.92	0.48
1:A:320:GLN:OE1	1:A:669:ARG:HG3	2.13	0.48
1:A:668:GLU:HB2	4:A:2134:HOH:O	2.12	0.48
1:B:305:TRP:CE3	1:B:311:ILE:HG23	2.49	0.48
1:B:402:TRP:HE3	1:B:403:GLU:O	1.97	0.48
1:B:692:ALA:O	1:B:695:PHE:HB2	2.14	0.47
1:A:528:MET:HG2	1:A:574:ILE:CG2	2.45	0.47
1:A:603:VAL:HG12	1:A:639:VAL:HG22	1.95	0.47
1:B:48:TYR:CD2	1:B:49:LEU:CD1	2.97	0.47
1:B:139:LYS:O	1:B:140:ARG:C	2.56	0.47
1:B:659:TRP:CE3	1:B:667:THR:HG23	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:689:MET:SD	1:B:689:MET:N	2.84	0.47
1:A:103:ASN:OD1	1:A:117:GLU:OE2	2.33	0.47
1:A:217:SER:O	1:A:218:PRO:C	2.54	0.47
1:B:389:ILE:HG22	1:B:390:ASP:N	2.28	0.47
1:B:540:TYR:CD1	1:B:540:TYR:N	2.83	0.47
1:B:620:ASP:C	1:B:622:LYS:N	2.69	0.47
3:A:1771:FPB:H2	4:A:2133:HOH:O	2.14	0.47
1:A:428:GLY:C	1:A:429:ARG:HG2	2.40	0.47
1:A:750:HIS:CG	1:B:724:VAL:HG22	2.50	0.47
1:B:46:THR:O	1:B:47:ASP:C	2.56	0.47
1:A:57:LEU:HA	1:A:480:TYR:CE1	2.49	0.47
1:A:121:VAL:O	1:A:128:TYR:HB2	2.15	0.47
1:A:163:LYS:NZ	1:A:273:THR:CG2	2.78	0.47
1:A:271:VAL:HG23	1:A:284:SER:OG	2.13	0.47
1:A:438:ASP:OD1	1:A:440:THR:OG1	2.26	0.47
1:B:661:TYR:HB2	1:B:715:GLN:NE2	2.29	0.47
1:B:48:TYR:CD2	1:B:49:LEU:HD13	2.50	0.47
1:B:173:TYR:CE2	1:B:184:ARG:HG3	2.50	0.47
1:B:236:ILE:HD11	1:B:254:VAL:HB	1.97	0.47
1:B:453:ARG:NE	1:B:479:LEU:CD1	2.71	0.47
1:B:562:ASN:HD21	1:B:564:ALA:HB3	1.80	0.47
1:B:636:THR:O	1:B:637:SER:C	2.58	0.47
1:B:637:SER:O	1:B:638:MET:C	2.58	0.47
1:A:633:GLY:C	1:A:655:PRO:HB3	2.40	0.47
1:B:167:VAL:HG21	1:B:196:ASN:O	2.15	0.47
1:B:347:GLU:O	1:B:354:VAL:HG21	2.14	0.47
1:A:602:GLU:OE2	1:A:631:TYR:OH	2.28	0.47
1:B:483:HIS:HB3	1:B:489:LYS:O	2.14	0.47
1:A:532:PRO:CD	1:A:569:SER:HA	2.44	0.46
1:B:443:THR:HG22	1:B:445:LEU:HD23	1.97	0.46
1:B:653:VAL:O	1:B:654:ALA:HB3	2.15	0.46
1:A:175:LYS:O	1:A:176:ILE:C	2.57	0.46
1:A:201:TRP:CE3	1:A:202:VAL:HA	2.50	0.46
1:A:247:GLN:HB3	4:A:2063:HOH:O	2.15	0.46
1:A:603:VAL:HG13	1:A:639:VAL:HG22	1.88	0.46
1:A:668:GLU:CB	4:A:2134:HOH:O	2.63	0.46
1:B:271:VAL:CG1	1:B:272:ASN:N	2.77	0.46
1:B:363:HIS:CG	1:B:407:ILE:HG21	2.50	0.46
1:A:168:TRP:CE3	1:A:169:ASN:OD1	2.68	0.46
1:B:113:PHE:CZ	1:B:178:PRO:HG2	2.50	0.46
1:B:761:GLN:HA	4:B:2157:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:MET:HE3	1:A:755:MET:HB2	1.50	0.46
4:A:2068:HOH:O	1:B:245:SER:HB3	2.15	0.46
1:B:198:ILE:HB	1:B:211:TYR:CE1	2.51	0.46
1:B:520:ASN:O	1:B:521:GLU:HB3	2.14	0.46
1:B:609:ALA:O	1:B:610:ALA:C	2.58	0.46
1:B:240:PHE:HA	4:B:2051:HOH:O	2.16	0.46
1:B:392:LYS:HD3	1:B:393:ASP:OD2	2.14	0.46
1:B:446:SER:HB2	1:B:457:TYR:CE2	2.51	0.46
1:B:486:VAL:CG1	1:B:487:ASN:OD1	2.64	0.46
1:A:127:SER:CB	1:A:211:TYR:CG	2.99	0.46
1:A:221:THR:O	1:A:273:THR:HB	2.16	0.46
1:A:374:ILE:C	1:A:375:ILE:CD1	2.88	0.46
1:A:418:ILE:HD11	1:A:459:VAL:HG12	1.96	0.46
1:A:605:ASP:O	1:A:606:GLN:C	2.57	0.46
1:B:459:VAL:HG12	4:B:2085:HOH:O	2.16	0.46
1:B:551:CYS:HA	1:B:584:GLY:CA	2.46	0.46
1:B:595:ASN:CB	1:B:597:ARG:HH21	2.28	0.46
1:B:668:GLU:HG2	1:B:673:LEU:HD23	1.96	0.46
1:A:466:LYS:HA	1:A:466:LYS:CE	2.46	0.46
