



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:26 PM UTC

PDB ID : 1TCM / pdb_00001tcm
Title : CYCLODEXTRIN GLYCOSYLTRANSFERASE W616A MUTANT FROM BACILLUS CIRCULANS STRAIN 251
Authors : Knegt, R.M.A.; Dijkstra, B.W.
Deposited on : 1996-10-07
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

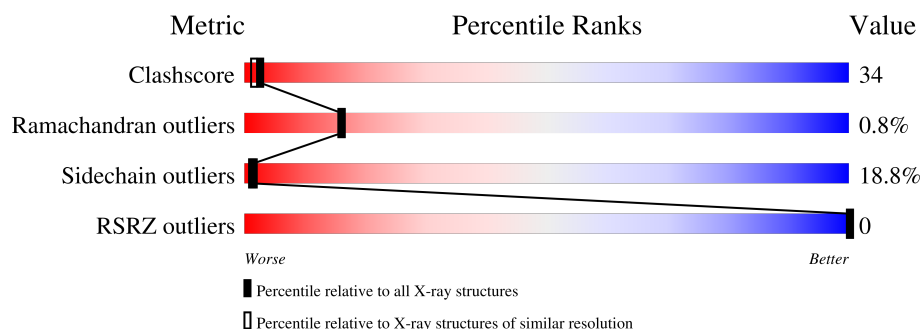
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	686	
1	B	686	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10779 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 CYCLODEXTRIN GLYCOSYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	686	Total	C	N	O	S	0	0	0
			5255	3313	899	1027	16			
1	B	686	Total	C	N	O	S	0	0	0
			5255	3313	899	1027	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	616	ALA	TRP	engineered mutation	UNP P43379
B	616	ALA	TRP	engineered mutation	UNP P43379

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		
2	B	2	Total	Ca	0	0
			2	2		

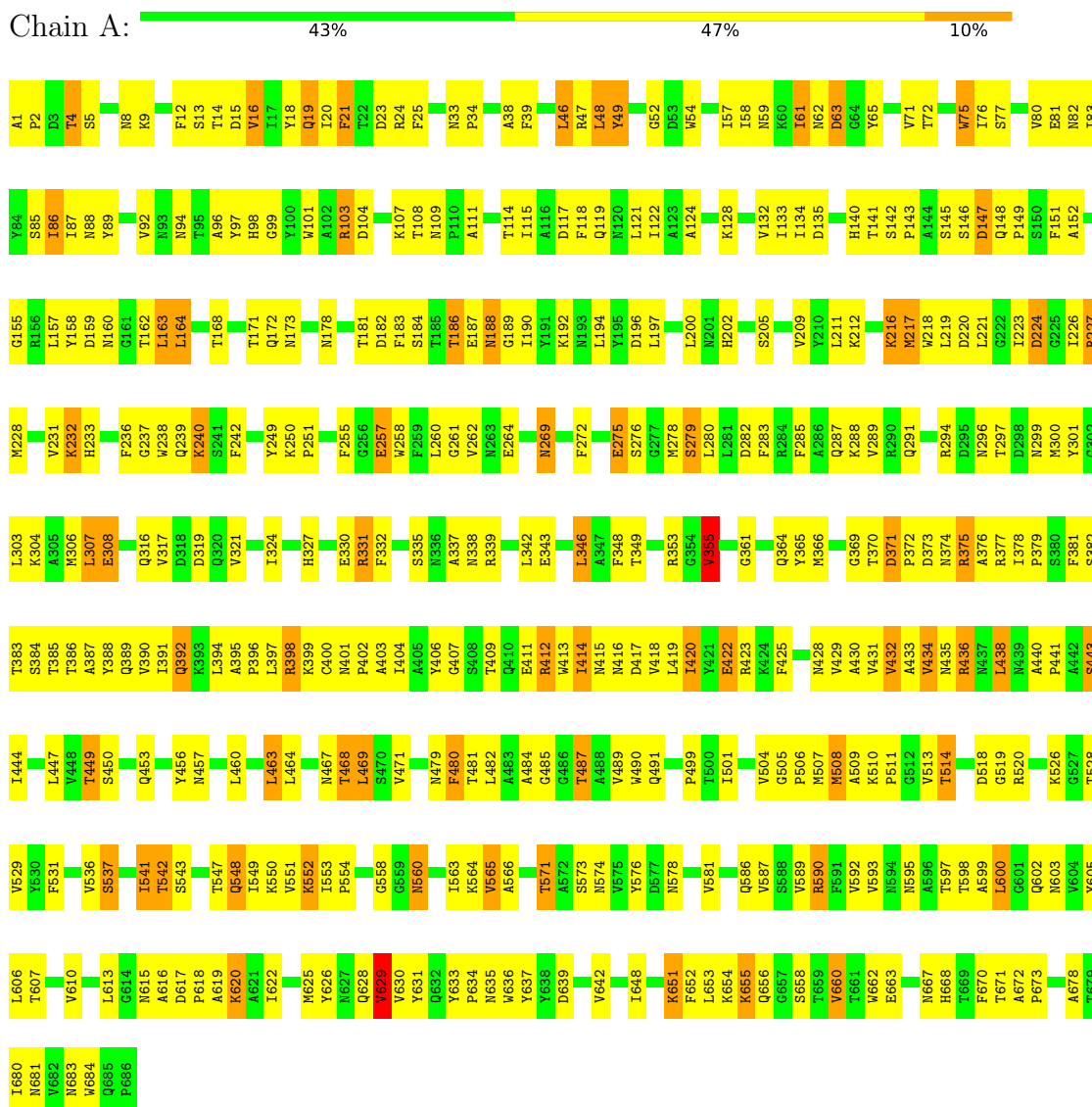
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	119	Total	O	0	0
			119	119		
3	B	146	Total	O	0	0
			146	146		

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: CYCLODEXTRIN GLYCOSYLTRANSFERASE



Y631	I563	L469	N401	R331	H233	D159	I87	A1
Q632	K564	G474	F402	F332	M234	L163	N88	P2
Y633	A565		A403	R333	P235		Y89	D3
P634	A566		I404	A334	P236		T4	T4
N635	N567	L482	A405	S335	G237	T168	S5	S5
N636	A568	G485	Y406	N336	W238	N169	V6	V6
Y637	A569		G407	A337	Q239	D170	S7	S7
Y638	G570		S408	R338	K240	T171	N8	N8
D639	T571	V489	T409	R339		Q172	A96	
V640	A572		Q410	R340	M243	N173	F12	F12
S641		T493	E411	K341		L174	H98	
V642	V575	A494	R412	L342	N248	F175	D15	D15
P643	Y576	A495	W413	E343	Y249	H176	Y16	Y16
	D577	T496	I414		K250	H177	I17	I17
R646	N578		N415	T351	P251	M178	Y18	Y18
T647	F579	G502	N416	S352	V252	G179	A102	A102
I648		H503	D417	R353	F253	G180	R103	R103
E649	L582	V504	V418	G354	T254	T181	K106	K106
F650		G505	L419	V355	F255	D182	K107	K107
K651	D585	P506	I420	P356	G256	F183	R24	R24
F652	Q586	M507	Y421	A357	E257	S184	T25	T25
L653	V587	M508	E422	I358		T185	N109	N109
K654	S588	A509	R423	Y359	L260	T186	P110	P110
K655	V589	K510	K424	Y360		E187	A111	A111
	R590	P511	F425	G361	N269	N188	Y112	Y112
S658	F591	G512	G426	T362	H270		G113	G113
T659	V592	V513	S427		K271	K192	T114	T114
V660	V593	T514	N428	Y365		N193	I115	I115
T661	N594	I515	V429	M366	G277	L194	F118	F118
V662		T516	A430		M278	Y195		
E663	T597	I517	V431	G369	S279	D196	L121	L121
	T598	A599	V432	T370	L280	A198	I122	I122
S666	A599	R520	A433	D371		D199	I130	I130
N667	L600	K526	N434	P372	K288	L200	K131	K131
H668			N435	D373	V289	N201	V132	V132
T669			R436	N374	R290	H202	D53	D53
F670	N603	Y530	N437	R375	Q291	N203	W54	W54
	Y604	F531	L438	A376	V292	N204	Q55	Q55
P673	L606	V536	N439	R377	F293	S205	G56	G56
	T607	S537	A440	I378	R294	T206	I57	I57
A678	G608	G538	S443			P138	P138	
T679	S609	A539	I444	S382	D298	Y210	K60	K60
I680	D540	D540	S445	T383	N299	L211	M69	M69
N681	T541	I541	G446	S384	M300	K212	G70	G70
W684	T542	T542	L447	T385	L303	D213	V71	V71
Q685	W544	W544	V448		K304	A214	T72	T72
P686			T449	Y388		I215	A144	A144
	D617		S450	Q389	Q316	K216	A73	A73
P618	P618	T547	L451	V390	V317	M217	I74	I74
A619	Q548	Q548	P452	I391	D318	Q148	W75	W75
K620	I549	I549	Y456	Q392	L219	P149	I76	I76
A621				K393	T223		S77	S77
T622	K652	K652	V459	L394	D224	A152	Q78	Q78
	T553	T553	P554	A395	G225	F153	P79	P79
Y626	P554	P554	L464	P396	T322	N154	V80	V80
N627	A555	A555	N465	L397	F323		E81	E81
Q628	V556	V556	T468	R398	I324		N82	N82
V629				K399		L157		
V630		N562		C400	E330	Y158	I86	I86

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.70Å 84.80Å 118.30Å 90.00° 107.00° 90.00°	Depositor
Resolution (Å)	6.50 – 2.20 6.50 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.50-2.20) 70.7 (6.50-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.21Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.193 , 0.250 0.240 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	15.3	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10779	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% 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: CA

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	0.67	1/5383 (0.0%)	1.03	10/7336 (0.1%)
1	B	0.68	1/5383 (0.0%)	1.02	14/7336 (0.2%)
All	All	0.67	2/10766 (0.0%)	1.03	24/14672 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	SER	C-O	-6.80	1.16	1.24
1	B	494	ALA	C-O	-6.31	1.15	1.23

