



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:15 PM UTC

PDB ID : 6IWR / pdb_00006iwr
Title : Crystal structure of GalNAc-T7 with UDP, GalNAc and Mn2+
Authors : Yu, C.; Yin, Y.X.
Deposited on : 2018-12-06
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

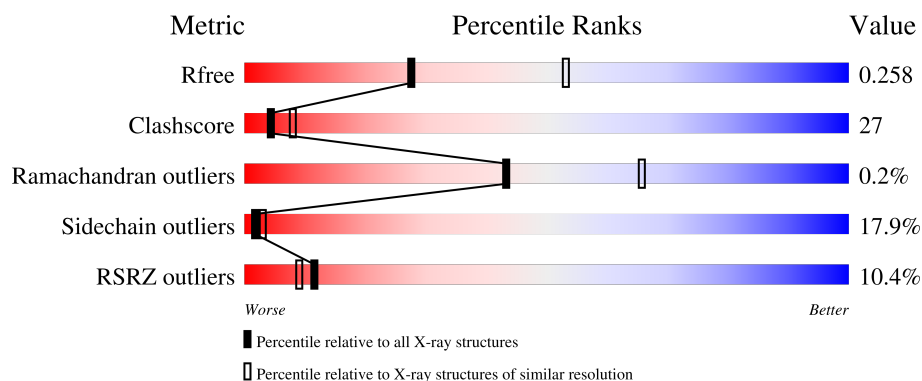
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	597	
1	B	597	
1	C	597	
1	D	597	
1	E	597	

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Mol	Chain	Length	Quality of chain
1	F	597	16% 51% 32% 8% 9%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 27098 atoms, of which 26 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 N-acetylgalactosaminyltransferase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	546	Total	C	N	O	S	0	0	0
			4440	2855	757	805	23			
1	B	546	Total	C	N	O	S	0	0	0
			4440	2855	757	805	23			
1	C	546	Total	C	N	O	S	0	0	0
			4440	2855	757	805	23			
1	D	538	Total	C	N	O	S	0	0	0
			4380	2814	748	795	23			
1	E	546	Total	C	N	O	S	0	0	0
			4440	2855	757	805	23			
1	F	546	Total	C	N	O	S	0	0	0
			4440	2855	757	805	23			

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

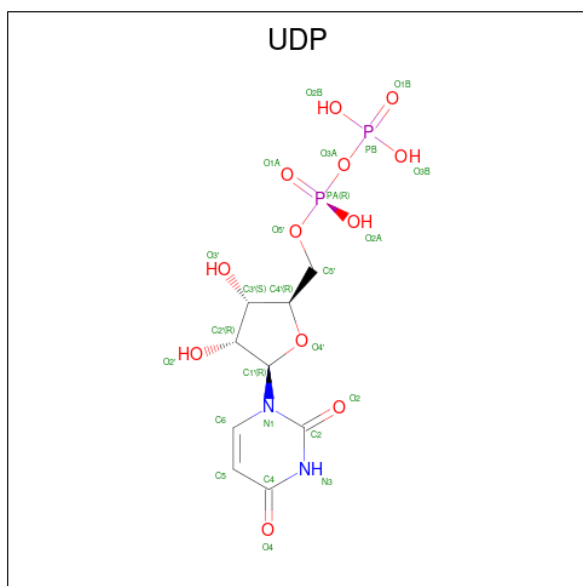
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		
2	E	1	Total	Mn	0	0
			1	1		
2	F	1	Total	Mn	0	0
			1	1		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



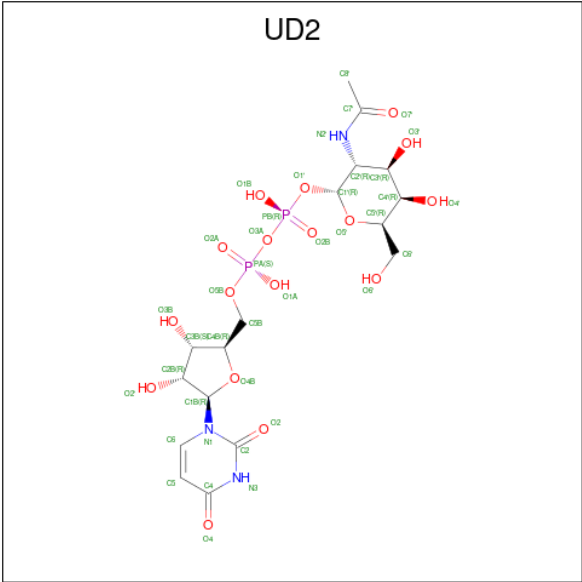
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	H	N	O	0	0
			30	8	15	1	6		

- Molecule 4 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	H	N	O	P	
			36	9	11	2	12	2	

- Molecule 5 is URIDINE-DIPHOSPHATE-N-ACETYLGLACTOSAMINE (CCD ID: UD2) (formula: $C_{17}H_{27}N_3O_{17}P_2$).



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

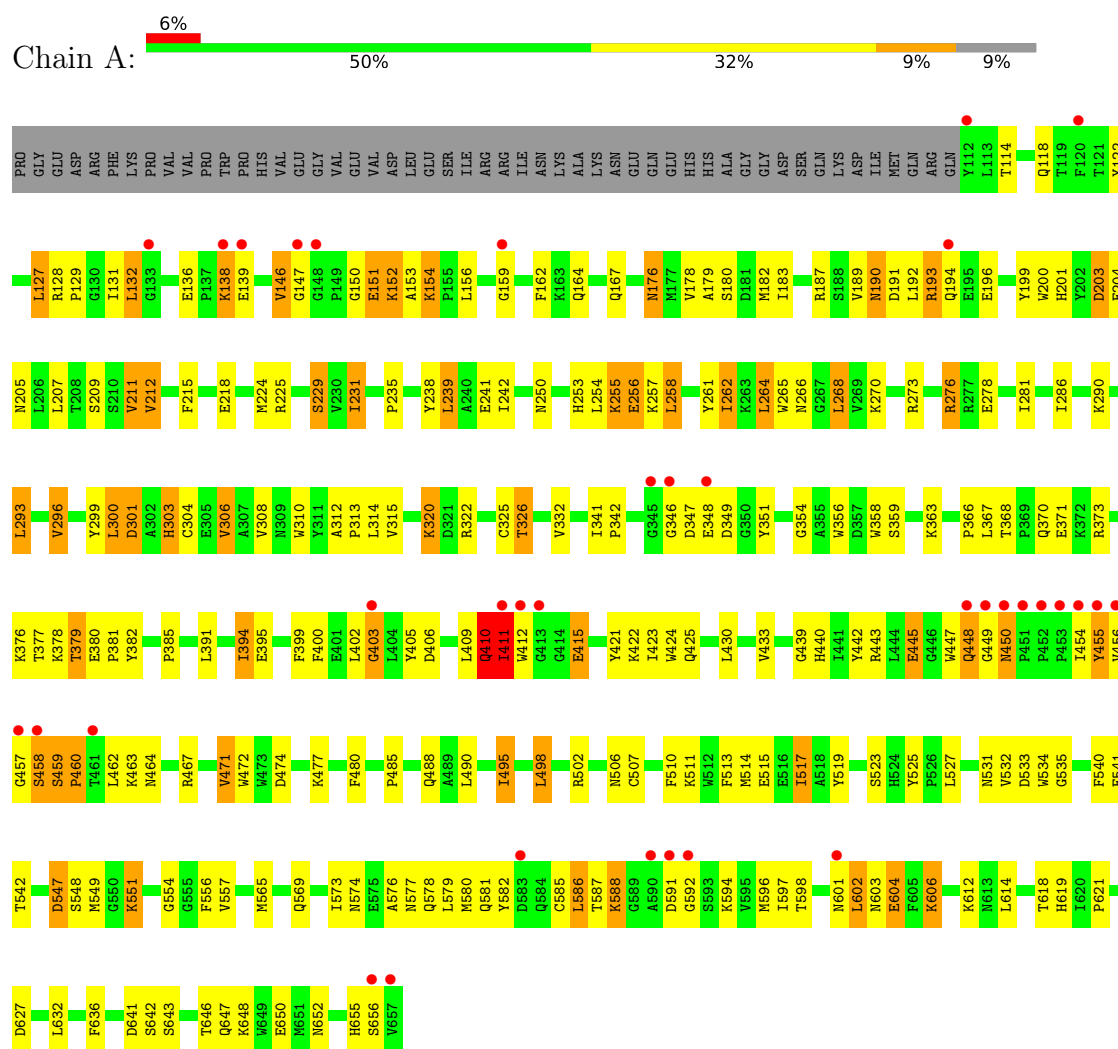
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	100	Total	O	0	0
			100	100		
6	B	77	Total	O	0	0
			77	77		
6	C	60	Total	O	0	0
			60	60		
6	D	55	Total	O	0	0
			55	55		
6	E	68	Total	O	0	0
			68	68		
6	F	47	Total	O	0	0
			47	47		

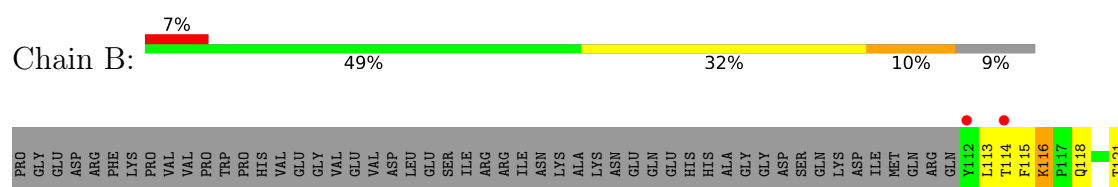
3 Residue-property plots [i](#)

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.

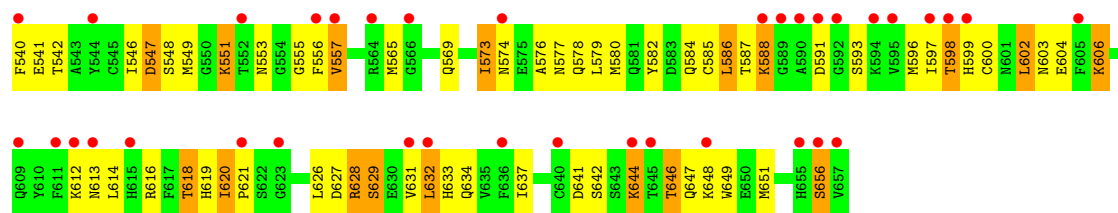
• Molecule 1: N-acetylgalactosaminyltransferase 7



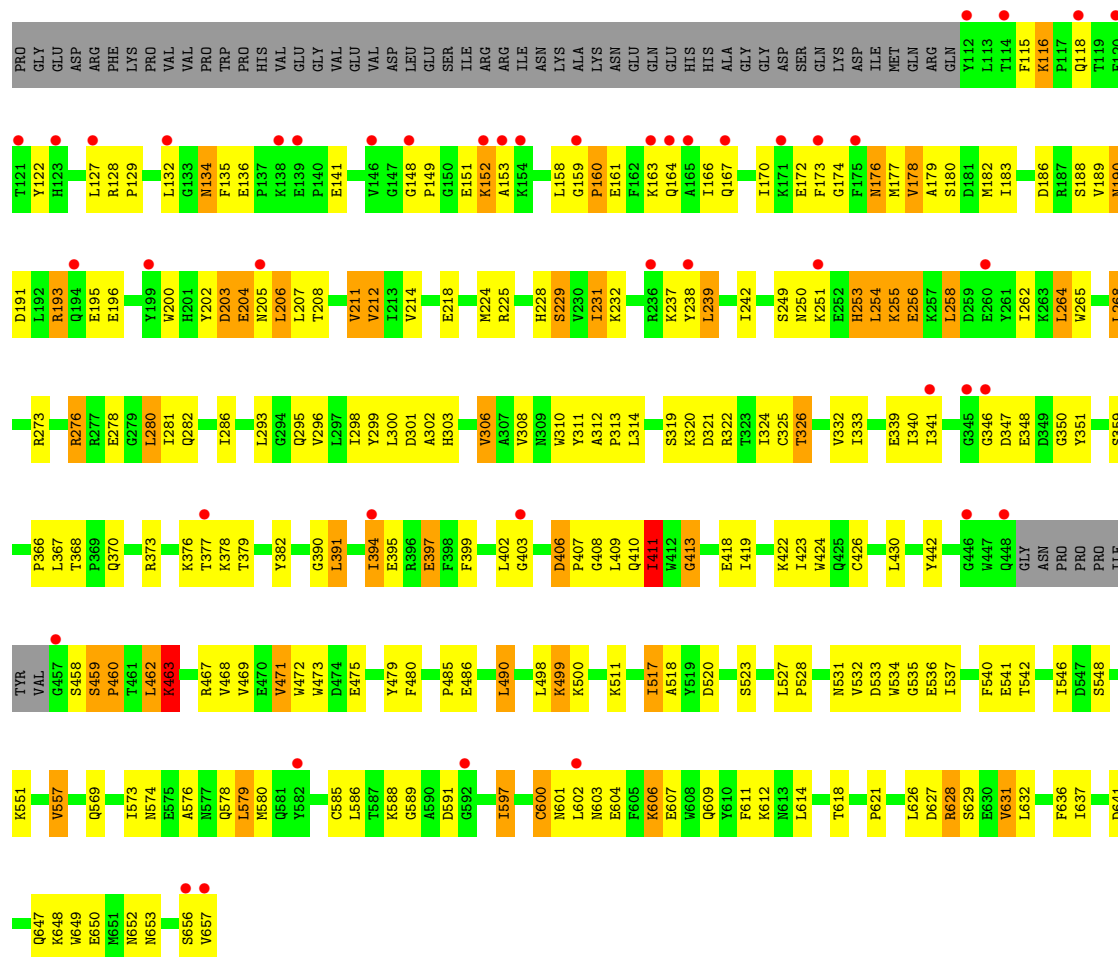
• Molecule 1: N-acetylgalactosaminyltransferase 7