1:A:639:VAL:O	1:A:639:VAL:CG1	2.62	0.46
1:B:558:VAL:HG23	1:B:559:PHE:N	2.30	0.46
1:B:716:SER:O	1:B:717:ALA:C	2.59	0.46
1:A:170:ASN:HA	1:A:198:ILE:HD11	1.98	0.46
1:A:541:PRO:HG2	1:A:573:ILE:HG12	1.98	0.46
1:B:125:ARG:HG2	1:B:126:HIS:ND1	2.30	0.46
1:B:227:GLN:O	1:B:266:VAL:HG23	2.16	0.46
1:B:633:GLY:CA	1:B:655:PRO:HB3	2.45	0.46
1:A:630:SER:OG	1:A:740:HIS:NE2	2.45	0.46
1:A:763:PHE:C	1:A:765:LEU:N	2.74	0.46
1:B:449:LEU:O	1:B:450:ASN:HB2	2.14	0.46
1:B:485:SER:O	1:B:486:VAL:C	2.59	0.46
1:B:629:TRP:O	1:B:632:GLY:CA	2.64	0.46
1:B:236:ILE:HD12	1:B:236:ILE:C	2.29	0.46
1:B:321:ASN:OD1	1:B:349:SER:O	2.33	0.46
1:A:721:LYS:HA	4:B:2152:HOH:O	2.16	0.45
1:A:750:HIS:HE1	1:B:728:VAL:O	1.99	0.45
1:B:592:HIS:C	1:B:594:ILE:H	2.25	0.45
1:A:258:LYS:HD3	1:A:661:TYR:O	2.17	0.45
1:B:600:THR:HG22	1:B:601:PHE:H	1.67	0.45
1:A:147:ARG:HD3	2:A:1767:NAG:H83	1.98	0.45
1:A:542:LEU:HD23	1:A:542:LEU:C	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:HIS:O	1:B:534:PHE:C	2.60	0.45
1:A:79:PHE:CD2	1:A:86:SER:HB3	2.52	0.45
1:A:201:TRP:O	1:A:201:TRP:CD2	2.70	0.45
1:A:266:VAL:CG2	1:A:267:LYS:N	2.79	0.45
1:A:414:TYR:HA	1:A:434:ILE:O	2.17	0.45
1:A:744:SER:O	1:A:745:SER:C	2.60	0.45
1:B:43:TYR:CE2	1:B:565:THR:HG21	2.51	0.45
1:B:462:SER:C	1:B:463:LYS:O	2.57	0.45
1:B:703:ILE:HG21	1:B:751:ILE:HD12	1.97	0.45
1:A:61:ARG:NH1	1:A:105:TYR:HE1	2.14	0.45
1:A:361:GLU:H	1:A:361:GLU:HG3	1.25	0.45
1:A:389:ILE:HD13	1:A:389:ILE:HA	1.79	0.45
1:B:621:ASN:CA	1:B:624:ILE:HD11	2.45	0.45
1:A:316:LEU:HD23	1:A:316:LEU:C	2.42	0.45
1:B:306:ALA:C	1:B:307:THR:HG22	2.41	0.45
1:B:446:SER:O	1:B:447:CYS:C	2.58	0.45
1:B:463:LYS:C	1:B:465:ALA:N	2.73	0.45
1:B:675:THR:C	1:B:680:LEU:HB2	2.42	0.45
1:A:327:ILE:HG12	1:A:389:ILE:HD11	1.98	0.45
1:A:179:ASN:OD1	1:A:180:LEU:HD23	2.17	0.45
1:A:693:GLU:CD	1:A:726:VAL:CG2	2.90	0.45
1:A:271:VAL:HG22	1:A:284:SER:OG	2.17	0.45
1:A:597:ARG:C	1:A:600:THR:CG2	2.81	0.45
1:B:720:SER:HA	1:B:723:LEU:CD1	2.34	0.45
1:A:71:LYS:HE3	1:A:105:TYR:HE2	1.81	0.45
1:A:174:VAL:HG12	1:A:175:LYS:N	2.31	0.45
1:B:228:PHE:HA	1:B:265:THR:O	2.17	0.45
1:B:302:ASP:OD1	1:B:302:ASP:C	2.60	0.45
1:B:431:LEU:HD12	1:B:432:TYR:N	2.32	0.45
1:B:765:LEU:HA	1:B:766:PRO:HD3	1.70	0.45
1:A:693:GLU:OE1	1:A:696:LYS:HE3	2.17	0.44
1:B:184:ARG:HD3	1:B:187:TRP:CE2	2.51	0.44
1:B:293:MET:CG	1:B:315:TRP:HB2	2.48	0.44
1:B:513:LYS:O	1:B:527:GLN:HA	2.18	0.44
1:B:613:PHE:C	1:B:619:VAL:HG21	2.41	0.44
1:B:761:GLN:HG2	4:B:2156:HOH:O	2.16	0.44
1:A:156:THR:HG23	1:A:216:TRP:HE1	1.82	0.44
1:A:375:ILE:HG22	1:A:396:PHE:HZ	1.82	0.44
1:B:133:ASP:HA	4:B:2029:HOH:O	2.17	0.44
1:B:621:ASN:C	1:B:621:ASN:ND2	2.76	0.44
1:B:143:ILE:O	1:B:143:ILE:HG13	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:ASP:O	1:B:332:GLU:C	2.60	0.44
1:B:503:MET:O	1:B:506:ASN:HB2	2.18	0.44
1:B:558:VAL:CG2	1:B:559:PHE:N	2.81	0.44
1:A:68:TYR:CZ	1:A:79:PHE:CB	3.01	0.44
1:A:712:HIS:C	1:A:714:GLN:H	2.26	0.44
1:B:60:LEU:CD1	1:B:469:GLN:NE2	2.80	0.44
1:B:310:ARG:HD3	1:B:327:ILE:HG21	1.96	0.44
1:B:668:GLU:HG2	1:B:673:LEU:CD2	2.48	0.44