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	ALA	N-CA-C	10.78	123.11	108.23
1	B	658	SER	N-CA-C	-8.59	102.34	113.17
1	B	494	ALA	CA-C-O	-8.02	112.52	121.51
1	B	395	ALA	O-C-N	7.46	126.27	120.38
1	B	599	ALA	N-CA-C	-7.31	98.07	108.96
1	A	335	SER	CA-C-O	7.17	128.37	120.63
1	A	349	THR	N-CA-C	6.76	119.49	111.71
1	B	599	ALA	CA-C-O	-6.67	114.31	121.45
1	B	76	ILE	N-CA-C	6.43	118.42	109.29
1	B	600	LEU	N-CA-C	6.13	118.89	110.24
1	B	668	HIS	N-CA-C	-5.80	103.28	110.41
1	A	668	HIS	N-CA-C	-5.56	102.25	110.48
1	B	277	GLY	N-CA-C	-5.52	106.90	115.67
1	A	275	GLU	N-CA-C	5.44	120.19	113.50
1	B	80	VAL	N-CA-C	5.40	115.93	110.05
1	A	648	ILE	N-CA-C	5.38	116.33	108.53
1	B	542	THR	N-CA-C	5.36	119.31	112.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	660	VAL	N-CA-C	5.31	115.61	108.17
1	B	292	VAL	N-CA-C	5.28	117.18	111.58
1	B	333	HIS	N-CA-C	5.26	116.83	108.67
1	B	474	GLY	N-CA-C	-5.22	108.06	115.43
1	A	414	ILE	N-CA-C	5.16	115.00	107.88
1	A	586	GLN	N-CA-C	5.12	117.66	110.14
1	A	355	VAL	N-CA-C	5.04	112.54	107.55

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5255	0	5020	372	0
1	B	5255	0	5020	332	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	119	0	0	10	0
3	B	146	0	0	14	0
All	All	10779	0	10040	700	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 34.