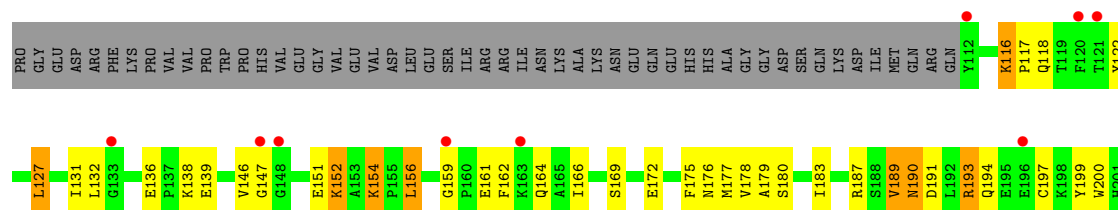


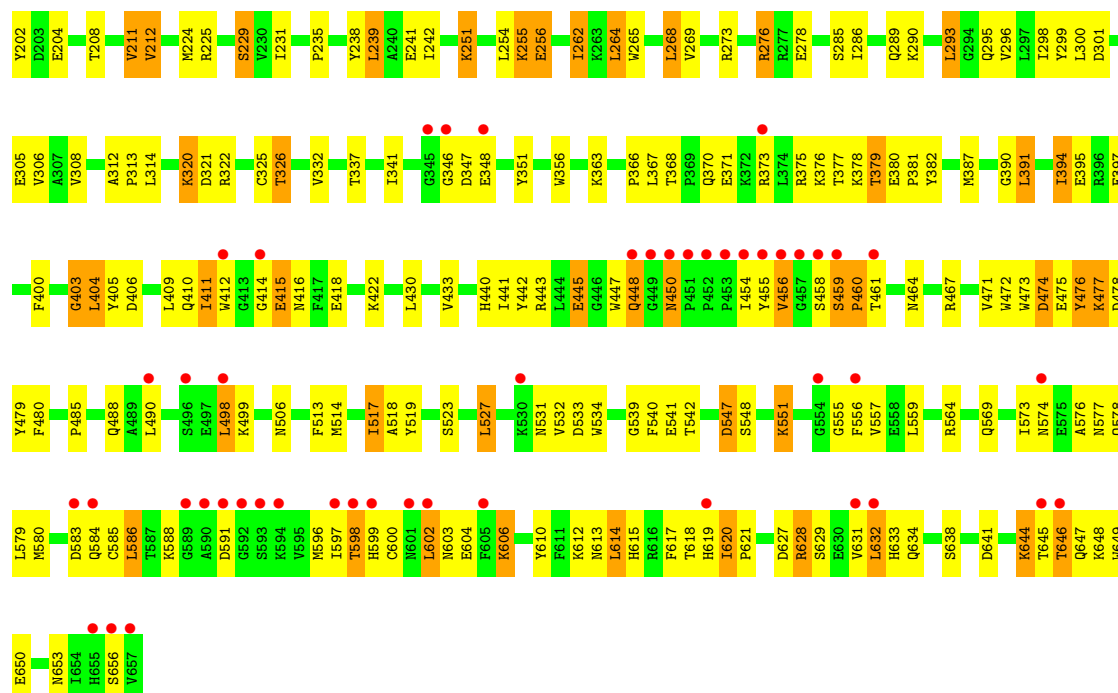


● Molecule 1: N-acetylgalactosaminyltransferase 7

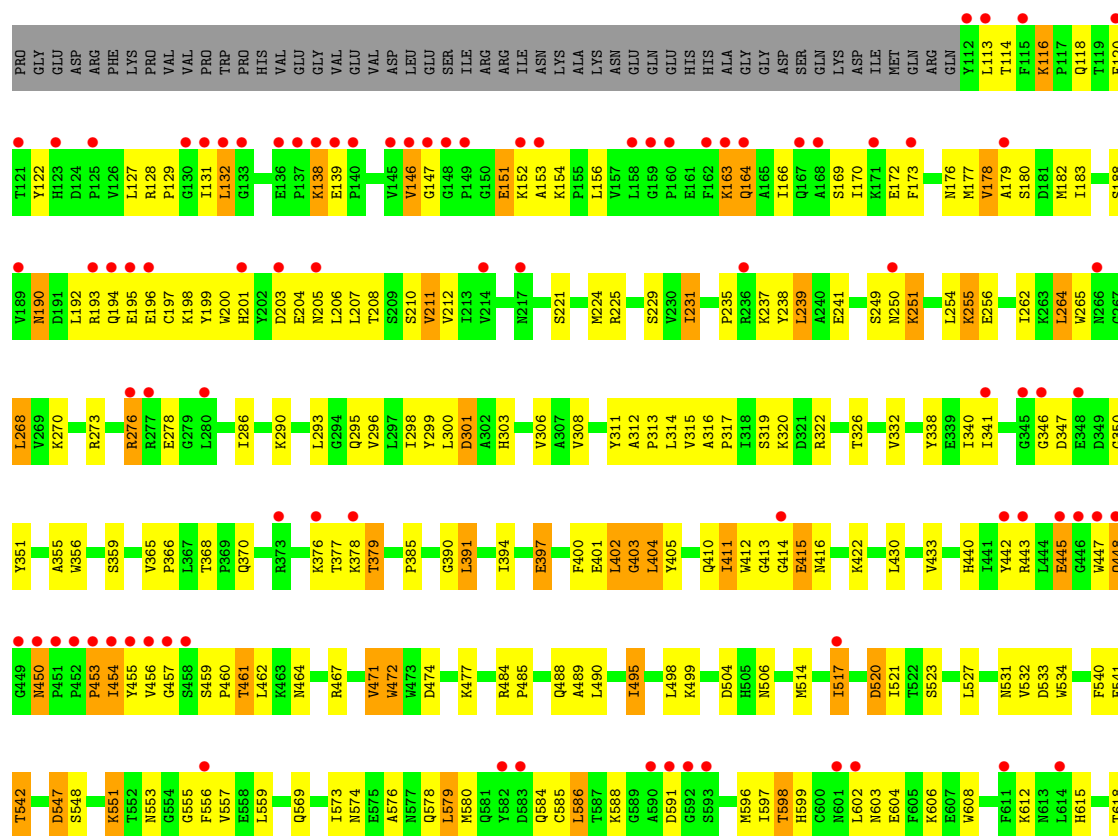


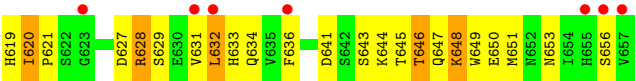
● Molecule 1: N-acetylgalactosaminyltransferase 7





• Molecule 1: N-acetylgalactosaminyltransferase 7





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	137.44Å 158.26Å 251.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.25 – 2.60 49.25 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.7 (49.25-2.60) 95.7 (49.25-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.61Å)	Xtriage
Refinement program	PHENIX (dev_2400: ???)	Depositor
R, R_{free}	0.220 , 0.258 0.222 , 0.258	Depositor DCC
R_{free} test set	8025 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	43.2	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27098	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: UDP, UD2, MN, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.55	1/4569 (0.0%)	0.79	5/6192 (0.1%)
1	B	0.53	1/4569 (0.0%)	0.75	3/6192 (0.0%)
1	C	0.54	3/4569 (0.1%)	0.78	8/6192 (0.1%)
1	D	0.55	6/4504 (0.1%)	0.79	10/6098 (0.2%)
1	E	0.49	3/4569 (0.1%)	0.74	7/6192 (0.1%)
1	F	0.45	2/4569 (0.0%)	0.69	7/6192 (0.1%)
All	All	0.52	16/27349 (0.1%)	0.76	40/37058 (0.1%)

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
1	E	0	1
1	F	0	1
All	All	0	5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	451	PRO	C-N	6.14	1.41	1.33
1	E	116	LYS	C-N	5.90	1.40	1.33
1	F	459	SER	C-N	5.55	1.40	1.34
1	D	407	PRO	N-CD	5.42	1.55	1.47
1	D	159	GLY	C-N	5.40	1.40	1.33
1	D	303	HIS	CA-CB	-5.36	1.48	1.53
1	C	452	PRO	N-CD	5.30	1.55	1.47
1	D	460	PRO	N-CD	5.29	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	117	PRO	N-CD	5.28	1.55	1.47
1	D	160	PRO	N-CD	5.22	1.55	1.47
1	B	460	PRO	N-CD	5.17	1.54	1.47
1	C	460	PRO	N-CD	5.16	1.54	1.47
1	E	460	PRO	N-CD	5.13	1.54	1.47
1	D	600	CYS	CA-CB	5.12	1.62	1.53
1	F	489	ALA	C-N	-5.07	1.23	1.33
1	A	460	PRO	N-CD	5.07	1.54	1.47

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	402	LEU	N-CA-C	9.71	121.95	111.36
1	C	451	PRO	CA-C-N	-9.64	112.72	119.66
1	C	451	PRO	C-N-CA	-9.64	112.72	119.66
1	E	403	GLY	N-CA-C	9.61	129.67	115.64
1	F	403	GLY	N-CA-C	9.44	124.38	111.54
1	C	405	TYR	N-CA-C	-9.38	93.97	108.42
1	D	203	ASP	N-CA-C	-9.28	96.54	110.28
1	D	403	GLY	N-CA-C	8.72	133.84	113.18
1	B	148	GLY	C-N-CD	-7.82	103.39	120.60
1	B	412	TRP	N-CA-C	-7.57	97.81	109.24
1	E	403	GLY	CA-C-N	7.53	130.22	120.44
1	E	403	GLY	C-N-CA	7.53	130.22	120.44
1	C	452	PRO	O-C-N	7.33	124.60	121.15
1	D	413	GLY	N-CA-C	7.18	121.17	112.48
1	D	204	GLU	N-CA-C	-7.15	98.64	109.79
1	E	116	LYS	CA-C-N	-6.93	113.52	120.31
1	E	116	LYS	C-N-CA	-6.93	113.52	120.31
1	D	411	ILE	N-CA-C	6.93	117.07	110.42
1	E	476	TYR	N-CA-C	-6.58	105.25	113.28
1	F	402	LEU	CA-C-N	6.29	126.73	120.31
1	F	402	LEU	C-N-CA	6.29	126.73	120.31
1	A	411	ILE	N-CA-C	6.25	116.42	110.42
1	D	463	LYS	N-CA-C	-6.23	104.38	112.23
1	A	203	ASP	N-CA-C	6.11	118.73	111.71
1	C	452	PRO	CA-C-N	-5.70	112.72	119.84
1	C	452	PRO	C-N-CA	-5.70	112.72	119.84
1	E	405	TYR	N-CA-C	-5.60	100.28	109.40
1	C	163	LYS	N-CA-C	5.55	117.01	111.07
1	A	403	GLY	N-CA-C	5.50	126.21	113.18
1	F	472	TRP	N-CA-C	5.49	120.10	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	458	SER	N-CA-C	5.37	117.13	111.28
1	F	459	SER	CA-C-N	-5.36	113.00	118.85
1	F	459	SER	C-N-CA	-5.36	113.00	118.85
1	F	405	TYR	N-CA-C	-5.30	101.52	109.95
1	D	159	GLY	CA-C-N	-5.22	113.53	119.28
1	D	159	GLY	C-N-CA	-5.22	113.53	119.28
1	C	582	TYR	CB-CA-C	-5.18	110.18	117.23
1	D	459	SER	CA-C-N	-5.18	113.30	119.05
1	D	459	SER	C-N-CA	-5.18	113.30	119.05
1	A	257	LYS	N-CA-C	-5.06	105.76	111.28

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	410	GLN	Peptide
1	B	402	LEU	Peptide
1	B	413	GLY	Peptide
1	E	403	GLY	Peptide
1	F	402	LEU	Peptide

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	4440	0	4325	228	0
1	B	4440	0	4325	265	0
1	C	4440	0	4325	252	0
1	D	4380	0	4265	234	0
1	E	4440	0	4325	210	0
1	F	4440	0	4325	236	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	15	15	15	1	0
4	D	25	11	11	2	0
5	D	39	0	25	3	0
6	A	100	0	0	8	0
6	B	77	0	0	7	0
6	C	60	0	0	2	0
6	D	55	0	0	10	0
6	E	68	0	0	2	0
6	F	47	0	0	4	0
All	All	27072	26	25941	1407	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 27.

