



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:35 PM UTC

PDB ID : 2Z87 / pdb_00002z87
Title : Crystal structure of chondroitin polymerase from Escherichia coli strain K4 (K4CP) complexed with UDP-GalNAc and UDP
Authors : Osawa, T.; Sugiura, N.; Shimada, H.; Hirooka, R.; Tsuji, A.; Kimura, M.; Kimata, K.; Kakuta, Y.
Deposited on : 2007-09-03
Resolution : 3.00 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

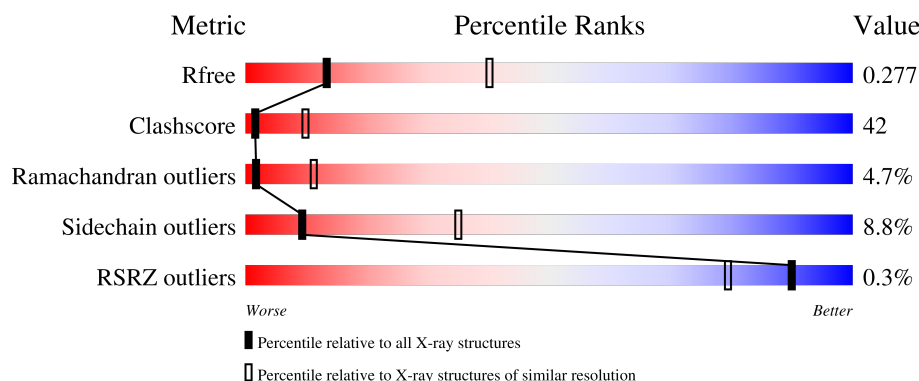
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

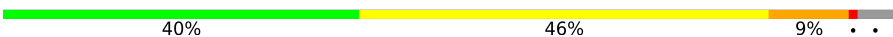
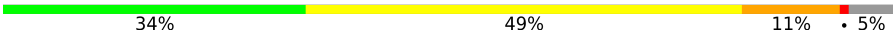
The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	624	
1	B	624	

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
3	UDP	A	684	-	-	X	-

2 Entry composition [i](#)

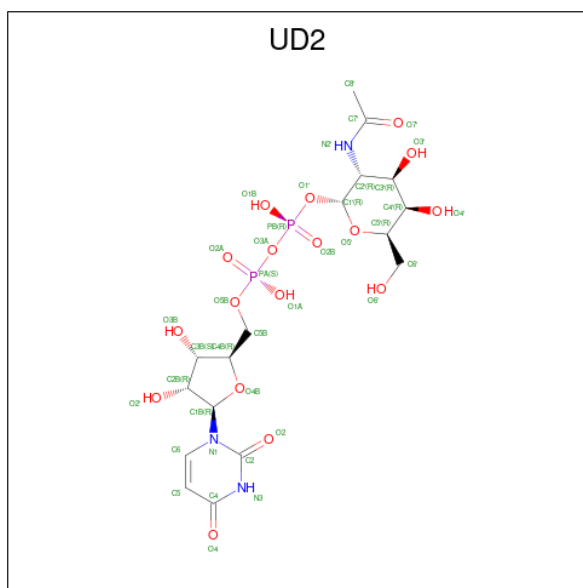
There are 5 unique types of molecules in this entry. The entry contains 9983 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Chondroitin synthase.

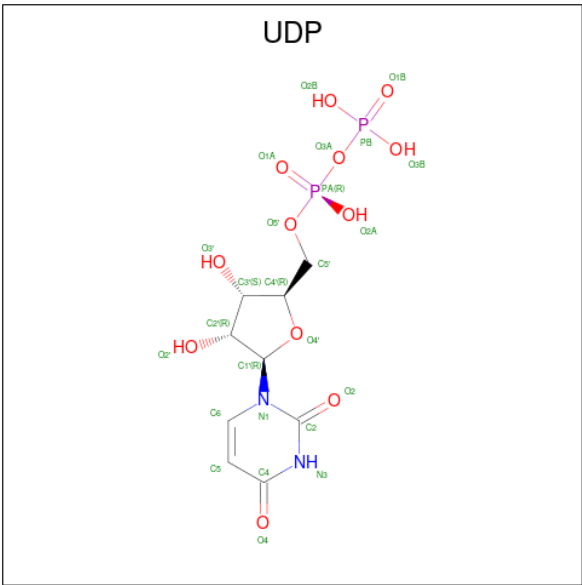
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	601	Total	C	N	O	S	25	0	0
			4894	3119	835	916	24			
1	B	591	Total	C	N	O	S	25	0	0
			4816	3071	822	899	24			

- Molecule 2 is URIDINE-DIPHOSPHATE-N-ACETYLGALACTOSAMINE (CCD ID: UD2) (formula: $C_{17}H_{27}N_3O_{17}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
2	B	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mn	0	0
			2	2		
4	B	2	Total	Mn	0	0
			2	2		

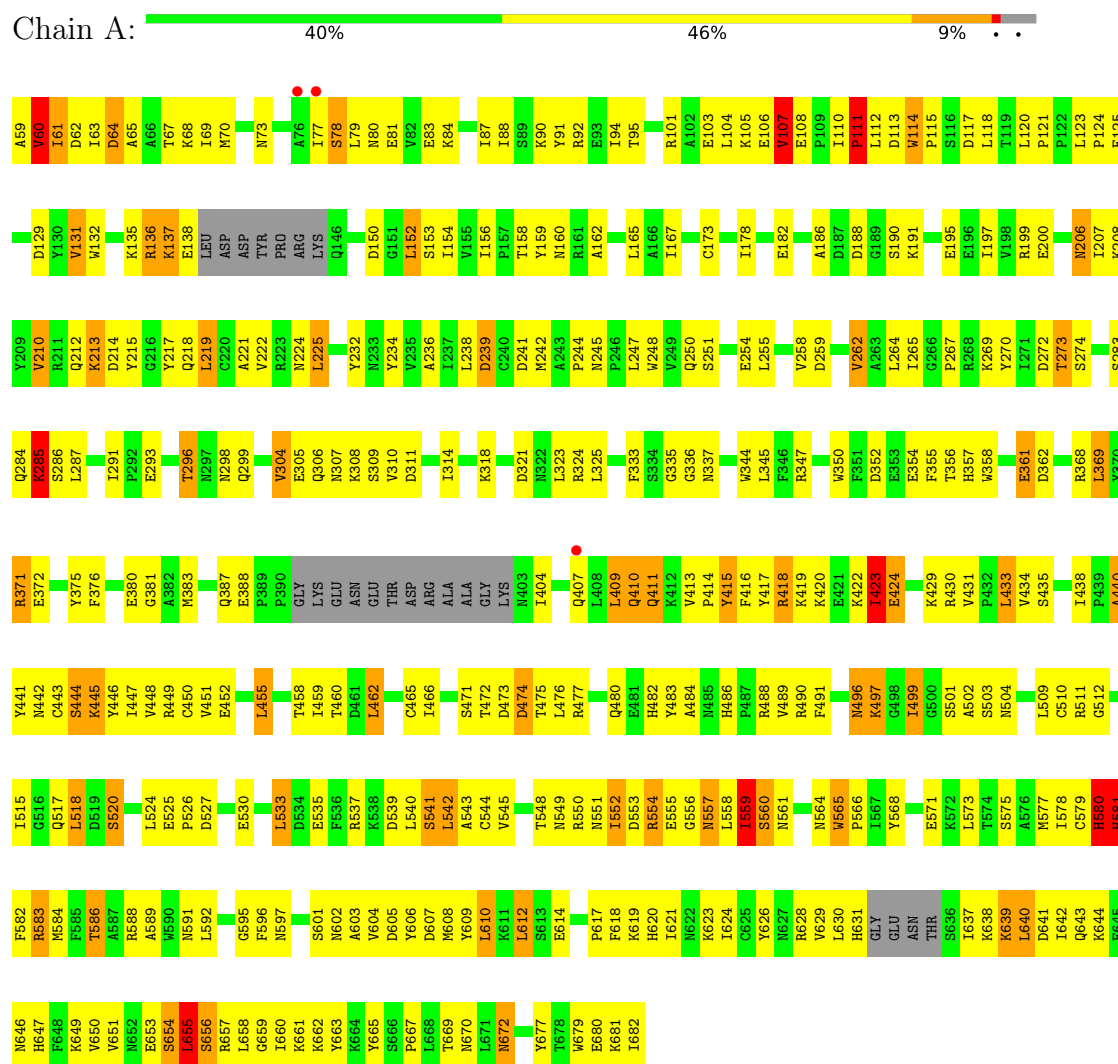
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	78	Total	O	0	0
			78	78		
5	B	63	Total	O	0	0
			63	63		

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: Chondroitin synthase



• Molecule 1: Chondroitin synthase



L630	H631	GLY	GLU	N634	K638	K639	L642	Q643	K644	E645	N646	H647	F648	K649	V650	V651	N652	E653	S654	L655	S656	R657	L658	G659	I660	K661	K662	Y663	K664	Y665	S666	L668	T669	N670	L671	N672	Y677	K681	I682																		
G562	Y563	N564	W565	K497	G498	I499	S503	N504	T505	R508	L509	C510	R511	G512	F513	Y514	Q517	L518	D519	D522	L524	E525	F526	D527	A528	V529	E530	L531	C532	L533	F536	R537	R538	D539	L540	S541	L542	A543	C544	V545	N549	R550	N551	I552	D553	R554	E555	G556	N557	L558	I559	S560	N561				
K422	I423	A426	T427	L428	K429	R430	V431	P432	L433	V434	S435	I436	Y437	I438	N442	I447	V448	R449	C450	V451	F452	S453	T458	L462	F463	V464	C465	L466	C467	D468	D469	C470	S471	T472	D473	D474	T475	L476	R477	Q480	E481	H482	Y483	A484	N485	H486	P487	V488	V489	R490	F491	S492	S493				
Q494	K495	N496	K497	G498	I499	S503	N504	T505	R508	L509	C510	R511	G512	F513	Y514	Q517	L518	D519	D522	L524	E525	F526	D527	A528	V529	E530	L531	C532	L533	F536	R537	R538	D539	L540	S541	L542	A543	C544	V545	N549	R550	N551	I552	D553	R554	E555	G556	N557	L558	I559	S560	N561					
T356	R357	W358	G359	K360	E361	D362	N363	E364	Y367	F368	L369	Y370	R371	F376	R377	S378	E380	Y385	H386	Q387	E388	P389	P390	G391	K392	GLU	ASN	GLU	L466	C467	D468	D469	C470	S471	T472	D473	D474	T475	L476	R477	Q480	E481	H482	Y483	A484	N485	H486	P487	V488	V489	R490	F491	S492	S493			
S286	L287	I288	N289	E290	I291	P292	E293	I294	I295	T296	N297	ASN	GLN	VAL	ALA	ALA	GLY	LYS	VAL	GLU	Q306	N307	K308	S309	V310	D311	W312	R313	I314	K318	N319	T320	D321	N322	L323	M324	L325	C326	N327	T328	P329	F330	R331	F332	F333	S334	G335	G336	N337	V338	A341	W344	L345	W350	F351	K420	D352
N206	I207	K208	Y209	V210	R211	Q212	Y215	G216	Y217	Q218	L219	C220	A221	V222	R223	N224	L225	G226	L227	L238	D239	C240	D241	M242	N245	P246	L247	V248	V249	Q250	S251	Y252	M253	E254	L255	V258	V262	I265	G266	P267	R268	K269	Y270	I271	T273	Y278	L279	S283	K285								
A59	V60	I61	D62	I63	D64	A65	A66	T67	K68	I69	LEU	ASP	TYR	PRO	ARG	A74	K75	L79	N80	E81	V82	E83	K84	N85	E86	I87	I88	S89	K90	Y91	R92	E93	I94	T95	A96	A102	E103	L104	K105	E106	V107	E108	F109	I110	P111	W114	P115	L118	T119	L120	P121	R122	L123	P124	E125	S126	
D129	Y130	V131	W132	K135	R136	K137	GLU	LEU	ASP	TYR	PRO	ARG	A74	LYS	Q146	D150	G151	L152	V155	I156	P157	T158	Y159	N160	R161	L164	L165	A166	I167	L172	Q175	K176	T177	I178	V185	A186	D187	D188	K191	E192	N193	I194	E195	V198	R199	E200	F201	E202									

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.37Å 109.28Å 85.58Å 90.00° 103.47° 90.00°	Depositor
Resolution (Å)	19.96 – 3.00 19.96 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.3 (19.96-3.00) 93.0 (19.96-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.199 , 0.283 0.198 , 0.277	Depositor DCC
R_{free} test set	1440 reflections (4.39%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.565	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9983	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, UDP, UD2

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	0.87	18/4998 (0.4%)	1.10	44/6761 (0.7%)
1	B	0.84	17/4919 (0.3%)	1.05	33/6651 (0.5%)
All	All	0.86	35/9917 (0.4%)	1.07	77/13412 (0.6%)

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
1	B	0	2
All	All	0	3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	581	HIS	C-O	-21.11	0.98	1.23
1	A	581	HIS	C-O	-19.92	0.99	1.24
1	A	582	PHE	C-O	-16.67	1.04	1.23
1	A	583	ARG	C-O	-16.63	1.02	1.23
1	A	581	HIS	CA-C	-15.62	1.33	1.52
1	B	583	ARG	C-O	-15.59	1.04	1.24
1	A	582	PHE	CA-C	-14.54	1.35	1.52
1	B	581	HIS	CA-C	-13.81	1.35	1.53
1	B	583	ARG	CA-C	-13.74	1.36	1.52
1	A	583	ARG	CZ-NH1	-13.65	1.13	1.32
1	B	582	PHE	C-O	-12.66	1.07	1.23
1	B	583	ARG	CZ-NH1	-11.79	1.16	1.32
1	B	582	PHE	CE1-CZ	-10.43	1.07	1.38
1	A	581	HIS	CA-CB	-10.35	1.39	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	582	PHE	CE1-CZ	-9.82	1.09	1.38
1	A	582	PHE	CE2-CZ	-9.72	1.09	1.38
1	B	583	ARG	CZ-NH2	-9.64	1.21	1.33
1	A	583	ARG	CZ-NH2	-9.47	1.21	1.33
1	B	582	PHE	CE2-CZ	-9.31	1.10	1.38
1	B	582	PHE	CG-CD2	-9.22	1.19	1.38
1	B	582	PHE	CA-C	-9.04	1.41	1.52
1	A	582	PHE	CG-CD2	-8.84	1.20	1.38
1	A	583	ARG	CA-C	-8.82	1.42	1.52
1	A	582	PHE	CD2-CE2	-7.96	1.14	1.38
1	B	581	HIS	CA-CB	-7.88	1.42	1.53
1	A	582	PHE	CD1-CE1	-7.66	1.15	1.38
1	B	582	PHE	CG-CD1	-7.66	1.22	1.38
1	A	581	HIS	N-CA	-7.30	1.37	1.46
1	B	582	PHE	CD2-CE2	-7.01	1.17	1.38
1	B	583	ARG	NE-CZ	-6.78	1.25	1.33
1	A	583	ARG	NE-CZ	-6.71	1.25	1.33
1	A	582	PHE	CG-CD1	-6.42	1.25	1.38
1	B	581	HIS	N-CA	-5.38	1.39	1.46
1	A	581	HIS	CE1-NE2	-5.20	1.27	1.32
1	B	583	ARG	N-CA	-5.01	1.40	1.46