All (700) 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:413:TRP:HB3	1:A:420:ILE:HG13	1.19	1.14
1:A:285:PHE:HA	1:A:306:MET:HE2	1.25	1.09
1:A:38:ALA:HB2	1:A:86:ILE:HD11	1.35	1.07
1:A:618:PRO:HG3	1:A:662:TRP:HZ2	1.28	0.98
1:B:409:THR:HG23	1:B:423:ARG:HD3	1.48	0.95
1:B:299:ASN:HA	1:B:436:ARG:NH2	1.84	0.93
1:B:106:LYS:HB3	1:B:217:MET:HE1	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:MET:HG3	1:B:419:LEU:HB2	1.51	0.91
1:B:383:THR:HG22	1:B:388:TYR:CZ	2.06	0.90
1:A:432:VAL:HG13	1:A:489:VAL:HG22	1.53	0.89
1:B:517:ILE:HD13	1:B:563:ILE:HD11	1.54	0.89
1:B:240:LYS:HG2	1:B:508:MET:HE1	1.55	0.88
1:B:526:LYS:HE2	1:B:541:ILE:HB	1.56	0.86
1:B:25:PHE:CE2	1:B:60:LYS:HG3	2.10	0.86
1:B:25:PHE:HE2	1:B:60:LYS:HG3	1.37	0.86
1:B:48:LEU:HD12	1:B:95:THR:HG23	1.56	0.86
1:B:194:LEU:HB3	1:B:197:LEU:HD12	1.58	0.85
1:B:395:ALA:HB3	1:B:396:PRO:HD3	1.56	0.85
1:A:140:HIS:CD2	1:A:197:LEU:HD13	2.12	0.85
1:B:517:ILE:CD1	1:B:563:ILE:HD11	2.06	0.85
1:A:12:PHE:CE2	1:A:133:ILE:HD11	2.12	0.84
1:B:12:PHE:CE2	1:B:133:ILE:HD11	2.14	0.83
1:B:249:TYR:CE2	1:B:250:LYS:HD2	2.13	0.83
1:B:409:THR:HG23	1:B:423:ARG:CD	2.07	0.83
1:A:432:VAL:HG13	1:A:489:VAL:CG2	2.07	0.83
1:A:501:ILE:HD11	1:A:565:VAL:HG22	1.62	0.81
1:B:423:ARG:HG3	1:B:423:ARG:HH11	1.45	0.81
1:B:633:TYR:CD1	1:B:634:PRO:HA	2.16	0.80
1:A:395:ALA:HB3	1:A:396:PRO:HD3	1.62	0.80
1:A:260:LEU:HD22	1:A:264:GLU:HG2	1.63	0.79
1:A:331:ARG:NH1	1:A:366:MET:HE2	1.97	0.79
1:A:38:ALA:CB	1:A:86:ILE:HD11	2.12	0.79
1:A:285:PHE:HA	1:A:306:MET:CE	2.11	0.79
1:A:633:TYR:CD2	1:A:634:PRO:HA	2.17	0.79
1:B:633:TYR:HA	1:B:635:ASN:H	1.46	0.79
1:B:317:VAL:HG21	1:B:353:ARG:HD2	1.63	0.79
1:A:618:PRO:HG3	1:A:662:TRP:CZ2	2.16	0.79
1:B:317:VAL:HG22	1:B:353:ARG:HG3	1.65	0.78
1:A:251:PRO:HB3	1:A:506:PRO:HG3	1.63	0.78
1:B:17:ILE:HB	1:B:357:ALA:HA	1.64	0.78
1:A:389:GLN:HA	1:A:392:GLN:HG2	1.66	0.77
1:B:554:PRO:HB2	1:B:556:VAL:HG13	1.66	0.77
1:B:299:ASN:HA	1:B:436:ARG:HH22	1.48	0.77
1:A:240:LYS:HE3	1:A:508:MET:SD	2.26	0.76
1:B:300:MET:HB3	1:B:414:ILE:HD11	1.66	0.76
1:A:361:GLY:O	1:A:366:MET:HG3	1.86	0.76
1:B:351:THR:HG22	3:B:768:HOH:O	1.86	0.75
1:B:248:ASN:OD1	1:B:510:LYS:HG2	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:LEU:HD12	1:B:485:GLY:HA3	1.68	0.75
1:A:262:VAL:HG13	1:A:291:GLN:OE1	1.86	0.75
1:B:69:MET:HG3	1:B:388:TYR:CE2	2.21	0.75
1:A:598:THR:HG22	1:A:654:LYS:HE2	1.67	0.74
1:A:183:PHE:HA	3:A:711:HOH:O	1.86	0.74
1:A:589:VAL:HG22	1:A:678:ALA:HB3	1.69	0.74
1:A:536:VAL:HG11	1:A:551:VAL:HG21	1.68	0.74
1:B:289:VAL:HG11	1:B:324:ILE:HG22	1.69	0.74
1:B:251:PRO:HB3	1:B:506:PRO:HG3	1.69	0.73
1:A:386:THR:O	1:A:390:VAL:HG23	1.89	0.73
1:A:536:VAL:HG11	1:A:551:VAL:CG2	2.17	0.73
1:B:142:SER:HB2	1:B:143:PRO:HD2	1.69	0.73
1:A:520:ARG:HH11	1:A:520:ARG:HG2	1.53	0.73
1:A:38:ALA:O	1:A:49:TYR:HB2	1.89	0.72
1:A:673:PRO:HG2	1:A:678:ALA:HB2	1.71	0.72
1:B:138:PRO:HG2	1:B:228:MET:HE1	1.72	0.72
1:B:140:HIS:CD2	1:B:197:LEU:HD22	2.25	0.72
1:B:251:PRO:HB3	1:B:506:PRO:CG	2.20	0.72
1:B:108:THR:HG23	1:B:115:ILE:HD13	1.71	0.72
1:B:507:MET:HE3	1:B:579:PHE:HA	1.72	0.72
1:B:108:THR:CG2	1:B:115:ILE:HD13	2.19	0.71
1:B:642:VAL:HG12	1:B:643:PRO:HD2	1.73	0.71
1:B:4:THR:HG22	1:B:399:LYS:HD2	1.70	0.71
1:A:543:SER:OG	1:A:550:LYS:HB2	1.91	0.71
1:A:157:LEU:O	1:A:164:LEU:HB2	1.91	0.71
1:B:594:ASN:HA	1:B:635:ASN:HD22	1.55	0.70
1:B:564:LYS:HG2	1:B:565:VAL:N	2.05	0.70
1:B:590:ARG:HG3	1:B:639:ASP:OD1	1.92	0.70
1:A:220:ASP:OD1	1:A:250:LYS:HE2	1.92	0.69
1:B:250:LYS:O	1:B:252:VAL:HG13	1.91	0.69
1:A:108:THR:HG22	1:A:218:TRP:HH2	1.58	0.69
1:A:143:PRO:HB3	1:A:196:ASP:OD2	1.93	0.69
1:B:24:ARG:HG3	1:B:375:ARG:O	1.93	0.69
1:B:8:ASN:O	1:B:131:LYS:HE2	1.92	0.69
1:A:216:LYS:HG3	1:A:249:TYR:CE2	2.26	0.69
1:A:374:ASN:OD1	1:A:375:ARG:HD2	1.93	0.69
1:A:520:ARG:HD3	1:A:547:THR:HG22	1.74	0.68
1:B:226:ILE:HD12	1:B:252:VAL:CG2	2.22	0.68
1:B:594:ASN:HA	1:B:635:ASN:ND2	2.08	0.68
1:A:590:ARG:HB2	1:A:639:ASP:OD1	1.94	0.68
1:B:106:LYS:CB	1:B:217:MET:HE1	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:GLN:O	1:B:393:LYS:HG2	1.94	0.68
1:A:397:LEU:HD23	1:A:400:CYS:SG	2.34	0.68
1:B:317:VAL:HG21	1:B:353:ARG:HH11	1.58	0.67
1:B:46:LEU:HD22	1:B:376:ALA:HA	1.76	0.67
1:A:75:TRP:HA	1:A:133:ILE:O	1.95	0.67
1:B:592:VAL:HG22	1:B:637:TYR:HB3	1.76	0.67
1:A:108:THR:CG2	1:A:115:ILE:HD13	2.24	0.67
1:B:633:TYR:HA	1:B:635:ASN:N	2.09	0.67
1:A:21:PHE:HE2	1:A:327:HIS:HB3	1.60	0.67
1:A:460:LEU:CD1	1:A:464:LEU:HD12	2.24	0.67
1:B:654:LYS:HE2	1:B:684:TRP:CZ2	2.30	0.67
1:B:24:ARG:HH12	1:B:46:LEU:HB3	1.58	0.67
1:B:331:ARG:HD3	3:B:790:HOH:O	1.95	0.67
1:B:585:ASP:C	1:B:586:GLN:HG2	2.20	0.67
1:B:394:LEU:HD21	1:B:489:VAL:HG21	1.76	0.67
1:A:518:ASP:OD1	1:A:548:GLN:HB2	1.95	0.66
1:A:12:PHE:HA	1:A:15:ASP:OD2	1.95	0.66
1:B:563:ILE:HG23	1:B:576:TYR:HB3	1.76	0.66
1:A:299:ASN:OD1	1:A:301:TYR:HB2	1.94	0.66
1:A:316:GLN:HB2	3:A:696:HOH:O	1.95	0.66
1:B:414:ILE:HG13	1:B:415:ASN:N	2.09	0.66
1:A:261:GLY:O	1:A:264:GLU:HB3	1.96	0.66
1:A:12:PHE:O	1:A:355:VAL:HG13	1.96	0.66
1:A:217:MET:HE1	1:A:218:TRP:CE2	2.30	0.66
1:B:4:THR:CG2	1:B:399:LYS:HD2	2.25	0.66
1:A:304:LYS:HG2	1:A:308:GLU:OE2	1.96	0.66
1:B:26:SER:O	1:B:52:GLY:HA2	1.96	0.65
1:B:227:ARG:HG2	1:B:255:PHE:CE2	2.30	0.65
1:B:575:VAL:HG12	1:B:577:ASP:OD1	1.96	0.65
1:B:149:PRO:HG3	1:B:168:THR:HG21	1.78	0.65
1:A:308:GLU:HA	3:A:803:HOH:O	1.97	0.65
1:A:260:LEU:HB2	1:A:283:PHE:CB	2.26	0.65
1:B:290:ARG:HH11	1:B:290:ARG:HB3	1.61	0.65
1:A:108:THR:HG23	1:A:115:ILE:HD13	1.78	0.65
1:A:19:GLN:HG3	1:A:75:TRP:CE3	2.32	0.65
1:B:633:TYR:CG	1:B:634:PRO:HA	2.31	0.65
1:A:260:LEU:HB2	1:A:283:PHE:HB3	1.78	0.64
1:B:4:THR:HG22	1:B:399:LYS:CD	2.28	0.64
1:A:285:PHE:O	1:A:289:VAL:HG23	1.97	0.64
1:A:12:PHE:HB3	1:A:355:VAL:HG11	1.78	0.64
1:B:48:LEU:HD12	1:B:95:THR:CG2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ILE:CD1	1:A:223:ILE:HG21	2.28	0.64
1:A:272:PHE:CD2	1:A:280:LEU:HD21	2.33	0.64
1:A:420:ILE:HD12	1:A:447:LEU:CD1	2.27	0.64
1:A:134:ILE:HD13	1:A:223:ILE:HG21	1.80	0.64
1:B:178:ASN:HB3	1:B:192:LYS:HE2	1.79	0.64
1:A:509:ALA:HB1	1:A:513:VAL:HG21	1.79	0.63
1:A:192:LYS:HE3	1:A:629:VAL:CG1	2.28	0.63
1:A:413:TRP:HB3	1:A:420:ILE:CG1	2.12	0.63
1:B:540:ASP:O	1:B:552:LYS:HG3	1.98	0.63
1:B:331:ARG:CZ	1:B:366:MET:HE2	2.28	0.63
1:A:304:LYS:HE3	1:A:411:GLU:HB3	1.81	0.63
1:A:531:PHE:CD2	1:A:554:PRO:HG3	2.33	0.63
1:B:341:LYS:HG2	1:B:438:LEU:HD21	1.79	0.63
1:A:501:ILE:HD11	1:A:565:VAL:CG2	2.29	0.63
1:B:108:THR:HG23	1:B:115:ILE:CD1	2.29	0.63
1:B:226:ILE:HD12	1:B:252:VAL:HG21	1.81	0.63
1:B:240:LYS:CG	1:B:508:MET:HE1	2.27	0.63
1:B:410:GLN:HE21	1:B:412:ARG:HD2	1.63	0.63
1:A:8:ASN:HB3	3:A:785:HOH:O	1.99	0.62
1:A:513:VAL:HB	1:A:553:ILE:HD12	1.79	0.62
1:A:87:ILE:HD13	1:A:143:PRO:HG2	1.81	0.62
1:A:670:PHE:CE2	1:A:680:ILE:HD11	2.34	0.62
1:B:447:LEU:HB3	3:B:806:HOH:O	1.98	0.62
1:A:300:MET:SD	1:A:303:LEU:HD23	2.39	0.62
1:A:316:GLN:O	1:A:319:ASP:HB2	1.99	0.62
1:B:204:ASN:OD1	1:B:206:THR:HB	1.99	0.62
1:A:142:SER:HB2	1:A:143:PRO:HD2	1.81	0.62
1:A:560:ASN:ND2	1:A:578:ASN:HA	2.14	0.62
1:A:87:ILE:HD12	1:A:101:TRP:CZ3	2.35	0.62
1:A:192:LYS:HE3	1:A:629:VAL:HG13	1.79	0.62
1:A:285:PHE:CD1	1:A:306:MET:HE1	2.35	0.62
1:B:673:PRO:HG3	1:B:678:ALA:HB2	1.80	0.62
1:A:178:ASN:O	1:A:192:LYS:HE2	1.99	0.62
1:A:633:TYR:CG	1:A:634:PRO:HA	2.35	0.62
1:A:216:LYS:HE3	1:A:219:LEU:HD12	1.81	0.62
1:A:463:LEU:HD12	1:A:463:LEU:O	2.00	0.62
1:B:435:ASN:O	1:B:485:GLY:HA2	1.99	0.61
1:B:300:MET:CG	1:B:419:LEU:HB2	2.29	0.61
1:B:12:PHE:HB3	1:B:355:VAL:HG11	1.83	0.61
1:B:87:ILE:HG21	1:B:89:TYR:CE2	2.35	0.61
1:B:417:ASP:O	1:B:436:ARG:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:THR:HG23	1:A:115:ILE:CD1	2.30	0.61
1:B:300:MET:HE2	1:B:436:ARG:HG2	1.82	0.61