All (1407) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:VAL:HG23	1:B:458:SER:CA	1.41	1.47
1:F:453:PRO:HB2	1:F:455:TYR:CZ	1.56	1.37
1:F:453:PRO:HB2	1:F:455:TYR:CE2	1.62	1.34
1:B:454:ILE:HG22	1:B:457:GLY:CA	1.62	1.27
1:C:454:ILE:O	1:C:458:SER:HA	1.39	1.22
1:B:456:VAL:CG2	1:B:458:SER:HA	1.71	1.20
1:B:449:GLY:HA2	6:B:821:HOH:O	1.44	1.17
1:F:414:GLY:HA2	1:F:415:GLU:HB3	1.25	1.17
1:F:453:PRO:CB	1:F:455:TYR:CZ	2.26	1.16
1:C:379:THR:CG2	1:C:435:CYS:SG	2.33	1.15
1:A:281:ILE:HG12	1:A:415:GLU:HG2	1.18	1.14
1:B:456:VAL:CG2	1:B:458:SER:CA	2.24	1.14
1:E:564:ARG:HD3	6:E:849:HOH:O	1.46	1.13
1:E:414:GLY:HA2	1:E:415:GLU:HB3	1.28	1.10
1:E:346:GLY:HA3	1:E:366:PRO:HB3	1.31	1.10
1:B:454:ILE:HG22	1:B:457:GLY:HA3	1.22	1.09
1:B:458:SER:HB2	1:B:463:LYS:HD2	1.21	1.09
1:D:347:ASP:HB3	1:D:351:TYR:H	1.12	1.09
1:B:455:TYR:C	1:B:457:GLY:HA2	1.78	1.08
1:B:414:GLY:HA2	1:B:415:GLU:HB3	1.35	1.07
1:F:453:PRO:CB	1:F:455:TYR:CE2	2.37	1.07
1:A:455:TYR:HB2	1:A:456:VAL:HG22	1.35	1.06
1:B:454:ILE:CG2	1:B:457:GLY:HA3	1.83	1.06
1:B:456:VAL:HG23	1:B:458:SER:HA	1.23	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:547:ASP:HB2	1:C:569:GLN:HG2	1.39	1.04
1:C:379:THR:HG23	1:C:435:CYS:SG	1.95	1.04
1:B:454:ILE:HG22	1:B:457:GLY:HA2	1.39	1.04
1:B:456:VAL:HG23	1:B:458:SER:N	1.71	1.04
1:E:456:VAL:HG12	1:E:458:SER:HB3	1.38	1.03
1:C:191:ASP:OD1	1:C:193:ARG:HG2	1.57	1.02
1:B:456:VAL:N	1:B:457:GLY:C	2.18	1.02
1:D:161:GLU:OE2	1:D:161:GLU:N	1.92	1.02
1:D:579:LEU:HD13	1:D:586:LEU:HD12	1.39	1.02
1:C:414:GLY:HA2	1:C:415:GLU:HB3	1.37	1.02
1:E:456:VAL:HG12	1:E:458:SER:CB	1.88	1.02
1:A:455:TYR:HB2	1:A:456:VAL:CG2	1.90	1.01
1:B:456:VAL:HG23	1:B:458:SER:C	1.83	1.01
1:C:565:MET:HE2	1:D:163:LYS:NZ	1.76	1.00
1:D:411:ILE:HD11	1:D:460:PRO:HG3	1.43	1.00
1:B:584:GLN:HG3	1:B:598:THR:O	1.61	1.00
1:F:547:ASP:HB2	1:F:569:GLN:HG2	1.36	1.00
1:A:547:ASP:HB2	1:A:569:GLN:HG2	1.41	0.99
1:A:346:GLY:HA3	1:A:366:PRO:HB3	1.41	0.99
1:C:163:LYS:HE3	5:D:704:UD2:O2A	1.63	0.99
1:B:456:VAL:N	1:B:457:GLY:O	1.97	0.98
1:B:346:GLY:HA3	1:B:366:PRO:HB3	1.44	0.97
1:A:377:THR:HG22	1:A:379:THR:H	1.29	0.96
1:E:641:ASP:H	1:E:647:GLN:HE22	1.12	0.96
1:E:547:ASP:HB2	1:E:569:GLN:HG2	1.46	0.96
1:B:514:MET:HE2	1:B:514:MET:HA	1.48	0.96
1:B:456:VAL:CG2	1:B:458:SER:C	2.40	0.95
1:C:346:GLY:HA3	1:C:366:PRO:HB3	1.49	0.95
1:B:456:VAL:HG21	1:B:458:SER:O	1.66	0.94
1:B:458:SER:CB	1:B:463:LYS:HD2	1.97	0.94
1:B:547:ASP:HB2	1:B:569:GLN:HG2	1.45	0.94
1:F:641:ASP:H	1:F:647:GLN:HE22	0.97	0.94
1:B:458:SER:H	1:B:459:SER:HA	1.29	0.94
1:B:132:LEU:HD23	1:B:199:TYR:HE1	1.32	0.94
1:C:411:ILE:HD12	1:C:412:TRP:N	1.81	0.94
1:F:410:GLN:H	1:F:464:ASN:HD21	1.06	0.94
1:B:458:SER:HB2	1:B:463:LYS:CD	1.98	0.93
1:C:632:LEU:CD1	1:C:634:GLN:HB2	1.98	0.93
1:B:132:LEU:HD23	1:B:199:TYR:CE1	2.03	0.93
1:E:404:LEU:HD22	1:E:404:LEU:H	1.28	0.93
1:F:453:PRO:HG2	1:F:455:TYR:HE2	1.33	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:641:ASP:H	1:C:647:GLN:HE22	1.07	0.92
1:A:341:ILE:CG2	1:B:632:LEU:HB2	2.00	0.92
1:C:282:GLN:HG3	1:C:410:GLN:NE2	1.85	0.91
1:B:132:LEU:CD2	1:B:199:TYR:CE1	2.53	0.91
1:C:462:LEU:HD11	1:C:487:SER:HB3	1.52	0.91
1:E:632:LEU:CD1	1:E:634:GLN:HB2	2.00	0.91
1:A:281:ILE:CG1	1:A:415:GLU:HG2	2.00	0.90
1:F:193:ARG:HD2	1:F:197:CYS:SG	2.11	0.90
1:C:412:TRP:O	1:C:461:THR:HG22	1.71	0.90
1:F:414:GLY:HA2	1:F:415:GLU:CB	2.01	0.90
1:D:631:VAL:HG22	1:D:632:LEU:HD12	1.52	0.89
1:F:377:THR:HG22	1:F:379:THR:H	1.38	0.89
1:E:414:GLY:HA2	1:E:415:GLU:CB	2.01	0.89
1:B:641:ASP:H	1:B:647:GLN:HE22	1.17	0.89
1:B:414:GLY:HA2	1:B:415:GLU:CB	1.99	0.89
1:C:151:GLU:HA	1:C:152:LYS:O	1.71	0.89
1:C:454:ILE:O	1:C:458:SER:CA	2.21	0.89
1:A:422:LYS:HG2	1:A:472:TRP:CZ2	2.08	0.88
1:F:347:ASP:HB3	1:F:351:TYR:H	1.35	0.88
1:F:453:PRO:HG2	1:F:455:TYR:CE2	2.08	0.88
1:A:276:ARG:HD2	1:A:278:GLU:OE2	1.73	0.88
1:A:641:ASP:H	1:A:647:GLN:HE22	1.16	0.88
1:C:467:ARG:O	1:C:471:VAL:HG12	1.73	0.88
1:F:453:PRO:CG	1:F:455:TYR:CE2	2.57	0.88
1:E:455:TYR:HB2	1:E:456:VAL:HG22	1.55	0.87
1:B:377:THR:HG22	1:B:379:THR:H	1.37	0.87
1:E:224:MET:HA	1:E:224:MET:HE3	1.56	0.87
1:B:458:SER:CB	1:B:463:LYS:CD	2.53	0.86
1:D:163:LYS:O	1:D:167:GLN:HG3	1.74	0.86
1:A:485:PRO:O	1:A:488:GLN:HG3	1.75	0.86
1:F:314:LEU:HD12	1:F:326:THR:HG22	1.57	0.86
1:B:467:ARG:O	1:B:471:VAL:HG12	1.76	0.86
1:C:163:LYS:CE	5:D:704:UD2:O2A	2.23	0.86
1:E:414:GLY:HA3	1:E:416:ASN:H	1.40	0.86
1:E:619:HIS:CE1	1:E:621:PRO:HG2	2.11	0.86
1:A:511:LYS:HE3	1:A:515:GLU:OE2	1.77	0.85
1:E:346:GLY:CA	1:E:366:PRO:HB3	2.07	0.85
1:E:459:SER:OG	1:E:460:PRO:CD	2.24	0.85
1:E:346:GLY:HA3	1:E:366:PRO:CB	2.04	0.85
1:A:458:SER:OG	1:A:462:LEU:HB2	1.75	0.84
1:A:458:SER:OG	1:A:462:LEU:CB	2.26	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:LYS:HB3	1:D:253:HIS:CD2	2.11	0.84
1:B:632:LEU:HD11	1:B:634:GLN:CD	2.03	0.84
1:F:632:LEU:CD1	1:F:634:GLN:HB2	2.08	0.84
1:B:458:SER:OG	1:B:463:LYS:HG3	1.76	0.84
1:D:160:PRO:HA	1:D:163:LYS:HE3	1.58	0.84
1:C:118:GLN:HE22	1:C:322:ARG:H	1.25	0.84
1:D:347:ASP:HB3	1:D:351:TYR:N	1.93	0.84
1:C:565:MET:HE2	1:D:163:LYS:HZ1	1.40	0.83
1:B:632:LEU:CD1	1:B:634:GLN:HB2	2.09	0.83
1:B:619:HIS:CE1	1:B:621:PRO:HG2	2.13	0.83
1:A:191:ASP:OD1	1:A:193:ARG:HG2	1.76	0.83
1:B:422:LYS:HG2	1:B:472:TRP:CZ2	2.13	0.83
1:E:410:GLN:H	1:E:464:ASN:HD21	1.23	0.83
1:B:458:SER:CB	1:B:463:LYS:HG3	2.09	0.83
1:E:467:ARG:O	1:E:471:VAL:HG12	1.78	0.83
1:A:347:ASP:HB3	1:A:351:TYR:H	1.42	0.83
1:B:132:LEU:CD2	1:B:199:TYR:HE1	1.89	0.82
1:A:281:ILE:HG12	1:A:415:GLU:CG	2.07	0.82
1:C:414:GLY:HA2	1:C:415:GLU:CB	2.09	0.82
1:A:632:LEU:HD23	1:B:342:PRO:HG2	1.61	0.82
1:C:454:ILE:O	1:C:457:GLY:HA3	1.78	0.82
1:D:127:LEU:HD11	1:D:196:GLU:HG2	1.60	0.82
1:B:456:VAL:N	1:B:457:GLY:CA	2.43	0.82
1:E:459:SER:OG	1:E:460:PRO:HD2	1.80	0.81
1:B:347:ASP:HB3	1:B:351:TYR:H	1.46	0.81
1:E:632:LEU:HD13	1:E:632:LEU:C	2.06	0.81
1:F:454:ILE:HG23	1:F:457:GLY:CA	2.10	0.81
1:D:348:GLU:OE1	1:D:348:GLU:N	2.13	0.81
1:B:458:SER:HB3	1:B:459:SER:O	1.80	0.81
1:C:122:TYR:CE1	1:C:203:ASP:HB3	2.16	0.80
1:C:314:LEU:HD12	1:C:326:THR:CG2	2.12	0.80
1:B:632:LEU:HD13	1:B:632:LEU:C	2.07	0.80
1:F:193:ARG:CD	1:F:197:CYS:HB3	2.12	0.80
1:B:458:SER:OG	1:B:463:LYS:CG	2.29	0.79
1:D:251:LYS:HB3	1:D:253:HIS:NE2	1.96	0.79
1:F:485:PRO:O	1:F:488:GLN:HG3	1.82	0.79
1:C:632:LEU:HD13	1:C:632:LEU:C	2.06	0.79
1:D:347:ASP:HB2	1:D:351:TYR:O	1.82	0.79
1:F:193:ARG:CD	1:F:197:CYS:CB	2.60	0.79
1:E:513:PHE:CE1	1:E:517:ILE:HD11	2.18	0.79
1:F:410:GLN:N	1:F:464:ASN:HD21	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:619:HIS:CE1	1:F:621:PRO:HG2	2.18	0.79
1:C:196:GLU:OE1	1:C:379:THR:HB	1.83	0.79
1:D:422:LYS:HG2	1:D:472:TRP:CZ2	2.18	0.78
1:B:414:GLY:HA3	1:B:416:ASN:H	1.46	0.78
1:B:455:TYR:C	1:B:457:GLY:CA	2.55	0.78
1:C:632:LEU:HD11	1:C:634:GLN:HB2	1.62	0.78
1:D:641:ASP:H	1:D:647:GLN:HE22	1.29	0.78
1:B:196:GLU:OE2	1:B:377:THR:HG23	1.84	0.78
1:A:347:ASP:HB2	1:A:351:TYR:O	1.83	0.77
1:F:151:GLU:HA	1:F:152:LYS:C	2.09	0.77
1:C:379:THR:HG21	1:C:435:CYS:SG	2.22	0.77
1:F:193:ARG:NE	1:F:197:CYS:HB3	1.99	0.77
1:A:314:LEU:HD12	1:A:326:THR:CG2	2.14	0.77
1:D:609:GLN:HG2	1:D:618:THR:HG23	1.65	0.77
1:F:193:ARG:HD2	1:F:197:CYS:HB3	1.67	0.77
1:F:410:GLN:H	1:F:464:ASN:ND2	1.83	0.77
1:F:193:ARG:HD2	1:F:197:CYS:CB	2.14	0.77
1:C:632:LEU:HD22	1:C:633:HIS:H	1.50	0.76
1:B:118:GLN:HE22	1:B:322:ARG:H	1.33	0.76
1:A:346:GLY:CA	1:A:366:PRO:HB3	2.15	0.76
1:C:628:ARG:HG3	1:C:628:ARG:HH11	1.50	0.76
1:F:467:ARG:O	1:F:471:VAL:HG12	1.84	0.76
1:A:349:ASP:CG	6:A:810:HOH:O	2.26	0.76
1:D:373:ARG:CZ	6:D:805:HOH:O	2.33	0.76
1:D:628:ARG:HG2	1:D:628:ARG:HH11	1.50	0.76
1:B:485:PRO:O	1:B:488:GLN:HG3	1.85	0.76
1:D:411:ILE:CD1	1:D:460:PRO:HG3	2.16	0.76
1:A:346:GLY:HA3	1:A:366:PRO:CB	2.16	0.76
1:D:251:LYS:CB	1:D:253:HIS:NE2	2.49	0.76
1:B:347:ASP:HB2	1:B:351:TYR:O	1.84	0.75
1:B:456:VAL:CG2	1:B:458:SER:O	2.33	0.75
1:B:586:LEU:N	1:B:586:LEU:HD23	2.01	0.75
1:C:122:TYR:CZ	1:C:203:ASP:HB3	2.19	0.75
1:C:377:THR:HG22	1:C:379:THR:H	1.51	0.75
1:C:619:HIS:CE1	1:C:621:PRO:HG2	2.21	0.75
1:F:414:GLY:HA3	1:F:416:ASN:OD1	1.86	0.75
1:B:458:SER:CB	1:B:463:LYS:CG	2.65	0.75
1:E:414:GLY:CA	1:E:416:ASN:H	2.00	0.75
1:C:565:MET:HE2	1:D:163:LYS:HZ2	1.49	0.75
1:F:347:ASP:HB3	1:F:351:TYR:N	2.02	0.75
1:F:628:ARG:HD2	1:F:646:THR:HG22	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:GLN:HE22	1:A:349:ASP:CG	1.95	0.75
1:D:158:LEU:CD1	1:D:178:VAL:CG2	2.65	0.75
1:F:193:ARG:CG	1:F:197:CYS:SG	2.75	0.74
1:F:314:LEU:HD12	1:F:326:THR:CG2	2.17	0.74
1:A:314:LEU:CD1	1:A:326:THR:HG22	2.17	0.74
1:B:414:GLY:HA3	1:B:416:ASN:OD1	1.88	0.74
1:D:314:LEU:O	1:D:326:THR:HG21	1.87	0.74
1:F:574:ASN:HB3	1:F:576:ALA:H	1.53	0.74