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	565	TRP	CA-C-N	12.14	135.02	119.84
1	A	565	TRP	C-N-CA	12.14	135.02	119.84
1	A	417	TYR	N-CA-C	10.99	123.01	111.14
1	A	583	ARG	NE-CZ-NH2	9.63	127.86	119.20
1	B	291	ILE	CA-C-N	8.39	128.15	119.76
1	B	291	ILE	C-N-CA	8.39	128.15	119.76
1	A	581	HIS	CA-C-O	-8.25	111.19	120.43
1	B	656	SER	N-CA-C	-8.06	103.00	112.92
1	B	62	ASP	N-CA-C	7.88	117.55	108.49
1	A	207	ILE	N-CA-C	7.66	120.51	108.87
1	B	541	SER	N-CA-C	-7.61	103.07	111.36
1	B	610	LEU	N-CA-C	-7.49	101.26	112.04
1	A	656	SER	N-CA-C	-7.46	103.44	112.54
1	B	358	TRP	N-CA-C	7.36	120.26	109.07
1	A	610	LEU	N-CA-C	-7.33	102.68	111.69
1	A	520	SER	N-CA-C	7.31	119.88	111.11
1	B	108	GLU	CA-C-N	7.25	128.91	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	108	GLU	C-N-CA	7.25	128.91	119.84
1	A	581	HIS	CA-C-N	7.21	134.44	121.89
1	A	581	HIS	C-N-CA	7.21	134.44	121.89
1	A	552	ILE	N-CA-C	7.18	119.90	108.85
1	A	191	LYS	N-CA-C	-7.11	103.23	112.68
1	A	582	PHE	N-CA-C	-7.05	95.78	108.48
1	B	582	PHE	N-CA-C	-6.90	97.38	108.55
1	A	274	SER	N-CA-C	6.89	119.67	111.33
1	B	417	TYR	N-CA-C	6.65	118.53	111.28
1	B	107	VAL	N-CA-C	6.55	116.53	108.53
1	A	445	LYS	N-CA-C	6.55	119.42	111.82
1	A	131	VAL	N-CA-C	-6.49	104.43	110.53
1	A	541	SER	N-CA-C	-6.44	105.72	113.97
1	B	583	ARG	N-CA-C	-6.33	97.48	107.93
1	B	581	HIS	CA-C-N	6.23	133.22	121.69
1	B	581	HIS	C-N-CA	6.23	133.22	121.69
1	A	206	ASN	N-CA-C	-6.23	100.28	109.62
1	B	447	ILE	N-CA-C	6.21	117.77	111.00
1	A	78	SER	N-CA-C	6.17	119.56	110.30
1	B	565	TRP	N-CA-C	-6.16	99.68	109.04
1	B	412	LYS	N-CA-C	6.09	119.66	112.72
1	A	107	VAL	N-CA-C	6.02	121.86	109.34
1	B	423	ILE	N-CA-C	6.01	116.07	110.42
1	B	208	LYS	N-CA-C	-5.96	100.48	109.95
1	B	672	ASN	N-CA-C	5.95	119.73	112.23
1	A	239	ASP	N-CA-C	-5.91	102.32	110.35
1	A	472	THR	N-CA-C	-5.89	105.67	112.92
1	A	411	GLN	N-CA-C	5.86	117.75	111.36
1	A	583	ARG	NE-CZ-NH1	-5.86	115.64	121.50
1	A	581	HIS	CB-CA-C	-5.83	100.48	110.22
1	A	515	ILE	N-CA-C	5.82	116.25	107.75
1	B	581	HIS	CB-CA-C	-5.73	101.69	111.31
1	B	581	HIS	CA-C-O	-5.62	114.77	120.84
1	B	206	ASN	N-CA-C	-5.62	97.77	108.17
1	A	114	TRP	CA-C-N	5.57	125.58	119.90
1	A	114	TRP	C-N-CA	5.57	125.58	119.90
1	B	90	LYS	N-CA-C	-5.55	104.25	111.02
1	A	369	LEU	N-CA-C	-5.52	105.35	111.36
1	A	455	LEU	N-CA-C	-5.45	105.37	112.23
1	A	440	ALA	N-CA-C	5.42	117.24	108.41
1	B	657	ARG	N-CA-C	-5.39	105.44	112.23
1	A	524	LEU	N-CA-C	5.36	118.66	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	677	TYR	N-CA-C	5.35	117.82	109.52
1	A	525	GLU	CA-C-N	5.34	126.52	119.84
1	A	525	GLU	C-N-CA	5.34	126.52	119.84
1	B	310	VAL	N-CA-C	5.31	116.37	108.46
1	A	580	HIS	CA-C-N	-5.30	115.15	122.30
1	A	580	HIS	C-N-CA	-5.30	115.15	122.30
1	A	165	LEU	N-CA-C	-5.28	104.99	111.75
1	A	420	LYS	N-CA-C	5.28	117.97	110.10
1	B	132	TRP	N-CA-C	-5.25	105.45	111.07
1	A	449	ARG	N-CA-C	-5.24	105.25	111.69
1	A	296	THR	N-CA-C	5.20	117.38	108.90
1	B	415	TYR	N-CA-C	5.19	117.61	111.33
1	A	173	CYS	N-CA-C	-5.17	106.12	112.90
1	A	667	PRO	N-CA-C	-5.14	103.70	111.41
1	A	672	ASN	N-CA-C	5.11	117.63	111.40
1	B	584	MET	N-CA-C	-5.05	100.47	109.06
1	B	580	HIS	CA-C-N	-5.05	115.83	122.85
1	B	580	HIS	C-N-CA	-5.05	115.83	122.85

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	581	HIS	Peptide
1	B	581	HIS	Peptide
1	B	582	PHE	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	4894	0	4853	373	0
1	B	4816	0	4775	448	0
2	A	39	0	25	0	0
2	B	39	0	25	1	0
3	A	25	0	11	8	0
3	B	25	0	11	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	78	0	0	47	0
5	B	63	0	0	28	0
All	All	9983	0	9700	820	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 42.