1:A:589:VAL:HG11	1:A:680:ILE:CD1	2.30	0.61
1:A:505:GLY:HA2	1:A:506:PRO:C	2.24	0.61
1:A:551:VAL:HG22	1:A:552:LYS:N	2.15	0.61
1:A:537:SER:HA	1:A:541:ILE:HD11	1.82	0.61
1:A:304:LYS:HE3	1:A:411:GLU:CB	2.31	0.61
1:B:423:ARG:HG3	1:B:423:ARG:NH1	2.15	0.61
1:A:420:ILE:HG21	1:A:447:LEU:HD11	1.83	0.61
1:B:504:VAL:HB	1:B:576:TYR:CE2	2.35	0.61
1:A:383:THR:HG22	1:A:388:TYR:CZ	2.35	0.60
1:B:182:ASP:OD2	1:B:184:SER:HB3	2.01	0.60
1:B:429:VAL:HG12	1:B:430:ALA:N	2.16	0.60
1:A:457:ASN:HA	1:A:468:THR:HG22	1.82	0.60
1:B:82:ASN:O	1:B:103:ARG:HD2	2.01	0.60
1:B:300:MET:HG3	1:B:419:LEU:CB	2.29	0.60
1:B:390:VAL:HG13	1:B:394:LEU:HD12	1.83	0.60
1:B:609:SER:HA	3:B:812:HOH:O	2.01	0.60
1:A:58:ILE:HG23	1:A:124:ALA:CB	2.31	0.60
1:A:602:GLN:HB2	1:A:656:GLN:HB3	1.84	0.60
1:A:511:PRO:HA	1:A:553:ILE:HG22	1.82	0.60
1:B:633:TYR:CA	1:B:635:ASN:H	2.14	0.60
1:A:81:GLU:CD	1:A:103:ARG:HD3	2.27	0.59
1:B:603:ASN:O	1:B:654:LYS:HA	2.02	0.59
1:B:414:ILE:HG13	1:B:415:ASN:H	1.66	0.59
1:A:469:LEU:HD21	1:A:471:VAL:CG2	2.32	0.59
1:B:142:SER:HB2	1:B:143:PRO:CD	2.32	0.59
1:B:147:ASP:C	1:B:149:PRO:HD3	2.28	0.59
1:B:106:LYS:HB3	1:B:217:MET:CE	2.27	0.59
1:B:403:ALA:O	1:B:423:ARG:HB3	2.02	0.59
1:A:272:PHE:HD2	1:A:280:LEU:HD21	1.68	0.59
1:A:592:VAL:HB	1:A:681:ASN:HA	1.83	0.59
1:A:625:MET:HE1	1:A:652:PHE:HE2	1.66	0.59
1:B:136:PHE:O	1:B:138:PRO:HD3	2.03	0.59
1:A:403:ALA:HA	1:A:425:PHE:CB	2.33	0.59
1:A:589:VAL:HG11	1:A:680:ILE:HD11	1.84	0.59
1:B:28:GLY:O	1:B:55:GLN:HG2	2.02	0.59
1:B:632:GLN:O	1:B:635:ASN:HB2	2.02	0.59
1:B:1:ALA:HB1	1:B:2:PRO:HD2	1.85	0.59
1:B:108:THR:O	1:B:110:PRO:HD3	2.03	0.59
1:B:617:ASP:OD2	1:B:620:LYS:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:ASP:OD1	1:A:436:ARG:HD2	2.03	0.59
1:B:195:TYR:HA	3:B:732:HOH:O	2.03	0.58
1:B:616:ALA:O	1:B:618:PRO:HD3	2.03	0.58
1:B:444:ILE:HD13	1:B:482:LEU:HB2	1.85	0.58
1:B:235:PRO:O	1:B:239:GLN:HG3	2.03	0.58
1:B:369:GLY:O	1:B:374:ASN:HB3	2.04	0.58
1:B:138:PRO:HB3	1:B:211:LEU:HD13	1.85	0.58
1:B:194:LEU:HD21	1:B:233:HIS:CD2	2.39	0.58
1:A:291:GLN:O	1:A:296:ASN:HA	2.03	0.57
1:A:364:GLN:OE1	1:A:385:THR:HG21	2.03	0.57
1:A:413:TRP:CZ3	1:A:418:VAL:HG11	2.39	0.57
1:A:653:LEU:CD1	1:A:655:LYS:HG2	2.34	0.57
1:A:435:ASN:O	1:A:485:GLY:HA2	2.03	0.57
1:A:514:THR:HB	3:A:746:HOH:O	2.03	0.57
1:B:57:ILE:HG21	1:B:121:LEU:HD11	1.86	0.57
1:A:260:LEU:CD2	1:A:264:GLU:HG2	2.32	0.57
1:A:499:PRO:O	1:A:573:SER:HB2	2.04	0.57
1:A:422:GLU:HB2	1:A:431:VAL:HG22	1.87	0.57
1:B:417:ASP:HA	1:B:436:ARG:HD2	1.86	0.57
1:A:361:GLY:HA3	1:A:366:MET:SD	2.44	0.57
1:B:517:ILE:HB	1:B:549:ILE:HB	1.87	0.57
1:A:653:LEU:HD12	1:A:653:LEU:C	2.29	0.57
1:B:317:VAL:CG2	1:B:353:ARG:HD2	2.34	0.57
1:B:630:VAL:HG23	1:B:637:TYR:OH	2.03	0.57
1:A:511:PRO:HA	1:A:553:ILE:CG2	2.35	0.57
1:B:318:ASP:HB2	3:B:722:HOH:O	2.03	0.57
1:B:353:ARG:HG2	1:B:354:GLY:N	2.17	0.57
1:B:403:ALA:O	1:B:407:GLY:HA3	2.04	0.57
1:A:34:PRO:HG2	1:A:49:TYR:CG	2.39	0.57
1:A:307:LEU:HD13	1:A:409:THR:HG21	1.86	0.57
1:B:136:PHE:C	1:B:138:PRO:HD3	2.29	0.57
1:A:464:LEU:HD12	1:A:487:THR:HG21	1.87	0.57
1:A:122:ILE:HD13	1:A:132:VAL:HG21	1.85	0.56
1:A:403:ALA:HB2	1:A:428:ASN:O	2.05	0.56
1:B:421:TYR:CZ	1:B:432:VAL:HB	2.40	0.56
1:A:9:LYS:HG2	1:A:224:ASP:HA	1.86	0.56
1:A:566:ALA:HA	1:A:571:THR:O	2.05	0.56
1:B:366:MET:SD	1:B:379:PRO:HD3	2.46	0.56
1:B:398:ARG:NH1	1:B:404:ILE:HG22	2.20	0.56
1:A:188:ASN:O	1:A:192:LYS:HG3	2.06	0.56
1:A:205:SER:O	1:A:209:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:ALA:O	1:A:602:GLN:HB3	2.05	0.56
1:B:219:LEU:HD13	1:B:250:LYS:HB2	1.88	0.56
1:B:517:ILE:HD11	1:B:563:ILE:HD11	1.87	0.56
1:A:654:LYS:HG3	1:A:684:TRP:CH2	2.41	0.56
1:A:19:GLN:HG3	1:A:75:TRP:CZ3	2.41	0.56
1:B:630:VAL:HG12	1:B:631:TYR:CE1	2.41	0.56
1:A:397:LEU:HA	1:A:400:CYS:SG	2.45	0.56
1:A:403:ALA:HA	1:A:425:PHE:HB3	1.88	0.56
1:A:467:ASN:HD21	1:A:480:PHE:HD2	1.52	0.56
1:A:504:VAL:HG11	1:A:563:ILE:HD12	1.88	0.56
1:B:531:PHE:CE2	1:B:554:PRO:HD3	2.41	0.56
1:A:403:ALA:O	1:A:423:ARG:HB3	2.06	0.56
1:A:520:ARG:HG2	1:A:520:ARG:NH1	2.19	0.55
1:A:670:PHE:CZ	1:A:680:ILE:HD11	2.41	0.55
1:A:499:PRO:HB2	1:A:573:SER:HB3	1.87	0.55
1:B:237:GLY:HA3	1:B:639:ASP:O	2.06	0.55
1:A:218:TRP:CE3	1:A:221:LEU:HD12	2.42	0.55
1:A:316:GLN:NE2	1:A:507:MET:HE2	2.21	0.55
1:B:243:MET:SD	1:B:254:THR:HG21	2.47	0.55
1:A:402:PRO:HG3	1:A:520:ARG:NH2	2.21	0.55
1:A:342:LEU:C	1:A:342:LEU:HD23	2.31	0.55
1:A:19:GLN:HG3	1:A:75:TRP:CD2	2.41	0.55
1:A:403:ALA:O	1:A:407:GLY:HA3	2.06	0.55
1:A:414:ILE:HG13	1:A:418:VAL:O	2.06	0.55
1:B:187:GLU:OE2	1:B:626:TYR:HB3	2.07	0.55
1:A:415:ASN:OD1	1:A:418:VAL:HB	2.07	0.54
1:A:460:LEU:O	1:A:463:LEU:HB2	2.07	0.54
1:A:227:ARG:NH1	1:A:257:GLU:HB2	2.22	0.54
1:B:406:TYR:HB2	1:B:425:PHE:CD2	2.42	0.54
1:A:444:ILE:N	1:A:444:ILE:HD12	2.22	0.54
1:A:558:GLY:HA2	1:A:581:VAL:O	2.08	0.54
1:A:605:TYR:CD1	1:A:655:LYS:HG3	2.42	0.54
1:B:188:ASN:O	1:B:192:LYS:HB2	2.07	0.54
1:A:307:LEU:HD11	3:A:693:HOH:O	2.07	0.54
1:B:290:ARG:HH11	1:B:290:ARG:CB	2.20	0.54
1:A:514:THR:OG1	1:A:552:LYS:HG3	2.08	0.54
1:B:1:ALA:HB1	1:B:2:PRO:CD	2.38	0.54
1:A:282:ASP:OD2	1:A:285:PHE:HB2	2.08	0.54
1:A:24:ARG:NH1	1:A:46:LEU:HD22	2.22	0.54
1:A:411:GLU:C	1:A:412:ARG:HG2	2.33	0.54
1:A:630:VAL:HB	1:A:637:TYR:CE2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:511:PRO:HA	1:B:553:ILE:HB	1.89	0.54
1:B:339:ARG:HD3	3:B:781:HOH:O	2.07	0.53
1:B:552:LYS:NZ	1:B:552:LYS:HB3	2.22	0.53
1:A:227:ARG:C	1:A:227:ARG:HD2	2.32	0.53
1:A:300:MET:HB3	1:A:414:ILE:HD11	1.90	0.53
1:B:223:ILE:HD12	1:B:225:GLY:O	2.08	0.53
1:B:303:LEU:HD23	1:B:419:LEU:CD2	2.39	0.53
1:B:650:PHE:CE1	1:B:670:PHE:HD1	2.26	0.53
1:A:158:TYR:CE2	1:A:163:LEU:HG	2.44	0.53
1:B:330:GLU:HB3	1:B:369:GLY:HA2	1.89	0.53
1:B:585:ASP:HA	3:B:766:HOH:O	2.07	0.53
1:A:54:TRP:HE1	1:A:76:ILE:HD12	1.73	0.53
1:A:62:ASN:HD22	1:A:128:LYS:HD2	1.73	0.53
1:B:418:VAL:HG13	1:B:434:VAL:O	2.07	0.53
1:A:92:VAL:HG23	1:A:94:ASN:HD21	1.73	0.53
1:B:585:ASP:O	1:B:586:GLN:HG2	2.08	0.53
1:A:223:ILE:HG13	1:A:223:ILE:O	2.07	0.53
1:A:135:ASP:OD1	1:A:227:ARG:HB3	2.09	0.53
1:A:560:ASN:HD21	1:A:578:ASN:HA	1.72	0.53
1:A:429:VAL:HG12	1:A:430:ALA:H	1.73	0.53
1:A:429:VAL:HG12	1:A:430:ALA:N	2.24	0.53
1:B:88:ASN:HB3	3:B:721:HOH:O	2.07	0.53
1:B:414:ILE:HD12	1:B:419:LEU:HD13	1.89	0.53
1:B:290:ARG:HH11	1:B:290:ARG:CG	2.22	0.53
1:B:317:VAL:HG22	1:B:353:ARG:CG	2.37	0.53
1:B:526:LYS:O	1:B:568:ALA:HB2	2.09	0.53
1:B:652:PHE:HB3	1:B:684:TRP:HZ3	1.74	0.53
1:B:317:VAL:CG2	1:B:353:ARG:HH11	2.21	0.52
1:A:324:ILE:HD12	1:A:332:PHE:CD2	2.44	0.52
1:A:383:THR:HG22	1:A:388:TYR:CE2	2.45	0.52
1:A:231:VAL:HG12	1:A:239:GLN:OE1	2.09	0.52
1:A:339:ARG:O	1:A:343:GLU:HG3	2.10	0.52
1:B:651:LYS:HG3	1:B:652:PHE:H	1.74	0.52
1:A:81:GLU:CG	1:A:103:ARG:HD3	2.40	0.52
1:A:186:THR:O	1:A:190:ILE:HG13	2.09	0.52
1:B:513:VAL:O	1:B:553:ILE:HG13	2.09	0.52
1:B:567:ASN:C	1:B:569:ALA:H	2.16	0.52
1:A:262:VAL:HG13	1:A:291:GLN:CD	2.34	0.52
1:B:615:ASN:HA	3:B:812:HOH:O	2.09	0.52
1:A:147:ASP:O	1:A:148:GLN:HG2	2.10	0.52
1:A:303:LEU:HD11	1:A:348:PHE:CZ	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:THR:HG22	1:B:193:ASN:O	2.10	0.52
1:B:289:VAL:CG1	1:B:324:ILE:HG22	2.38	0.52
1:A:142:SER:HB2	1:A:143:PRO:CD	2.39	0.52
1:B:506:PRO:HD2	1:B:515:ILE:HG22	1.91	0.52
1:A:371:ASP:HB2	1:A:375:ARG:CZ	2.40	0.52
1:A:61:ILE:HG22	1:A:62:ASN:N	2.24	0.51
1:A:228:MET:HE2	1:A:242:PHE:CD2	2.44	0.51
1:A:504:VAL:HG11	1:A:563:ILE:CD1	2.40	0.51
1:B:53:ASP:HB2	1:B:112:TYR:O	2.10	0.51
1:A:317:VAL:C	1:A:319:ASP:H	2.18	0.51
1:A:300:MET:SD	1:A:419:LEU:HB2	2.50	0.51
1:A:187:GLU:OE2	1:A:629:VAL:HG23	2.11	0.51
1:B:562:ASN:OD1	1:B:577:ASP:HB3	2.09	0.51
1:B:187:GLU:CD	1:B:626:TYR:HB3	2.36	0.51
1:B:339:ARG:HB3	1:B:365:TYR:CE2	2.46	0.51