1:B:708:ASP:CG	1:B:711:VAL:O	2.60	0.44
1:B:744:SER:OG	1:B:747:ALA:HB3	2.15	0.44
1:B:750:HIS:O	1:B:753:THR:HB	2.17	0.44
1:A:197:GLY:O	1:A:198:ILE:HG23	2.18	0.44
1:A:470:LEU:HA	1:A:470:LEU:HD23	1.53	0.44
1:A:706:THR:OG1	1:A:736:THR:HA	2.18	0.44
1:B:141:GLN:CG	1:B:142:LEU:N	2.77	0.44
1:B:158:SER:HB2	1:B:159:PRO:CD	2.48	0.44
1:B:500:LEU:O	1:B:504:LEU:HG	2.17	0.44
1:A:498:SER:O	1:A:501:ASP:CB	2.65	0.44
1:B:132:TYR:CZ	1:B:155:VAL:HG21	2.53	0.44
1:A:614:SER:HB3	1:A:624:ILE:HD11	2.00	0.44
1:B:459:VAL:HG13	4:B:2097:HOH:O	2.17	0.44
1:A:206:GLU:OE1	1:A:206:GLU:CA	2.59	0.43
1:A:638:MET:C	1:A:640:LEU:N	2.76	0.43
1:A:658:ARG:HG3	1:A:660:GLU:OE1	2.18	0.43
1:A:692:ALA:HB1	1:A:726:VAL:HG11	1.90	0.43
1:B:332:GLU:CG	1:B:333:SER:N	2.64	0.43
1:B:610:ALA:HA	1:B:613:PHE:HB2	2.00	0.43
1:B:738:GLU:CD	1:B:744:SER:HB3	2.38	0.43
1:A:718:GLN:OE1	1:A:718:GLN:HA	2.18	0.43
1:B:271:VAL:CG2	1:B:284:SER:OG	2.66	0.43
1:B:334:SER:HB2	1:B:336:ARG:HG3	2.00	0.43
1:B:538:LYS:CG	4:B:2113:HOH:O	2.60	0.43
1:B:562:ASN:ND2	1:B:565:THR:H	2.15	0.43
1:B:739:ASP:OD1	1:B:739:ASP:C	2.61	0.43
1:A:132:TYR:CZ	1:A:155:VAL:CG2	3.01	0.43
1:A:314:GLN:HA	1:A:324:VAL:O	2.19	0.43
1:A:481:THR:OG1	1:A:483:HIS:HE1	2.00	0.43
1:B:639:VAL:HG12	1:B:640:LEU:N	2.33	0.43
1:B:530:LEU:HD22	1:B:534:PHE:CE1	2.53	0.43
1:B:744:SER:OG	1:B:747:ALA:HB2	2.16	0.43
1:A:111:GLY:O	1:A:137:LEU:HD11	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:LYS:CD	1:B:393:ASP:CG	2.89	0.43
1:A:180:LEU:HB3	1:A:181:PRO:CD	2.49	0.43
1:A:383:HIS:HB3	1:A:398:THR:OG1	2.19	0.43
1:A:436:LEU:HA	1:A:436:LEU:HD23	1.23	0.43
1:A:712:HIS:HB3	4:A:2144:HOH:O	2.18	0.43
1:B:214:LEU:CD1	1:B:225:TYR:HB3	2.48	0.43
1:B:472:CYS:HB3	1:B:479:LEU:CB	2.49	0.43
1:B:522:THR:HG22	1:B:523:LYS:N	2.32	0.43
1:A:270:VAL:HG23	1:A:287:ILE:HD12	1.99	0.43
1:A:55:LEU:HD22	1:A:478:PRO:HG2	2.01	0.43
1:A:93:SER:HB2	1:A:96:ASP:OD2	2.18	0.43
1:A:741:GLY:O	1:A:742:ILE:C	2.60	0.43
1:A:748:HIS:CE1	1:A:752:TYR:CE2	3.06	0.43
1:B:68:TYR:CD1	1:B:68:TYR:C	2.96	0.43
1:A:57:LEU:HA	1:A:480:TYR:CZ	2.54	0.43
1:A:423:LYS:O	1:A:424:GLY:C	2.62	0.43
1:A:641:GLY:O	1:A:694:ASN:HB2	2.19	0.43
1:A:765:LEU:HA	1:A:766:PRO:HD2	1.76	0.43
1:A:263:ASN:HD22	1:A:264:PRO:HD2	1.84	0.43
1:A:487:ASN:O	1:A:488:ASP:HB2	2.18	0.43
1:A:578:PHE:CD2	1:A:578:PHE:C	2.97	0.43
1:A:602:GLU:HG2	1:A:603:VAL:N	2.34	0.43
1:A:691:ARG:O	1:A:692:ALA:C	2.62	0.43
1:B:134:ILE:HG21	1:B:178:PRO:HB3	2.01	0.43
1:B:271:VAL:HG12	1:B:272:ASN:N	2.33	0.43
1:B:534:PHE:HZ	1:B:618:PHE:CG	2.36	0.43
1:B:750:HIS:CD2	1:B:750:HIS:C	2.96	0.43
1:A:547:TYR:CE1	3:A:1771:FPB:C26	3.02	0.42
1:A:651:ILE:HD13	1:A:755:MET:HG3	1.98	0.42
1:B:55:LEU:N	1:B:55:LEU:HD23	2.33	0.42
1:B:556:ASP:CG	1:B:558:VAL:HG13	2.44	0.42
1:A:145:GLU:O	1:A:146:GLU:HB2	2.19	0.42
1:A:631:TYR:CD1	1:A:635:VAL:HG23	2.54	0.42
1:B:71:LYS:HA	1:B:75:ASN:O	2.19	0.42
1:B:90:LEU:HD12	1:B:90:LEU:HA	1.90	0.42
1:B:459:VAL:HG23	1:B:470:LEU:HD23	2.01	0.42
1:B:602:GLU:O	1:B:606:GLN:HG2	2.19	0.42
1:B:666:TYR:CZ	3:B:1771:FPB:H2	2.53	0.42
1:A:540:TYR:HB2	1:A:574:ILE:HD11	2.01	0.42