All (820) 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:539:ASP:HB3	1:A:542:LEU:HD22	1.20	1.18
1:A:273:THR:HG21	1:A:387:GLN:HE21	0.99	1.07
3:A:684:UDP:H5'1	3:A:684:UDP:O1B	1.54	1.05
1:B:423:ILE:H	1:B:423:ILE:HD12	1.20	1.04
1:B:466:ILE:HA	5:B:709:HOH:O	1.59	1.01
1:B:549:ASN:HB3	1:B:626:TYR:HB3	1.42	0.98
1:B:107:VAL:HG12	1:B:108:GLU:H	1.27	0.98
1:B:90:LYS:HE3	1:B:94:ILE:HD12	1.47	0.96
1:A:418:ARG:HH11	1:A:418:ARG:HB2	1.27	0.96
1:A:411:GLN:HE22	1:A:430:ARG:H	1.05	0.95
1:A:273:THR:HG21	1:A:387:GLN:NE2	1.81	0.94
1:B:107:VAL:HG11	1:B:565:TRP:CH2	2.01	0.94
1:B:555:GLU:HB3	5:B:718:HOH:O	1.67	0.94
1:A:605:ASP:HB3	5:A:711:HOH:O	1.67	0.93
1:B:186:ALA:HB1	1:B:222:VAL:HG22	1.51	0.93
1:A:649:LYS:HD3	5:A:757:HOH:O	1.67	0.93
1:A:423:ILE:HD12	1:A:423:ILE:H	1.34	0.92
1:B:433:LEU:HD13	1:B:434:VAL:HG23	1.48	0.91
1:A:267:PRO:HG2	1:A:383:MET:HE2	1.50	0.91
1:A:586:THR:HG22	1:A:589:ALA:H	1.32	0.91
1:B:273:THR:HG22	5:B:742:HOH:O	1.72	0.89
1:B:646:ASN:O	1:B:650:VAL:HG23	1.73	0.88
1:B:420:LYS:HE3	1:B:537:ARG:HH22	1.37	0.88
1:A:557:ASN:N	1:A:557:ASN:HD22	1.72	0.87
1:B:453:SER:HB3	5:B:731:HOH:O	1.75	0.87
1:A:554:ARG:H	1:A:554:ARG:HD3	1.40	0.85
1:A:206:ASN:HB3	5:A:706:HOH:O	1.74	0.85
1:B:120:LEU:HD12	5:B:738:HOH:O	1.76	0.84
1:B:411:GLN:NE2	1:B:430:ARG:H	1.75	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:LEU:HA	5:B:705:HOH:O	1.78	0.84
1:B:605:ASP:HB3	5:B:693:HOH:O	1.77	0.84
1:B:414:PRO:HB2	1:B:433:LEU:HD23	1.59	0.83
1:A:411:GLN:NE2	1:A:430:ARG:H	1.78	0.82
1:B:177:THR:HA	1:B:250:GLN:HE21	1.45	0.81
1:A:643:GLN:HG3	1:A:644:LYS:N	1.94	0.81
1:B:660:ILE:HD11	5:B:738:HOH:O	1.81	0.81
1:B:161:ARG:HH21	1:B:392:LYS:HE2	1.45	0.80
1:A:549:ASN:HB3	1:A:626:TYR:HB3	1.63	0.80
3:A:684:UDP:PB	3:A:684:UDP:C5'	2.68	0.80
1:A:433:LEU:HD13	1:A:434:VAL:HG23	1.63	0.79
1:B:411:GLN:HE22	1:B:430:ARG:H	1.29	0.79
1:B:414:PRO:HA	1:B:418:ARG:HB2	1.64	0.79
1:B:107:VAL:HG12	1:B:108:GLU:N	1.96	0.79
1:A:208:LYS:HE3	1:B:212:GLN:HB3	1.64	0.78
1:A:640:LEU:O	1:A:643:GLN:HG2	1.83	0.78
3:A:684:UDP:O1B	3:A:684:UDP:C5'	2.30	0.78
1:A:264:LEU:HD21	5:A:691:HOH:O	1.81	0.78
1:B:120:LEU:HA	5:B:738:HOH:O	1.84	0.78
1:B:130:TYR:CE2	1:B:377:ARG:HD2	2.18	0.78
1:A:375:TYR:HA	5:A:748:HOH:O	1.83	0.77
1:A:639:LYS:HD3	1:B:639:LYS:HZ2	1.49	0.77
1:A:539:ASP:HB3	1:A:542:LEU:CD2	2.08	0.76
1:A:105:LYS:HB2	1:A:566:PRO:HG2	1.67	0.76
1:B:219:LEU:O	1:B:222:VAL:HG12	1.86	0.76
1:B:559:ILE:HG22	1:B:560:SER:N	2.01	0.75
1:A:245:ASN:ND2	1:A:247:LEU:H	1.83	0.75
1:A:418:ARG:HH21	1:A:429:LYS:HB3	1.52	0.75
1:B:606:TYR:O	1:B:610:LEU:HB2	1.86	0.75
1:A:438:ILE:HG23	1:A:518:LEU:O	1.86	0.75
1:A:59:ALA:O	1:A:60:VAL:HG13	1.87	0.75
1:B:653:GLU:OE2	1:B:665:TYR:HB3	1.87	0.75
1:B:497:LYS:NZ	1:B:497:LYS:HB2	2.02	0.74
1:A:517:GLN:HE22	1:A:583:ARG:HH11	1.35	0.74
1:A:323:LEU:HD12	5:A:742:HOH:O	1.87	0.74
1:A:443:CYS:CB	1:A:520:SER:HB2	2.18	0.74
1:B:294:ILE:HD12	1:B:295:ILE:N	2.02	0.74
1:B:418:ARG:HE	1:B:429:LYS:HG3	1.52	0.74
1:A:612:LEU:HB3	1:A:618:PHE:HZ	1.53	0.74
1:B:152:LEU:HG	1:B:253:MET:SD	2.27	0.73
1:B:410:GLN:NE2	1:B:418:ARG:HA	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:612:LEU:HG	5:A:737:HOH:O	1.87	0.73
1:A:91:TYR:CE2	1:A:423:ILE:HG12	2.22	0.73
1:A:662:LYS:HG3	1:A:663:TYR:HD1	1.54	0.73
1:A:352:ASP:HB3	1:A:355:PHE:CD2	2.24	0.72
1:A:423:ILE:HD12	1:A:423:ILE:N	2.03	0.72
1:B:111:PRO:HG3	1:B:572:LYS:HD2	1.70	0.72
1:B:79:LEU:HD21	1:B:83:GLU:HB3	1.70	0.72
1:A:418:ARG:HE	1:A:429:LYS:HG3	1.54	0.71
1:B:115:PRO:HB2	1:B:118:LEU:HB2	1.72	0.71
1:B:61:ILE:HD13	1:B:62:ASP:N	2.04	0.71
1:B:656:SER:HA	5:B:685:HOH:O	1.91	0.71
1:A:610:LEU:HD22	5:A:732:HOH:O	1.89	0.70
1:B:529:VAL:O	1:B:533:LEU:HB2	1.92	0.70
1:A:649:LYS:O	1:A:653:GLU:HG2	1.91	0.70
1:A:557:ASN:N	1:A:557:ASN:ND2	2.39	0.70
1:A:418:ARG:CZ	5:A:738:HOH:O	2.39	0.70
1:B:655:LEU:CD2	1:B:658:LEU:HG	2.22	0.70
1:A:152:LEU:HD21	1:A:236:ALA:HB2	1.74	0.70
3:A:684:UDP:C5'	3:A:684:UDP:O2B	2.39	0.70
1:B:288:ILE:HG13	1:B:385:TYR:CD2	2.27	0.70
1:B:433:LEU:CD1	1:B:434:VAL:HG23	2.21	0.70
1:B:649:LYS:HG3	5:B:706:HOH:O	1.91	0.70
1:B:255:LEU:O	1:B:258:VAL:HG22	1.92	0.70
1:B:360:GLY:HA2	1:B:409:LEU:HD11	1.74	0.69
1:A:643:GLN:HG3	1:A:644:LYS:H	1.56	0.69
1:B:517:GLN:HE22	1:B:583:ARG:HH11	1.37	0.69
1:B:499:ILE:HD11	1:B:604:VAL:CB	2.23	0.69
1:A:656:SER:HA	5:A:722:HOH:O	1.92	0.69
1:B:136:ARG:O	1:B:137:LYS:HG2	1.93	0.69
1:A:404:ILE:HD12	1:A:407:GLN:NE2	2.08	0.69
1:A:309:SER:HB2	5:A:753:HOH:O	1.92	0.68
1:A:559:ILE:HG13	1:A:559:ILE:O	1.93	0.68
1:B:607:ASP:O	1:B:611:LYS:HG3	1.93	0.68
1:A:612:LEU:HB3	1:A:618:PHE:CZ	2.28	0.68
1:B:360:GLY:CA	1:B:409:LEU:HD11	2.24	0.68
1:A:323:LEU:HB2	5:A:742:HOH:O	1.92	0.68
1:A:414:PRO:HA	1:A:418:ARG:NH1	2.09	0.68
1:A:78:SER:HA	5:A:751:HOH:O	1.94	0.68
1:B:286:SER:C	5:B:729:HOH:O	2.36	0.68
1:A:162:ALA:HB1	1:A:197:ILE:HG13	1.75	0.68
1:A:490:ARG:HH12	1:A:509:LEU:HD22	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:LEU:HD12	5:A:715:HOH:O	1.94	0.68
1:B:572:LYS:CG	1:B:578:ILE:HD13	2.24	0.68
1:B:669:THR:HG23	1:B:671:LEU:H	1.57	0.68
1:A:610:LEU:HB2	5:A:732:HOH:O	1.93	0.68
1:A:443:CYS:SG	1:A:520:SER:HB2	2.34	0.67
1:B:504:ASN:ND2	1:B:596:PHE:HB2	2.10	0.67
1:A:61:ILE:HD13	1:A:62:ASP:N	2.10	0.67
1:A:643:GLN:O	1:A:646:ASN:HB3	1.93	0.66
3:A:684:UDP:H5'1	3:A:684:UDP:PB	2.34	0.66
1:B:550:ARG:HA	1:B:562:GLY:H	1.60	0.66
1:A:137:LYS:HG3	1:A:138:GLU:H	1.59	0.66
1:A:154:ILE:HD13	1:A:248:TRP:HZ3	1.60	0.66
1:B:217:TYR:CD2	1:B:357:HIS:HA	2.31	0.66
1:A:553:ASP:HB3	1:A:557:ASN:N	2.11	0.66
1:B:357:HIS:O	1:B:357:HIS:ND1	2.27	0.66
1:B:669:THR:HG23	1:B:671:LEU:HG	1.77	0.66
1:A:84:LYS:O	1:A:88:ILE:HG13	1.96	0.65
1:B:536:PHE:CE1	1:B:545:VAL:HG22	2.31	0.65
1:B:161:ARG:HE	1:B:392:LYS:HE2	1.61	0.65
1:B:69:ILE:HG22	1:B:73:ASN:HD21	1.61	0.65
1:B:552:ILE:HD13	1:B:558:LEU:HA	1.77	0.65
1:A:69:ILE:HD11	1:A:88:ILE:HA	1.79	0.65
1:A:434:VAL:HB	1:A:462:LEU:HB2	1.79	0.65
1:A:553:ASP:HB3	1:A:557:ASN:H	1.61	0.65
1:A:123:LEU:HB3	1:A:124:PRO:HD2	1.79	0.65
1:B:91:TYR:HA	1:B:94:ILE:HG22	1.77	0.64
1:B:462:LEU:HD12	1:B:529:VAL:HG11	1.79	0.64
1:A:238:LEU:HD13	1:A:248:TRP:CZ2	2.33	0.64
1:A:682:ILE:HD11	5:A:710:HOH:O	1.96	0.64
1:B:504:ASN:O	1:B:508:ARG:HB2	1.96	0.64
1:A:458:THR:OG1	1:A:530:GLU:HB2	1.96	0.64
1:A:131:VAL:HG23	1:A:324:ARG:HD2	1.78	0.64
1:A:414:PRO:HB3	5:A:738:HOH:O	1.97	0.64
1:B:476:LEU:O	1:B:480:GLN:HG3	1.98	0.64
1:A:121:PRO:HD2	1:A:658:LEU:HD22	1.79	0.64
1:A:416:PHE:N	5:A:736:HOH:O	2.31	0.64
1:A:497:LYS:HB2	1:A:497:LYS:HZ2	1.63	0.64
1:A:527:ASP:HA	5:A:761:HOH:O	1.98	0.64
1:B:358:TRP:O	1:B:359:GLY:O	2.16	0.64
1:A:620:HIS:CD2	1:A:621:ILE:O	2.50	0.64
1:A:105:LYS:HB2	1:A:566:PRO:CG	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:PHE:HD2	5:A:748:HOH:O	1.80	0.63
1:B:294:ILE:HD12	1:B:295:ILE:C	2.23	0.63
1:B:499:ILE:HD11	1:B:604:VAL:HB	1.79	0.63
1:B:565:TRP:NE1	1:B:572:LYS:HG2	2.14	0.63
1:B:549:ASN:HA	1:B:624:ILE:HG23	1.81	0.63
1:B:669:THR:CG2	1:B:671:LEU:H	2.11	0.63
1:B:410:GLN:HE22	1:B:418:ARG:HA	1.63	0.63
1:A:411:GLN:HB2	5:A:747:HOH:O	1.98	0.62
1:A:273:THR:HB	1:A:387:GLN:HG2	1.80	0.62
1:A:218:GLN:HB3	1:A:221:ALA:HB3	1.80	0.62
1:A:551:ASN:O	1:A:552:ILE:HD13	2.00	0.62
1:A:551:ASN:HB2	1:A:560:SER:HB3	1.82	0.62
1:A:352:ASP:HB3	1:A:355:PHE:HD2	1.65	0.62
1:B:595:GLY:C	1:B:608:MET:HE1	2.25	0.62
1:A:483:TYR:CD1	1:A:489:VAL:HG21	2.34	0.62
1:B:586:THR:HG22	1:B:588:ARG:N	2.15	0.62
1:B:107:VAL:CG1	1:B:108:GLU:H	2.09	0.61
1:B:266:GLY:HA3	1:B:337:ASN:ND2	2.15	0.61
1:A:595:GLY:C	1:A:608:MET:HE1	2.25	0.61
1:B:410:GLN:HE21	1:B:418:ARG:HD3	1.63	0.61
1:B:528:ALA:HB2	1:B:625:CYS:HB3	1.82	0.61
1:A:69:ILE:HG22	1:A:73:ASN:HD21	1.65	0.61
1:A:435:SER:CB	1:A:510:CYS:HB3	2.31	0.61
1:B:423:ILE:H	1:B:423:ILE:CD1	1.95	0.61
1:B:90:LYS:O	1:B:94:ILE:HB	2.01	0.61
1:B:191:LYS:HE2	5:B:708:HOH:O	2.00	0.61
1:B:215:TYR:CE2	1:B:218:GLN:HG3	2.35	0.61
1:A:628:ARG:HG2	1:A:629:VAL:O	2.01	0.61
1:A:92:ARG:HG3	1:A:92:ARG:HH11	1.66	0.61
1:B:416:PHE:HD2	1:B:417:TYR:CE1	2.18	0.61
1:B:418:ARG:HB2	1:B:418:ARG:HH11	1.64	0.60
1:B:494:GLN:NE2	1:B:497:LYS:NZ	2.49	0.60
3:A:684:UDP:O2B	3:A:684:UDP:H5'2	2.00	0.60
1:A:361:GLU:OE2	1:A:362:ASP:N	2.35	0.60
1:B:161:ARG:NH2	1:B:392:LYS:HE2	2.15	0.60
1:A:418:ARG:NH2	5:A:738:HOH:O	2.34	0.60
1:A:654:SER:C	1:A:656:SER:H	2.09	0.60
1:A:418:ARG:HH21	1:A:429:LYS:CB	2.14	0.60
1:A:550:ARG:CD	1:A:552:ILE:HD11	2.32	0.60
1:B:499:ILE:HD11	1:B:604:VAL:HG11	1.84	0.60
1:B:79:LEU:HD22	1:B:84:LYS:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:THR:OG1	1:B:530:GLU:HB2	2.02	0.59
1:B:577:MET:CE	1:B:579:CYS:HB3	2.32	0.59
1:A:418:ARG:HH11	1:A:418:ARG:CB	2.10	0.59
1:B:91:TYR:O	1:B:94:ILE:HG22	2.03	0.59
1:A:60:VAL:HG23	1:A:61:ILE:H	1.66	0.59
1:A:91:TYR:HE2	1:A:423:ILE:HG12	1.66	0.59
1:A:224:ASN:OD1	1:A:350:TRP:HB3	2.02	0.59
1:A:548:THR:HG22	1:A:623:LYS:O	2.01	0.59
1:A:646:ASN:O	1:A:650:VAL:HG23	2.01	0.59
1:B:539:ASP:HB3	1:B:542:LEU:HD22	1.83	0.59
1:B:167:ILE:HG21	1:B:387:GLN:NE2	2.18	0.59
1:A:64:ASP:O	1:A:67:THR:HG22	2.01	0.59
1:A:304:VAL:HB	5:A:762:HOH:O	2.03	0.59
1:A:368:ARG:O	1:A:372:GLU:HG2	2.02	0.59
1:B:655:LEU:HD21	1:B:658:LEU:HG	1.83	0.59
1:A:308:LYS:O	1:A:310:VAL:HG13	2.03	0.59
1:A:578:ILE:HB	5:A:724:HOH:O	2.01	0.59
1:A:558:LEU:HD12	1:A:559:ILE:H	1.67	0.58
1:B:549:ASN:CB	1:B:626:TYR:HB3	2.24	0.58
1:B:72:SER:C	1:B:74:ALA:N	2.60	0.58
1:B:371:ARG:NH2	1:B:512:GLY:O	2.36	0.58
1:A:131:VAL:CG2	1:A:324:ARG:HD2	2.34	0.58
1:A:554:ARG:HA	1:A:629:VAL:HG13	1.85	0.58
1:B:289:ASN:HB2	5:B:729:HOH:O	2.03	0.58
1:B:576:ALA:O	1:B:578:ILE:HG23	2.03	0.58
1:A:114:TRP:CZ2	1:A:571:GLU:HG3	2.39	0.58
1:A:639:LYS:HD3	1:B:639:LYS:NZ	2.17	0.58
1:B:511:ARG:HG3	1:B:511:ARG:HH11	1.69	0.58
1:A:480:GLN:C	1:A:482:HIS:H	2.09	0.58
1:B:542:LEU:HA	1:B:617:PRO:HG2	1.84	0.58
1:A:299:GLN:HE21	1:A:304:VAL:HG22	1.69	0.58
1:A:409:LEU:O	1:A:411:GLN:N	2.36	0.58
1:A:517:GLN:HE22	1:A:583:ARG:NH1	2.01	0.58
1:B:65:ALA:O	1:B:68:LYS:N	2.37	0.58
1:A:124:PRO:HD3	1:A:132:TRP:CE2	2.38	0.58
1:B:63:ILE:HG13	1:B:64:ASP:N	2.17	0.58
1:B:358:TRP:CD1	2:B:683:UD2:H6'1	2.39	0.58
1:B:494:GLN:NE2	1:B:497:LYS:HZ2	2.01	0.58
1:A:423:ILE:H	1:A:423:ILE:CD1	2.05	0.57
1:A:577:MET:HA	5:A:715:HOH:O	2.03	0.57
1:B:466:ILE:N	1:B:466:ILE:HD12	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ASN:HB3	1:B:192:GLU:OE2	2.04	0.57
1:A:69:ILE:HG22	1:A:73:ASN:ND2	2.19	0.57
1:B:509:LEU:HD23	1:B:509:LEU:O	2.04	0.57
1:B:245:ASN:ND2	1:B:247:LEU:H	2.02	0.57
1:A:559:ILE:O	1:A:560:SER:HB2	2.03	0.57
1:B:328:THR:O	1:B:331:ARG:HG3	2.04	0.57
1:A:269:LYS:HG3	1:A:383:MET:SD	2.45	0.57
1:B:499:ILE:HD11	1:B:604:VAL:CG1	2.35	0.57
1:A:642:ILE:O	1:A:646:ASN:HB2	2.05	0.57
1:B:67:THR:HG23	1:B:68:LYS:N	2.20	0.57
1:B:265:ILE:HD13	1:B:332:PHE:O	2.04	0.57
1:B:363:ASN:HD22	1:B:409:LEU:HD23	1.70	0.57
1:A:68:LYS:HG2	1:A:87:ILE:HD13	1.85	0.57
1:A:371:ARG:NH2	1:A:512:GLY:O	2.38	0.57
1:B:611:LYS:HG2	1:B:657:ARG:NH1	2.19	0.57
1:B:224:ASN:OD1	1:B:350:TRP:HB3	2.05	0.56
1:B:552:ILE:HG22	1:B:553:ASP:N	2.19	0.56
1:A:605:ASP:CG	1:A:606:TYR:N	2.62	0.56
1:A:137:LYS:O	1:A:138:GLU:HB3	2.04	0.56
1:A:186:ALA:HB1	1:A:222:VAL:HG22	1.86	0.56
1:A:565:TRP:N	1:A:580:HIS:NE2	2.52	0.56
1:A:637:ILE:O	1:A:640:LEU:HD13	2.05	0.56
1:B:87:ILE:O	1:B:90:LYS:HB3	2.04	0.56
1:B:159:TYR:O	1:B:160:ASN:HB2	2.05	0.56
1:B:388:GLU:OE2	1:B:389:PRO:HD2	2.06	0.56
1:B:492:ILE:HG12	1:B:493:SER:N	2.20	0.56
1:A:212:GLN:NE2	5:A:744:HOH:O	2.38	0.56
1:A:273:THR:CG2	1:A:387:GLN:HE21	1.94	0.56
1:A:443:CYS:HB3	1:A:520:SER:HB2	1.87	0.56
1:A:662:LYS:HG3	1:A:663:TYR:CD1	2.38	0.56
1:B:177:THR:HA	1:B:250:GLN:NE2	2.18	0.56
1:B:474:ASP:O	1:B:475:THR:C	2.46	0.56
1:B:638:LYS:O	1:B:642:ILE:HG12	2.06	0.56
1:A:649:LYS:HD2	1:A:665:TYR:HE1	1.70	0.56
1:B:420:LYS:CE	1:B:537:ARG:HH22	2.15	0.56
1:B:654:SER:C	1:B:656:SER:H	2.13	0.56
1:A:620:HIS:HD2	1:A:621:ILE:N	2.03	0.56
1:B:499:ILE:HD12	1:B:499:ILE:C	2.31	0.56
1:A:639:LYS:HE2	1:A:639:LYS:O	2.05	0.56