1:A:5:SER:HA	3:A:801:HOH:O	2.10	0.51
1:B:73:ALA:HA	1:B:130:ILE:HG23	1.93	0.51
1:B:607:THR:OG1	1:B:616:ALA:HA	2.11	0.51
1:A:543:SER:HG	1:A:550:LYS:HB2	1.75	0.51
1:B:251:PRO:CB	1:B:506:PRO:HG3	2.40	0.51
1:B:290:ARG:O	1:B:294:ARG:HB3	2.11	0.51
1:B:592:VAL:HG22	1:B:637:TYR:CB	2.39	0.51
1:A:600:LEU:C	1:A:602:GLN:H	2.18	0.50
1:B:526:LYS:HE2	1:B:541:ILE:CB	2.36	0.50
1:B:652:PHE:HB2	1:B:684:TRP:CZ3	2.46	0.50
1:A:38:ALA:CA	1:A:86:ILE:HD11	2.42	0.50
1:A:87:ILE:CD1	1:A:143:PRO:HG2	2.41	0.50
1:A:260:LEU:HB2	1:A:283:PHE:HB2	1.92	0.50
1:B:361:GLY:O	1:B:366:MET:HG3	2.10	0.50
1:A:1:ALA:HB1	1:A:2:PRO:HD2	1.92	0.50
1:A:16:VAL:HG12	1:A:16:VAL:O	2.11	0.50
1:A:331:ARG:CD	1:A:366:MET:HB2	2.41	0.50
1:B:223:ILE:HD11	1:B:226:ILE:HD11	1.94	0.50
1:A:65:TYR:HB2	3:A:761:HOH:O	2.12	0.50
1:A:236:PHE:CZ	1:A:258:TRP:CZ3	3.00	0.50
1:A:464:LEU:HD12	1:A:487:THR:CG2	2.42	0.50
1:A:553:ILE:HG23	1:A:554:PRO:HD2	1.93	0.50
1:B:19:GLN:NE2	1:B:359:TYR:CD1	2.80	0.50
1:B:331:ARG:NH1	1:B:366:MET:HE2	2.26	0.50
1:B:653:LEU:HD12	1:B:660:VAL:HB	1.92	0.50
1:A:617:ASP:HB3	1:A:620:LYS:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:TRP:CH2	1:B:662:TRP:CD1	3.00	0.50
1:B:643:PRO:HB2	1:B:646:LYS:HG2	1.93	0.50
1:A:605:TYR:CE1	1:A:655:LYS:HG3	2.47	0.50
1:A:633:TYR:HA	1:A:635:ASN:N	2.26	0.50
1:A:236:PHE:N	1:A:236:PHE:CD1	2.80	0.50
1:A:480:PHE:N	1:A:480:PHE:CD1	2.80	0.49
1:B:251:PRO:HB3	1:B:506:PRO:HG2	1.92	0.49
1:A:378:ILE:HG21	1:A:381:PHE:CZ	2.47	0.49
1:B:395:ALA:HB3	1:B:396:PRO:CD	2.36	0.49
1:B:427:SER:H	1:B:496:THR:HG23	1.77	0.49
1:A:549:ILE:HG22	1:A:550:LYS:N	2.26	0.49
1:A:617:ASP:OD2	1:A:619:ALA:HB3	2.12	0.49
1:B:34:PRO:HG2	1:B:49:TYR:CG	2.46	0.49
1:A:140:HIS:HD2	1:A:197:LEU:HD22	1.76	0.49
1:A:226:ILE:HG22	1:A:227:ARG:N	2.27	0.49
1:B:101:TRP:HB3	1:B:142:SER:CB	2.42	0.49
1:A:172:GLN:O	1:A:173:ASN:HB2	2.12	0.49
1:B:564:LYS:HD2	1:B:572:ALA:HB1	1.94	0.49
1:A:432:VAL:HG13	1:A:489:VAL:HG23	1.94	0.49
1:B:17:ILE:CD1	1:B:133:ILE:HD12	2.42	0.49
1:A:457:ASN:HA	1:A:468:THR:CG2	2.42	0.49
1:B:201:ASN:OD1	1:B:203:ASN:HB3	2.12	0.49
1:B:636:TRP:CD1	1:B:636:TRP:N	2.80	0.49
1:A:4:THR:HG22	1:A:399:LYS:HD2	1.93	0.49
1:B:106:LYS:CA	1:B:217:MET:HE1	2.42	0.49
1:A:464:LEU:CD1	1:A:487:THR:HG21	2.43	0.49
1:A:87:ILE:HG21	1:A:89:TYR:CZ	2.48	0.49
1:A:339:ARG:HB3	1:A:365:TYR:CE2	2.47	0.49
1:B:269:ASN:C	1:B:269:ASN:HD22	2.21	0.49
1:B:201:ASN:C	1:B:203:ASN:H	2.21	0.48
1:B:330:GLU:CB	1:B:369:GLY:HA2	2.43	0.48
1:A:82:ASN:OD1	1:A:99:GLY:HA2	2.13	0.48
1:A:602:GLN:HA	1:A:655:LYS:O	2.13	0.48
1:B:139:ASN:HB3	3:B:695:HOH:O	2.12	0.48
1:B:509:ALA:HA	1:B:582:LEU:HD12	1.94	0.48
1:A:610:VAL:CG2	1:A:613:LEU:HB2	2.42	0.48
1:B:383:THR:HG22	1:B:388:TYR:CE2	2.48	0.48
1:A:75:TRP:CE2	1:A:227:ARG:HG3	2.48	0.48
1:A:202:HIS:HB3	1:A:238:TRP:CD1	2.48	0.48
1:A:300:MET:HE1	1:A:434:VAL:HG12	1.96	0.48
1:A:504:VAL:HB	1:A:576:TYR:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:PHE:O	1:A:663:GLU:HB2	2.12	0.48
1:B:101:TRP:HB3	1:B:142:SER:HB3	1.96	0.48
1:B:610:VAL:HG11	1:B:648:ILE:HG13	1.96	0.48
1:A:662:TRP:CZ3	1:B:662:TRP:CD1	3.02	0.48
1:A:118:PHE:O	1:A:121:LEU:HB3	2.14	0.48
1:A:531:PHE:CE2	1:A:554:PRO:HD3	2.48	0.48
1:A:18:TYR:CE1	1:A:20:ILE:HG12	2.48	0.48
1:A:33:ASN:ND2	1:A:39:PHE:CZ	2.81	0.48
1:A:108:THR:HG22	1:A:218:TRP:CH2	2.43	0.48
1:A:420:ILE:HG23	1:A:433:ALA:HB2	1.95	0.48
1:B:642:VAL:HG12	1:B:643:PRO:CD	2.43	0.48
1:B:659:THR:O	1:B:659:THR:HG22	2.14	0.48
1:A:47:ARG:NE	1:A:372:PRO:HG3	2.29	0.48
1:B:598:THR:HG23	1:B:636:TRP:HZ2	1.78	0.48
1:A:287:GLN:HA	1:A:287:GLN:OE1	2.14	0.48
1:B:610:VAL:HG11	1:B:648:ILE:CG1	2.44	0.48
1:B:652:PHE:CB	1:B:684:TRP:HZ3	2.27	0.48
1:A:228:MET:HE2	1:A:242:PHE:CE2	2.48	0.47
1:B:38:ALA:O	1:B:49:TYR:HB2	2.14	0.47
1:B:288:LYS:HE3	1:B:298:ASP:OD2	2.14	0.47
1:A:181:THR:OG1	1:A:189:GLY:HA2	2.15	0.47
1:A:316:GLN:HE21	1:A:507:MET:HG3	1.79	0.47
1:A:508:MET:HB3	1:A:508:MET:HE2	1.64	0.47
1:B:172:GLN:HB3	1:B:174:LEU:HD21	1.95	0.47
1:A:134:ILE:HD11	1:A:223:ILE:HD13	1.95	0.47
1:B:159:ASP:OD1	1:B:210:TYR:HE1	1.97	0.47
1:A:440:ALA:O	1:A:484:ALA:HA	2.14	0.47
1:A:519:GLY:O	1:A:547:THR:HA	2.14	0.47
1:B:24:ARG:HA	1:B:24:ARG:HD3	1.55	0.47
1:A:389:GLN:CA	1:A:392:GLN:HG2	2.42	0.47
1:B:12:PHE:O	1:B:355:VAL:HG13	2.15	0.47
1:A:48:LEU:HD12	1:A:48:LEU:HA	1.80	0.47
1:A:456:TYR:HB3	1:A:490:TRP:HB3	1.96	0.47
1:A:464:LEU:HB3	1:A:487:THR:HB	1.97	0.47
1:B:333:HIS:HE1	1:B:337:ALA:O	1.95	0.47
1:B:502:GLY:O	1:B:503:HIS:HB2	2.13	0.47
1:B:650:PHE:N	1:B:650:PHE:CD1	2.83	0.47
1:B:459:VAL:HG23	1:B:489:VAL:O	2.14	0.47
1:B:504:VAL:HG12	1:B:505:GLY:N	2.30	0.47
1:A:651:LYS:HB2	1:A:651:LYS:HE2	1.60	0.46
1:B:434:VAL:HG12	1:B:435:ASN:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:VAL:O	1:A:541:ILE:HD11	2.14	0.46
1:B:219:LEU:HD12	1:B:249:TYR:HD2	1.80	0.46
1:B:506:PRO:O	1:B:579:PHE:HE2	1.98	0.46
1:A:108:THR:HG21	1:A:115:ILE:HD13	1.94	0.46
1:A:413:TRP:CE3	1:A:418:VAL:HG11	2.50	0.46
1:A:236:PHE:N	1:A:236:PHE:HD1	2.13	0.46
1:A:589:VAL:CG1	1:A:680:ILE:HD12	2.45	0.46
1:B:75:TRP:CZ2	1:B:227:ARG:HG3	2.50	0.46
1:B:541:ILE:O	1:B:541:ILE:HG22	2.16	0.46
1:B:564:LYS:HG2	1:B:565:VAL:H	1.75	0.46
1:A:14:THR:O	1:A:398:ARG:HB2	2.16	0.46
1:A:447:LEU:HD21	1:A:449:THR:CG2	2.46	0.46
1:B:366:MET:HE3	1:B:366:MET:HB3	1.77	0.46
1:B:651:LYS:HE3	1:B:663:GLU:O	2.16	0.46
1:A:369:GLY:H	1:A:373:ASP:HB2	1.79	0.46
1:A:398:ARG:HE	1:A:398:ARG:HB3	1.48	0.46
1:B:24:ARG:NH1	1:B:46:LEU:HB3	2.28	0.46
1:B:300:MET:CE	1:B:436:ARG:HG2	2.44	0.46
1:A:83:ILE:HD12	1:A:85:SER:OG	2.16	0.46
1:A:140:HIS:CD2	1:A:197:LEU:HD22	2.51	0.46
1:A:285:PHE:CE1	1:A:348:PHE:HE1	2.33	0.46
1:B:19:GLN:HG3	1:B:75:TRP:CE3	2.50	0.46
1:A:417:ASP:O	1:A:436:ARG:HG3	2.16	0.46
1:A:528:THR:OG1	1:A:537:SER:HB3	2.15	0.46
1:A:610:VAL:HG23	1:A:613:LEU:H	1.81	0.46
1:B:146:SER:O	1:B:168:THR:HG23	2.16	0.46
1:A:25:PHE:HD2	1:A:57:ILE:HG13	1.81	0.46
1:A:182:ASP:OD2	1:A:184:SER:HB3	2.15	0.46
1:A:202:HIS:HB3	1:A:238:TRP:NE1	2.31	0.46
1:A:300:MET:CE	1:A:434:VAL:HG12	2.45	0.46
1:B:510:LYS:O	1:B:513:VAL:HG23	2.15	0.46
1:B:600:LEU:HD22	1:B:600:LEU:HA	1.71	0.46
1:B:610:VAL:CG1	1:B:648:ILE:HG13	2.46	0.46
1:B:673:PRO:CG	1:B:678:ALA:HB2	2.44	0.46
1:A:61:ILE:HG22	1:A:62:ASN:ND2	2.30	0.46
1:B:98:HIS:ND1	1:B:100:TYR:HB2	2.31	0.46
1:A:430:ALA:HA	1:A:491:GLN:HA	1.98	0.45
1:A:467:ASN:ND2	1:A:480:PHE:HD2	2.14	0.45
1:B:134:ILE:HD12	1:B:135:ASP:O	2.16	0.45
1:A:285:PHE:CZ	1:A:348:PHE:HE1	2.34	0.45
1:A:610:VAL:HG22	1:A:613:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:THR:O	1:B:323:PHE:HB3	2.16	0.45
1:A:38:ALA:HB2	1:A:86:ILE:CD1	2.25	0.45
1:A:187:GLU:OE1	1:A:626:TYR:HB3	2.16	0.45
1:A:438:LEU:HD12	1:A:438:LEU:HA	1.82	0.45
1:B:236:PHE:CD1	1:B:236:PHE:N	2.80	0.45
1:B:397:LEU:O	1:B:401:ASN:HB3	2.17	0.45
1:A:216:LYS:CE	1:A:219:LEU:HD12	2.44	0.45
1:A:526:LYS:HE2	1:A:541:ILE:HB	1.97	0.45
1:B:336:ASN:N	1:B:336:ASN:HD22	2.14	0.45
1:B:444:ILE:HD12	1:B:444:ILE:N	2.30	0.45
1:A:103:ARG:HG2	1:A:104:ASP:N	2.32	0.45
1:A:593:VAL:HG12	1:A:636:TRP:HB2	1.97	0.45
1:A:630:VAL:HB	1:A:637:TYR:CZ	2.52	0.45
1:B:290:ARG:HH12	1:B:294:ARG:NH1	2.14	0.45
1:A:14:THR:O	1:A:399:LYS:HD3	2.16	0.45
1:A:81:GLU:HB2	1:A:108:THR:O	2.17	0.45
1:A:200:LEU:HD13	1:A:211:LEU:HD11	1.98	0.45
1:A:615:ASN:O	1:A:616:ALA:HB3	2.17	0.45
1:A:653:LEU:HD13	1:A:655:LYS:HG2	1.97	0.45
1:B:215:ILE:O	1:B:219:LEU:HG	2.17	0.45
1:B:57:ILE:HG13	3:B:764:HOH:O	2.17	0.45
1:B:224:ASP:O	1:B:252:VAL:HB	2.17	0.45
1:B:365:TYR:HE1	1:B:385:THR:HB	1.82	0.45
1:A:655:LYS:HB3	1:A:655:LYS:HE2	1.46	0.45
1:B:331:ARG:NH1	1:B:366:MET:CE	2.80	0.45
1:B:452:PRO:HD2	1:B:456:TYR:OH	2.17	0.45
1:B:548:GLN:HG2	1:B:549:ILE:N	2.32	0.45
1:B:652:PHE:CB	1:B:684:TRP:CZ3	3.00	0.45