1:B:177:GLU:CG	1:B:180:LEU:CD2	2.97	0.42
1:B:219:ASN:H	1:B:308:GLN:HE22	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:TRP:CH2	1:B:755:MET:HE3	2.54	0.42
1:B:598:LEU:HD22	1:B:631:TYR:OH	2.20	0.42
1:B:621:ASN:C	1:B:624:ILE:CD1	2.92	0.42
1:B:700:TYR:OH	1:B:702:LEU:HD13	2.18	0.42
1:A:153:GLN:HB3	1:A:211:TYR:CE2	2.55	0.42
1:A:190:LYS:O	1:A:191:GLU:C	2.62	0.42
1:A:701:LEU:HD12	1:A:701:LEU:C	2.44	0.42
1:B:134:ILE:HD13	1:B:178:PRO:HB3	2.01	0.42
1:B:326:ASP:OD2	1:B:339:CYS:HB3	2.18	0.42
1:B:550:PRO:O	1:B:551:CYS:HB3	2.18	0.42
1:B:558:VAL:HG23	1:B:559:PHE:H	1.85	0.42
1:A:117:GLU:HG3	1:A:132:TYR:CZ	2.54	0.42
1:A:594:ILE:O	1:A:595:ASN:C	2.62	0.42
1:B:295:ILE:CG2	1:B:296:GLY:N	2.82	0.42
1:B:386:TYR:CB	1:B:397:ILE:HD11	2.46	0.42
1:B:402:TRP:O	1:B:402:TRP:CD2	2.71	0.42
1:B:630:SER:HB3	1:B:631:TYR:H	1.50	0.42
1:A:174:VAL:O	1:A:182:SER:HB2	2.19	0.42
1:A:263:ASN:ND2	1:A:264:PRO:HD2	2.34	0.42
1:A:346:ILE:HG22	1:A:347:GLU:N	2.32	0.42
1:B:60:LEU:HD13	1:B:469:GLN:NE2	2.35	0.42
1:B:453:ARG:O	1:B:453:ARG:HG2	2.19	0.42
1:B:509:MET:HA	1:B:510:PRO:HD3	1.91	0.42
1:B:739:ASP:O	1:B:742:ILE:HG13	2.20	0.42
1:A:48:TYR:CD1	1:A:562:ASN:HA	2.55	0.42
1:A:134:ILE:O	1:A:143:ILE:HB	2.18	0.42
1:B:156:THR:CG2	4:B:2019:HOH:O	2.51	0.42
1:A:520:ASN:ND2	4:A:2111:HOH:O	2.52	0.42
1:B:242:SER:OG	1:B:243:ASP:N	2.53	0.42
1:B:438:ASP:CG	1:B:441:LYS:HG2	2.45	0.42
1:B:466:LYS:HB3	1:B:467:TYR:CD1	2.55	0.42
1:A:256:TYR:CD1	1:A:256:TYR:C	2.97	0.42
1:A:446:SER:HB2	1:A:457:TYR:CD2	2.53	0.42
1:B:125:ARG:O	1:B:125:ARG:CG	2.68	0.42
1:B:172:ILE:HG22	1:B:185:ILE:CG1	2.49	0.42
1:B:562:ASN:C	1:B:562:ASN:ND2	2.77	0.42
1:B:664:SER:O	1:B:665:VAL:C	2.61	0.42
1:A:191:GLU:O	1:A:193:ILE:HD12	2.20	0.42
1:A:415:LEU:CD2	1:A:434:ILE:HD11	2.40	0.42
1:A:311:ILE:CD1	1:A:337:TRP:CZ3	3.03	0.41
1:B:125:ARG:HD2	1:B:126:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:SER:OG	1:B:361:GLU:N	2.53	0.41
1:B:389:ILE:HD12	1:B:389:ILE:HA	1.66	0.41
1:B:403:GLU:N	1:B:420:ASN:HD21	2.18	0.41
1:A:630:SER:C	1:A:632:GLY:N	2.76	0.41
1:A:648:LYS:HD3	1:A:762:CYS:SG	2.60	0.41
1:B:214:LEU:HG	1:B:223:LEU:HD21	2.02	0.41
1:B:258:LYS:NZ	1:B:712:HIS:ND1	2.68	0.41
1:B:293:MET:HE2	1:B:324:VAL:CG2	2.50	0.41
1:B:500:LEU:HD22	1:B:504:LEU:HG	2.01	0.41
1:B:690:SER:CA	4:B:2139:HOH:O	2.65	0.41
1:A:499:ALA:HB3	4:A:2005:HOH:O	2.20	0.41
1:A:526:TYR:HB2	1:A:577:SER:O	2.20	0.41
1:B:292:SER:HB2	1:B:317:ARG:NH2	2.35	0.41
1:B:679:ASN:HD22	1:B:679:ASN:HA	1.64	0.41
1:B:730:PHE:CE2	1:B:732:ALA:HB2	2.55	0.41
1:A:58:TYR:CZ	1:A:494:LEU:HB3	2.56	0.41
1:A:248:TYR:CE2	1:B:234:PRO:HB2	2.56	0.41
1:A:357:PHE:CZ	1:A:551:CYS:HB3	2.55	0.41
1:B:374:ILE:C	1:B:375:ILE:HD12	2.46	0.41
1:B:487:ASN:O	1:B:488:ASP:C	2.63	0.41
1:B:680:LEU:HD22	1:B:684:ARG:HD2	2.00	0.41
1:A:132:TYR:CZ	1:A:155:VAL:HG21	2.55	0.41
1:A:392:LYS:O	1:A:393:ASP:HB2	2.20	0.41
1:A:656:VAL:CG1	1:A:657:SER:H	2.29	0.41
1:A:747:ALA:O	1:A:751:ILE:HG22	2.19	0.41
1:B:44:THR:O	1:B:45:LEU:C	2.64	0.41
1:B:126:HIS:N	1:B:204:GLU:OE2	2.50	0.41