1:B:69:ILE:HG22	1:B:73:ASN:ND2	2.21	0.56
1:B:411:GLN:HE22	1:B:430:ARG:N	2.02	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:544:CYS:HB3	1:B:618:PHE:CE1	2.41	0.56
1:B:586:THR:HG22	1:B:588:ARG:H	1.70	0.56
1:B:131:VAL:CG2	1:B:324:ARG:HD2	2.36	0.56
1:A:267:PRO:CG	1:A:383:MET:HE2	2.28	0.56
1:B:167:ILE:HB	1:B:387:GLN:HE22	1.70	0.56
1:B:215:TYR:CZ	1:B:218:GLN:HG3	2.40	0.56
1:B:668:LEU:O	1:B:668:LEU:HG	2.05	0.55
1:A:539:ASP:C	1:A:541:SER:H	2.14	0.55
1:A:596:PHE:CG	1:A:608:MET:HE3	2.40	0.55
1:A:213:LYS:HE3	1:B:202:GLU:O	2.07	0.55
1:A:568:TYR:CD2	1:A:618:PHE:HB2	2.41	0.55
1:B:185:VAL:HG21	1:B:198:VAL:HG22	1.88	0.55
1:B:218:GLN:HB3	1:B:221:ALA:HB3	1.89	0.55
1:B:255:LEU:CD1	1:B:379:VAL:HG22	2.36	0.55
1:B:390:PRO:O	1:B:392:LYS:N	2.39	0.55
1:A:217:TYR:CE2	1:A:357:HIS:HA	2.42	0.55
1:A:558:LEU:HD12	1:A:559:ILE:N	2.22	0.55
1:A:620:HIS:CD2	1:A:621:ILE:N	2.75	0.55
1:B:114:TRP:CZ2	1:B:118:LEU:HD13	2.41	0.55
1:A:497:LYS:HB2	1:A:497:LYS:NZ	2.22	0.55
1:A:596:PHE:HA	1:A:608:MET:CE	2.36	0.55
1:B:64:ASP:OD1	1:B:67:THR:HG21	2.07	0.55
1:B:418:ARG:NH2	1:B:431:VAL:O	2.40	0.55
1:A:501:SER:O	1:A:502:ALA:C	2.50	0.55
1:A:135:LYS:O	1:A:137:LYS:N	2.40	0.55
1:B:318:LYS:HB2	1:B:318:LYS:NZ	2.22	0.55
1:A:311:ASP:HB3	1:A:314:ILE:HG13	1.89	0.54
1:A:550:ARG:CZ	1:A:624:ILE:HG21	2.37	0.54
1:B:80:ASN:HD21	1:B:83:GLU:HB2	1.71	0.54
1:B:123:LEU:HB3	1:B:124:PRO:HD2	1.88	0.54
1:B:653:GLU:OE2	1:B:665:TYR:N	2.39	0.54
1:A:208:LYS:HE3	1:B:212:GLN:CB	2.35	0.54
1:A:543:ALA:HB2	5:A:739:HOH:O	2.07	0.54
1:B:67:THR:HA	1:B:70:MET:HE3	1.88	0.54
1:B:198:VAL:HG11	1:B:209:TYR:HB2	1.89	0.54
1:B:333:PHE:O	1:B:362:ASP:HB3	2.06	0.54
1:A:553:ASP:OD1	1:A:555:GLU:HB3	2.08	0.54
1:A:597:ASN:HB2	1:A:607:ASP:OD2	2.07	0.54
1:B:92:ARG:O	1:B:96:ALA:N	2.41	0.54
1:B:72:SER:O	1:B:74:ALA:N	2.40	0.54
1:B:114:TRP:CZ2	1:B:120:LEU:HD13	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:LEU:O	1:B:291:ILE:HG13	2.07	0.54
1:B:568:TYR:CE2	1:B:618:PHE:HB2	2.42	0.54
1:A:137:LYS:O	1:A:138:GLU:CB	2.56	0.54
1:A:255:LEU:O	1:A:258:VAL:HG22	2.08	0.54
1:A:550:ARG:HG3	1:A:552:ILE:HD11	1.90	0.54
1:B:178:ILE:H	1:B:250:GLN:HE22	1.54	0.54
1:B:638:LYS:NZ	1:B:639:LYS:HD2	2.23	0.54
1:A:462:LEU:CD2	1:A:488:ARG:HH21	2.20	0.54
1:B:525:GLU:HG3	1:B:625:CYS:HA	1.89	0.54
1:B:513:PHE:CZ	1:B:586:THR:HG23	2.42	0.54
1:B:470:GLY:N	1:B:494:GLN:O	2.41	0.54
1:A:214:ASP:OD1	1:A:214:ASP:C	2.50	0.54
1:A:284:GLN:C	1:A:286:SER:H	2.15	0.54
1:B:311:ASP:HB3	1:B:314:ILE:HG13	1.90	0.54
1:B:352:ASP:OD2	1:B:412:LYS:NZ	2.40	0.54
1:B:495:LYS:O	1:B:497:LYS:HG3	2.07	0.54
1:A:124:PRO:HB3	1:A:132:TRP:CD2	2.43	0.54
1:B:497:LYS:HB2	1:B:497:LYS:HZ3	1.72	0.54
1:B:577:MET:HE3	1:B:579:CYS:HB3	1.89	0.54
1:B:657:ARG:C	1:B:659:GLY:H	2.16	0.54
1:B:84:LYS:HG2	1:B:88:ILE:HD11	1.90	0.53
1:B:72:SER:C	1:B:74:ALA:H	2.16	0.53
1:B:412:LYS:HA	1:B:431:VAL:HB	1.91	0.53
1:B:434:VAL:HG22	1:B:514:TYR:HB2	1.90	0.53
1:A:80:ASN:OD1	1:A:83:GLU:HB2	2.08	0.53
1:A:80:ASN:OD1	1:A:83:GLU:OE1	2.26	0.53
1:A:245:ASN:HD21	1:A:247:LEU:HB2	1.73	0.53
1:A:106:GLU:O	1:A:107:VAL:HG13	2.06	0.53
1:A:345:LEU:HD13	1:A:350:TRP:CZ3	2.43	0.53
1:B:65:ALA:O	1:B:66:ALA:C	2.51	0.53
1:B:423:ILE:HA	1:B:426:ALA:HB2	1.90	0.53
1:B:559:ILE:HG22	1:B:560:SER:H	1.71	0.53
1:A:444:SER:O	1:A:447:ILE:HG22	2.08	0.53
1:B:568:TYR:CG	1:B:569:SER:N	2.76	0.53
1:B:653:GLU:OE1	1:B:664:LYS:HG3	2.07	0.53
1:A:423:ILE:HG13	5:A:714:HOH:O	2.08	0.53
1:A:577:MET:HE2	1:A:605:ASP:OD2	2.08	0.53
1:B:341:ALA:HB3	1:B:344:TRP:CD1	2.43	0.53
1:B:527:ASP:O	1:B:531:LEU:HG	2.09	0.53
1:A:296:THR:O	1:A:306:GLN:HA	2.09	0.53
1:B:130:TYR:CZ	1:B:324:ARG:HB2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:THR:N	1:B:329:PRO:CD	2.70	0.53
1:B:392:LYS:HB2	1:B:392:LYS:NZ	2.23	0.53
1:B:186:ALA:HA	1:B:210:VAL:HG23	1.90	0.53
1:A:554:ARG:H	1:A:554:ARG:CD	2.16	0.52
1:B:295:ILE:HG12	1:B:308:LYS:HA	1.89	0.52
1:B:553:ASP:O	1:B:554:ARG:C	2.50	0.52
1:B:503:SER:O	1:B:505:THR:N	2.42	0.52
1:A:450:CYS:SG	1:A:518:LEU:HD22	2.49	0.52
1:B:105:LYS:HB3	1:B:566:PRO:HG3	1.92	0.52
1:B:238:LEU:HD13	1:B:248:TRP:CZ2	2.44	0.52
1:B:409:LEU:O	1:B:410:GLN:C	2.53	0.52
1:A:110:ILE:O	1:A:111:PRO:C	2.51	0.52
1:A:199:ARG:HH21	1:B:211:ARG:HH21	1.57	0.52
1:B:411:GLN:NE2	1:B:430:ARG:HB2	2.25	0.52
1:B:284:GLN:C	1:B:286:SER:H	2.18	0.52
1:A:114:TRP:CE2	1:A:571:GLU:HG3	2.45	0.52
1:A:442:ASN:HA	1:A:473:ASP:OD2	2.10	0.52
1:B:71:CYS:O	1:B:75:LYS:HG3	2.09	0.52
1:A:91:TYR:O	1:A:94:ILE:HG22	2.09	0.52
1:A:649:LYS:HB2	5:A:757:HOH:O	2.09	0.52
1:A:62:ASP:CG	1:A:63:ILE:H	2.18	0.52
1:A:565:TRP:H	1:A:580:HIS:CE1	2.27	0.52
1:B:545:VAL:HG12	1:B:619:LYS:HB3	1.91	0.52
1:B:557:ASN:N	1:B:557:ASN:HD22	2.08	0.52
1:A:296:THR:HB	1:A:309:SER:OG	2.09	0.52
1:A:499:ILE:O	1:A:499:ILE:HD12	2.10	0.52
1:B:490:ARG:HH12	1:B:511:ARG:NH1	2.08	0.52
1:A:490:ARG:NH2	1:A:511:ARG:HD3	2.25	0.51
1:A:552:ILE:HG22	1:A:553:ASP:O	2.11	0.51
1:B:483:TYR:C	1:B:485:ASN:H	2.18	0.51
1:A:64:ASP:OD2	1:A:67:THR:HB	2.10	0.51
1:A:418:ARG:HH21	1:A:429:LYS:CG	2.23	0.51
1:A:517:GLN:NE2	1:A:583:ARG:HH11	2.05	0.51
1:B:131:VAL:HG23	1:B:324:ARG:HD2	1.92	0.51
1:B:483:TYR:C	1:B:485:ASN:N	2.68	0.51
1:A:132:TRP:CH2	1:A:136:ARG:HD2	2.46	0.51
1:A:647:HIS:O	1:A:651:VAL:HG23	2.10	0.51
1:B:571:GLU:H	1:B:571:GLU:CD	2.18	0.51
1:A:415:TYR:CG	1:A:416:PHE:N	2.75	0.51
1:A:535:GLU:O	1:A:542:LEU:HD23	2.10	0.51
1:A:559:ILE:O	1:A:560:SER:CB	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:LEU:N	5:B:729:HOH:O	2.43	0.51
1:B:466:ILE:HD12	1:B:466:ILE:H	1.75	0.51
1:B:649:LYS:HD2	1:B:649:LYS:N	2.26	0.51
1:A:462:LEU:HD23	1:A:488:ARG:HH21	1.76	0.51
1:B:107:VAL:HG11	1:B:565:TRP:CZ2	2.43	0.51
1:B:541:SER:HB2	5:B:703:HOH:O	2.11	0.51
1:B:450:CYS:SG	1:B:518:LEU:HD13	2.51	0.51
1:A:67:THR:HB	1:A:488:ARG:HH11	1.75	0.51
1:B:647:HIS:O	1:B:648:PHE:C	2.54	0.51
1:A:178:ILE:HG12	1:A:250:GLN:HE22	1.75	0.51
1:B:94:ILE:HG23	1:B:95:THR:HG23	1.93	0.51
1:A:653:GLU:OE2	1:A:665:TYR:O	2.28	0.51
1:B:60:VAL:O	1:B:61:ILE:HB	2.11	0.51
1:B:363:ASN:HD22	1:B:409:LEU:CD2	2.23	0.51
1:B:411:GLN:HE21	1:B:411:GLN:CA	2.24	0.51
1:B:523:PHE:HA	5:B:731:HOH:O	2.10	0.51
1:B:662:LYS:HG3	1:B:663:TYR:HD1	1.76	0.51
3:A:684:UDP:O2B	3:A:684:UDP:O5'	2.29	0.50
1:B:602:ASN:O	1:B:603:ALA:HB3	2.10	0.50
1:A:154:ILE:CD1	1:A:248:TRP:HZ3	2.24	0.50
1:A:557:ASN:ND2	1:A:557:ASN:H	2.08	0.50
1:B:643:GLN:HG3	1:B:644:LYS:N	2.24	0.50
1:B:107:VAL:HG23	1:B:566:PRO:HG2	1.93	0.50
1:B:559:ILE:CG2	1:B:560:SER:N	2.70	0.50
1:A:250:GLN:HA	1:A:250:GLN:NE2	2.26	0.50
1:A:642:ILE:HG12	5:A:712:HOH:O	2.12	0.50
1:B:334:SER:O	1:B:338:VAL:HG13	2.11	0.50
1:B:367:TYR:O	1:B:370:TYR:HB3	2.12	0.50
1:B:552:ILE:CG2	1:B:553:ASP:N	2.75	0.50
1:B:620:HIS:C	1:B:620:HIS:CD2	2.89	0.50
1:A:167:ILE:HD12	1:A:387:GLN:NE2	2.27	0.50
1:A:657:ARG:C	1:A:659:GLY:H	2.20	0.50
1:A:190:SER:O	1:B:199:ARG:NH2	2.44	0.50
1:A:435:SER:HB3	1:A:510:CYS:HB3	1.92	0.50
1:A:661:LYS:HD3	5:A:693:HOH:O	2.09	0.50
1:B:327:ASN:HD22	1:B:540:LEU:HB2	1.76	0.50
1:B:438:ILE:N	5:B:709:HOH:O	2.31	0.50
1:B:458:THR:OG1	1:B:527:ASP:HA	2.12	0.50
1:A:544:CYS:HA	1:A:584:MET:O	2.11	0.50
1:B:438:ILE:HG12	1:B:518:LEU:O	2.12	0.50
1:A:460:THR:HB	5:A:730:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:MET:HE3	1:B:579:CYS:O	2.11	0.50
1:B:80:ASN:O	1:B:82:VAL:N	2.45	0.50
1:B:167:ILE:CG2	1:B:387:GLN:NE2	2.75	0.50
1:A:504:ASN:ND2	1:A:596:PHE:HB2	2.27	0.49
1:B:188:ASP:OD1	1:B:218:GLN:HB2	2.12	0.49
1:B:363:ASN:ND2	1:B:417:TYR:CE2	2.80	0.49
1:B:483:TYR:HB3	1:B:489:VAL:HB	1.94	0.49
1:A:212:GLN:HA	5:A:708:HOH:O	2.12	0.49
1:A:490:ARG:HH12	1:A:509:LEU:CD2	2.25	0.49
1:A:617:PRO:C	1:A:618:PHE:HD1	2.20	0.49
3:A:684:UDP:O1B	3:A:684:UDP:O2A	2.29	0.49
1:B:420:LYS:HE3	1:B:537:ARG:NH2	2.18	0.49
1:A:564:ASN:O	1:A:566:PRO:HD3	2.13	0.49
1:A:630:LEU:O	1:A:631:HIS:C	2.54	0.49
1:B:596:PHE:CE1	1:B:608:MET:HE3	2.48	0.49
1:B:306:GLN:O	1:B:307:ASN:CB	2.60	0.49
1:B:319:ASN:C	1:B:321:ASP:H	2.19	0.49
1:B:409:LEU:O	1:B:412:LYS:N	2.46	0.49
1:B:413:VAL:C	1:B:418:ARG:HH12	2.20	0.49
1:B:536:PHE:HE1	1:B:545:VAL:HG22	1.77	0.49
1:B:565:TRP:CZ2	1:B:572:LYS:HE2	2.48	0.49
3:B:1:UDP:O2A	3:B:1:UDP:O1B	2.30	0.49
1:B:503:SER:C	1:B:505:THR:N	2.68	0.49
1:B:549:ASN:O	1:B:562:GLY:N	2.45	0.49
1:A:197:ILE:O	1:A:200:GLU:HB2	2.11	0.49
1:A:499:ILE:HG13	1:A:604:VAL:HG21	1.94	0.49
1:B:531:LEU:HB3	1:B:621:ILE:HD13	1.95	0.49
1:A:559:ILE:HD11	1:A:630:LEU:HD23	1.94	0.49
1:A:568:TYR:CE2	1:A:618:PHE:HB2	2.47	0.49
1:A:497:LYS:NZ	1:A:501:SER:OG	2.45	0.49
1:B:206:ASN:ND2	5:B:697:HOH:O	2.45	0.49
1:B:360:GLY:O	1:B:364:GLU:N	2.46	0.49
1:A:448:VAL:O	1:A:452:GLU:HG2	2.13	0.49
1:A:88:ILE:O	1:A:91:TYR:HB3	2.13	0.49
1:B:152:LEU:HD12	1:B:249:VAL:HG13	1.94	0.49
1:B:156:ILE:HG23	1:B:238:LEU:O	2.13	0.49
1:B:503:SER:C	1:B:505:THR:H	2.20	0.49
1:A:344:TRP:CZ3	1:A:347:ARG:HD2	2.47	0.48
1:A:465:CYS:HA	1:A:490:ARG:O	2.13	0.48
1:B:225:LEU:C	1:B:225:LEU:HD23	2.38	0.48
1:B:655:LEU:HD22	1:B:658:LEU:HG	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:668:LEU:O	1:B:668:LEU:CG	2.61	0.48
1:B:490:ARG:HH22	1:B:511:ARG:NH1	2.11	0.48
1:A:614:GLU:CD	1:A:655:LEU:HD21	2.38	0.48
1:B:663:TYR:OH	1:B:681:LYS:HD2	2.13	0.48
1:A:296:THR:HG22	1:A:307:ASN:O	2.14	0.48
1:B:223:ARG:CZ	1:B:335:GLY:HA3	2.44	0.48
1:B:655:LEU:HD23	1:B:657:ARG:HG3	1.95	0.48
1:A:283:SER:OG	1:A:284:GLN:N	2.45	0.48
1:B:188:ASP:CG	1:B:188:ASP:O	2.56	0.48
1:B:91:TYR:CE1	1:B:95:THR:HG21	2.49	0.48
1:A:208:LYS:HE3	1:B:212:GLN:HE21	1.78	0.48
1:A:352:ASP:HB3	1:A:355:PHE:CE2	2.48	0.48
1:A:553:ASP:O	1:A:556:GLY:N	2.42	0.48
1:B:450:CYS:O	1:B:451:VAL:C	2.57	0.48
1:A:251:SER:OG	1:A:381:GLY:HA3	2.14	0.48
1:B:409:LEU:O	1:B:411:GLN:N	2.47	0.48
1:A:669:THR:HG22	1:A:670:ASN:N	2.28	0.48
1:B:477:ARG:NH1	1:B:477:ARG:HB3	2.29	0.48
1:A:273:THR:O	1:A:273:THR:HG23	2.13	0.48
1:A:477:ARG:HD2	1:A:477:ARG:O	2.13	0.48
1:B:220:CYS:O	1:B:221:ALA:C	2.57	0.48
1:B:360:GLY:HA3	1:B:409:LEU:HD11	1.95	0.48
1:B:490:ARG:HH12	1:B:511:ARG:HH11	1.61	0.48
1:A:466:ILE:O	1:A:491:PHE:HA	2.13	0.47
1:B:161:ARG:NE	1:B:392:LYS:HE2	2.28	0.47
1:B:477:ARG:O	1:B:481:GLU:HG2	2.13	0.47
1:A:460:THR:HG21	5:A:714:HOH:O	2.14	0.47
1:B:64:ASP:CG	1:B:67:THR:HG22	2.39	0.47
1:B:91:TYR:HA	1:B:94:ILE:CG2	2.44	0.47
1:B:414:PRO:HA	1:B:418:ARG:NH1	2.29	0.47
1:B:499:ILE:CD1	1:B:604:VAL:HG11	2.44	0.47
1:A:162:ALA:HB1	1:A:197:ILE:CG1	2.42	0.47
1:A:642:ILE:CD1	1:A:672:ASN:HD21	2.27	0.47
1:B:474:ASP:O	1:B:477:ARG:N	2.48	0.47
1:B:542:LEU:HD21	1:B:619:LYS:HB2	1.95	0.47
1:A:503:SER:O	1:A:504:ASN:C	2.58	0.47
1:A:614:GLU:OE2	1:A:655:LEU:HD21	2.14	0.47
1:A:677:TYR:HE2	1:A:679:TRP:NE1	2.13	0.47
1:B:94:ILE:CG2	1:B:95:THR:HG23	2.45	0.47
1:B:565:TRP:CE2	1:B:572:LYS:HE2	2.49	0.47
1:B:79:LEU:HD23	1:B:80:ASN:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:GLN:HB3	1:B:221:ALA:CB	2.44	0.47
1:A:371:ARG:O	1:A:591:ASN:ND2	2.48	0.47
1:A:459:ILE:O	1:A:462:LEU:HD22	2.14	0.47
1:A:545:VAL:HA	1:A:619:LYS:O	2.14	0.47
1:A:558:LEU:C	1:A:559:ILE:CG2	2.87	0.47
1:A:605:ASP:CG	1:A:606:TYR:H	2.22	0.47
1:B:114:TRP:HZ2	1:B:120:LEU:HD13	1.79	0.47
1:B:577:MET:HE2	1:B:583:ARG:NH2	2.29	0.47
1:B:589:ALA:O	1:B:590:TRP:C	2.57	0.47
1:A:496:ASN:C	1:A:496:ASN:ND2	2.73	0.47
1:B:497:LYS:HB2	1:B:497:LYS:HZ2	1.77	0.47
1:A:267:PRO:HG2	1:A:383:MET:CE	2.34	0.46
1:B:64:ASP:OD2	1:B:67:THR:HG22	2.15	0.46
1:A:232:TYR:HB3	5:A:709:HOH:O	2.14	0.46
1:A:460:THR:N	5:A:759:HOH:O	2.47	0.46
1:A:605:ASP:O	1:A:609:TYR:HD2	1.99	0.46
1:A:620:HIS:CD2	1:A:620:HIS:C	2.92	0.46
1:B:136:ARG:O	1:B:137:LYS:CB	2.63	0.46
1:A:92:ARG:HG3	1:A:92:ARG:NH1	2.29	0.46
1:A:459:ILE:HD11	1:A:530:GLU:HG3	1.98	0.46
1:A:496:ASN:C	1:A:496:ASN:HD22	2.23	0.46
1:B:410:GLN:HE22	1:B:419:LYS:H	1.63	0.46
1:B:449:ARG:HD2	5:B:686:HOH:O	2.15	0.46
1:B:564:ASN:HA	1:B:580:HIS:CD2	2.51	0.46
1:B:126:SER:HB2	1:B:327:ASN:OD1	2.15	0.46
1:B:164:ILE:HG21	1:B:241:ASP:CB	2.46	0.46
1:A:285:LYS:HB2	1:A:285:LYS:NZ	2.30	0.46