1:F:632:LEU:HD12	6:F:807:HOH:O	1.86	0.74
1:A:467:ARG:O	1:A:471:VAL:HG12	1.87	0.74
1:D:471:VAL:HG22	1:D:472:TRP:CD1	2.23	0.73
1:A:457:GLY:C	1:A:459:SER:HB2	2.12	0.73
1:A:547:ASP:HB2	1:A:569:GLN:CG	2.17	0.73
1:E:422:LYS:HG2	1:E:472:TRP:CZ2	2.24	0.73
1:C:632:LEU:HB2	1:D:341:ILE:CG2	2.19	0.73
1:C:347:ASP:HB3	1:C:351:TYR:H	1.53	0.72
1:B:458:SER:HB3	1:B:459:SER:C	2.15	0.72
1:F:411:ILE:HG22	1:F:412:TRP:N	2.03	0.72
1:D:390:GLY:C	1:D:391:LEU:HD23	2.14	0.72
1:E:628:ARG:HD2	1:E:646:THR:HG22	1.69	0.72
1:D:122:TYR:CZ	1:D:203:ASP:HB3	2.25	0.72
1:D:160:PRO:HA	1:D:163:LYS:HG3	1.71	0.72
1:C:414:GLY:HA3	1:C:416:ASN:OD1	1.88	0.72
1:B:584:GLN:HG2	1:B:597:ILE:HG23	1.70	0.72
1:A:196:GLU:OE2	1:A:377:THR:HG23	1.89	0.72
1:A:224:MET:HE2	1:A:261:TYR:HE2	1.55	0.72
1:A:547:ASP:CB	1:A:569:GLN:HG2	2.18	0.72
1:C:191:ASP:OD1	1:C:193:ARG:CG	2.38	0.72
1:D:200:TRP:HZ2	1:D:377:THR:HG21	1.55	0.71
1:F:632:LEU:C	1:F:632:LEU:HD13	2.15	0.71
1:B:455:TYR:CA	1:B:457:GLY:HA2	2.20	0.71
1:C:203:ASP:OD2	1:C:205:ASN:HB2	1.90	0.71
1:C:540:PHE:O	1:C:542:THR:HG23	1.89	0.71
1:C:632:LEU:HB2	1:D:341:ILE:HG22	1.72	0.71
1:D:314:LEU:CD1	1:D:326:THR:HG22	2.20	0.71
1:C:224:MET:HA	1:C:224:MET:HE3	1.73	0.71
1:D:118:GLN:NE2	1:D:322:ARG:H	1.87	0.71
1:B:191:ASP:OD1	1:B:193:ARG:HG2	1.91	0.71
1:A:224:MET:HE2	1:A:261:TYR:CE2	2.25	0.71
1:C:136:GLU:OE1	1:C:193:ARG:NH2	2.21	0.71
1:F:332:VAL:HG13	1:F:442:TYR:HD2	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:VAL:HG11	1:A:565:MET:HE1	1.73	0.71
1:E:632:LEU:HD13	1:E:634:GLN:HB2	1.73	0.71
1:D:207:LEU:HD13	1:D:319:SER:OG	1.89	0.71
1:D:255:LYS:C	1:D:256:GLU:HG2	2.13	0.71
1:E:377:THR:HG22	1:E:379:THR:H	1.56	0.70
1:F:193:ARG:CD	1:F:197:CYS:SG	2.79	0.70
1:F:314:LEU:CD1	1:F:326:THR:HG22	2.20	0.70
1:C:513:PHE:CE1	1:C:517:ILE:HD11	2.26	0.70
1:D:580:MET:HG2	1:D:585:CYS:SG	2.32	0.70
1:E:406:ASP:OD1	1:E:498:LEU:HD11	1.91	0.70
1:A:574:ASN:HB3	1:A:576:ALA:H	1.55	0.70
1:F:453:PRO:CB	1:F:455:TYR:OH	2.38	0.70
1:D:629:SER:OG	1:D:632:LEU:HD13	1.91	0.70
1:F:414:GLY:CA	1:F:415:GLU:HB3	2.12	0.70
1:B:514:MET:HE2	1:B:518:ALA:HB3	1.74	0.70
1:C:399:PHE:CE1	1:C:404:LEU:O	2.45	0.70
1:F:632:LEU:HD11	1:F:634:GLN:CD	2.16	0.70
1:C:314:LEU:CD1	1:C:326:THR:CG2	2.70	0.69
1:F:347:ASP:HB2	1:F:351:TYR:O	1.92	0.69
1:A:459:SER:HB3	1:A:460:PRO:CD	2.23	0.69
1:E:314:LEU:CD1	1:E:326:THR:HG22	2.22	0.69
1:A:332:VAL:HG13	1:A:442:TYR:HD2	1.56	0.69
1:B:450:ASN:N	1:B:450:ASN:HD22	1.89	0.69
1:C:118:GLN:NE2	1:C:322:ARG:H	1.90	0.69
1:E:628:ARG:HG3	1:E:628:ARG:HH11	1.58	0.69
1:C:632:LEU:HD13	1:C:634:GLN:HB2	1.75	0.69
1:D:141:GLU:OE1	1:D:232:LYS:NZ	2.22	0.69
1:D:332:VAL:HG13	1:D:442:TYR:CD2	2.28	0.69
1:F:422:LYS:HG2	1:F:472:TRP:CZ2	2.27	0.69
1:B:203:ASP:OD2	1:B:205:ASN:HB2	1.93	0.69
1:B:584:GLN:HG3	1:B:598:THR:C	2.17	0.68
1:C:450:ASN:N	1:C:450:ASN:HD22	1.91	0.68
1:F:122:TYR:CZ	1:F:203:ASP:HB3	2.28	0.68
1:F:454:ILE:HG23	1:F:457:GLY:N	2.08	0.68
1:C:602:LEU:HD22	1:C:602:LEU:O	1.93	0.68
1:D:411:ILE:HD11	1:D:460:PRO:CG	2.23	0.68
1:E:456:VAL:HG12	1:E:458:SER:OG	1.93	0.68
1:A:132:LEU:HD23	1:A:199:TYR:CE1	2.29	0.68
1:A:458:SER:N	1:A:459:SER:HA	2.06	0.68
1:E:347:ASP:HB2	1:E:351:TYR:O	1.92	0.68
1:B:414:GLY:CA	1:B:416:ASN:H	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:193:ARG:HE	1:F:197:CYS:HB3	1.57	0.68
1:C:314:LEU:CD1	1:C:326:THR:HG22	2.24	0.68
1:D:314:LEU:HD12	1:D:326:THR:CG2	2.23	0.68
1:E:471:VAL:HG13	1:E:472:TRP:CD1	2.28	0.68
1:B:346:GLY:HA3	1:B:366:PRO:CB	2.23	0.68
1:D:208:THR:OG1	1:D:295:GLN:HG3	1.94	0.68
1:F:540:PHE:CD2	1:F:541:GLU:HG3	2.29	0.68
1:E:514:MET:HA	1:E:514:MET:HE2	1.75	0.68
1:A:286:ILE:CG2	1:A:290:LYS:HD2	2.24	0.68
1:B:212:VAL:HG21	1:B:299:TYR:CE1	2.28	0.68
1:F:203:ASP:O	1:F:204:GLU:HB2	1.92	0.68
1:F:411:ILE:HG22	1:F:412:TRP:H	1.56	0.68
1:A:450:ASN:N	1:A:450:ASN:HD22	1.92	0.67
1:C:282:GLN:NE2	1:C:409:LEU:O	2.24	0.67
1:E:450:ASN:N	1:E:450:ASN:HD22	1.92	0.67
1:B:346:GLY:CA	1:B:366:PRO:HB3	2.23	0.67
1:F:574:ASN:HB3	1:F:576:ALA:N	2.09	0.67
1:F:628:ARG:HG3	1:F:628:ARG:HH11	1.60	0.67
1:B:456:VAL:HG23	1:B:457:GLY:C	2.20	0.67
1:C:347:ASP:HB2	1:C:351:TYR:O	1.94	0.67
1:C:422:LYS:HG2	1:C:472:TRP:CZ2	2.30	0.67
1:C:641:ASP:HB3	1:C:644:LYS:HG3	1.76	0.67
1:E:314:LEU:HD12	1:E:326:THR:CG2	2.23	0.66
1:D:164:GLN:OE1	1:D:164:GLN:HA	1.94	0.66
1:E:632:LEU:HD11	1:E:634:GLN:HB2	1.76	0.66
1:D:200:TRP:CZ2	1:D:377:THR:HG21	2.29	0.66
1:B:414:GLY:CA	1:B:415:GLU:HB3	2.21	0.66
1:B:547:ASP:HB2	1:B:569:GLN:CG	2.21	0.66
1:C:346:GLY:HA3	1:C:366:PRO:CB	2.22	0.66
1:B:559:LEU:O	1:B:633:HIS:HB3	1.96	0.66
1:C:586:LEU:N	1:C:586:LEU:HD23	2.10	0.66
1:E:314:LEU:O	1:E:326:THR:HG21	1.95	0.66
1:B:458:SER:N	1:B:459:SER:HA	2.06	0.66
1:C:118:GLN:HE22	1:C:322:ARG:N	1.94	0.66
1:D:251:LYS:CB	1:D:253:HIS:CD2	2.79	0.66
1:D:333:ILE:HG12	1:D:340:ILE:HG12	1.77	0.66
1:E:632:LEU:HD22	1:E:633:HIS:H	1.60	0.66
1:F:122:TYR:CE2	1:F:203:ASP:HB3	2.31	0.66
1:B:514:MET:CE	1:B:518:ALA:HB3	2.26	0.65
1:C:632:LEU:HD22	1:C:633:HIS:N	2.10	0.65
1:E:176:ASN:C	1:E:176:ASN:HD22	2.04	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:410:GLN:N	1:E:464:ASN:HD21	1.94	0.65
1:E:574:ASN:HB2	1:E:578:GLN:H	1.61	0.65
1:C:325:CYS:HB2	1:C:394:ILE:HG23	1.77	0.65
1:C:574:ASN:HB3	1:C:576:ALA:H	1.60	0.65
1:D:158:LEU:CD1	1:D:178:VAL:HG23	2.27	0.65
1:E:627:ASP:OD1	1:E:646:THR:HB	1.95	0.65
1:C:511:LYS:HE3	1:C:515:GLU:OE2	1.97	0.65
1:D:179:ALA:O	1:D:183:ILE:HG13	1.97	0.65
1:A:354:GLY:O	1:A:385:PRO:HD2	1.97	0.65
1:B:458:SER:H	1:B:459:SER:CA	2.05	0.65
1:D:467:ARG:O	1:D:471:VAL:HG13	1.97	0.65
1:E:547:ASP:HB2	1:E:569:GLN:CG	2.24	0.65
1:F:632:LEU:HD13	1:F:634:GLN:HB2	1.77	0.65
1:D:135:PHE:CE2	1:D:202:TYR:HB2	2.32	0.65
1:D:490:LEU:C	1:D:490:LEU:HD12	2.20	0.65
1:E:211:VAL:HG22	1:E:242:ILE:HG12	1.79	0.65
1:B:118:GLN:NE2	1:B:322:ARG:H	1.95	0.64
1:B:447:TRP:CD1	1:B:448:GLN:H	2.15	0.64
1:E:514:MET:HE2	1:E:518:ALA:HB3	1.78	0.64
1:E:414:GLY:CA	1:E:415:GLU:HB3	2.14	0.64
1:F:414:GLY:HA3	1:F:416:ASN:H	1.61	0.64
1:A:373:ARG:HD2	1:A:373:ARG:O	1.97	0.64
1:A:255:LYS:O	1:A:256:GLU:HB2	1.96	0.64
1:E:276:ARG:HD2	1:E:278:GLU:OE2	1.98	0.64
1:E:586:LEU:N	1:E:586:LEU:HD23	2.12	0.64
1:F:450:ASN:HD22	1:F:450:ASN:N	1.94	0.64
1:A:458:SER:OG	1:A:462:LEU:HB3	1.97	0.64
1:A:540:PHE:CD2	1:A:541:GLU:HG3	2.32	0.64
1:D:533:ASP:OD2	1:D:612:LYS:HE2	1.98	0.64
1:F:255:LYS:O	1:F:256:GLU:HB2	1.97	0.64
1:D:486:GLU:OE1	1:D:486:GLU:N	2.23	0.64
1:E:127:LEU:HD23	1:E:199:TYR:O	1.98	0.64
1:E:347:ASP:HB3	1:E:351:TYR:H	1.63	0.64
1:E:404:LEU:HD22	1:E:404:LEU:N	2.09	0.64
1:F:231:ILE:HD12	1:F:265:TRP:CD1	2.33	0.64
1:C:190:ASN:N	1:C:190:ASN:HD22	1.96	0.64
1:B:632:LEU:CD1	1:B:632:LEU:C	2.71	0.64
1:D:424:TRP:CE2	1:D:517:ILE:HD13	2.33	0.64
1:D:314:LEU:HD12	1:D:326:THR:HG22	1.80	0.63
1:B:632:LEU:HD13	1:B:634:GLN:HB2	1.78	0.63
1:D:127:LEU:CD1	1:D:196:GLU:HG2	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:586:LEU:HD23	1:F:586:LEU:N	2.13	0.63
1:A:341:ILE:HG22	1:B:632:LEU:HB2	1.78	0.63
1:A:510:PHE:CZ	1:A:514:MET:HE3	2.33	0.63
1:E:118:GLN:HE22	1:E:322:ARG:H	1.45	0.63
1:F:301:ASP:OD2	1:F:303:HIS:NE2	2.31	0.63
1:F:332:VAL:HG13	1:F:442:TYR:CD2	2.32	0.63
1:D:211:VAL:HG22	1:D:242:ILE:HG12	1.78	0.63
1:E:373:ARG:HD2	1:E:373:ARG:O	1.98	0.63
1:F:239:LEU:HD13	1:F:268:LEU:HD11	1.81	0.63
1:A:200:TRP:HZ2	1:A:377:THR:HG21	1.64	0.63
1:A:449:GLY:CA	6:A:802:HOH:O	2.47	0.63
1:C:151:GLU:HA	1:C:152:LYS:C	2.16	0.63
1:A:190:ASN:C	1:A:190:ASN:HD22	2.06	0.63
1:A:258:LEU:HD12	1:A:258:LEU:O	1.99	0.63
1:A:533:ASP:OD2	1:A:612:LYS:HE2	1.98	0.63
1:A:314:LEU:CD1	1:A:326:THR:CG2	2.76	0.63
1:F:454:ILE:O	1:F:457:GLY:N	2.32	0.63
1:B:628:ARG:HG2	1:B:649:TRP:CH2	2.34	0.62
1:C:207:LEU:CD1	1:C:319:SER:HA	2.29	0.62
1:A:632:LEU:CD2	1:B:342:PRO:HG2	2.27	0.62
1:C:180:SER:HB2	1:C:338:TYR:CZ	2.33	0.62
1:C:447:TRP:CD1	1:C:448:GLN:H	2.16	0.62
1:B:458:SER:HB3	1:B:463:LYS:HG3	1.81	0.62
1:D:176:ASN:C	1:D:176:ASN:HD22	2.06	0.62
1:D:368:THR:HB	1:D:370:GLN:OE1	1.99	0.62
1:D:628:ARG:HG2	1:D:649:TRP:CH2	2.34	0.62
1:C:390:GLY:C	1:C:391:LEU:HD23	2.24	0.62
1:E:118:GLN:NE2	1:E:321:ASP:HA	2.14	0.62
1:C:485:PRO:HG3	1:C:531:ASN:ND2	2.14	0.62
1:F:200:TRP:HZ2	1:F:377:THR:HG21	1.65	0.62
1:F:356:TRP:CZ2	1:F:514:MET:HE1	2.35	0.62
1:B:414:GLY:HA2	1:B:415:GLU:OE2	2.00	0.62
1:C:411:ILE:HD12	1:C:411:ILE:C	2.25	0.62
1:F:299:TYR:O	1:F:391:LEU:HA	2.00	0.62
1:D:176:ASN:HD21	1:D:178:VAL:HG22	1.64	0.62
1:D:532:VAL:HB	1:D:573:ILE:HG23	1.82	0.62
1:C:534:TRP:HA	1:C:651:MET:HE2	1.82	0.62
1:D:122:TYR:CE1	1:D:203:ASP:HB3	2.35	0.62
1:F:454:ILE:C	1:F:457:GLY:H	2.07	0.62
1:A:176:ASN:C	1:A:176:ASN:HD22	2.07	0.61