1:A:101:TRP:HA	1:A:141:THR:O	2.17	0.45
1:A:147:ASP:C	1:A:148:GLN:HG2	2.41	0.45
1:A:406:TYR:HB2	1:A:425:PHE:CD2	2.52	0.45
1:B:426:GLY:HA3	1:B:496:THR:HG21	1.99	0.45
1:B:505:GLY:HA2	1:B:506:PRO:C	2.42	0.45
1:B:530:TYR:O	1:B:563:ILE:HA	2.17	0.45
1:B:648:ILE:HG22	1:B:649:GLU:N	2.31	0.45
1:A:269:ASN:C	1:A:269:ASN:HD22	2.25	0.44
1:A:387:ALA:O	1:A:391:ILE:HG13	2.17	0.44
1:B:317:VAL:CG2	1:B:353:ARG:NH1	2.80	0.44
1:B:397:LEU:HD11	1:B:459:VAL:HG11	1.99	0.44
1:A:15:ASP:HB3	1:A:72:THR:OG1	2.16	0.44
1:A:444:ILE:N	1:A:444:ILE:CD1	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:TRP:CH2	1:B:662:TRP:NE1	2.86	0.44
1:B:520:ARG:HD3	1:B:547:THR:HG22	1.99	0.44
1:A:59:ASN:O	1:A:63:ASP:HB3	2.17	0.44
1:A:610:VAL:HG23	1:A:613:LEU:N	2.32	0.44
1:B:25:PHE:HE2	1:B:60:LYS:CG	2.19	0.44
1:A:58:ILE:HG23	1:A:124:ALA:HB1	2.00	0.44
1:A:420:ILE:HG21	1:A:447:LEU:CD1	2.48	0.44
1:B:98:HIS:HB2	1:B:100:TYR:CD2	2.52	0.44
1:B:429:VAL:HG12	1:B:430:ALA:H	1.79	0.44
1:B:648:ILE:CG2	1:B:649:GLU:N	2.80	0.44
1:A:81:GLU:HG2	1:A:103:ARG:HD3	2.00	0.44
1:A:92:VAL:HG23	1:A:94:ASN:ND2	2.32	0.44
1:A:228:MET:CE	1:A:242:PHE:CD2	3.01	0.44
1:A:551:VAL:CG2	1:A:552:LYS:N	2.80	0.44
1:A:407:GLY:HA2	1:A:425:PHE:HB2	1.99	0.44
1:B:290:ARG:HH12	1:B:294:ARG:HH11	1.66	0.44
1:B:647:THR:O	1:B:647:THR:HG22	2.17	0.44
1:A:440:ALA:HA	1:A:441:PRO:HD3	1.73	0.44
1:B:71:VAL:O	1:B:71:VAL:HG12	2.18	0.44
1:B:78:GLN:HA	1:B:79:PRO:HD3	1.72	0.44
1:B:383:THR:HG22	1:B:388:TYR:CE1	2.51	0.44
1:B:630:VAL:CG2	1:B:637:TYR:CE2	3.01	0.44
1:A:24:ARG:NH2	1:A:97:TYR:CE2	2.85	0.44
1:A:149:PRO:HG3	1:A:168:THR:HG21	2.00	0.44
1:A:662:TRP:CD1	1:B:651:LYS:HE2	2.53	0.44
1:B:426:GLY:HA3	1:B:496:THR:CG2	2.47	0.44
1:B:504:VAL:CG1	1:B:505:GLY:N	2.80	0.44
1:A:54:TRP:O	1:A:58:ILE:HG13	2.18	0.44
1:A:520:ARG:CD	1:A:547:THR:HG22	2.47	0.44
1:A:82:ASN:HD22	1:A:82:ASN:N	2.16	0.43
1:A:303:LEU:HD21	1:A:348:PHE:CE2	2.53	0.43
1:A:537:SER:HA	1:A:541:ILE:CD1	2.47	0.43
1:B:87:ILE:CG2	1:B:89:TYR:CE2	3.01	0.43
1:A:114:THR:H	1:A:117:ASP:HB2	1.83	0.43
1:A:251:PRO:HB3	1:A:506:PRO:CG	2.42	0.43
1:A:413:TRP:CZ3	1:A:418:VAL:CG1	3.01	0.43
1:B:598:THR:HG23	1:B:636:TRP:CZ2	2.53	0.43
1:A:651:LYS:HB2	3:A:765:HOH:O	2.17	0.43
1:A:232:LYS:HG3	1:A:258:TRP:CE2	2.53	0.43
1:B:6:VAL:O	1:B:6:VAL:HG22	2.18	0.43
1:B:219:LEU:HD13	1:B:250:LYS:CB	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:LEU:O	1:B:465:ASN:HB2	2.17	0.43
1:A:413:TRP:CE3	1:A:418:VAL:CG1	3.01	0.43
1:B:429:VAL:CG1	1:B:430:ALA:N	2.80	0.43
1:A:403:ALA:HA	1:A:425:PHE:HB2	1.99	0.43
1:B:86:ILE:HG21	1:B:93:ASN:ND2	2.33	0.43
1:A:23:ASP:HA	1:A:52:GLY:HA3	1.99	0.43
1:A:46:LEU:HD11	1:A:376:ALA:HB2	2.01	0.43
1:A:151:PHE:O	1:A:152:ALA:HB3	2.19	0.43
1:A:481:THR:O	1:A:481:THR:HG22	2.17	0.43
1:B:339:ARG:O	1:B:343:GLU:HG3	2.18	0.43
1:B:536:VAL:CG1	1:B:540:ASP:HB2	2.48	0.43
1:B:617:ASP:HB2	1:B:620:LYS:NZ	2.34	0.43
1:B:12:PHE:HA	1:B:15:ASP:OD1	2.19	0.43
1:B:187:GLU:OE1	1:B:628:GLN:HG3	2.19	0.43
1:B:331:ARG:HE	1:B:331:ARG:HB3	1.45	0.43
1:B:554:PRO:HB2	1:B:556:VAL:CG1	2.44	0.43
1:A:115:ILE:O	1:A:119:GLN:HG3	2.19	0.42
1:A:272:PHE:O	1:A:276:SER:HB3	2.19	0.42
1:B:278:MET:O	1:B:278:MET:HG2	2.19	0.42
1:B:684:TRP:O	1:B:686:PRO:HD3	2.19	0.42
1:A:378:ILE:HG21	1:A:381:PHE:CE1	2.53	0.42
1:A:467:ASN:ND2	1:A:480:PHE:CD2	2.81	0.42
1:B:49:TYR:CE1	1:B:97:TYR:HA	2.54	0.42
1:B:185:THR:OG1	1:B:188:ASN:HB2	2.19	0.42
1:B:290:ARG:CG	1:B:290:ARG:NH1	2.81	0.42
1:B:339:ARG:HB3	1:B:365:TYR:CD2	2.54	0.42
1:B:468:THR:CG2	1:B:469:LEU:N	2.82	0.42
1:B:243:MET:HE1	1:B:254:THR:OG1	2.19	0.42
1:B:439:ASN:O	1:B:440:ALA:HB2	2.19	0.42
1:B:680:ILE:H	1:B:680:ILE:HG12	1.53	0.42
1:A:460:LEU:HD11	1:A:464:LEU:HD12	2.00	0.42
1:A:549:ILE:CG2	1:A:550:LYS:N	2.81	0.42
1:A:346:LEU:HD23	1:A:346:LEU:HA	1.77	0.42
1:A:633:TYR:HA	1:A:634:PRO:C	2.45	0.42
1:B:19:GLN:HG3	1:B:75:TRP:CD2	2.54	0.42
1:B:82:ASN:OD1	1:B:99:GLY:HA2	2.18	0.42
1:A:565:VAL:HG23	1:A:573:SER:OG	2.20	0.42
1:B:122:ILE:HD12	1:B:122:ILE:HA	1.74	0.42
1:B:176:HIS:HB3	1:B:178:ASN:ND2	2.34	0.42
1:B:234:MET:HE3	1:B:239:GLN:CD	2.44	0.42
1:B:393:LYS:HG2	1:B:393:LYS:H	1.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:526:LYS:HA	1:B:544:TRP:CD2	2.54	0.42
1:A:21:PHE:CE2	1:A:327:HIS:HB3	2.47	0.42
1:A:159:ASP:O	1:A:160:ASN:HB3	2.20	0.42
1:A:397:LEU:HD23	1:A:397:LEU:HA	1.80	0.42
1:A:479:ASN:N	1:A:479:ASN:HD22	2.18	0.42
1:B:45:ASN:C	1:B:47:ARG:H	2.28	0.42
1:B:257:GLU:HB2	1:B:281:LEU:HD12	2.01	0.42
1:A:388:TYR:O	1:A:392:GLN:HB3	2.19	0.42
1:B:548:GLN:O	1:B:549:ILE:HG13	2.20	0.42
1:B:240:LYS:HD3	1:B:641:SER:HB3	2.01	0.42
1:B:507:MET:CE	1:B:579:PHE:HA	2.47	0.42
1:A:1:ALA:HB1	1:A:2:PRO:CD	2.50	0.42
1:A:283:PHE:O	1:A:287:GLN:HG2	2.20	0.42
1:A:371:ASP:HA	1:A:374:ASN:OD1	2.20	0.42
1:A:401:ASN:OD1	1:A:428:ASN:HB3	2.20	0.42
1:A:440:ALA:C	1:A:484:ALA:HB2	2.44	0.42
1:B:646:LYS:HA	1:B:646:LYS:HD3	1.39	0.42
1:A:631:TYR:HB2	1:A:637:TYR:CD1	2.55	0.41
1:A:251:PRO:CB	1:A:506:PRO:HG3	2.44	0.41
1:A:667:ASN:HA	3:A:765:HOH:O	2.19	0.41
1:B:17:ILE:HB	1:B:357:ALA:CA	2.43	0.41
1:B:157:LEU:HD11	1:B:210:TYR:CE2	2.54	0.41
1:B:374:ASN:HA	3:B:790:HOH:O	2.21	0.41
1:B:654:LYS:CE	1:B:684:TRP:CZ2	3.00	0.41
1:A:142:SER:OG	1:A:155:GLY:HA2	2.20	0.41
1:A:216:LYS:HA	1:A:219:LEU:HB2	2.02	0.41
1:A:613:LEU:HA	1:A:622:ILE:HD11	2.02	0.41
1:A:96:ALA:HA	1:A:98:HIS:CE1	2.55	0.41
1:A:226:ILE:CG2	1:A:227:ARG:N	2.84	0.41
1:A:285:PHE:CZ	1:A:348:PHE:CE1	3.09	0.41
1:B:255:PHE:CD2	1:B:321:VAL:HG21	2.55	0.41
1:B:548:GLN:HG2	1:B:549:ILE:H	1.84	0.41
1:A:236:PHE:HZ	1:A:258:TRP:CH2	2.38	0.41
1:B:87:ILE:HD11	1:B:152:ALA:HB2	2.01	0.41
1:B:339:ARG:H	1:B:339:ARG:HG3	1.62	0.41
1:B:393:LYS:HE3	1:B:393:LYS:HB3	1.97	0.41
1:A:412:ARG:HE	1:A:412:ARG:HB3	1.45	0.41
1:A:672:ALA:HA	1:A:673:PRO:HD3	1.81	0.41
1:B:417:ASP:CB	1:B:436:ARG:HD2	2.51	0.41
1:A:114:THR:O	1:A:117:ASP:HB2	2.21	0.41
1:A:300:MET:HE1	1:A:434:VAL:CG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:ILE:HD12	1:A:447:LEU:HD13	2.01	0.41
1:B:101:TRP:HA	1:B:141:THR:O	2.21	0.41
1:B:210:TYR:CD2	1:B:211:LEU:HD23	2.55	0.41
1:A:75:TRP:HB2	1:A:133:ILE:HB	2.01	0.41
1:A:228:MET:CE	1:A:242:PHE:CE2	3.03	0.41
1:A:378:ILE:O	1:A:378:ILE:HG23	2.21	0.41
1:B:409:THR:HG23	1:B:423:ARG:HD2	1.96	0.41
1:B:618:PRO:O	1:B:655:LYS:HE3	2.20	0.41
1:A:378:ILE:HA	1:A:379:PRO:HD3	1.93	0.41
1:A:435:ASN:HB2	1:A:482:LEU:CD2	2.51	0.41
1:B:517:ILE:HD13	1:B:563:ILE:CD1	2.39	0.41
1:A:385:THR:O	1:A:389:GLN:HG3	2.20	0.40
1:A:402:PRO:HG3	1:A:520:ARG:CZ	2.51	0.40
1:B:170:ASP:HB3	1:B:177:HIS:NE2	2.36	0.40
1:B:411:GLU:HA	1:B:421:TYR:HA	2.02	0.40
1:A:236:PHE:CZ	1:A:258:TRP:HZ3	2.39	0.40
1:A:443:SER:C	1:A:444:ILE:HD12	2.46	0.40
1:B:54:TRP:CZ3	1:B:118:PHE:HB2	2.56	0.40
1:B:180:GLY:HA2	1:B:193:ASN:HB2	2.03	0.40
1:B:237:GLY:HA2	3:B:762:HOH:O	2.21	0.40
1:B:322:THR:C	1:B:323:PHE:HD1	2.29	0.40
1:B:605:TYR:CE1	1:B:655:LYS:HB2	2.56	0.40
1:A:237:GLY:HA3	1:A:639:ASP:O	2.22	0.40
1:A:617:ASP:CG	1:A:620:LYS:HZ2	2.28	0.40
1:B:69:MET:O	1:B:391:ILE:HG22	2.22	0.40
1:B:280:LEU:H	1:B:320:GLN:HE21	1.68	0.40
1:A:75:TRP:CD1	1:A:75:TRP:C	3.00	0.40
1:A:109:ASN:OD1	1:A:111:ALA:HB3	2.22	0.40
1:A:194:LEU:HD21	1:A:233:HIS:CE1	2.56	0.40
1:A:278:MET:HG3	1:A:279:SER:O	2.22	0.40
1:A:353:ARG:O	1:A:353:ARG:HG2	2.21	0.40
1:A:366:MET:HE2	1:A:366:MET:HB3	1.85	0.40
1:B:371:ASP:HA	1:B:372:PRO:HA	1.54	0.40
1:A:219:LEU:HD23	1:A:219:LEU:HA	1.86	0.40
1:A:255:PHE:CD2	1:A:321:VAL:HG21	2.57	0.40
1:A:603:ASN:O	1:A:654:LYS:HA	2.21	0.40
1:B:564:LYS:HE2	1:B:564:LYS:HB3	1.78	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	684/686 (100%)	608 (89%)	72 (10%)	4 (1%)	21	23
1	B	684/686 (100%)	602 (88%)	75 (11%)	7 (1%)	12	11
All	All	1368/1372 (100%)	1210 (88%)	147 (11%)	11 (1%)	16	16