1:A:299:GLN:NE2	1:A:304:VAL:HG22	2.29	0.46
1:B:306:GLN:O	1:B:307:ASN:HB3	2.16	0.46
1:B:472:THR:OG1	1:B:473:ASP:N	2.48	0.46
1:B:543:ALA:HB2	1:B:616:GLY:HA3	1.97	0.46
1:A:415:TYR:C	5:A:736:HOH:O	2.58	0.46
1:B:649:LYS:CD	1:B:649:LYS:H	2.29	0.46
1:A:125:GLU:OE1	1:A:324:ARG:NH2	2.48	0.46
1:B:63:ILE:CG1	1:B:64:ASP:N	2.76	0.46
1:B:72:SER:O	1:B:75:LYS:N	2.49	0.46
1:B:295:ILE:HA	1:B:309:SER:OG	2.16	0.46
1:B:433:LEU:HD22	1:B:433:LEU:O	2.16	0.46
1:B:577:MET:SD	1:B:606:TYR:CD1	3.09	0.46
1:A:262:VAL:HG13	5:A:691:HOH:O	2.15	0.46
1:B:649:LYS:CG	5:B:706:HOH:O	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:VAL:HG12	5:A:736:HOH:O	2.16	0.46
1:B:420:LYS:NZ	1:B:537:ARG:HH12	2.14	0.46
1:B:552:ILE:HG22	1:B:553:ASP:O	2.15	0.46
1:A:596:PHE:N	1:A:608:MET:HE1	2.31	0.46
1:B:166:ALA:HB1	1:B:278:TYR:CD2	2.51	0.46
1:A:414:PRO:O	1:A:418:ARG:HB3	2.16	0.45
1:A:602:ASN:O	1:A:603:ALA:HB3	2.16	0.45
1:B:130:TYR:CD2	1:B:377:ARG:HD2	2.51	0.45
1:B:483:TYR:O	1:B:485:ASN:N	2.49	0.45
1:A:443:CYS:O	1:A:447:ILE:HB	2.15	0.45
1:B:79:LEU:HD23	1:B:80:ASN:O	2.16	0.45
1:B:649:LYS:O	1:B:653:GLU:HG2	2.16	0.45
1:A:356:THR:OG1	1:A:358:TRP:HD1	1.99	0.45
1:A:418:ARG:NH2	1:A:431:VAL:O	2.48	0.45
1:A:434:VAL:HB	1:A:462:LEU:CB	2.45	0.45
1:A:480:GLN:C	1:A:482:HIS:N	2.74	0.45
1:B:67:THR:HG23	1:B:68:LYS:H	1.80	0.45
1:B:480:GLN:C	1:B:482:HIS:H	2.24	0.45
1:A:65:ALA:HB1	1:A:87:ILE:HG22	1.99	0.45
1:A:219:LEU:O	1:A:222:VAL:HG12	2.17	0.45
1:A:677:TYR:HE2	1:A:679:TRP:HE1	1.65	0.45
1:A:680:GLU:O	1:A:680:GLU:HG3	2.16	0.45
1:B:410:GLN:NE2	1:B:418:ARG:HD3	2.30	0.45
1:B:437:TYR:CZ	1:B:517:GLN:HG3	2.52	0.45
1:B:442:ASN:HD21	1:B:472:THR:HG23	1.81	0.45
1:B:438:ILE:C	5:B:709:HOH:O	2.59	0.45
1:A:108:GLU:H	1:A:108:GLU:HG2	1.40	0.45
1:A:550:ARG:CG	1:A:552:ILE:HD11	2.47	0.45
1:B:67:THR:O	1:B:68:LYS:C	2.60	0.45
1:B:136:ARG:O	1:B:137:LYS:CG	2.63	0.45
1:B:572:LYS:HG3	1:B:578:ILE:HG21	1.98	0.45
1:A:511:ARG:HD2	1:A:511:ARG:N	2.31	0.45
1:A:656:SER:O	1:A:659:GLY:N	2.46	0.45
1:B:392:LYS:HB2	1:B:392:LYS:HZ2	1.82	0.45
1:B:518:LEU:HG	1:B:524:LEU:HD12	1.99	0.45
1:A:655:LEU:HD22	1:A:658:LEU:HG	1.98	0.45
1:B:284:GLN:O	1:B:286:SER:N	2.50	0.45
1:B:466:ILE:O	1:B:491:PHE:HA	2.16	0.45
1:B:596:PHE:CD1	1:B:608:MET:HE3	2.52	0.45
1:B:653:GLU:C	1:B:655:LEU:N	2.74	0.45
1:A:188:ASP:OD1	1:A:218:GLN:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:LEU:C	1:A:559:ILE:HG22	2.42	0.45
1:B:160:ASN:OD1	1:B:192:GLU:HG3	2.17	0.45
1:B:199:ARG:O	1:B:202:GLU:HG3	2.17	0.45
1:B:631:HIS:O	1:B:634:ASN:N	2.49	0.45
1:A:61:ILE:HD13	1:A:61:ILE:C	2.42	0.45
1:A:423:ILE:N	1:A:423:ILE:CD1	2.73	0.45
1:A:486:HIS:CE1	1:A:488:ARG:HB2	2.52	0.45
1:B:654:SER:C	1:B:656:SER:N	2.74	0.45
1:A:114:TRP:HA	1:A:115:PRO:HD3	1.89	0.44
1:A:156:ILE:HA	1:A:238:LEU:O	2.16	0.44
1:A:606:TYR:HE1	5:A:715:HOH:O	1.98	0.44
1:B:217:TYR:CE2	1:B:357:HIS:HA	2.51	0.44
1:B:187:ASP:C	1:B:187:ASP:OD2	2.58	0.44
1:B:296:THR:HG22	1:B:297:ASN:N	2.32	0.44
1:A:250:GLN:HA	1:A:250:GLN:HE21	1.83	0.44
1:A:445:LYS:HE2	1:A:446:TYR:OH	2.18	0.44
1:A:451:VAL:HG12	1:A:455:LEU:HD11	2.00	0.44
1:B:102:ALA:O	1:B:103:GLU:C	2.60	0.44
1:B:255:LEU:HD12	1:B:379:VAL:CG2	2.47	0.44
1:B:296:THR:CG2	1:B:297:ASN:N	2.80	0.44
1:B:418:ARG:HB2	1:B:418:ARG:NH1	2.30	0.44
1:B:583:ARG:NH1	1:B:609:TYR:HE2	2.15	0.44
1:A:159:TYR:CE2	1:A:160:ASN:ND2	2.85	0.44
1:B:85:ASN:HA	1:B:88:ILE:HD12	2.00	0.44
1:B:522:ASP:OD1	1:B:628:ARG:HA	2.18	0.44
1:B:553:ASP:O	1:B:555:GLU:N	2.50	0.44
1:B:586:THR:CG2	1:B:588:ARG:HB3	2.47	0.44
1:B:129:ASP:OD1	1:B:129:ASP:C	2.60	0.44
1:B:164:ILE:CG2	1:B:241:ASP:HA	2.47	0.44
1:A:150:ASP:OD2	1:A:150:ASP:N	2.47	0.44
1:A:321:ASP:OD1	1:A:324:ARG:NH1	2.50	0.44
1:B:323:LEU:C	1:B:325:LEU:N	2.76	0.44
1:A:94:ILE:HG23	1:A:95:THR:HG23	2.00	0.44
1:A:251:SER:HA	1:A:254:GLU:OE2	2.17	0.44
1:B:175:GLN:HE22	1:B:248:TRP:H	1.64	0.44
1:B:284:GLN:C	1:B:286:SER:N	2.75	0.44
1:A:73:ASN:OD1	1:A:424:GLU:O	2.35	0.44
1:A:210:VAL:CG2	1:A:225:LEU:HD13	2.48	0.44
1:A:409:LEU:HB3	1:A:413:VAL:HB	1.99	0.44
1:A:440:ALA:HB1	1:A:443:CYS:SG	2.58	0.44
1:B:322:ASN:O	1:B:323:LEU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:LEU:HD13	1:B:434:VAL:CG2	2.33	0.44
1:A:242:MET:HG3	1:A:336:GLY:O	2.18	0.44
1:A:451:VAL:HG12	1:A:455:LEU:CD1	2.47	0.44
1:B:211:ARG:HG2	1:B:211:ARG:HH11	1.82	0.44
1:B:388:GLU:HA	1:B:389:PRO:HD3	1.76	0.44
1:A:118:LEU:HD21	1:A:660:ILE:HD13	2.00	0.43
1:A:545:VAL:HG12	1:A:619:LYS:HB3	2.00	0.43
1:A:550:ARG:HD2	1:A:552:ILE:HD11	1.99	0.43
1:B:361:GLU:O	1:B:362:ASP:C	2.60	0.43
1:B:564:ASN:HA	1:B:580:HIS:NE2	2.33	0.43
1:B:645:GLU:O	1:B:649:LYS:HD3	2.18	0.43
1:A:67:THR:HA	1:A:70:MET:HE3	1.99	0.43
1:A:545:VAL:O	1:A:545:VAL:HG23	2.18	0.43
1:B:294:ILE:CD1	1:B:295:ILE:N	2.78	0.43
1:B:565:TRP:CE3	1:B:565:TRP:HA	2.52	0.43
1:A:418:ARG:NH2	1:A:429:LYS:HB3	2.27	0.43
1:A:551:ASN:C	1:A:552:ILE:HD13	2.44	0.43
1:A:588:ARG:O	1:A:592:LEU:HG	2.17	0.43
1:B:150:ASP:OD2	1:B:150:ASP:N	2.51	0.43
1:B:666:SER:C	5:B:706:HOH:O	2.61	0.43
1:B:135:LYS:O	1:B:136:ARG:C	2.61	0.43
1:B:477:ARG:HA	1:B:480:GLN:OE1	2.18	0.43
1:B:558:LEU:C	1:B:558:LEU:HD13	2.43	0.43
1:A:61:ILE:HD11	5:A:754:HOH:O	2.19	0.43
1:A:103:GLU:H	1:A:103:GLU:HG3	1.58	0.43
1:A:238:LEU:HD21	1:A:244:PRO:HD3	1.99	0.43
1:A:445:LYS:HE2	1:A:446:TYR:CZ	2.54	0.43
1:B:84:LYS:O	1:B:85:ASN:C	2.62	0.43
1:B:552:ILE:HG13	1:B:627:ASN:HB3	2.01	0.43
1:B:610:LEU:HD12	1:B:610:LEU:HA	1.85	0.43
1:B:648:PHE:O	1:B:651:VAL:HB	2.19	0.43
1:A:101:ARG:HG2	1:A:101:ARG:HH11	1.84	0.43
1:A:129:ASP:HA	1:A:324:ARG:HG2	1.99	0.43
1:A:414:PRO:O	1:A:415:TYR:O	2.36	0.43
1:B:464:VAL:HG12	1:B:466:ILE:HD11	2.01	0.43
1:A:117:ASP:O	1:A:662:LYS:NZ	2.34	0.43
1:A:287:LEU:O	1:A:291:ILE:HG13	2.19	0.43
1:A:490:ARG:NH1	1:A:509:LEU:HD22	2.30	0.43
1:A:669:THR:HG22	1:A:670:ASN:H	1.84	0.43
1:B:79:LEU:HD23	1:B:79:LEU:C	2.43	0.43
1:B:241:ASP:CG	5:B:746:HOH:O	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:ASP:OD1	1:B:628:ARG:HG3	2.19	0.43
1:B:657:ARG:C	1:B:659:GLY:N	2.74	0.43
1:A:255:LEU:HB2	1:A:264:LEU:HD11	2.00	0.43
1:A:476:LEU:O	1:A:476:LEU:HD12	2.18	0.43
1:A:643:GLN:CG	1:A:644:LYS:N	2.71	0.43
1:B:172:LEU:HA	1:B:175:GLN:HG2	2.01	0.43
1:B:206:ASN:CB	5:B:697:HOH:O	2.66	0.43
1:A:153:SER:HA	1:A:182:GLU:HG2	2.00	0.43
1:A:284:GLN:O	1:A:286:SER:N	2.50	0.43
1:B:270:TYR:HB3	1:B:296:THR:OG1	2.19	0.43
1:B:572:LYS:HG2	1:B:578:ILE:HD13	2.01	0.43
1:A:80:ASN:O	1:A:81:GLU:C	2.61	0.42
1:A:265:ILE:HD13	1:A:333:PHE:HA	2.01	0.42
1:A:270:TYR:O	1:A:293:GLU:HA	2.19	0.42
1:A:404:ILE:HD12	1:A:407:GLN:HE21	1.82	0.42
1:B:575:SER:O	1:B:576:ALA:HB2	2.18	0.42
1:A:124:PRO:HB3	1:A:132:TRP:CE3	2.54	0.42
1:A:441:TYR:CE2	1:A:471:SER:HA	2.54	0.42
1:A:474:ASP:O	1:A:475:THR:C	2.62	0.42
1:A:490:ARG:HH21	1:A:511:ARG:HD3	1.83	0.42
1:A:573:LEU:C	1:A:575:SER:H	2.28	0.42
1:B:68:LYS:HG2	1:B:87:ILE:HD13	2.00	0.42
1:B:84:LYS:O	1:B:87:ILE:HB	2.19	0.42
1:B:110:ILE:O	1:B:111:PRO:C	2.62	0.42
1:B:270:TYR:O	1:B:293:GLU:HA	2.20	0.42
1:A:167:ILE:HB	1:A:387:GLN:HE22	1.85	0.42
1:A:409:LEU:O	1:A:410:GLN:C	2.62	0.42
1:B:291:ILE:HG23	1:B:292:PRO:HD2	2.02	0.42
1:B:449:ARG:HD3	1:B:523:PHE:HB3	2.00	0.42
1:B:653:GLU:O	1:B:656:SER:HB3	2.18	0.42
1:A:539:ASP:C	1:A:541:SER:N	2.77	0.42
1:B:125:GLU:OE1	1:B:324:ARG:NH2	2.51	0.42
1:B:225:LEU:C	1:B:225:LEU:CD2	2.92	0.42
1:B:549:ASN:CA	1:B:624:ILE:HG23	2.48	0.42
1:A:152:LEU:CD2	1:A:236:ALA:HB2	2.47	0.42
1:A:553:ASP:O	1:A:554:ARG:C	2.62	0.42
1:B:155:VAL:O	1:B:157:PRO:HD3	2.20	0.42
1:B:223:ARG:NH2	1:B:335:GLY:HA3	2.34	0.42
1:B:583:ARG:NH1	1:B:609:TYR:CE2	2.88	0.42
1:A:219:LEU:HA	1:A:222:VAL:HG12	2.02	0.42
1:B:82:VAL:O	1:B:83:GLU:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:PRO:CG	1:B:572:LYS:HD2	2.45	0.42
1:B:312:TRP:CZ2	1:B:313:ARG:HG2	2.54	0.42
1:B:352:ASP:OD1	1:B:352:ASP:C	2.63	0.42
1:B:503:SER:HB3	1:B:596:PHE:CE1	2.54	0.42
1:B:557:ASN:N	1:B:557:ASN:ND2	2.67	0.42
1:B:630:LEU:HD12	1:B:630:LEU:HA	1.88	0.42
1:A:113:ASP:OD1	1:A:677:TYR:OH	2.27	0.42
1:A:258:VAL:HG23	1:A:259:ASP:N	2.35	0.42
1:A:376:PHE:CD2	5:A:748:HOH:O	2.56	0.42
1:A:533:LEU:O	1:A:537:ARG:HD3	2.20	0.42
1:B:63:ILE:CG1	1:B:64:ASP:H	2.33	0.42
1:B:318:LYS:HB2	1:B:318:LYS:HZ3	1.85	0.42
1:B:414:PRO:CA	1:B:418:ARG:NH1	2.83	0.42
1:B:486:HIS:ND1	1:B:487:PRO:HD2	2.34	0.42
1:B:577:MET:HE1	1:B:579:CYS:HB3	2.02	0.42
1:A:460:THR:CB	5:A:730:HOH:O	2.67	0.42
1:A:640:LEU:C	1:A:643:GLN:HG2	2.45	0.42
1:B:81:GLU:HG2	1:B:85:ASN:ND2	2.35	0.42
1:B:525:GLU:CG	1:B:625:CYS:HA	2.50	0.42
1:B:662:LYS:HG3	1:B:663:TYR:CD1	2.54	0.42
1:A:552:ILE:CG2	1:A:553:ASP:N	2.82	0.41
1:A:653:GLU:OE2	1:A:665:TYR:HB3	2.20	0.41
1:B:67:THR:HB	1:B:488:ARG:HD3	2.02	0.41
1:B:329:PRO:HB2	1:B:376:PHE:HB2	2.02	0.41
1:B:552:ILE:CD1	1:B:558:LEU:HA	2.49	0.41
1:B:603:ALA:O	1:B:604:VAL:C	2.63	0.41
1:B:614:GLU:CD	1:B:655:LEU:HD21	2.45	0.41
1:B:658:LEU:HD23	1:B:658:LEU:HA	1.73	0.41
1:A:239:ASP:HB3	1:A:241:ASP:OD1	2.20	0.41
1:A:350:TRP:CD1	1:A:350:TRP:N	2.88	0.41
1:A:418:ARG:HH21	1:A:429:LYS:HG3	1.85	0.41
1:B:158:THR:HG21	1:B:194:ILE:HD12	2.03	0.41
1:B:238:LEU:O	1:B:239:ASP:C	2.63	0.41
1:B:519:ASP:HB2	1:B:522:ASP:OD2	2.21	0.41
1:A:429:LYS:HA	1:A:429:LYS:HD3	1.69	0.41
1:A:550:ARG:HG3	1:A:550:ARG:O	2.19	0.41
1:A:620:HIS:HD2	1:A:621:ILE:O	2.02	0.41
1:B:177:THR:CA	1:B:250:GLN:HE21	2.25	0.41
1:B:272:ASP:OD2	1:B:272:ASP:N	2.48	0.41
1:A:69:ILE:HD13	1:A:88:ILE:HG12	2.02	0.41
1:A:552:ILE:HG22	1:A:553:ASP:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:GLU:HB2	5:B:691:HOH:O	2.21	0.41
1:B:323:LEU:O	1:B:325:LEU:N	2.54	0.41
1:B:435:SER:CB	1:B:510:CYS:HB3	2.50	0.41
1:A:215:TYR:CE1	1:A:218:GLN:HG3	2.55	0.41
1:A:234:TYR:N	5:A:709:HOH:O	2.53	0.41
1:B:645:GLU:O	1:B:645:GLU:HG3	2.19	0.41
1:B:91:TYR:CA	1:B:94:ILE:HG22	2.48	0.41
1:A:114:TRP:CZ2	1:A:118:LEU:HD12	2.55	0.41
1:A:156:ILE:HG23	1:A:238:LEU:O	2.20	0.41
1:A:354:GLU:CD	1:A:430:ARG:HH22	2.28	0.41
1:B:121:PRO:HA	1:B:122:PRO:HD3	1.85	0.41
1:B:363:ASN:ND2	1:B:417:TYR:HE2	2.18	0.41
1:B:523:PHE:CE1	1:B:627:ASN:ND2	2.89	0.41
1:B:601:SER:HB2	1:B:647:HIS:HE1	1.86	0.41
1:A:199:ARG:NH2	1:B:211:ARG:HH21	2.18	0.41
1:A:471:SER:HB3	1:A:473:ASP:OD2	2.21	0.41
1:B:345:LEU:HD23	1:B:345:LEU:HA	1.95	0.41
1:B:649:LYS:N	1:B:649:LYS:CD	2.84	0.41
1:A:560:SER:OG	1:A:561:ASN:N	2.54	0.41
1:B:81:GLU:HG2	1:B:85:ASN:HD21	1.86	0.41
1:B:242:MET:HE1	1:B:268:ARG:HB3	2.02	0.41
1:B:423:ILE:HD12	1:B:423:ILE:N	2.06	0.41
1:B:92:ARG:O	1:B:96:ALA:HB2	2.21	0.41
1:B:126:SER:CA	5:B:737:HOH:O	2.68	0.41
1:B:284:GLN:NE2	1:B:287:LEU:HD22	2.35	0.41
1:B:356:THR:OG1	1:B:357:HIS:N	2.53	0.41
1:A:90:LYS:HA	1:A:90:LYS:HD2	1.90	0.40
1:A:212:GLN:HB2	5:A:708:HOH:O	2.20	0.40
1:A:418:ARG:HB2	1:A:418:ARG:NH1	2.11	0.40
1:B:227:LEU:HD23	1:B:227:LEU:HA	1.94	0.40
1:A:79:LEU:HD21	1:A:83:GLU:CD	2.45	0.40
1:A:213:LYS:CE	1:B:202:GLU:O	2.69	0.40
1:A:475:THR:N	5:A:750:HOH:O	2.54	0.40
1:B:283:SER:OG	1:B:284:GLN:N	2.54	0.40
1:B:389:PRO:HA	1:B:390:PRO:HD3	1.83	0.40
1:A:422:LYS:HD3	5:A:743:HOH:O	2.20	0.40
1:B:80:ASN:C	1:B:82:VAL:N	2.80	0.40
1:B:124:PRO:HD3	1:B:132:TRP:CE2	2.57	0.40
1:B:248:TRP:CZ2	1:B:252:TYR:HE2	2.39	0.40
1:B:296:THR:HG22	1:B:297:ASN:O	2.21	0.40
1:A:61:ILE:CD1	1:A:62:ASP:N	2.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:ARG:C	1:A:659:GLY:N	2.79	0.40
1:B:72:SER:O	1:B:73:ASN:C	2.64	0.40
1:B:164:ILE:HG21	1:B:241:ASP:HB3	2.03	0.40
1:B:164:ILE:HG22	1:B:241:ASP:HA	2.03	0.40
1:B:427:THR:CG2	5:B:741:HOH:O	2.69	0.40
1:B:563:TYR:CD1	1:B:564:ASN:N	2.89	0.40
1:A:639:LYS:O	1:A:640:LEU:C	2.64	0.40
1:A:655:LEU:CD2	1:A:658:LEU:HG	2.52	0.40
1:B:238:LEU:HA	1:B:336:GLY:O	2.21	0.40
1:B:418:ARG:NE	1:B:429:LYS:HG3	2.28	0.40
1:B:511:ARG:HH11	1:B:511:ARG:CG	2.32	0.40
1:B:572:LYS:HB3	1:B:578:ILE:HD13	2.03	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	593/624 (95%)	507 (86%)	63 (11%)	23 (4%)	2	14
1	B	581/624 (93%)	472 (81%)	77 (13%)	32 (6%)	1	8
All	All	1174/1248 (94%)	979 (83%)	140 (12%)	55 (5%)	2	11