1:B:416:TYR:CD2	1:B:461:PHE:CZ	3.08	0.41
1:B:595:ASN:O	1:B:597:ARG:CZ	2.67	0.41
1:B:630:SER:OG	1:B:740:HIS:NE2	2.20	0.41
1:A:656:VAL:CG1	1:A:657:SER:N	2.81	0.41
1:A:687:THR:O	1:A:688:VAL:C	2.61	0.41
1:B:80:ASN:HB3	1:B:85:ASN:OD1	2.21	0.41
1:B:279:VAL:HB	1:B:280:THR:H	1.73	0.41
1:B:701:LEU:HD21	1:B:703:ILE:HD11	2.02	0.41
1:B:146:GLU:HG3	1:B:179:ASN:O	2.21	0.41
1:B:418:ILE:HA	1:B:430:ASN:O	2.21	0.41
1:B:603:VAL:O	1:B:607:ILE:HG13	2.21	0.41
1:A:132:TYR:CE1	1:A:155:VAL:CG2	3.02	0.41
1:A:724:VAL:HG22	1:B:750:HIS:CE1	2.48	0.41
1:B:105:TYR:CD2	1:B:105:TYR:N	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:635:VAL:O	1:B:636:THR:C	2.63	0.41
1:B:682:HIS:CE1	1:B:686:SER:HB3	2.56	0.41
1:A:263:ASN:HD22	1:A:263:ASN:HA	1.62	0.41
1:A:343:ARG:O	1:A:345:HIS:ND1	2.52	0.41
1:A:477:LEU:HD21	1:A:504:LEU:HD12	2.03	0.41
1:A:550:PRO:O	1:A:551:CYS:CB	2.69	0.41
1:A:752:TYR:HA	1:A:755:MET:HE3	2.03	0.41
1:B:49:LEU:HD13	1:B:49:LEU:N	2.36	0.41
1:B:106:SER:OG	1:B:157:TRP:CD1	2.74	0.41
1:B:120:TYR:HE2	1:B:128:TYR:CG	2.38	0.41
1:B:162:HIS:HD2	1:B:178:PRO:HD3	1.86	0.41
1:B:377:ASN:ND2	1:B:377:ASN:C	2.76	0.41
1:B:633:GLY:C	1:B:655:PRO:HB3	2.45	0.41
1:B:704:HIS:HD2	1:B:705:GLY:O	2.04	0.41
1:A:49:LEU:HG	1:A:749:GLN:HG2	2.03	0.41
1:A:266:VAL:CG2	1:A:267:LYS:H	2.34	0.41
1:A:327:ILE:HD12	1:A:343:ARG:CB	2.51	0.41
1:B:122:LYS:HE3	1:B:122:LYS:HB3	1.70	0.41
1:A:41:LYS:O	1:A:508:GLN:HG3	2.21	0.40
1:A:420:ASN:C	1:A:420:ASN:HD22	2.29	0.40
1:A:525:TRP:H	1:A:525:TRP:CD1	2.39	0.40
1:B:472:CYS:CB	1:B:479:LEU:HB2	2.50	0.40
1:B:543:LEU:HD21	1:B:627:TRP:CD1	2.53	0.40
1:A:248:TYR:HA	1:A:249:PRO:HD3	1.91	0.40
1:A:656:VAL:CG1	1:A:715:GLN:HE22	2.33	0.40
1:B:467:TYR:HD2	1:B:484:SER:HA	1.85	0.40
1:B:679:ASN:O	1:B:683:TYR:HD1	2.04	0.40
1:B:695:PHE:HB3	1:B:728:VAL:HG11	2.04	0.40
1:A:52:THR:O	1:A:52:THR:HG22	2.21	0.40
1:A:179:ASN:OD1	1:A:179:ASN:C	2.64	0.40
1:A:188:THR:O	1:A:189:GLY:C	2.65	0.40
1:A:477:LEU:HD23	1:A:559:PHE:CE2	2.57	0.40
1:A:500:LEU:O	1:A:503:MET:HB2	2.20	0.40
1:A:629:TRP:O	1:A:630:SER:HB2	2.21	0.40
1:A:751:ILE:C	1:A:755:MET:HE2	2.44	0.40
1:B:219:ASN:H	1:B:308:GLN:NE2	2.19	0.40
1:B:285:ILE:N	1:B:285:ILE:CD1	2.84	0.40
1:B:541:PRO:HB2	1:B:763:PHE:CE2	2.57	0.40
1:A:61:ARG:O	1:A:68:TYR:HA	2.21	0.40
1:A:206:GLU:OE2	3:A:1771:FPB:N18	2.53	0.40
1:A:315:TRP:O	1:A:323:SER:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:LEU:CD1	1:A:557:THR:HG23	2.51	0.40
1:A:713:PHE:N	4:A:2144:HOH:O	2.54	0.40
1:B:229:ASN:OD1	1:B:231:THR:OG1	2.26	0.40
1:B:623:ARG:NH1	1:B:763:PHE:O	2.50	0.40
1:B:684:ARG:NH1	4:B:2136:HOH:O	2.15	0.40
1:A:361:GLU:OE1	1:A:363:HIS:NE2	2.55	0.40
1:A:607:ILE:CG1	1:A:639:VAL:HG13	2.52	0.40
1:B:677:GLU:N	1:B:677:GLU:OE2	2.41	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	726/728 (100%)	626 (86%)	88 (12%)	12 (2%)	7	12
1	B	726/728 (100%)	624 (86%)	82 (11%)	20 (3%)	4	6
All	All	1452/1456 (100%)	1250 (86%)	170 (12%)	32 (2%)	5	9

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	713	PHE
1	A	764	SER
1	B	140	ARG
1	B	219	ASN
1	B	279	VAL