1:B:176:ASN:C	1:B:176:ASN:HD22	2.08	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:VAL:HG22	1:B:299:TYR:CD1	2.36	0.61
1:B:255:LYS:O	1:B:256:GLU:HB2	2.00	0.61
1:B:584:GLN:CG	1:B:598:THR:O	2.42	0.61
1:C:332:VAL:HG13	1:C:442:TYR:HD2	1.64	0.61
1:B:122:TYR:CZ	1:B:203:ASP:HB2	2.35	0.61
1:B:454:ILE:CG2	1:B:457:GLY:CA	2.50	0.61
1:D:173:PHE:CD2	1:D:177:MET:HG3	2.34	0.61
1:F:368:THR:HB	1:F:370:GLN:OE1	1.99	0.61
1:C:255:LYS:O	1:C:256:GLU:HB2	1.98	0.61
1:C:485:PRO:O	1:C:488:GLN:HG3	1.99	0.61
1:D:377:THR:HG22	1:D:379:THR:H	1.65	0.61
1:C:414:GLY:HA2	1:C:415:GLU:OE2	2.00	0.61
1:C:546:ILE:CD1	1:C:626:LEU:HD21	2.30	0.61
1:A:180:SER:OG	1:A:225:ARG:NH1	2.33	0.61
1:B:628:ARG:HG3	1:B:628:ARG:HH11	1.66	0.61
1:B:632:LEU:HD13	1:B:632:LEU:O	2.01	0.61
1:D:253:HIS:CD2	1:D:253:HIS:H	2.18	0.61
1:F:169:SER:HB2	1:F:177:MET:HB2	1.83	0.61
1:D:158:LEU:HD11	1:D:178:VAL:HG23	1.82	0.61
1:F:520:ASP:OD1	1:F:520:ASP:N	2.33	0.61
1:B:176:ASN:ND2	1:B:179:ALA:H	1.99	0.60
1:D:152:LYS:H	1:D:152:LYS:HD3	1.65	0.60
1:C:628:ARG:HH11	1:C:628:ARG:CG	2.14	0.60
1:E:533:ASP:OD2	1:E:612:LYS:HE2	2.02	0.60
1:F:377:THR:HG22	1:F:378:LYS:N	2.16	0.60
1:C:180:SER:OG	1:C:225:ARG:NH1	2.35	0.60
1:D:499:LYS:HE2	6:D:847:HOH:O	2.01	0.60
1:E:580:MET:HE3	1:E:585:CYS:SG	2.42	0.60
1:B:574:ASN:HB2	1:B:578:GLN:H	1.65	0.60
1:E:235:PRO:HB2	1:E:238:TYR:HD2	1.65	0.60
1:E:404:LEU:H	1:E:404:LEU:CD2	1.94	0.60
1:F:132:LEU:HD23	1:F:199:TYR:HE1	1.66	0.60
1:F:454:ILE:O	1:F:456:VAL:HA	2.01	0.60
1:B:314:LEU:HD12	1:B:326:THR:CG2	2.32	0.60
1:C:346:GLY:CA	1:C:366:PRO:HB3	2.28	0.60
1:D:641:ASP:H	1:D:647:GLN:NE2	1.99	0.60
1:C:159:GLY:HA2	1:C:162:PHE:H	1.66	0.60
1:D:191:ASP:OD1	1:D:193:ARG:HG2	2.01	0.60
1:E:459:SER:OG	1:E:460:PRO:HD3	1.99	0.60
1:F:356:TRP:HZ2	1:F:514:MET:HE1	1.67	0.60
1:F:453:PRO:CG	1:F:455:TYR:CZ	2.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:GLN:NE2	1:A:322:ARG:H	2.00	0.60
1:A:551:LYS:HE3	1:A:556:PHE:O	2.02	0.60
1:B:193:ARG:NH1	1:B:308:VAL:HG22	2.17	0.60
1:C:136:GLU:CD	1:C:193:ARG:HH22	2.06	0.60
1:C:546:ILE:HD11	1:C:626:LEU:HD21	1.83	0.60
1:D:251:LYS:HB2	1:D:254:LEU:HD22	1.83	0.60
1:C:628:ARG:NH1	1:C:646:THR:O	2.35	0.60
1:D:458:SER:HB3	1:D:463:LYS:NZ	2.17	0.60
1:B:514:MET:HA	1:B:514:MET:CE	2.28	0.59
1:E:551:LYS:HG2	1:E:555:GLY:HA3	1.84	0.59
1:B:128:ARG:HG3	1:B:201:HIS:CD2	2.37	0.59
1:E:118:GLN:HE22	1:E:322:ARG:N	1.99	0.59
1:A:159:GLY:HA2	1:A:162:PHE:H	1.66	0.59
1:A:574:ASN:HB2	1:A:578:GLN:H	1.66	0.59
1:E:208:THR:OG1	1:E:295:GLN:HG3	2.03	0.59
1:E:410:GLN:H	1:E:464:ASN:ND2	1.98	0.59
1:C:462:LEU:CD1	1:C:487:SER:HB3	2.28	0.59
1:D:190:ASN:HD22	1:D:190:ASN:C	2.05	0.59
1:A:619:HIS:CE1	1:A:621:PRO:HG2	2.38	0.59
1:B:131:ILE:O	1:B:199:TYR:HD1	1.85	0.59
1:B:455:TYR:C	1:B:457:GLY:O	2.46	0.59
1:D:280:LEU:HD13	4:D:702:UDP:H5'1	1.84	0.59
1:F:533:ASP:OD2	1:F:612:LYS:HE2	2.01	0.59
1:F:603:ASN:HA	1:F:606:LYS:HD2	1.85	0.59
1:A:406:ASP:HB2	1:A:498:LEU:HD21	1.85	0.59
1:A:627:ASP:OD1	1:A:646:THR:HB	2.03	0.59
1:B:314:LEU:CD1	1:B:326:THR:CG2	2.80	0.59
1:C:377:THR:HB	1:C:380:GLU:HG2	1.84	0.59
1:D:347:ASP:O	1:D:350:GLY:N	2.30	0.59
1:B:211:VAL:HA	1:B:298:ILE:O	2.03	0.59
1:B:456:VAL:CA	1:B:457:GLY:C	2.76	0.58
1:C:246:ASP:OD1	1:C:249:SER:OG	2.20	0.58
1:C:628:ARG:HD2	1:C:646:THR:HG22	1.84	0.58
1:D:160:PRO:CA	1:D:163:LYS:HE3	2.32	0.58
1:F:254:LEU:O	1:F:273:ARG:NH2	2.36	0.58
1:A:154:LYS:HD2	6:A:874:HOH:O	2.04	0.58
1:A:347:ASP:HB3	1:A:351:TYR:N	2.16	0.58
1:A:513:PHE:CE1	1:A:517:ILE:HD11	2.38	0.58
1:C:551:LYS:HE3	1:C:556:PHE:O	2.04	0.58
1:C:632:LEU:HD11	1:C:634:GLN:CD	2.28	0.58
1:F:212:VAL:HG21	1:F:299:TYR:CE2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:VAL:HG22	1:C:442:TYR:CE2	2.38	0.58
1:F:180:SER:OG	1:F:225:ARG:NH1	2.36	0.58
1:B:314:LEU:O	1:B:326:THR:HG21	2.03	0.58
1:C:186:ASP:OD1	1:C:228:HIS:ND1	2.30	0.58
1:C:628:ARG:HG2	1:C:649:TRP:CH2	2.38	0.58
1:E:632:LEU:CD1	1:E:632:LEU:C	2.73	0.58
1:C:276:ARG:HD2	1:C:278:GLU:OE2	2.04	0.58
1:C:514:MET:HE2	1:C:514:MET:HA	1.84	0.58
1:D:485:PRO:HG3	1:D:531:ASN:ND2	2.18	0.58
1:F:207:LEU:CD1	1:F:319:SER:OG	2.52	0.58
1:A:580:MET:HG2	1:A:585:CYS:SG	2.44	0.58
1:C:455:TYR:HA	1:C:457:GLY:HA3	1.84	0.58
1:E:400:PHE:HA	1:E:404:LEU:HD13	1.85	0.58
1:B:485:PRO:HG3	1:B:531:ASN:ND2	2.19	0.58
1:C:414:GLY:HA3	1:C:416:ASN:H	1.69	0.58
1:D:127:LEU:HD11	1:D:196:GLU:CG	2.33	0.58
1:D:135:PHE:HE2	1:D:202:TYR:HB2	1.68	0.58
1:D:204:GLU:O	1:D:205:ASN:HB2	2.03	0.58
1:E:172:GLU:HG3	1:E:251:LYS:HZ3	1.66	0.58
1:C:212:VAL:HG22	1:C:299:TYR:CD1	2.38	0.58
1:F:190:ASN:C	1:F:190:ASN:HD22	2.11	0.58
1:C:176:ASN:C	1:C:176:ASN:HD22	2.10	0.57
1:C:203:ASP:O	1:C:204:GLU:HB2	2.03	0.57
1:E:540:PHE:CD2	1:E:541:GLU:HG3	2.39	0.57
1:D:178:VAL:O	1:D:182:MET:HG2	2.04	0.57
1:A:449:GLY:N	6:A:802:HOH:O	2.32	0.57
1:D:251:LYS:HB2	1:D:254:LEU:CD2	2.33	0.57
1:E:255:LYS:O	1:E:256:GLU:HB2	2.04	0.57
1:F:627:ASP:HB3	1:F:636:PHE:CE1	2.38	0.57
1:A:447:TRP:CD1	1:A:448:GLN:H	2.23	0.57
1:D:377:THR:HG22	1:D:378:LYS:N	2.19	0.57
1:F:193:ARG:HE	1:F:197:CYS:CB	2.18	0.57
1:D:281:ILE:HD12	1:D:410:GLN:O	2.04	0.57
1:E:190:ASN:C	1:E:190:ASN:HD22	2.12	0.57
1:A:455:TYR:HB2	1:A:456:VAL:HG23	1.82	0.57
1:A:532:VAL:HB	1:A:573:ILE:HG23	1.86	0.57
1:B:190:ASN:C	1:B:190:ASN:HD22	2.11	0.57
1:C:454:ILE:O	1:C:457:GLY:CA	2.49	0.57
1:D:609:GLN:HG2	1:D:618:THR:CG2	2.33	0.57
1:C:314:LEU:O	1:C:326:THR:HG21	2.04	0.57
1:B:377:THR:HG22	1:B:378:LYS:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:373:ARG:NE	6:D:805:HOH:O	2.38	0.56
1:A:535:GLY:HA3	1:A:652:ASN:O	2.06	0.56
1:C:412:TRP:HE3	1:C:461:THR:HG21	1.70	0.56
1:F:264:LEU:HD23	1:F:264:LEU:O	2.05	0.56
1:A:203:ASP:O	1:A:204:GLU:HB2	2.05	0.56
1:A:332:VAL:HG13	1:A:442:TYR:CD2	2.38	0.56
1:A:467:ARG:NH2	1:A:495:ILE:HD12	2.20	0.56
1:B:212:VAL:CG2	1:B:299:TYR:CD1	2.88	0.56
1:E:314:LEU:CD1	1:E:326:THR:CG2	2.83	0.56
1:F:196:GLU:CB	6:F:837:HOH:O	2.53	0.56
1:F:208:THR:OG1	1:F:295:GLN:HG3	2.04	0.56
1:E:191:ASP:OD1	1:E:193:ARG:CG	2.53	0.56
1:F:632:LEU:HD11	1:F:634:GLN:HB2	1.86	0.56
1:A:356:TRP:CZ2	1:A:514:MET:HE1	2.40	0.56
1:B:118:GLN:HE22	1:B:322:ARG:N	2.00	0.56
1:B:422:LYS:HG2	1:B:472:TRP:HZ2	1.70	0.56
1:F:231:ILE:HD12	1:F:265:TRP:NE1	2.21	0.56
1:F:641:ASP:OD1	1:F:643:SER:OG	2.23	0.56
1:C:533:ASP:OD2	1:C:612:LYS:HE2	2.06	0.56
1:D:118:GLN:HE22	1:D:322:ARG:N	2.04	0.56
1:A:122:TYR:O	1:A:320:LYS:HG2	2.06	0.56
1:B:254:LEU:O	1:B:273:ARG:NH2	2.39	0.56
1:B:281:ILE:HD12	1:B:410:GLN:O	2.05	0.56
1:E:615:HIS:O	1:E:648:LYS:HA	2.05	0.56
1:A:325:CYS:HB2	1:A:394:ILE:HG23	1.88	0.56
1:B:224:MET:HE2	1:B:261:TYR:HE2	1.69	0.56
1:F:152:LYS:O	1:F:188:SER:O	2.24	0.56
1:F:390:GLY:C	1:F:391:LEU:HD23	2.31	0.56
1:F:632:LEU:CD1	1:F:632:LEU:C	2.78	0.56
1:B:276:ARG:HD2	1:B:278:GLU:OE2	2.05	0.56
1:B:455:TYR:N	1:B:457:GLY:HA2	2.21	0.56
1:C:414:GLY:CA	1:C:415:GLU:HB3	2.21	0.56
1:A:235:PRO:HB2	1:A:238:TYR:HD2	1.70	0.56
1:B:347:ASP:HB3	1:B:351:TYR:N	2.17	0.56
1:C:574:ASN:HB2	1:C:578:GLN:H	1.71	0.56
1:F:574:ASN:HB2	1:F:578:GLN:H	1.69	0.56
1:C:207:LEU:HD13	1:C:319:SER:OG	2.06	0.55
1:D:127:LEU:HB2	1:D:200:TRP:CD2	2.41	0.55
1:D:332:VAL:HG13	1:D:442:TYR:HD2	1.70	0.55
1:C:479:TYR:CD1	1:C:528:PRO:HD2	2.41	0.55
1:C:629:SER:O	1:C:632:LEU:O	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:611:PHE:CD1	1:E:204:GLU:HB2	2.40	0.55
1:D:264:LEU:O	1:D:264:LEU:HD23	2.05	0.55
1:F:641:ASP:H	1:F:647:GLN:NE2	1.82	0.55
1:B:406:ASP:HB2	1:B:498:LEU:HD21	1.88	0.55
1:D:160:PRO:HA	1:D:163:LYS:CE	2.33	0.55
1:E:191:ASP:OD1	1:E:193:ARG:HG3	2.07	0.55
1:F:173:PHE:CD2	1:F:177:MET:HG3	2.41	0.55
1:A:306:VAL:HG21	1:A:310:TRP:CD2	2.42	0.55
1:A:314:LEU:O	1:A:326:THR:HG21	2.07	0.55
1:C:406:ASP:HB2	1:C:498:LEU:HD21	1.88	0.55
1:E:118:GLN:NE2	1:E:322:ARG:H	2.03	0.55
1:E:189:VAL:HG12	1:E:190:ASN:O	2.06	0.55
1:F:414:GLY:CA	1:F:416:ASN:H	2.20	0.55
1:A:367:LEU:HD13	1:A:382:TYR:CD1	2.42	0.55
1:C:258:LEU:HD12	1:C:262:ILE:HG12	1.88	0.55
1:C:632:LEU:CD1	1:C:632:LEU:C	2.76	0.55
1:D:115:PHE:HE2	1:D:426:CYS:O	1.90	0.55
1:D:148:GLY:HA2	1:D:151:GLU:HG3	1.89	0.55
1:D:152:LYS:O	1:D:188:SER:O	2.23	0.55
1:F:178:VAL:O	1:F:182:MET:HG2	2.06	0.55
1:A:574:ASN:HB3	1:A:576:ALA:N	2.22	0.55
1:B:152:LYS:CD	1:B:152:LYS:H	2.18	0.55
1:A:258:LEU:HD12	1:A:258:LEU:C	2.32	0.55
1:A:368:THR:HB	1:A:370:GLN:OE1	2.07	0.55
1:D:627:ASP:HB3	1:D:636:PHE:CE1	2.42	0.55
1:F:193:ARG:NE	1:F:197:CYS:CB	2.67	0.55
1:C:584:GLN:HG2	1:C:599:HIS:HA	1.88	0.55
1:D:467:ARG:O	1:D:471:VAL:CG1	2.54	0.55
1:A:183:ILE:CG2	1:A:187:ARG:HD3	2.37	0.55
1:B:586:LEU:HA	1:B:596:MET:O	2.07	0.55
1:C:447:TRP:C	1:C:448:GLN:HG2	2.32	0.55
1:E:348:GLU:OE1	1:E:348:GLU:HA	2.07	0.55
1:F:200:TRP:CZ2	1:F:377:THR:HG21	2.42	0.55
1:B:224:MET:HE2	1:B:261:TYR:CE2	2.42	0.54