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	VAL
1	A	136	ARG
1	A	137	LYS
1	A	337	ASN
1	A	410	GLN
1	A	415	TYR

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Mol	Chain	Res	Type
1	A	444	SER
1	A	638	LYS
1	A	641	ASP
1	B	61	ILE
1	B	63	ILE
1	B	65	ALA
1	B	359	GLY
1	B	420	LYS
1	B	422	LYS
1	B	426	ALA
1	B	527	ASP
1	B	580	HIS
1	A	285	LYS
1	A	423	ILE
1	A	474	ASP
1	A	560	SER
1	A	580	HIS
1	B	66	ALA
1	B	73	ASN
1	B	81	GLU
1	B	285	LYS
1	B	357	HIS
1	B	391	GLY
1	B	410	GLN
1	B	559	ILE
1	B	577	MET
1	B	638	LYS
1	B	648	PHE
1	A	335	GLY
1	A	484	ALA
1	A	640	LEU
1	B	504	ASN
1	B	576	ALA
1	A	111	PRO
1	A	526	PRO
1	A	655	LEU
1	B	85	ASN
1	B	160	ASN
1	B	311	ASP
1	B	320	THR
1	B	554	ARG
1	B	556	GLY

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Mol	Chain	Res	Type
1	A	64	ASP
1	B	481	GLU
1	B	484	ALA
1	A	540	LEU
1	A	559	ILE
1	B	475	THR
1	B	294	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	539/557 (97%)	485 (90%)	54 (10%)	7	29
1	B	530/557 (95%)	490 (92%)	40 (8%)	12	41
All	All	1069/1114 (96%)	975 (91%)	94 (9%)	9	35

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	VAL
1	A	61	ILE
1	A	77	ILE
1	A	104	LEU
1	A	107	VAL
1	A	111	PRO
1	A	112	LEU
1	A	120	LEU
1	A	152	LEU
1	A	158	THR
1	A	195	GLU
1	A	210	VAL
1	A	213	LYS
1	A	219	LEU
1	A	225	LEU
1	A	262	VAL

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Mol	Chain	Res	Type
1	A	272	ASP
1	A	273	THR
1	A	285	LYS
1	A	298	ASN
1	A	304	VAL
1	A	305	GLU
1	A	318	LYS
1	A	325	LEU
1	A	361	GLU
1	A	369	LEU
1	A	371	ARG
1	A	380	GLU
1	A	388	GLU
1	A	409	LEU
1	A	418	ARG
1	A	419	LYS
1	A	423	ILE
1	A	424	GLU
1	A	433	LEU
1	A	462	LEU
1	A	496	ASN
1	A	497	LYS
1	A	499	ILE
1	A	518	LEU
1	A	533	LEU
1	A	542	LEU
1	A	554	ARG
1	A	557	ASN
1	A	559	ILE
1	A	579	CYS
1	A	581	HIS
1	A	586	THR
1	A	601	SER
1	A	612	LEU
1	A	639	LYS
1	A	654	SER
1	A	655	LEU
1	A	681	LYS
1	B	61	ILE
1	B	71	CYS
1	B	82	VAL
1	B	93	GLU

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Mol	Chain	Res	Type
1	B	118	LEU
1	B	120	LEU
1	B	150	ASP
1	B	195	GLU
1	B	219	LEU
1	B	262	VAL
1	B	279	LEU
1	B	318	LYS
1	B	325	LEU
1	B	356	THR
1	B	358	TRP
1	B	361	GLU
1	B	369	LEU
1	B	380	GLU
1	B	392	LYS
1	B	411	GLN
1	B	418	ARG
1	B	423	ILE
1	B	433	LEU
1	B	449	ARG
1	B	468	ASP
1	B	497	LYS
1	B	499	ILE
1	B	509	LEU
1	B	518	LEU
1	B	537	ARG
1	B	542	LEU
1	B	574	THR
1	B	575	SER
1	B	581	HIS
1	B	605	ASP
1	B	628	ARG
1	B	645	GLU
1	B	654	SER
1	B	655	LEU
1	B	669	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	174	ASN