1	B	360	SER
1	B	486	VAL
1	B	630	SER
1	A	242	SER
1	A	572	ASN

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Mol	Chain	Res	Type
1	A	630	SER
1	B	95	PHE
1	B	521	GLU
1	A	146	GLU
1	A	176	ILE
1	A	356	ARG
1	A	366	LEU
1	B	218	PRO
1	B	332	GLU
1	B	342	ALA
1	B	615	LYS
1	B	748	HIS
1	A	119	ASN
1	A	708	ASP
1	B	243	ASP
1	B	320	GLN
1	B	464	GLU
1	B	569	SER
1	A	501	ASP
1	B	463	LYS
1	B	51	ASN
1	B	450	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	653/653 (100%)	519 (80%)	134 (20%)	1	1
1	B	653/653 (100%)	495 (76%)	158 (24%)	1	0
All	All	1306/1306 (100%)	1014 (78%)	292 (22%)	1	1

All (292) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	SER

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Mol	Chain	Res	Type
1	A	41	LYS
1	A	42	THR
1	A	44	THR
1	A	46	THR
1	A	49	LEU
1	A	50	LYS
1	A	57	LEU
1	A	60	LEU
1	A	63	ILE
1	A	71	LYS
1	A	73	GLU
1	A	75	ASN
1	A	88	VAL
1	A	90	LEU
1	A	102	ILE
1	A	103	ASN
1	A	115	LEU
1	A	116	LEU
1	A	122	LYS
1	A	133	ASP
1	A	134	ILE
1	A	137	LEU
1	A	140	ARG
1	A	141	GLN
1	A	142	LEU
1	A	143	ILE
1	A	147	ARG
1	A	148	ILE
1	A	152	THR
1	A	155	VAL
1	A	160	VAL
1	A	174	VAL
1	A	185	ILE
1	A	190	LYS
1	A	193	ILE
1	A	194	ILE
1	A	198	ILE
1	A	202	VAL
1	A	206	GLU
1	A	212	SER
1	A	223	LEU
1	A	228	PHE

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Mol	Chain	Res	Type
1	A	231	THR
1	A	246	LEU
1	A	250	LYS
1	A	254	VAL
1	A	258	LYS
1	A	263	ASN
1	A	266	VAL
1	A	267	LYS
1	A	281	ASN
1	A	287	ILE
1	A	288	THR
1	A	294	LEU
1	A	295	ILE
1	A	300	LEU
1	A	311	ILE
1	A	313	LEU
1	A	314	GLN
1	A	329	ASP
1	A	333	SER
1	A	336	ARG
1	A	340	LEU
1	A	341	VAL
1	A	343	ARG
1	A	350	THR
1	A	351	THR
1	A	354	VAL
1	A	358	ARG
1	A	361	GLU
1	A	366	LEU
1	A	373	LYS
1	A	374	ILE
1	A	375	ILE
1	A	377	ASN
1	A	385	CYS
1	A	389	ILE
1	A	391	LYS
1	A	397	ILE
1	A	399	LYS
1	A	405	ILE
1	A	418	ILE
1	A	419	SER
1	A	420	ASN

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Mol	Chain	Res	Type
1	A	431	LEU
1	A	433	LYS
1	A	434	ILE
1	A	440	THR
1	A	441	LYS
1	A	445	LEU
1	A	452	GLU
1	A	464	GLU
1	A	466	LYS
1	A	471	ARG
1	A	473	SER
1	A	479	LEU
1	A	482	LEU
1	A	485	SER
1	A	487	ASN
1	A	494	LEU
1	A	500	LEU
1	A	502	LYS
1	A	505	GLN
1	A	506	ASN
1	A	513	LYS
1	A	517	ILE
1	A	521	GLU
1	A	528	MET
1	A	536	LYS
1	A	544	LEU
1	A	546	VAL
1	A	566	TYR
1	A	569	SER
1	A	577	SER
1	A	594	ILE
1	A	600	THR
1	A	622	LYS
1	A	627	TRP
1	A	630	SER
1	A	663	ASP
1	A	665	VAL
1	A	677	GLU
1	A	679	ASN
1	A	699	GLU
1	A	702	LEU
1	A	715	GLN

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Mol	Chain	Res	Type
1	A	721	LYS
1	A	731	GLN
1	A	736	THR
1	A	745	SER
1	A	755	MET
1	A	761	GLN
1	A	765	LEU
1	B	39	SER
1	B	40	ARG
1	B	41	LYS
1	B	42	THR
1	B	46	THR
1	B	49	LEU
1	B	50	LYS
1	B	55	LEU
1	B	56	LYS
1	B	57	LEU
1	B	60	LEU
1	B	61	ARG
1	B	71	LYS
1	B	77	LEU
1	B	86	SER
1	B	87	SER
1	B	97	GLU
1	B	101	SER
1	B	102	ILE
1	B	106	SER
1	B	110	ASP
1	B	112	GLN
1	B	114	ILE
1	B	115	LEU
1	B	116	LEU
1	B	122	LYS
1	B	123	GLN
1	B	125	ARG
1	B	129	THR
1	B	133	ASP
1	B	139	LYS
1	B	141	GLN
1	B	143	ILE
1	B	144	THR
1	B	145	GLU