1:B:485:PRO:O	1:B:488:GLN:CG	2.55	0.54
1:E:459:SER:CB	1:E:460:PRO:CD	2.85	0.54
1:F:627:ASP:OD1	1:F:646:THR:HB	2.06	0.54
1:A:301:ASP:OD2	1:A:440:HIS:NE2	2.38	0.54
1:E:603:ASN:HA	1:E:606:LYS:HD2	1.89	0.54
1:C:411:ILE:HD12	1:C:412:TRP:H	1.69	0.54
1:D:540:PHE:CD2	1:D:541:GLU:HG3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:GLU:OE1	1:E:193:ARG:NH2	2.23	0.54
1:E:447:TRP:CD1	1:E:448:GLN:H	2.25	0.54
1:E:586:LEU:HD23	1:E:586:LEU:H	1.73	0.54
1:E:632:LEU:HD11	1:E:634:GLN:CD	2.32	0.54
1:B:603:ASN:HA	1:B:606:LYS:HD2	1.89	0.54
1:C:113:LEU:HD12	1:C:504:ASP:HB3	1.88	0.54
1:C:455:TYR:HD1	1:C:455:TYR:H	1.54	0.54
1:E:485:PRO:HG3	1:E:531:ASN:ND2	2.22	0.54
1:F:641:ASP:N	1:F:647:GLN:HE22	1.83	0.54
1:A:151:GLU:HA	1:A:153:ALA:H	1.72	0.54
1:A:167:GLN:NE2	6:A:805:HOH:O	2.41	0.54
1:D:116:LYS:NZ	1:D:397:GLU:HG2	2.23	0.54
1:E:180:SER:OG	1:E:225:ARG:NH1	2.41	0.54
1:F:551:LYS:HE3	1:F:556:PHE:O	2.08	0.54
1:C:176:ASN:ND2	1:C:179:ALA:H	2.06	0.54
1:C:457:GLY:HA2	1:C:458:SER:C	2.32	0.54
1:E:175:PHE:CE1	1:E:441:ILE:HG22	2.43	0.54
1:A:118:GLN:HE22	1:A:322:ARG:N	2.06	0.54
1:A:241:GLU:OE1	1:A:293:LEU:HD22	2.08	0.54
1:B:231:ILE:HD12	1:B:265:TRP:CD1	2.43	0.54
1:F:132:LEU:HD23	1:F:199:TYR:CE1	2.43	0.54
1:B:231:ILE:HD12	1:B:265:TRP:NE1	2.23	0.54
1:B:456:VAL:HG22	1:B:458:SER:HA	1.78	0.54
1:B:610:TYR:HB2	1:B:617:PHE:CE1	2.42	0.54
1:A:586:LEU:HD23	1:A:586:LEU:N	2.23	0.53
1:C:299:TYR:O	1:C:300:LEU:HD13	2.08	0.53
1:C:312:ALA:HB3	1:C:313:PRO:HD3	1.89	0.53
1:C:332:VAL:HG13	1:C:442:TYR:CD2	2.43	0.53
1:C:348:GLU:HA	1:C:348:GLU:OE1	2.08	0.53
1:D:158:LEU:HD12	1:D:178:VAL:CG2	2.38	0.53
1:D:628:ARG:HH11	1:D:628:ARG:CG	2.20	0.53
1:D:410:GLN:HB2	1:D:460:PRO:HB2	1.89	0.53
1:F:151:GLU:HA	1:F:152:LYS:O	2.08	0.53
1:F:322:ARG:NH1	1:F:401:GLU:OE1	2.40	0.53
1:A:449:GLY:HA2	6:A:802:HOH:O	2.07	0.53
1:A:604:GLU:HG2	6:A:847:HOH:O	2.07	0.53
1:B:447:TRP:O	1:B:448:GLN:HG2	2.09	0.53
1:F:176:ASN:HD22	1:F:176:ASN:C	2.17	0.53
1:B:312:ALA:HB3	1:B:313:PRO:HD3	1.91	0.53
1:C:200:TRP:HZ2	1:C:377:THR:HG21	1.74	0.53
1:A:286:ILE:HG22	1:A:290:LYS:HD2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:GLU:OE1	1:B:232:LYS:NZ	2.31	0.53
1:B:279:GLY:HA2	1:B:411:ILE:HD12	1.90	0.53
1:B:454:ILE:HG21	1:B:457:GLY:HA3	1.81	0.53
1:E:152:LYS:CD	1:E:152:LYS:H	2.21	0.53
1:E:628:ARG:HG2	1:E:649:TRP:CH2	2.44	0.53
1:B:447:TRP:C	1:B:448:GLN:HG2	2.33	0.53
1:D:116:LYS:O	1:D:322:ARG:NH2	2.42	0.53
1:A:176:ASN:ND2	1:A:179:ALA:H	2.06	0.53
1:A:212:VAL:HG21	1:A:299:TYR:CE1	2.43	0.53
1:A:458:SER:N	1:A:459:SER:CA	2.72	0.53
1:B:180:SER:OG	1:B:225:ARG:NH1	2.41	0.53
1:C:325:CYS:HB2	1:C:394:ILE:CG2	2.38	0.53
1:E:559:LEU:O	1:E:633:HIS:HB3	2.07	0.53
1:A:266:ASN:HD21	1:D:500:LYS:NZ	2.07	0.53
1:C:314:LEU:HD11	1:C:326:THR:HG22	1.90	0.53
1:C:414:GLY:CA	1:C:416:ASN:H	2.21	0.53
1:C:522:THR:HG22	1:C:527:LEU:HD13	1.91	0.53
1:F:551:LYS:HG2	1:F:555:GLY:HA3	1.91	0.53
1:A:118:GLN:HE22	1:A:322:ARG:H	1.56	0.52
1:B:533:ASP:OD2	1:B:612:LYS:HE2	2.09	0.52
1:C:207:LEU:HD11	1:C:319:SER:HA	1.90	0.52
1:D:207:LEU:CD1	1:D:319:SER:OG	2.56	0.52
1:E:254:LEU:O	1:E:273:ARG:NH2	2.42	0.52
1:E:455:TYR:CB	1:E:456:VAL:HG22	2.35	0.52
1:A:332:VAL:HG22	1:A:442:TYR:CE2	2.44	0.52
1:B:456:VAL:CG2	1:B:457:GLY:C	2.83	0.52
1:D:118:GLN:HE22	1:D:322:ARG:H	1.54	0.52
1:D:314:LEU:CD1	1:D:326:THR:CG2	2.86	0.52
1:D:535:GLY:HA3	1:D:652:ASN:O	2.09	0.52
1:F:559:LEU:O	1:F:633:HIS:HB3	2.10	0.52
1:F:163:LYS:HG3	1:F:164:GLN:N	2.23	0.52
1:A:200:TRP:CZ2	1:A:377:THR:HG21	2.44	0.52
1:A:457:GLY:HA3	1:A:459:SER:OG	2.09	0.52
1:D:127:LEU:HB2	1:D:200:TRP:CE3	2.44	0.52
1:D:536:GLU:HA	1:D:569:GLN:O	2.10	0.52
1:E:551:LYS:HE3	1:E:556:PHE:O	2.09	0.52
1:E:628:ARG:HH11	1:E:628:ARG:CG	2.22	0.52
1:E:641:ASP:HB3	1:E:644:LYS:HG3	1.92	0.52
1:F:454:ILE:HG23	1:F:457:GLY:HA3	1.90	0.52
1:F:547:ASP:HB2	1:F:569:GLN:CG	2.26	0.52
1:A:152:LYS:N	1:A:152:LYS:HD2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:574:ASN:HB3	1:D:576:ALA:H	1.75	0.52
1:E:411:ILE:N	1:E:411:ILE:CD1	2.73	0.52
1:A:576:ALA:O	1:A:577:ASN:HB2	2.10	0.52
1:B:628:ARG:HH11	1:B:628:ARG:CG	2.22	0.52
1:A:356:TRP:HZ2	1:A:514:MET:HE1	1.73	0.52
1:C:132:LEU:HD23	1:C:199:TYR:CE1	2.44	0.52
1:C:282:GLN:CG	1:C:410:GLN:NE2	2.66	0.52
1:C:301:ASP:OD2	1:C:440:HIS:NE2	2.32	0.52
1:E:632:LEU:HD22	1:E:633:HIS:N	2.24	0.52
1:A:424:TRP:CE2	1:A:517:ILE:HD13	2.45	0.52
1:A:447:TRP:C	1:A:448:GLN:HG2	2.35	0.52
1:D:603:ASN:O	1:D:606:LYS:HD2	2.09	0.52
1:E:152:LYS:CD	1:E:152:LYS:N	2.73	0.52
1:E:641:ASP:H	1:E:647:GLN:NE2	1.95	0.52
1:F:326:THR:HG23	1:F:433:VAL:CG2	2.40	0.52
1:F:540:PHE:O	1:F:542:THR:HG23	2.09	0.52
1:B:311:TYR:CZ	1:B:315:VAL:HG21	2.45	0.51
1:B:455:TYR:N	1:B:455:TYR:CD1	2.73	0.51
1:B:620:ILE:N	1:B:621:PRO:HD2	2.25	0.51
1:C:218:GLU:O	1:C:253:HIS:HE1	1.93	0.51
1:D:136:GLU:OE2	1:D:193:ARG:NH2	2.43	0.51
1:F:641:ASP:HB3	1:F:644:LYS:HG3	1.90	0.51
1:B:314:LEU:HD11	1:B:328:PRO:HD3	1.92	0.51
1:B:611:PHE:HB3	1:B:614:LEU:HB2	1.91	0.51
1:E:371:GLU:HG2	1:E:519:TYR:OH	2.09	0.51
1:F:453:PRO:CG	1:F:455:TYR:OH	2.58	0.51
1:A:239:LEU:HD13	1:A:268:LEU:HD11	1.92	0.51
1:D:473:TRP:CZ3	1:D:480:PHE:HB2	2.44	0.51
1:A:152:LYS:N	1:A:152:LYS:CD	2.73	0.51
1:D:251:LYS:HB2	1:D:253:HIS:NE2	2.25	0.51
1:E:574:ASN:HB3	1:E:576:ALA:H	1.76	0.51
1:A:152:LYS:CD	1:A:152:LYS:H	2.24	0.51
1:F:314:LEU:O	1:F:326:THR:HG21	2.10	0.51
1:A:410:GLN:N	1:A:464:ASN:HD21	2.09	0.51
1:B:632:LEU:HD11	1:B:634:GLN:CG	2.41	0.51
1:D:629:SER:HG	1:D:632:LEU:HD13	1.75	0.51
1:F:453:PRO:HB3	1:F:455:TYR:CZ	2.40	0.51
1:A:306:VAL:HG21	1:A:310:TRP:CE2	2.46	0.51
1:B:212:VAL:CG2	1:B:299:TYR:CE1	2.93	0.51
1:C:190:ASN:HD22	1:C:190:ASN:H	1.58	0.51
1:C:641:ASP:H	1:C:647:GLN:NE2	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:LEU:HD13	1:D:382:TYR:CD1	2.46	0.51
1:E:584:GLN:HG2	1:E:599:HIS:HA	1.92	0.51
1:B:641:ASP:OD1	1:B:643:SER:OG	2.23	0.51
1:A:264:LEU:O	1:A:264:LEU:HD22	2.11	0.51
1:A:548:SER:CB	1:A:581:GLN:OE1	2.59	0.51
1:B:264:LEU:HD22	1:B:264:LEU:O	2.11	0.51
1:B:455:TYR:C	1:B:457:GLY:C	2.79	0.51
1:C:347:ASP:HB3	1:C:351:TYR:N	2.25	0.51
1:C:447:TRP:C	1:C:448:GLN:CG	2.84	0.51
1:E:116:LYS:O	1:E:322:ARG:NH2	2.44	0.51
1:E:368:THR:HB	1:E:370:GLN:OE1	2.11	0.51
1:B:513:PHE:CE1	1:B:517:ILE:HD11	2.46	0.50
1:D:458:SER:O	1:D:459:SER:C	2.52	0.50
1:D:586:LEU:HD23	1:D:597:ILE:HG12	1.92	0.50
1:F:177:MET:HE1	1:F:221:SER:OG	2.11	0.50
1:B:576:ALA:O	1:B:577:ASN:HB2	2.10	0.50
1:D:586:LEU:CD2	1:D:597:ILE:HG13	2.41	0.50
1:E:231:ILE:HD12	1:E:265:TRP:NE1	2.26	0.50
1:A:641:ASP:OD1	1:A:643:SER:OG	2.28	0.50
1:B:270:LYS:NZ	6:B:804:HOH:O	2.36	0.50
1:B:563:HIS:O	1:B:565:MET:HG2	2.10	0.50
1:C:462:LEU:HD12	1:C:490:LEU:HD22	1.92	0.50
1:D:118:GLN:NE2	1:D:322:ARG:N	2.58	0.50
1:D:254:LEU:O	1:D:258:LEU:HB2	2.11	0.50
1:E:346:GLY:HA3	1:E:366:PRO:CA	2.40	0.50
1:E:387:MET:HG3	1:E:387:MET:O	2.11	0.50
1:F:193:ARG:HG2	1:F:197:CYS:SG	2.49	0.50
1:A:314:LEU:HD12	1:A:326:THR:HG22	1.82	0.50
1:A:549:MET:HB2	1:A:551:LYS:HD3	1.94	0.50
1:E:619:HIS:NE2	1:E:621:PRO:HG2	2.26	0.50
1:E:629:SER:O	1:E:632:LEU:O	2.30	0.50
1:B:500:LYS:NZ	1:C:266:ASN:HD21	2.10	0.50
1:D:406:ASP:OD1	1:D:408:GLY:N	2.43	0.50
1:B:540:PHE:CD2	1:B:541:GLU:HG3	2.47	0.50
1:B:627:ASP:HB3	1:B:636:PHE:CE1	2.46	0.50
1:B:629:SER:O	1:B:632:LEU:O	2.29	0.50
1:C:211:VAL:HG22	1:C:242:ILE:HG23	1.94	0.50
1:F:211:VAL:HA	1:F:298:ILE:O	2.12	0.50
1:B:551:LYS:HE3	1:B:556:PHE:O	2.12	0.50
1:C:485:PRO:HG3	1:C:531:ASN:HD21	1.75	0.50
1:D:321:ASP:HB3	1:D:324:ILE:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:224:MET:HE3	1:E:224:MET:CA	2.33	0.50
1:F:411:ILE:CD1	1:F:460:PRO:HG2	2.42	0.50
1:A:128:ARG:HG3	1:A:201:HIS:CD2	2.47	0.50
1:A:377:THR:HG22	1:A:379:THR:N	2.12	0.50
1:A:581:GLN:HG2	1:A:582:TYR:CD2	2.47	0.50
1:C:152:LYS:O	1:C:188:SER:O	2.30	0.50
1:E:122:TYR:O	1:E:320:LYS:HG2	2.12	0.50
1:E:172:GLU:HG3	1:E:251:LYS:NZ	2.26	0.50
1:F:193:ARG:HG2	1:F:197:CYS:HB2	1.93	0.50
1:F:629:SER:O	1:F:632:LEU:O	2.30	0.50
1:B:520:ASP:N	1:B:520:ASP:OD1	2.42	0.49
1:C:207:LEU:HD13	1:C:319:SER:HA	1.93	0.49
1:E:332:VAL:HG13	1:E:442:TYR:HD2	1.77	0.49
1:B:127:LEU:HD23	1:B:199:TYR:O	2.12	0.49
1:B:377:THR:CG2	1:B:378:LYS:N	2.75	0.49
1:B:116:LYS:NZ	1:B:397:GLU:OE1	2.45	0.49
1:B:218:GLU:O	1:B:253:HIS:HE1	1.96	0.49
1:B:424:TRP:CE2	1:B:517:ILE:HD13	2.47	0.49
1:F:453:PRO:HB2	1:F:455:TYR:CE1	2.33	0.49
1:D:207:LEU:N	1:D:207:LEU:HD12	2.28	0.49
1:A:127:LEU:HD23	1:A:199:TYR:O	2.13	0.49
1:D:206:LEU:HD12	1:D:238:TYR:CE2	2.47	0.49
1:A:231:ILE:HD12	1:A:265:TRP:CD1	2.47	0.49
1:A:348:GLU:HA	1:A:348:GLU:OE1	2.12	0.49
1:B:152:LYS:CD	1:B:152:LYS:N	2.76	0.49
1:B:615:HIS:O	1:B:648:LYS:HA	2.13	0.49
1:D:276:ARG:NH1	1:D:278:GLU:OE1	2.45	0.49