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	338	ASN
1	B	22	THR
1	B	539	ALA
1	A	46	LEU
1	A	629	VAL
1	B	585	ASP
1	A	542	THR
1	B	46	LEU
1	B	195	TYR
1	B	627	ASN
1	B	629	VAL

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	555/555 (100%)	451 (81%)	104 (19%)	1	1
1	B	555/555 (100%)	450 (81%)	105 (19%)	1	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1110/1110 (100%)	901 (81%)	209 (19%)	1 1

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	13	SER
1	A	16	VAL
1	A	19	GLN
1	A	21	PHE
1	A	48	LEU
1	A	49	TYR
1	A	61	ILE
1	A	63	ASP
1	A	71	VAL
1	A	75	TRP
1	A	77	SER
1	A	80	VAL
1	A	86	ILE
1	A	88	ASN
1	A	103	ARG
1	A	107	LYS
1	A	145	SER
1	A	146	SER
1	A	147	ASP
1	A	162	THR
1	A	163	LEU
1	A	164	LEU
1	A	171	THR
1	A	186	THR
1	A	188	ASN
1	A	212	LYS
1	A	216	LYS
1	A	217	MET
1	A	224	ASP
1	A	227	ARG
1	A	232	LYS
1	A	240	LYS
1	A	257	GLU
1	A	269	ASN
1	A	275	GLU
1	A	279	SER