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Mol	Chain	Res	Type
1	B	152	THR
1	B	155	VAL
1	B	156	THR
1	B	160	VAL
1	B	167	VAL
1	B	169	ASN
1	B	174	VAL
1	B	180	LEU
1	B	182	SER
1	B	184	ARG
1	B	188	THR
1	B	202	VAL
1	B	214	LEU
1	B	221	THR
1	B	223	LEU
1	B	232	GLU
1	B	235	LEU
1	B	236	ILE
1	B	239	SER
1	B	244	GLU
1	B	246	LEU
1	B	250	LYS
1	B	253	ARG
1	B	263	ASN
1	B	279	VAL
1	B	280	THR
1	B	281	ASN
1	B	283	THR
1	B	288	THR
1	B	294	LEU
1	B	295	ILE
1	B	299	TYR
1	B	300	LEU
1	B	307	THR
1	B	308	GLN
1	B	309	GLU
1	B	310	ARG
1	B	311	ILE
1	B	319	ILE
1	B	332	GLU
1	B	334	SER
1	B	336	ARG

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Mol	Chain	Res	Type
1	B	343	ARG
1	B	347	GLU
1	B	350	THR
1	B	351	THR
1	B	353	TRP
1	B	360	SER
1	B	361	GLU
1	B	366	LEU
1	B	370	SER
1	B	373	LYS
1	B	375	ILE
1	B	377	ASN
1	B	378	GLU
1	B	385	CYS
1	B	388	GLN
1	B	389	ILE
1	B	392	LYS
1	B	399	LYS
1	B	401	THR
1	B	410	LEU
1	B	412	SER
1	B	416	TYR
1	B	420	ASN
1	B	423	LYS
1	B	429	ARG
1	B	437	SER
1	B	440	THR
1	B	458	SER
1	B	459	VAL
1	B	466	LYS
1	B	473	SER
1	B	479	LEU
1	B	481	THR
1	B	483	HIS
1	B	485	SER
1	B	486	VAL
1	B	488	ASP
1	B	500	LEU
1	B	507	VAL
1	B	508	GLN
1	B	514	LEU
1	B	519	LEU

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Mol	Chain	Res	Type
1	B	536	LYS
1	B	538	LYS
1	B	543	LEU
1	B	546	VAL
1	B	554	LYS
1	B	558	VAL
1	B	560	ARG
1	B	562	ASN
1	B	566	TYR
1	B	569	SER
1	B	577	SER
1	B	594	ILE
1	B	596	ARG
1	B	612	GLN
1	B	619	VAL
1	B	621	ASN
1	B	622	LYS
1	B	626	ILE
1	B	636	THR
1	B	637	SER
1	B	639	VAL
1	B	646	VAL
1	B	648	LYS
1	B	663	ASP
1	B	677	GLU
1	B	679	ASN
1	B	684	ARG
1	B	690	SER
1	B	696	LYS
1	B	715	GLN
1	B	720	SER
1	B	723	LEU
1	B	724	VAL
1	B	733	MET
1	B	745	SER
1	B	751	ILE
1	B	753	THR
1	B	759	ILE
1	B	760	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	72	GLN
1	A	74	ASN
1	A	75	ASN
1	A	103	ASN
1	A	119	ASN
1	A	141	GLN
1	A	169	ASN
1	A	263	ASN
1	A	369	ASN
1	A	377	ASN
1	A	388	GLN
1	A	420	ASN
1	A	483	HIS
1	A	487	ASN
1	A	508	GLN
1	A	520	ASN
1	A	533	HIS
1	A	553	GLN
1	A	572	ASN
1	A	586	GLN
1	A	592	HIS
1	A	621	ASN
1	A	679	ASN
1	A	710	ASN
1	A	715	GLN
1	A	748	HIS
1	A	750	HIS
1	B	51	ASN
1	B	103	ASN
1	B	119	ASN
1	B	123	GLN
1	B	126	HIS
1	B	138	ASN
1	B	162	HIS
1	B	263	ASN
1	B	281	ASN
1	B	298	HIS
1	B	377	ASN
1	B	420	ASN
1	B	430	ASN
1	B	455	GLN
1	B	469	GLN

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Mol	Chain	Res	Type
1	B	505	GLN
1	B	562	ASN
1	B	595	ASN
1	B	621	ASN
1	B	679	ASN
1	B	682	HIS
1	B	710	ASN
1	B	715	GLN
1	B	749	GLN
1	B	750	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	1767	1	14,14,15	0.50	0	17,19,21	1.22	3 (17%)
3	FPB	B	1771	-	30,30,30	0.71	1 (3%)	35,40,40	1.34	5 (14%)
2	NAG	A	1768	1	14,14,15	0.68	0	17,19,21	1.85	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	1770	1	14,14,15	0.71	0	17,19,21	0.92	0
2	NAG	A	1769	1	14,14,15	0.45	0	17,19,21	1.77	2 (11%)
2	NAG	B	1768	1	14,14,15	0.64	0	17,19,21	1.74	3 (17%)
2	NAG	B	1769	1	14,14,15	0.48	0	17,19,21	1.15	1 (5%)
3	FPB	A	1771	-	30,30,30	0.87	1 (3%)	35,40,40	1.10	2 (5%)
2	NAG	A	1767	1	14,14,15	0.51	0	17,19,21	1.06	2 (11%)