1:D:346:GLY:HA3	1:D:366:PRO:HB3	1.93	0.49
1:E:176:ASN:ND2	1:E:179:ALA:H	2.10	0.49
1:E:285:SER:O	1:E:289:GLN:HG3	2.13	0.49
1:A:215:PHE:CE1	1:A:254:LEU:HD22	2.46	0.49
1:B:122:TYR:CE1	1:B:203:ASP:HB3	2.47	0.49
1:D:418:GLU:HG3	1:D:468:VAL:HG22	1.93	0.49
1:E:347:ASP:HB3	1:E:351:TYR:N	2.28	0.49
1:F:312:ALA:HB3	1:F:313:PRO:HD3	1.93	0.49
1:B:535:GLY:HA3	1:B:652:ASN:O	2.12	0.49
1:C:586:LEU:HD23	1:C:586:LEU:H	1.73	0.49
1:A:281:ILE:CD1	1:A:415:GLU:CG	2.91	0.49
1:A:286:ILE:HG23	1:A:290:LYS:HD2	1.95	0.49
1:A:457:GLY:C	1:A:459:SER:CB	2.86	0.49
1:B:450:ASN:N	1:B:450:ASN:ND2	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:406:ASP:CG	1:D:498:LEU:HD11	2.37	0.49
1:C:411:ILE:C	1:C:411:ILE:CD1	2.86	0.49
1:D:153:ALA:HB2	1:D:190:ASN:HB3	1.94	0.49
1:E:414:GLY:CA	1:E:416:ASN:N	2.74	0.49
1:A:150:GLY:O	1:A:153:ALA:HA	2.13	0.48
1:A:304:CYS:HA	1:A:439:GLY:O	2.13	0.48
1:B:406:ASP:OD2	1:B:409:LEU:HD13	2.13	0.48
1:C:462:LEU:HD11	1:C:487:SER:CB	2.35	0.48
1:C:536:GLU:HA	1:C:569:GLN:O	2.13	0.48
1:D:134:ASN:OD1	1:D:134:ASN:N	2.40	0.48
1:F:301:ASP:OD2	1:F:440:HIS:NE2	2.36	0.48
1:B:200:TRP:HZ2	1:B:377:THR:HG21	1.78	0.48
1:C:211:VAL:HA	1:C:298:ILE:O	2.12	0.48
1:D:160:PRO:HA	1:D:163:LYS:CG	2.41	0.48
1:D:607:GLU:HB2	1:D:621:PRO:HD3	1.93	0.48
1:F:301:ASP:H	1:F:391:LEU:CD2	2.26	0.48
1:B:447:TRP:C	1:B:448:GLN:CG	2.86	0.48
1:D:160:PRO:O	1:D:163:LYS:HG3	2.13	0.48
1:A:254:LEU:O	1:A:273:ARG:NH2	2.46	0.48
1:A:325:CYS:HB3	1:A:423:ILE:HD13	1.95	0.48
1:B:394:ILE:HG22	6:B:811:HOH:O	2.13	0.48
1:E:200:TRP:HZ2	1:E:377:THR:HG21	1.78	0.48
1:A:394:ILE:HD12	1:A:399:PHE:HB2	1.95	0.48
1:D:278:GLU:HG3	1:D:286:ILE:HD11	1.95	0.48
1:E:314:LEU:HD11	1:E:326:THR:HG22	1.96	0.48
1:F:180:SER:HB2	1:F:338:TYR:CZ	2.48	0.48
1:A:209:SER:OG	1:A:296:VAL:HG22	2.13	0.48
1:D:186:ASP:OD1	1:D:228:HIS:ND1	2.46	0.48
1:F:194:GLN:O	1:F:197:CYS:HB2	2.14	0.48
1:F:485:PRO:HG3	1:F:531:ASN:ND2	2.29	0.48
1:F:628:ARG:HH11	1:F:628:ARG:CG	2.25	0.48
1:C:212:VAL:HG21	1:C:299:TYR:CE1	2.49	0.48
1:C:375:ARG:NE	1:C:382:TYR:HB3	2.28	0.48
1:D:406:ASP:HB2	1:D:498:LEU:HD11	1.95	0.48
1:F:377:THR:CG2	1:F:378:LYS:N	2.77	0.48
1:A:225:ARG:O	1:A:229:SER:HB3	2.13	0.48
1:A:587:THR:OG1	1:A:588:LYS:N	2.45	0.48
1:B:454:ILE:HD12	1:B:460:PRO:HG2	1.96	0.48
1:D:458:SER:HB3	1:D:463:LYS:HZ1	1.78	0.48
1:E:136:GLU:CD	1:E:193:ARG:HH22	2.14	0.48
1:E:235:PRO:HB2	1:E:238:TYR:CD2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:513:PHE:CD2	1:E:514:MET:HE3	2.49	0.48
1:F:603:ASN:CA	1:F:606:LYS:HD2	2.43	0.48
1:A:371:GLU:HG2	1:A:519:TYR:OH	2.14	0.48
1:B:620:ILE:H	1:B:621:PRO:HD2	1.79	0.48
1:C:385:PRO:HA	1:C:517:ILE:CD1	2.44	0.48
1:C:513:PHE:CD1	1:C:517:ILE:HG12	2.49	0.48
1:D:158:LEU:HD12	1:D:166:ILE:HD11	1.96	0.48
1:E:532:VAL:HB	1:E:573:ILE:HG23	1.94	0.48
1:E:583:ASP:OD2	1:E:599:HIS:HD2	1.95	0.48
1:A:281:ILE:CD1	1:A:415:GLU:HG2	2.43	0.48
1:B:122:TYR:CE1	1:B:203:ASP:CB	2.97	0.48
1:B:579:LEU:HB2	1:B:608:TRP:CD1	2.49	0.48
1:C:264:LEU:HD13	1:C:265:TRP:CE2	2.48	0.48
1:F:453:PRO:O	1:F:455:TYR:CD2	2.66	0.48
1:A:458:SER:HG	1:A:462:LEU:HB2	1.77	0.47
1:A:554:GLY:O	1:A:596:MET:HG3	2.14	0.47
1:D:161:GLU:H	1:D:161:GLU:CD	1.98	0.47
1:F:412:TRP:O	1:F:461:THR:HB	2.13	0.47
1:A:314:LEU:HD11	1:A:326:THR:HG22	1.92	0.47
1:C:187:ARG:O	1:C:187:ARG:HG3	2.14	0.47
1:D:373:ARG:HD2	6:D:805:HOH:O	2.13	0.47
1:F:370:GLN:CD	1:F:370:GLN:H	2.21	0.47
1:B:400:PHE:O	1:B:403:GLY:HA3	2.15	0.47
1:B:447:TRP:CD1	1:B:448:GLN:N	2.81	0.47
1:C:193:ARG:NH1	1:C:308:VAL:HG22	2.29	0.47
1:C:454:ILE:O	1:C:458:SER:C	2.57	0.47
1:D:224:MET:HE3	1:D:224:MET:HA	1.96	0.47
1:D:239:LEU:HD13	1:D:268:LEU:HD11	1.96	0.47
1:D:373:ARG:NH1	6:D:805:HOH:O	2.46	0.47
1:E:539:GLY:CA	1:E:628:ARG:NH2	2.77	0.47
1:A:485:PRO:HG3	1:A:531:ASN:ND2	2.29	0.47
1:B:191:ASP:OD1	1:B:193:ARG:CG	2.62	0.47
1:B:224:MET:HE3	1:B:224:MET:HA	1.96	0.47
1:D:347:ASP:CB	1:D:351:TYR:H	2.03	0.47
1:E:603:ASN:CA	1:E:606:LYS:HD2	2.45	0.47
1:F:192:LEU:HD11	1:F:340:ILE:HG22	1.94	0.47
1:A:262:ILE:HD13	1:A:262:ILE:HA	1.56	0.47
1:A:459:SER:HB3	1:A:460:PRO:HD3	1.94	0.47
1:B:631:VAL:HG23	1:B:631:VAL:O	2.15	0.47
1:F:116:LYS:NZ	1:F:397:GLU:OE1	2.46	0.47
1:F:356:TRP:HZ2	1:F:514:MET:CE	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:GLY:N	6:B:807:HOH:O	2.48	0.47
1:B:641:ASP:HB3	1:B:644:LYS:HG3	1.96	0.47
1:E:367:LEU:HD13	1:E:382:TYR:CD1	2.49	0.47
1:E:450:ASN:HD22	1:E:450:ASN:H	1.60	0.47
1:A:306:VAL:CG2	1:A:310:TRP:CD2	2.98	0.47
1:A:602:LEU:HA	1:A:602:LEU:HD23	1.55	0.47
1:B:203:ASP:O	1:B:204:GLU:HG3	2.15	0.47
1:C:212:VAL:CG2	1:C:299:TYR:CE1	2.98	0.47
1:C:241:GLU:OE1	1:C:293:LEU:HD22	2.13	0.47
1:C:378:LYS:HB3	1:C:378:LYS:HE3	1.65	0.47
1:C:553:ASN:HA	1:C:598:THR:HA	1.96	0.47
1:C:586:LEU:N	1:C:586:LEU:CD2	2.76	0.47
1:E:375:ARG:NE	1:E:382:TYR:HB3	2.29	0.47
1:E:620:ILE:H	1:E:621:PRO:HD2	1.80	0.47
1:F:454:ILE:HG23	1:F:457:GLY:C	2.40	0.47
1:A:394:ILE:HD12	1:A:399:PHE:CG	2.49	0.47
1:A:502:ARG:HG3	1:A:507:CYS:HB2	1.97	0.47
1:D:413:GLY:HA2	3:D:701:NAG:O6	2.15	0.47
1:F:207:LEU:HD11	1:F:319:SER:HA	1.96	0.47
1:F:235:PRO:HB2	1:F:238:TYR:HD2	1.80	0.47
1:F:400:PHE:HA	1:F:404:LEU:CD1	2.45	0.47
1:A:373:ARG:O	1:A:373:ARG:CD	2.63	0.47
1:C:346:GLY:N	6:C:801:HOH:O	2.47	0.47
1:E:380:GLU:HB2	1:E:381:PRO:CD	2.45	0.47
1:F:146:VAL:HA	1:F:147:GLY:HA2	1.64	0.47
1:F:193:ARG:HG2	1:F:197:CYS:CB	2.45	0.47
1:F:207:LEU:HD13	1:F:319:SER:OG	2.14	0.47
1:A:596:MET:HE2	1:A:596:MET:HB3	1.71	0.47
1:B:377:THR:HG22	1:B:379:THR:N	2.17	0.47
1:B:616:ARG:HG2	1:B:618:THR:HG22	1.97	0.47
1:C:322:ARG:HH11	1:C:397:GLU:HB3	1.78	0.47
1:D:151:GLU:HA	1:D:152:LYS:C	2.40	0.47
1:E:620:ILE:N	1:E:621:PRO:HD2	2.30	0.47
1:F:180:SER:HB2	1:F:338:TYR:OH	2.15	0.47
1:F:346:GLY:HA3	1:F:366:PRO:HB3	1.95	0.47
1:F:586:LEU:HA	1:F:596:MET:O	2.15	0.47
1:B:314:LEU:HD12	1:B:326:THR:HG23	1.95	0.46
1:E:156:LEU:O	1:E:337:THR:HG22	2.14	0.46
1:F:118:GLN:NE2	1:F:322:ARG:H	2.12	0.46
1:F:122:TYR:OH	1:F:206:LEU:CD2	2.64	0.46
1:B:584:GLN:CG	1:B:598:THR:C	2.87	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:TYR:CZ	1:C:203:ASP:CB	2.95	0.46
1:C:602:LEU:HA	1:C:602:LEU:HD23	1.66	0.46
1:D:153:ALA:CB	1:D:190:ASN:HB3	2.45	0.46
1:F:212:VAL:CG2	1:F:299:TYR:CD2	2.97	0.46
1:F:447:TRP:CD1	1:F:448:GLN:H	2.33	0.46
1:F:453:PRO:HB3	1:F:455:TYR:OH	2.15	0.46
1:A:212:VAL:HG22	1:A:299:TYR:CD1	2.50	0.46
1:B:402:LEU:HA	1:B:402:LEU:HD23	1.75	0.46
1:B:586:LEU:N	1:B:586:LEU:CD2	2.76	0.46
1:C:208:THR:O	1:C:296:VAL:HG13	2.16	0.46
1:D:499:LYS:HG3	6:D:816:HOH:O	2.13	0.46
1:F:411:ILE:CG2	1:F:412:TRP:N	2.73	0.46
1:A:211:VAL:HG22	1:A:242:ILE:HG12	1.97	0.46
1:B:262:ILE:HD13	1:B:262:ILE:HA	1.68	0.46
1:C:576:ALA:O	1:C:577:ASN:HB2	2.16	0.46
1:C:593:SER:HB3	1:C:637:ILE:O	2.15	0.46
1:C:627:ASP:OD1	1:C:646:THR:HB	2.15	0.46
1:D:180:SER:OG	1:D:225:ARG:NH1	2.49	0.46
1:D:231:ILE:HD12	1:D:265:TRP:CD1	2.50	0.46
1:D:632:LEU:HD12	1:D:632:LEU:N	2.31	0.46
1:E:410:GLN:O	1:E:412:TRP:N	2.43	0.46
1:F:456:VAL:HG12	1:F:456:VAL:O	2.15	0.46
1:F:474:ASP:O	1:F:477:LYS:HG2	2.15	0.46
1:A:315:VAL:HG12	1:A:315:VAL:O	2.15	0.46
1:B:610:TYR:OH	1:B:612:LYS:HG3	2.16	0.46
1:C:490:LEU:HD12	1:C:656:SER:O	2.15	0.46
1:E:183:ILE:O	1:E:225:ARG:NH2	2.49	0.46
1:E:190:ASN:C	1:E:190:ASN:ND2	2.73	0.46
1:E:377:THR:HG22	1:E:378:LYS:N	2.31	0.46
1:F:138:LYS:HB2	1:F:138:LYS:HE3	1.62	0.46
1:F:316:ALA:N	1:F:317:PRO:HD2	2.30	0.46
1:A:258:LEU:CD1	1:A:262:ILE:HG12	2.45	0.46
1:A:474:ASP:O	1:A:477:LYS:HG2	2.15	0.46
1:C:286:ILE:CG2	1:C:290:LYS:HD2	2.45	0.46
1:D:225:ARG:O	1:D:229:SER:HB3	2.16	0.46
1:E:212:VAL:HG21	1:E:299:TYR:CE2	2.50	0.46
1:E:455:TYR:HA	1:E:456:VAL:HA	1.62	0.46
1:E:474:ASP:C	1:E:476:TYR:H	2.22	0.46
1:E:602:LEU:O	1:E:602:LEU:HD22	2.15	0.46
1:F:113:LEU:HD12	1:F:504:ASP:HB3	1.98	0.46
1:A:192:LEU:HD22	1:A:342:PRO:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:LYS:HE3	1:A:463:LYS:HB2	1.63	0.46
1:A:548:SER:HB2	1:A:581:GLN:OE1	2.16	0.46
1:B:235:PRO:HB2	1:B:238:TYR:HD2	1.80	0.46
1:B:316:ALA:HB3	1:B:317:PRO:HD3	1.98	0.46
1:B:385:PRO:HA	1:B:517:ILE:HD11	1.98	0.46
1:C:455:TYR:HA	1:C:456:VAL:HA	1.42	0.46
1:E:409:LEU:HD13	1:E:415:GLU:HB2	1.97	0.46
1:C:476:TYR:CE2	1:C:514:MET:HG3	2.50	0.46
1:C:596:MET:HE2	1:C:596:MET:HB3	1.73	0.46
1:D:586:LEU:HD23	1:D:597:ILE:CG1	2.46	0.46
1:E:200:TRP:CZ2	1:E:377:THR:HG21	2.51	0.46
1:B:314:LEU:HG	1:B:326:THR:HG21	1.98	0.46
1:E:574:ASN:ND2	1:E:578:GLN:OE1	2.49	0.46
1:E:614:LEU:HD23	1:E:614:LEU:HA	1.66	0.46
1:F:128:ARG:HB3	1:F:131:ILE:HD12	1.97	0.46
1:F:195:GLU:OE2	1:F:198:LYS:HE3	2.16	0.46
1:F:454:ILE:CG2	1:F:457:GLY:O	2.63	0.46
1:A:312:ALA:N	1:A:313:PRO:CD	2.78	0.46
1:B:549:MET:HB2	1:B:551:LYS:HD3	1.98	0.46
1:C:447:TRP:CD1	1:C:448:GLN:N	2.83	0.46