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Mol	Chain	Res	Type
1	A	288	LYS
1	A	294	ARG
1	A	297	THR
1	A	307	LEU
1	A	308	GLU
1	A	330	GLU
1	A	331	ARG
1	A	346	LEU
1	A	355	VAL
1	A	370	THR
1	A	371	ASP
1	A	375	ARG
1	A	377	ARG
1	A	382	SER
1	A	384	SER
1	A	392	GLN
1	A	394	LEU
1	A	398	ARG
1	A	404	ILE
1	A	412	ARG
1	A	416	ASN
1	A	420	ILE
1	A	422	GLU
1	A	432	VAL
1	A	434	VAL
1	A	436	ARG
1	A	438	LEU
1	A	443	SER
1	A	449	THR
1	A	450	SER
1	A	453	GLN
1	A	463	LEU
1	A	468	THR
1	A	469	LEU
1	A	480	PHE
1	A	487	THR
1	A	508	MET
1	A	510	LYS
1	A	514	THR
1	A	529	VAL
1	A	537	SER
1	A	541	ILE

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Mol	Chain	Res	Type
1	A	542	THR
1	A	548	GLN
1	A	552	LYS
1	A	560	ASN
1	A	564	LYS
1	A	565	VAL
1	A	571	THR
1	A	574	ASN
1	A	587	VAL
1	A	590	ARG
1	A	595	ASN
1	A	597	THR
1	A	600	LEU
1	A	606	LEU
1	A	607	THR
1	A	620	LYS
1	A	628	GLN
1	A	629	VAL
1	A	642	VAL
1	A	651	LYS
1	A	655	LYS
1	A	658	SER
1	A	660	VAL
1	A	671	THR
1	A	683	ASN
1	B	4	THR
1	B	5	SER
1	B	17	ILE
1	B	19	GLN
1	B	24	ARG
1	B	26	SER
1	B	46	LEU
1	B	48	LEU
1	B	57	ILE
1	B	69	MET
1	B	71	VAL
1	B	74	ILE
1	B	75	TRP
1	B	76	ILE
1	B	78	GLN
1	B	82	ASN
1	B	87	ILE

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Mol	Chain	Res	Type
1	B	88	ASN
1	B	90	SER
1	B	114	THR
1	B	122	ILE
1	B	134	ILE
1	B	135	ASP
1	B	145	SER
1	B	148	GLN
1	B	154	ASN
1	B	157	LEU
1	B	163	LEU
1	B	173	ASN
1	B	186	THR
1	B	194	LEU
1	B	199	ASP
1	B	200	LEU
1	B	205	SER
1	B	213	ASP
1	B	216	LYS
1	B	227	ARG
1	B	234	MET
1	B	257	GLU
1	B	260	LEU
1	B	269	ASN
1	B	271	LYS
1	B	278	MET
1	B	279	SER
1	B	288	LYS
1	B	290	ARG
1	B	300	MET
1	B	303	LEU
1	B	304	LYS
1	B	316	GLN
1	B	331	ARG
1	B	335	SER
1	B	336	ASN
1	B	339	ARG
1	B	341	LYS
1	B	342	LEU
1	B	353	ARG
1	B	362	THR
1	B	375	ARG

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Mol	Chain	Res	Type
1	B	377	ARG
1	B	378	ILE
1	B	382	SER
1	B	383	THR
1	B	393	LYS
1	B	404	ILE
1	B	409	THR
1	B	412	ARG
1	B	414	ILE
1	B	415	ASN
1	B	427	SER
1	B	436	ARG
1	B	438	LEU
1	B	443	SER
1	B	445	SER
1	B	448	VAL
1	B	450	SER
1	B	493	THR
1	B	496	THR
1	B	508	MET
1	B	514	THR
1	B	517	ILE
1	B	537	SER
1	B	542	THR
1	B	543	SER
1	B	552	LYS
1	B	571	THR
1	B	577	ASP
1	B	588	SER
1	B	597	THR
1	B	600	LEU
1	B	606	LEU
1	B	613	LEU
1	B	622	ILE
1	B	630	VAL
1	B	632	GLN
1	B	640	VAL
1	B	642	VAL
1	B	646	LYS
1	B	647	THR
1	B	651	LYS
1	B	658	SER

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Mol	Chain	Res	Type
1	B	660	VAL
1	B	666	SER
1	B	680	ILE
1	B	681	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	62	ASN
1	A	88	ASN
1	A	120	ASN
1	A	139	ASN
1	A	188	ASN
1	A	269	ASN
1	A	333	HIS
1	A	344	GLN
1	A	410	GLN
1	A	416	ASN
1	A	439	ASN
1	A	479	ASN
1	A	548	GLN
1	A	560	ASN
1	A	595	ASN
1	A	603	ASN
1	A	632	GLN
1	A	681	ASN
1	A	683	ASN
1	A	685	GLN
1	B	11	ASN
1	B	19	GLN
1	B	32	ASN
1	B	62	ASN
1	B	88	ASN
1	B	93	ASN
1	B	94	ASN
1	B	119	GLN
1	B	120	ASN
1	B	139	ASN
1	B	160	ASN
1	B	169	ASN
1	B	178	ASN

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Mol	Chain	Res	Type
1	B	202	HIS
1	B	233	HIS
1	B	263	ASN
1	B	269	ASN
1	B	316	GLN
1	B	336	ASN
1	B	392	GLN
1	B	410	GLN
1	B	416	ASN
1	B	479	ASN
1	B	578	ASN
1	B	594	ASN
1	B	632	GLN
1	B	635	ASN
1	B	681	ASN
1	B	685	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	686/686 (100%)	-1.73	0 100 100	2, 18, 35, 64	0
1	B	686/686 (100%)	-1.76	0 100 100	2, 16, 33, 53	0
All	All	1372/1372 (100%)	-1.75	0 100 100	2, 17, 34, 64	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	B	688	1/1	0.95	0.06	11,11,11,11	0
2	CA	B	687	1/1	0.99	0.01	15,15,15,15	0
2	CA	A	688	1/1	0.99	0.02	12,12,12,12	0
2	CA	A	687	1/1	1.00	0.01	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.