2	NAG	A	1770	1	14,14,15	0.53	0	17,19,21	1.32	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1767	1	-	5/6/23/26	0/1/1/1
3	FPB	B	1771	-	-	1/21/31/31	0/3/3/3
2	NAG	A	1768	1	-	4/6/23/26	0/1/1/1
2	NAG	B	1770	1	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	A	1769	1	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	B	1768	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1769	1	-	3/6/23/26	0/1/1/1
3	FPB	A	1771	-	-	0/21/31/31	0/3/3/3
2	NAG	A	1767	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1770	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1771	FPB	C22-N17	3.15	1.40	1.33
3	B	1771	FPB	C22-N17	2.08	1.38	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1768	NAG	C2-N2-C7	-5.21	115.91	122.90
2	A	1769	NAG	C4-C3-C2	-4.37	104.61	111.02
2	A	1769	NAG	C1-O5-C5	3.79	117.27	112.19
3	B	1771	FPB	C14-C15-N17	3.41	120.49	111.97
2	A	1770	NAG	O5-C1-C2	-3.41	106.02	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1768	NAG	C4-C3-C2	-3.12	106.45	111.02
2	A	1768	NAG	C1-O5-C5	3.07	116.31	112.19
2	A	1768	NAG	C6-C5-C4	-3.05	105.53	113.02
3	B	1771	FPB	C21-C14-C15	-2.94	101.19	112.17
2	B	1767	NAG	C4-C3-C2	-2.59	107.22	111.02
3	A	1771	FPB	C10-C11-C12	-2.45	108.61	112.67
3	B	1771	FPB	C10-C11-C12	2.45	116.73	112.67
2	B	1767	NAG	C3-C4-C5	-2.45	105.79	110.23
2	A	1770	NAG	C1-O5-C5	2.45	115.46	112.19
2	A	1770	NAG	C2-N2-C7	-2.31	119.80	122.90
2	A	1768	NAG	O3-C3-C2	2.25	114.08	109.40
3	B	1771	FPB	C2-C3-C5	2.25	120.49	116.62
3	B	1771	FPB	C4-C2-C3	-2.23	117.61	120.88
2	B	1768	NAG	O5-C5-C6	2.22	111.98	107.66
2	A	1768	NAG	C2-N2-C7	2.14	125.77	122.90
2	A	1767	NAG	O5-C5-C6	2.11	111.77	107.66
2	A	1768	NAG	C1-C2-N2	2.06	113.67	110.43
3	A	1771	FPB	C14-N13-C12	2.04	126.41	120.15
2	B	1769	NAG	O4-C4-C5	2.03	114.31	109.32
2	A	1767	NAG	O5-C1-C2	-2.02	108.17	111.29
2	B	1768	NAG	C3-C4-C5	-2.01	106.58	110.23
2	B	1767	NAG	O5-C1-C2	-2.01	108.18	111.29

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1769	NAG	C1
2	B	1770	NAG	C1

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1769	NAG	C8-C7-N2-C2
2	A	1769	NAG	O7-C7-N2-C2
2	B	1767	NAG	C1-C2-N2-C7
2	B	1767	NAG	C8-C7-N2-C2
2	B	1767	NAG	O7-C7-N2-C2
2	B	1770	NAG	C4-C5-C6-O6
2	B	1770	NAG	O5-C5-C6-O6
2	B	1768	NAG	C4-C5-C6-O6
2	B	1768	NAG	O5-C5-C6-O6
2	B	1767	NAG	O5-C5-C6-O6

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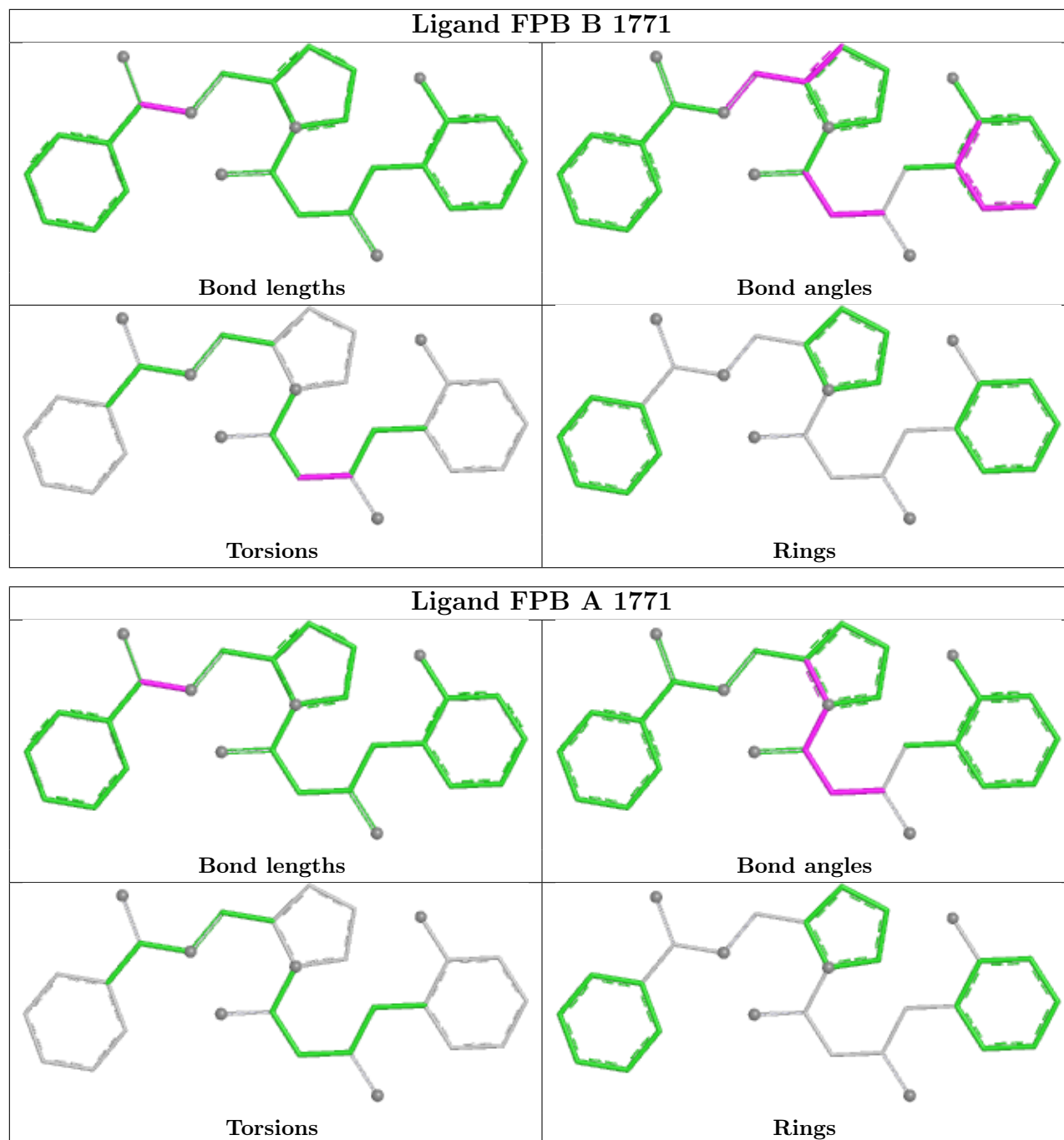
Mol	Chain	Res	Type	Atoms
2	A	1769	NAG	O5-C5-C6-O6
2	B	1767	NAG	C4-C5-C6-O6
2	A	1770	NAG	C8-C7-N2-C2
2	B	1770	NAG	C8-C7-N2-C2
2	A	1769	NAG	C4-C5-C6-O6
2	A	1768	NAG	C8-C7-N2-C2
2	A	1770	NAG	O7-C7-N2-C2
2	B	1770	NAG	O7-C7-N2-C2
2	A	1768	NAG	O7-C7-N2-C2
2	B	1769	NAG	C8-C7-N2-C2
2	B	1769	NAG	O7-C7-N2-C2
3	B	1771	FPB	C9-C10-C11-C12
2	A	1768	NAG	C4-C5-C6-O6
2	B	1769	NAG	O5-C5-C6-O6
2	A	1768	NAG	C1-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1771	FPB	4	0
2	B	1770	NAG	1	0
2	B	1769	NAG	1	0
3	A	1771	FPB	3	0
2	A	1767	NAG	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.