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Mol	Chain	Res	Type
1	A	175	GLN
1	A	212	GLN
1	A	245	ASN
1	A	250	GLN
1	A	289	ASN
1	A	297	ASN
1	A	299	GLN
1	A	363	ASN
1	A	387	GLN
1	A	407	GLN
1	A	411	GLN
1	A	494	GLN
1	A	496	ASN
1	A	517	GLN
1	A	551	ASN
1	A	557	ASN
1	A	620	HIS
1	A	631	HIS
1	A	643	GLN
1	B	80	ASN
1	B	85	ASN
1	B	174	ASN
1	B	175	GLN
1	B	212	GLN
1	B	245	ASN
1	B	250	GLN
1	B	284	GLN
1	B	289	ASN
1	B	297	ASN
1	B	363	ASN
1	B	387	GLN
1	B	410	GLN
1	B	411	GLN
1	B	494	GLN
1	B	496	ASN
1	B	504	ASN
1	B	517	GLN
1	B	551	ASN
1	B	557	ASN
1	B	620	HIS
1	B	631	HIS
1	B	634	ASN

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Mol	Chain	Res	Type
1	B	643	GLN
1	B	672	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	UDP	A	684	-	25,26,26	1.82	5 (20%)	38,40,40	2.34	11 (28%)
2	UD2	B	683	4	40,41,41	0.67	0	59,62,62	1.64	12 (20%)
2	UD2	A	683	4	40,41,41	0.75	0	59,62,62	1.68	11 (18%)
3	UDP	B	1	4	25,26,26	2.01	6 (24%)	38,40,40	2.04	10 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UDP	A	684	-	-	3/16/32/32	0/2/2/2
2	UD2	B	683	4	-	9/26/63/63	0/3/3/3
2	UD2	A	683	4	-	6/26/63/63	0/3/3/3
3	UDP	B	1	4	-	4/16/32/32	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	UDP	PA-O3A	-5.06	1.54	1.59
3	A	684	UDP	C4-N3	-3.91	1.31	1.38
3	B	1	UDP	C4-N3	-3.73	1.32	1.38
3	A	684	UDP	PA-O3A	-3.62	1.55	1.59
3	B	1	UDP	C5-C4	-3.53	1.36	1.43
3	B	1	UDP	C2-N3	-3.32	1.32	1.38
3	A	684	UDP	C2-N3	-3.11	1.32	1.38
3	B	1	UDP	C6-N1	-3.07	1.30	1.38
3	A	684	UDP	C6-N1	-2.84	1.31	1.38
3	A	684	UDP	C5-C4	-2.69	1.37	1.43
3	B	1	UDP	O4'-C4'	-2.42	1.39	1.45

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	684	UDP	N3-C2-N1	7.14	124.18	114.89
3	A	684	UDP	C4-N3-C2	-6.94	117.99	126.61
3	B	1	UDP	C4-N3-C2	-5.68	119.56	126.61
3	B	1	UDP	N3-C2-N1	5.29	121.78	114.89
2	A	683	UD2	C4-N3-C2	-4.46	121.08	126.61
2	B	683	UD2	C4-N3-C2	-4.41	121.13	126.61
2	B	683	UD2	N3-C2-N1	4.34	120.54	114.89
2	B	683	UD2	C3'-C2'-N2'	-4.29	102.71	110.62
2	A	683	UD2	N3-C2-N1	4.08	120.21	114.89
3	A	684	UDP	O3'-C3'-C2'	-3.94	99.17	111.82
2	A	683	UD2	O4B-C4B-C5B	-3.67	97.57	109.33
2	A	683	UD2	C5-C4-N3	3.58	119.81	114.80
3	A	684	UDP	C5-C4-N3	3.51	119.72	114.80
3	B	1	UDP	C5-C4-N3	3.36	119.51	114.80
3	A	684	UDP	O2-C2-N3	-3.25	115.49	121.49
2	B	683	UD2	C5-C4-N3	3.22	119.31	114.80
2	A	683	UD2	O1'-C1'-C2'	3.17	114.14	108.40
2	A	683	UD2	O4B-C1B-N1	3.11	115.41	108.36
3	B	1	UDP	O4-C4-C5	-3.10	119.81	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	683	UD2	O5'-C1'-C2'	-3.03	104.87	110.59
2	A	683	UD2	O4-C4-C5	-2.96	120.05	125.16
3	B	1	UDP	O3B-PB-O3A	-2.95	94.75	104.64
3	B	1	UDP	O4'-C1'-N1	-2.86	101.88	108.36
2	B	683	UD2	O5'-C1'-C2'	-2.75	105.40	110.59
2	B	683	UD2	O4-C4-C5	-2.70	120.50	125.16
3	A	684	UDP	O2'-C2'-C3'	-2.56	103.62	111.82
2	B	683	UD2	O5'-C5'-C6'	2.53	112.70	106.44
3	B	1	UDP	O2-C2-N3	-2.51	116.85	121.49
2	B	683	UD2	C6'-C5'-C4'	-2.51	106.85	113.02
3	A	684	UDP	O3'-C3'-C4'	-2.50	103.89	111.08
3	B	1	UDP	O2'-C2'-C3'	-2.48	103.86	111.82
3	A	684	UDP	O3A-PB-O1B	-2.40	98.42	111.04
2	A	683	UD2	O5'-C5'-C4'	2.37	113.97	109.70
2	A	683	UD2	C4'-C3'-C2'	-2.34	107.00	110.40
2	A	683	UD2	O1A-PA-O3A	2.30	113.50	107.27
3	B	1	UDP	O4'-C1'-C2'	-2.28	101.74	106.62
2	B	683	UD2	O3B-C3B-C4B	-2.19	104.79	111.08
2	B	683	UD2	C2B-C3B-C4B	2.18	106.82	102.61
3	A	684	UDP	C6-N1-C2	-2.16	118.37	121.00
3	A	684	UDP	C5-C6-N1	-2.14	118.36	121.84
2	B	683	UD2	O2-C2-N1	-2.13	120.03	122.80
3	A	684	UDP	O2B-PB-O1B	2.10	119.03	110.83
3	B	1	UDP	O3'-C3'-C2'	-2.10	105.09	111.82
2	B	683	UD2	O5'-C5'-C4'	2.02	113.34	109.70

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	683	UD2	C5B-O5B-PA-O1A
2	A	683	UD2	C5B-O5B-PA-O3A
2	B	683	UD2	C1'-C2'-N2'-C7'
2	B	683	UD2	C1'-O1'-PB-O3A
3	B	1	UDP	C5'-O5'-PA-O1A
3	B	1	UDP	C5'-O5'-PA-O2A
2	A	683	UD2	O5'-C5'-C6'-O6'
2	A	683	UD2	C3B-C4B-C5B-O5B
2	A	683	UD2	O4B-C4B-C5B-O5B
2	B	683	UD2	O5'-C5'-C6'-O6'
3	A	684	UDP	PB-O3A-PA-O5'
2	B	683	UD2	C1'-O1'-PB-O1B

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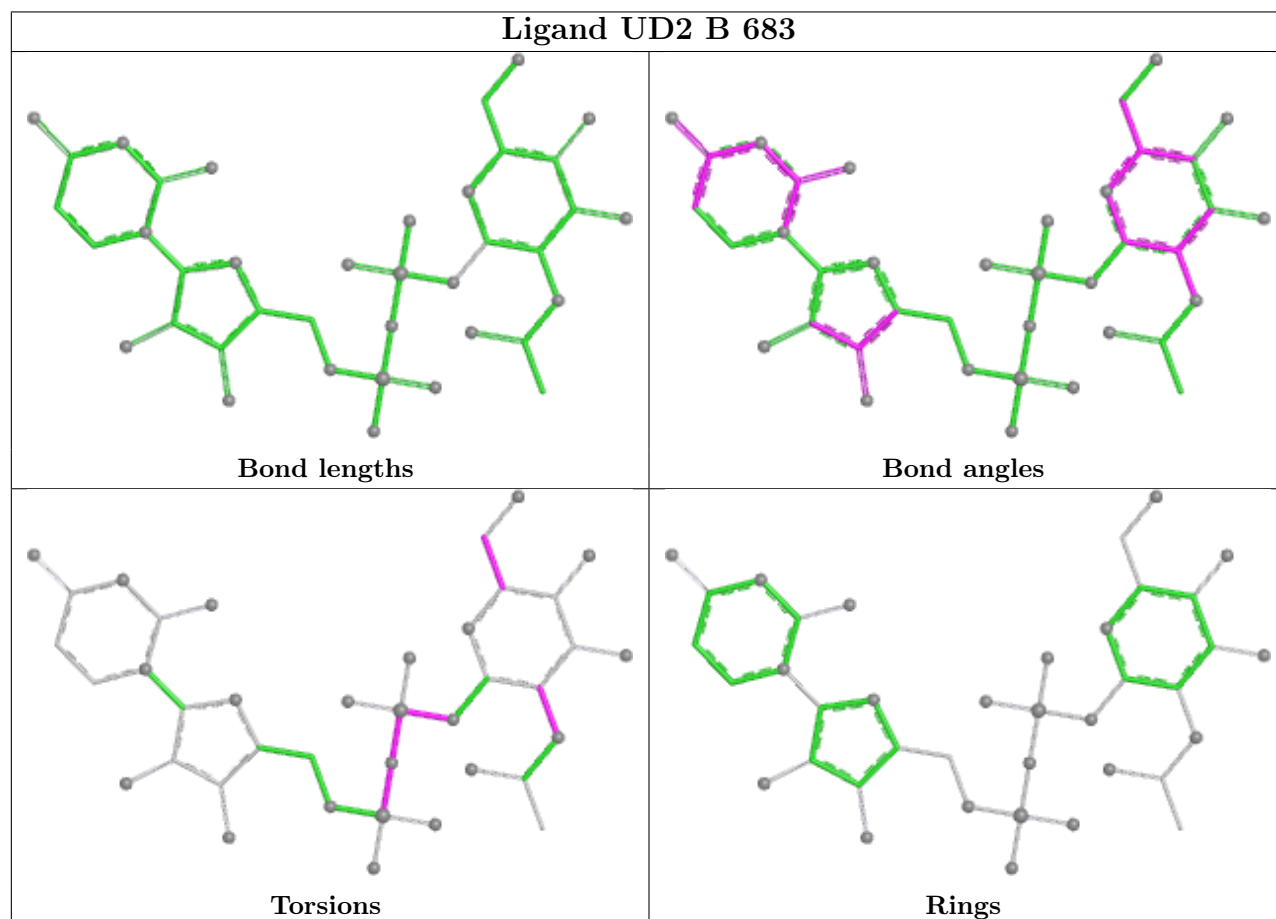
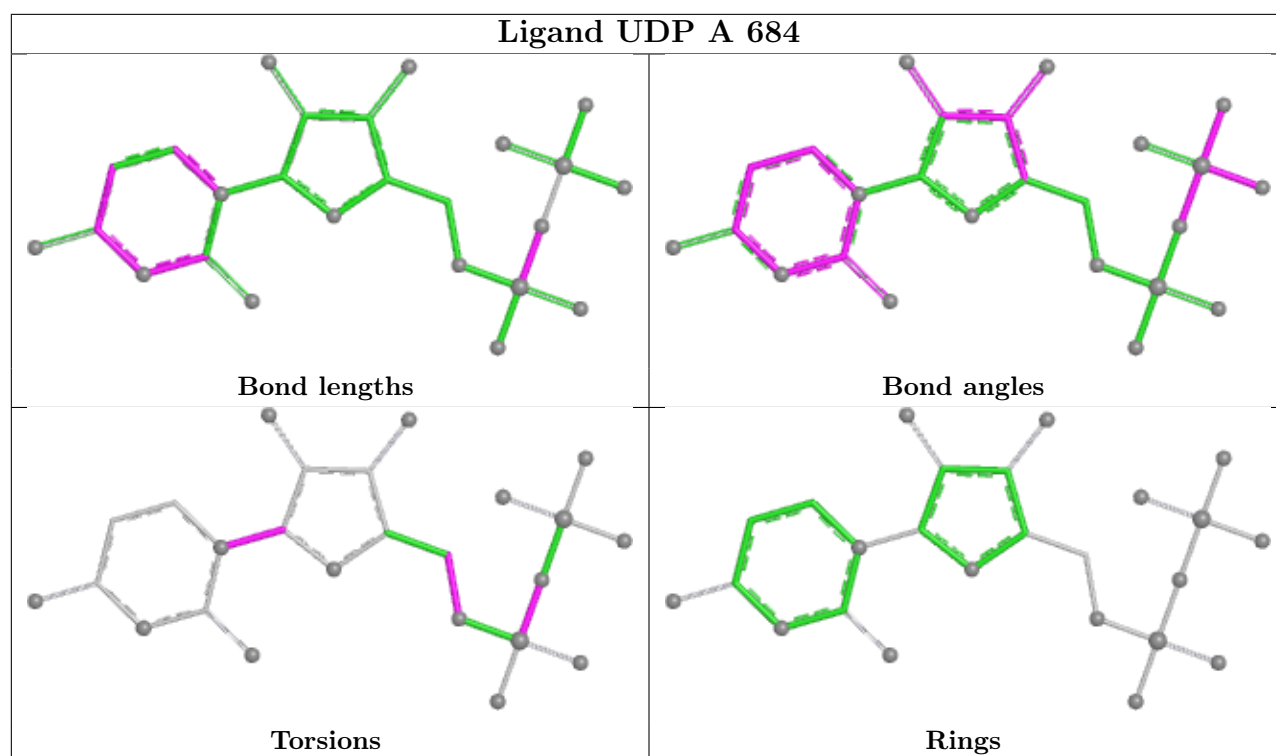
Mol	Chain	Res	Type	Atoms
3	B	1	UDP	C5'-O5'-PA-O3A
3	A	684	UDP	C4'-C5'-O5'-PA
2	A	683	UD2	C4'-C5'-C6'-O6'
2	B	683	UD2	C3'-C2'-N2'-C7'
2	B	683	UD2	PB-O3A-PA-O1A
2	B	683	UD2	PA-O3A-PB-O2B
2	B	683	UD2	PB-O3A-PA-O2A
2	B	683	UD2	PA-O3A-PB-O1B
3	A	684	UDP	C2'-C1'-N1-C6
3	B	1	UDP	PB-O3A-PA-O1A

There are no ring outliers.

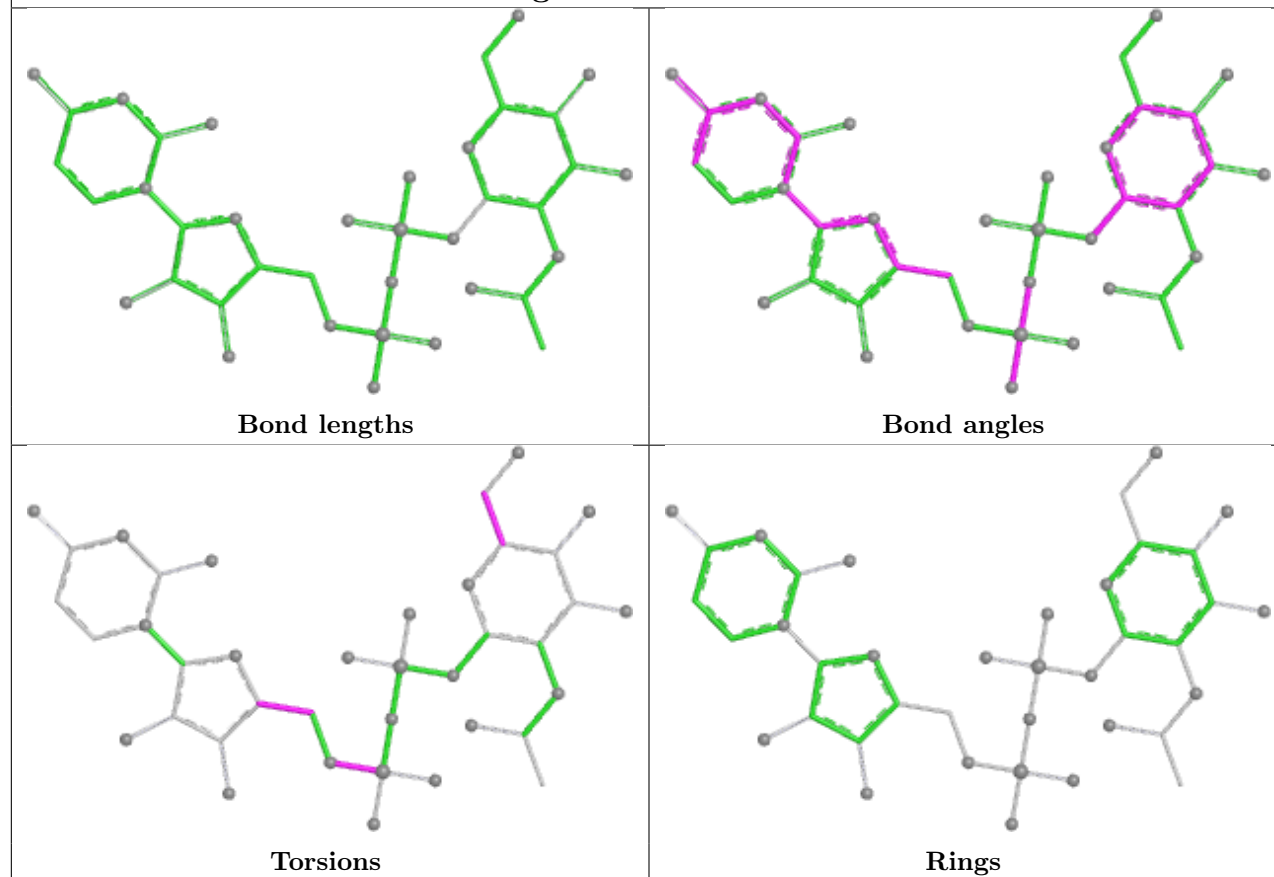
3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	684	UDP	8	0
2	B	683	UD2	1	0
3	B	1	UDP	1	0

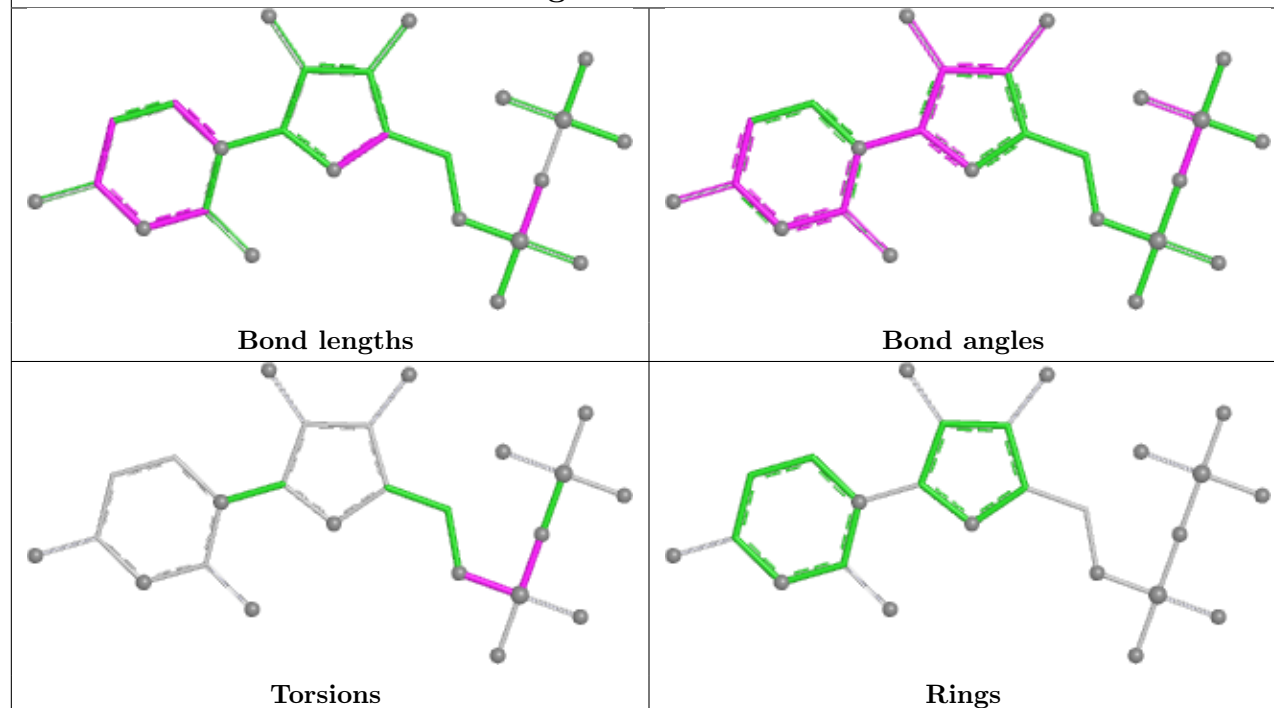
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



Ligand UD2 A 683



Ligand UDP B 1



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	601/624 (96%)	-0.59	3 (0%)	87 72	20, 49, 87, 122	22 (3%)
1	B	591/624 (94%)	-0.52	1 (0%)	91 83	20, 52, 95, 119	21 (3%)
All	All	1192/1248 (95%)	-0.56	4 (0%)	90 79	20, 50, 90, 122	43 (3%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	76	ALA	2.4
1	B	638	LYS	2.2
1	A	77	ILE	2.1
1	A	407	GLN	2.0

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.

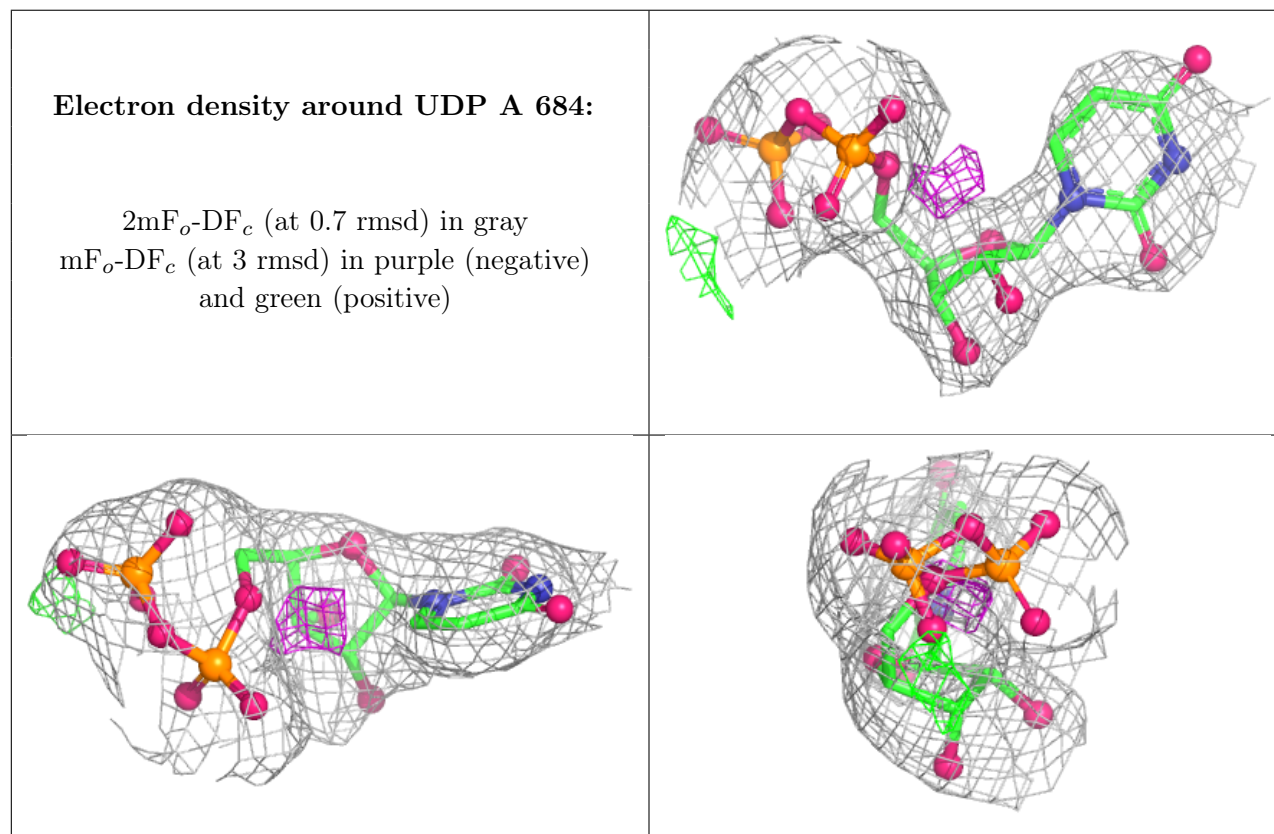
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
3	UDP	A	684	25/25	0.88	0.10	52,80,106,110	0

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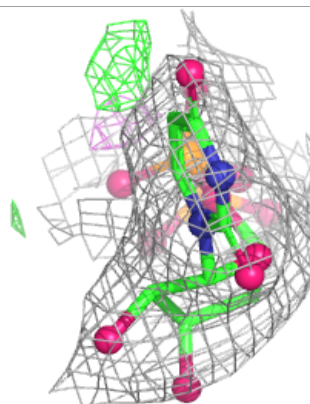
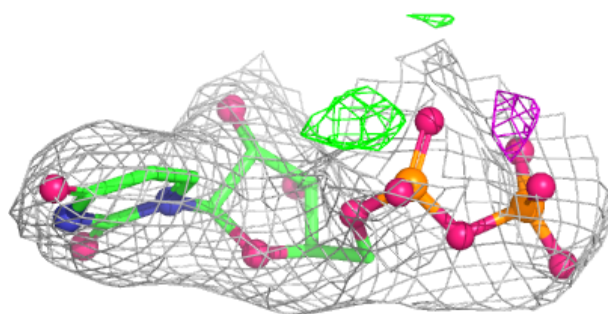
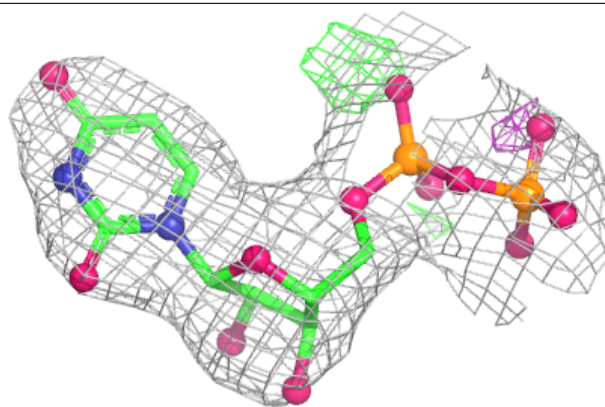
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	UDP	B	1	25/25	0.90	0.10	51,66,124,131	0
2	UD2	A	683	39/39	0.95	0.08	29,55,99,102	0
4	MN	A	2	1/1	0.95	0.06	62,62,62,62	0
2	UD2	B	683	39/39	0.96	0.08	29,55,72,79	0
4	MN	B	4	1/1	0.97	0.03	65,65,65,65	0
4	MN	A	1	1/1	0.98	0.03	47,47,47,47	0
4	MN	B	3	1/1	0.99	0.02	48,48,48,48	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

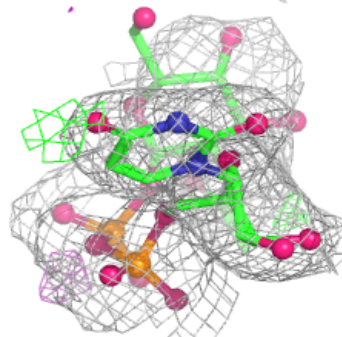
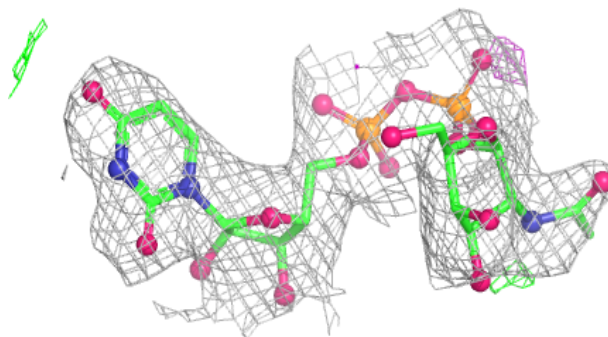
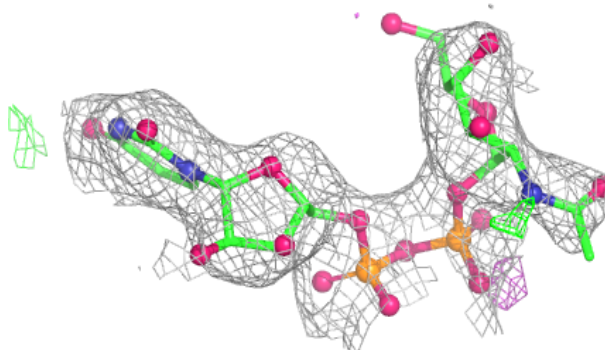


Electron density around UDP B 1:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

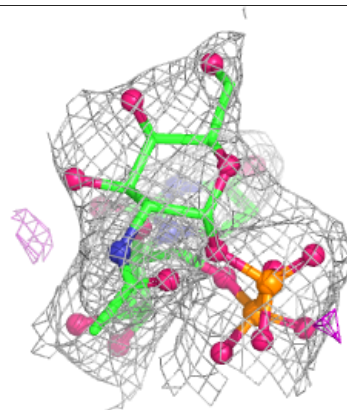
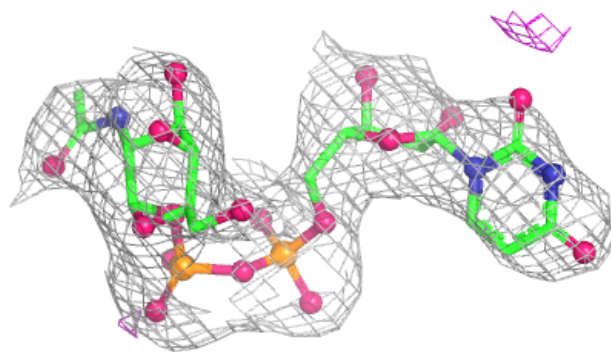
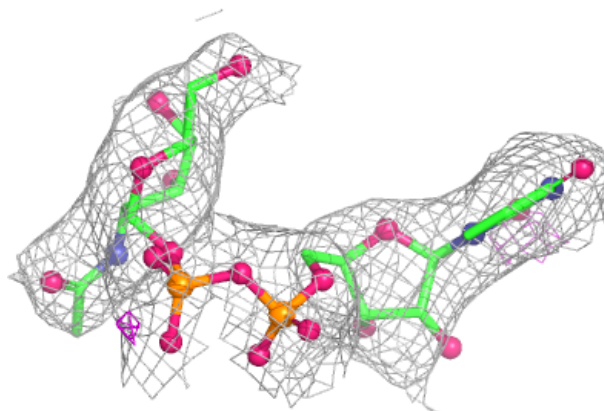
**Electron density around UD2 A 683:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around UD2 B 683:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.