1:C:450:ASN:HD22	1:C:450:ASN:H	1.63	0.46
1:D:231:ILE:HD12	1:D:265:TRP:NE1	2.31	0.46
1:D:588:LYS:HD2	1:D:589:GLY:O	2.15	0.46
1:E:596:MET:HE2	1:E:596:MET:HB3	1.69	0.46
1:A:422:LYS:HG2	1:A:472:TRP:HZ2	1.76	0.45
1:A:574:ASN:ND2	1:A:578:GLN:OE1	2.49	0.45
1:A:627:ASP:HB3	1:A:636:PHE:CE1	2.51	0.45
1:B:138:LYS:HB2	1:B:138:LYS:HE3	1.61	0.45
1:C:373:ARG:HD2	1:C:373:ARG:O	2.16	0.45
1:E:485:PRO:O	1:E:488:GLN:HG3	2.16	0.45
1:F:615:HIS:O	1:F:648:LYS:HA	2.17	0.45
1:A:138:LYS:HB2	1:A:138:LYS:HE3	1.52	0.45
1:A:394:ILE:HD12	1:A:399:PHE:CB	2.46	0.45
1:C:321:ASP:HB3	1:C:324:ILE:HG13	1.97	0.45
1:D:189:VAL:HG12	1:D:190:ASN:O	2.16	0.45
1:B:118:GLN:NE2	1:B:321:ASP:HA	2.30	0.45
1:B:146:VAL:HA	1:B:147:GLY:HA2	1.56	0.45
1:B:190:ASN:C	1:B:190:ASN:ND2	2.73	0.45
1:C:163:LYS:NZ	5:D:704:UD2:O2A	2.49	0.45
1:C:391:LEU:HD23	1:C:391:LEU:N	2.31	0.45
1:D:160:PRO:N	1:D:161:GLU:OE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:138:LYS:HB2	1:E:138:LYS:HE3	1.71	0.45
1:E:194:GLN:O	1:E:197:CYS:HB2	2.16	0.45
1:F:455:TYR:HA	1:F:456:VAL:HA	1.65	0.45
1:B:474:ASP:O	1:B:477:LYS:HG2	2.17	0.45
1:C:116:LYS:NZ	1:C:397:GLU:HG2	2.32	0.45
1:C:574:ASN:HB3	1:C:576:ALA:N	2.29	0.45
1:D:176:ASN:C	1:D:176:ASN:ND2	2.74	0.45
1:F:122:TYR:CD2	1:F:205:ASN:HB3	2.52	0.45
1:A:380:GLU:HB2	1:A:381:PRO:HD2	1.97	0.45
1:B:517:ILE:HG13	1:B:518:ALA:N	2.32	0.45
1:D:418:GLU:OE2	6:D:801:HOH:O	2.21	0.45
1:F:179:ALA:O	1:F:183:ILE:HG13	2.16	0.45
1:F:355:ALA:HB1	1:F:521:ILE:HG12	1.98	0.45
1:F:584:GLN:HB3	1:F:598:THR:O	2.16	0.45
1:D:278:GLU:HG3	1:D:286:ILE:CD1	2.46	0.45
1:B:192:LEU:HD13	1:B:342:PRO:HD3	1.99	0.45
1:B:387:MET:O	1:B:387:MET:HG3	2.17	0.45
1:D:253:HIS:H	1:D:253:HIS:HD2	1.63	0.45
1:D:377:THR:CG2	1:D:378:LYS:N	2.79	0.45
1:D:588:LYS:HG3	1:D:637:ILE:HD11	1.99	0.45
1:F:193:ARG:CG	1:F:197:CYS:CB	2.94	0.45
1:F:641:ASP:OD1	1:F:641:ASP:C	2.59	0.45
1:A:212:VAL:CG2	1:A:299:TYR:CD1	3.00	0.45
1:B:138:LYS:H	1:B:138:LYS:HG3	1.56	0.45
1:E:262:ILE:HD13	1:E:262:ILE:HA	1.54	0.45
1:E:586:LEU:N	1:E:586:LEU:CD2	2.78	0.45
1:F:454:ILE:CG2	1:F:457:GLY:CA	2.91	0.45
1:E:159:GLY:HA2	1:E:162:PHE:H	1.81	0.45
1:F:534:TRP:CH2	1:F:653:ASN:HB3	2.51	0.45
1:A:122:TYR:CE1	1:A:205:ASN:HB3	2.52	0.45
1:A:262:ILE:HD13	1:A:265:TRP:HZ3	1.82	0.45
1:B:641:ASP:HB2	6:B:809:HOH:O	2.15	0.45
1:C:511:LYS:NZ	6:C:803:HOH:O	2.49	0.45
1:D:459:SER:OG	1:D:462:LEU:HB2	2.17	0.45
1:E:191:ASP:OD1	1:E:193:ARG:HG2	2.16	0.45
1:E:455:TYR:O	1:E:455:TYR:CD1	2.70	0.45
1:F:196:GLU:HG3	6:F:837:HOH:O	2.16	0.45
1:F:264:LEU:O	1:F:264:LEU:CD2	2.65	0.45
1:F:495:ILE:HD12	1:F:495:ILE:HA	1.70	0.45
1:F:579:LEU:HB2	1:F:608:TRP:CD1	2.52	0.45
1:F:584:GLN:HG2	1:F:599:HIS:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:GLY:C	1:A:366:PRO:HB3	2.43	0.44
1:B:113:LEU:HD12	1:B:504:ASP:HB3	1.98	0.44
1:C:197:CYS:SG	1:C:379:THR:HG23	2.57	0.44
1:C:286:ILE:HG22	1:C:290:LYS:HD2	1.98	0.44
1:D:172:GLU:HG2	1:D:251:LYS:NZ	2.32	0.44
1:D:650:GLU:HG3	1:D:652:ASN:HD21	1.81	0.44
1:E:154:LYS:HE3	1:E:154:LYS:HB3	1.90	0.44
1:E:276:ARG:HD2	1:E:278:GLU:CD	2.42	0.44
1:E:404:LEU:N	1:E:404:LEU:CD2	2.73	0.44
1:A:400:PHE:O	1:A:403:GLY:CA	2.65	0.44
1:A:405:TYR:O	1:A:406:ASP:C	2.59	0.44
1:B:597:ILE:O	1:B:597:ILE:HG22	2.16	0.44
1:F:166:ILE:O	1:F:170:ILE:HG13	2.17	0.44
1:F:210:SER:OG	1:F:241:GLU:HG2	2.18	0.44
1:A:258:LEU:HD12	1:A:262:ILE:HG12	1.99	0.44
1:C:447:TRP:O	1:C:448:GLN:HG2	2.17	0.44
1:D:339:GLU:OE1	1:D:339:GLU:N	2.47	0.44
1:D:486:GLU:HA	1:D:534:TRP:CH2	2.52	0.44
1:A:358:TRP:O	1:A:480:PHE:HA	2.17	0.44
1:A:445:GLU:H	1:A:445:GLU:HG2	1.47	0.44
1:C:377:THR:HG22	1:C:378:LYS:N	2.31	0.44
1:C:421:TYR:HB3	1:C:425:GLN:HE21	1.82	0.44
1:C:513:PHE:CE1	1:C:517:ILE:CD1	2.98	0.44
1:D:128:ARG:O	1:D:129:PRO:C	2.59	0.44
1:D:214:VAL:HG12	4:D:702:UDP:H1'	1.99	0.44
1:D:262:ILE:HD13	1:D:262:ILE:HA	1.78	0.44
1:E:477:LYS:O	1:E:478:ASP:C	2.60	0.44
1:F:207:LEU:CD1	1:F:319:SER:HA	2.47	0.44
1:A:122:TYR:CD1	1:A:205:ASN:HB3	2.52	0.44
1:A:513:PHE:CD1	1:A:517:ILE:HG12	2.52	0.44
1:B:410:GLN:N	1:B:464:ASN:HD21	2.15	0.44
1:B:627:ASP:OD1	1:B:646:THR:HB	2.18	0.44
1:C:375:ARG:HE	1:C:382:TYR:HB3	1.81	0.44
1:D:469:VAL:HG22	1:D:473:TRP:CD2	2.52	0.44
1:E:189:VAL:CG1	1:E:190:ASN:N	2.80	0.44
1:E:202:TYR:OH	1:E:313:PRO:HG3	2.18	0.44
1:F:172:GLU:HG3	1:F:251:LYS:NZ	2.32	0.44
1:F:311:TYR:CZ	1:F:315:VAL:HG21	2.53	0.44
1:A:301:ASP:H	1:A:391:LEU:CD2	2.31	0.44
1:A:363:LYS:HD2	1:A:525:TYR:OH	2.18	0.44
1:B:332:VAL:HG22	1:B:442:TYR:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:596:MET:HE2	1:B:596:MET:HB3	1.71	0.44
1:C:192:LEU:HD13	1:C:342:PRO:HD3	2.00	0.44
1:D:498:LEU:HA	1:D:498:LEU:HD23	1.75	0.44
1:E:264:LEU:O	1:E:264:LEU:HD22	2.17	0.44
1:E:312:ALA:HB3	1:E:313:PRO:HD3	1.99	0.44
1:A:136:GLU:CD	1:A:193:ARG:HH22	2.24	0.44
1:A:138:LYS:H	1:A:138:LYS:HG3	1.59	0.44
1:B:172:GLU:CG	1:B:251:LYS:NZ	2.81	0.44
1:B:248:PHE:CE1	1:B:275:GLU:O	2.71	0.44
1:C:353:ARG:HG2	1:C:365:VAL:HG23	1.99	0.44
1:C:628:ARG:CG	1:C:628:ARG:NH1	2.75	0.44
1:D:211:VAL:HA	1:D:298:ILE:O	2.17	0.44
1:E:410:GLN:HB3	1:E:411:ILE:HD13	2.00	0.44
1:E:641:ASP:C	1:E:641:ASP:OD1	2.60	0.44
1:F:286:ILE:HG22	1:F:290:LYS:HD2	2.00	0.44
1:F:454:ILE:HG23	1:F:454:ILE:O	2.18	0.44
1:B:495:ILE:HD12	1:B:495:ILE:HA	1.67	0.44
1:C:551:LYS:HG2	1:C:555:GLY:HA3	1.99	0.44
1:D:190:ASN:C	1:D:190:ASN:ND2	2.75	0.44
1:D:312:ALA:HB3	1:D:313:PRO:HD3	1.99	0.44
1:E:225:ARG:O	1:E:229:SER:HB3	2.18	0.44
1:F:326:THR:HG23	1:F:433:VAL:HG23	1.99	0.44
1:A:341:ILE:CG2	1:B:632:LEU:CB	2.85	0.43
1:B:539:GLY:HA3	1:B:628:ARG:NH2	2.33	0.43
1:C:421:TYR:HB3	1:C:425:GLN:NE2	2.33	0.43
1:C:455:TYR:CD1	1:C:455:TYR:N	2.86	0.43
1:D:373:ARG:CD	6:D:805:HOH:O	2.65	0.43
1:A:467:ARG:CZ	1:A:495:ILE:CD1	2.95	0.43
1:B:116:LYS:HB3	1:B:116:LYS:HE2	1.81	0.43
1:B:357:ASP:C	1:B:357:ASP:OD1	2.60	0.43
1:B:573:ILE:HA	1:B:578:GLN:O	2.18	0.43
1:C:368:THR:HB	1:C:370:GLN:OE1	2.18	0.43
1:D:458:SER:HB2	1:D:657:VAL:O	2.19	0.43
1:A:457:GLY:CA	1:A:459:SER:HB2	2.49	0.43
1:B:177:MET:HE1	1:B:221:SER:OG	2.18	0.43
1:C:239:LEU:HD13	1:C:268:LEU:HD11	2.00	0.43
1:C:412:TRP:O	1:C:461:THR:CG2	2.54	0.43
1:D:211:VAL:CG2	1:D:242:ILE:HG12	2.46	0.43
1:F:548:SER:O	1:F:551:LYS:HB2	2.17	0.43
1:E:332:VAL:HG22	1:E:442:TYR:CE2	2.54	0.43
1:F:195:GLU:OE2	1:F:195:GLU:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:ASN:ND2	1:B:578:GLN:OE1	2.51	0.43
1:B:632:LEU:HD11	1:B:634:GLN:HB2	1.95	0.43
1:C:312:ALA:N	1:C:313:PRO:CD	2.82	0.43
1:C:462:LEU:CD1	1:C:487:SER:CB	2.94	0.43
1:D:282:GLN:HG2	6:D:815:HOH:O	2.16	0.43
1:D:394:ILE:HD12	1:D:399:PHE:CG	2.53	0.43
1:D:410:GLN:HG3	6:D:844:HOH:O	2.18	0.43
1:D:458:SER:HB3	1:D:463:LYS:HZ2	1.84	0.43
1:E:325:CYS:SG	1:E:394:ILE:HG23	2.59	0.43
1:E:370:GLN:H	1:E:370:GLN:CD	2.23	0.43
1:E:548:SER:O	1:E:551:LYS:HB2	2.19	0.43
1:F:532:VAL:HB	1:F:573:ILE:HG23	2.01	0.43
1:A:191:ASP:OD1	1:A:193:ARG:CG	2.58	0.43
1:A:218:GLU:O	1:A:253:HIS:HE1	2.01	0.43
1:A:394:ILE:CD1	1:A:399:PHE:CG	3.01	0.43
1:A:586:LEU:N	1:A:586:LEU:CD2	2.81	0.43
1:C:254:LEU:O	1:C:273:ARG:NH2	2.52	0.43
1:C:346:GLY:HA3	1:C:366:PRO:CA	2.48	0.43
1:C:549:MET:C	1:C:551:LYS:H	2.26	0.43
1:D:511:LYS:HB2	1:D:511:LYS:HE3	1.75	0.43
1:F:631:VAL:HG23	1:F:631:VAL:O	2.19	0.43
1:A:235:PRO:HB2	1:A:238:TYR:CD2	2.51	0.43
1:B:159:GLY:HA2	1:B:162:PHE:H	1.83	0.43
1:B:371:GLU:HG2	1:B:519:TYR:OH	2.19	0.43
1:C:193:ARG:HG2	1:C:193:ARG:H	1.61	0.43
1:C:580:MET:HG2	1:C:585:CYS:SG	2.59	0.43
1:C:632:LEU:HD11	1:C:634:GLN:CB	2.40	0.43
1:D:118:GLN:NE2	1:D:322:ARG:HG2	2.34	0.43
1:D:218:GLU:HG3	1:D:302:ALA:CB	2.47	0.43
1:B:209:SER:OG	1:B:296:VAL:HG22	2.18	0.43
1:C:358:TRP:O	1:C:480:PHE:HA	2.19	0.43
1:C:370:GLN:H	1:C:370:GLN:CD	2.26	0.43
1:C:539:GLY:HA3	1:C:628:ARG:NH2	2.33	0.43
1:D:153:ALA:HB2	1:D:190:ASN:CB	2.49	0.43
1:D:574:ASN:HB2	1:D:578:GLN:H	1.83	0.43
1:E:187:ARG:NH1	1:E:305:GLU:OE2	2.45	0.43
1:E:363:LYS:NZ	6:E:808:HOH:O	2.52	0.43
1:E:602:LEU:HD23	1:E:602:LEU:HA	1.71	0.43
1:F:276:ARG:HD2	1:F:278:GLU:OE2	2.19	0.43
1:F:365:VAL:HB	1:F:366:PRO:HD2	1.99	0.43
1:A:146:VAL:HA	1:A:147:GLY:HA2	1.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ILE:HG23	1:A:412:TRP:H	1.84	0.43
1:B:574:ASN:HB3	1:B:576:ALA:H	1.84	0.43
1:C:616:ARG:HG2	1:C:618:THR:HG22	2.01	0.43
1:D:135:PHE:CZ	1:D:204:GLU:HG2	2.54	0.43
1:F:262:ILE:C	1:F:264:LEU:N	2.77	0.43
1:F:359:SER:HB2	1:F:484:ARG:NH1	2.34	0.43
1:F:411:ILE:HD13	1:F:460:PRO:HG2	2.00	0.43
1:A:301:ASP:OD2	1:A:303:HIS:NE2	2.52	0.43
1:A:447:TRP:O	1:A:448:GLN:HG2	2.19	0.43
1:B:484:ARG:NH2	6:B:803:HOH:O	2.50	0.43
1:F:122:TYR:OH	1:F:206:LEU:HD21	2.19	0.43
1:F:195:GLU:CD	1:F:198:LYS:HE3	2.43	0.43
1:F:453:PRO:HG3	1:F:455:TYR:OH	2.19	0.43
1:A:281:ILE:CD1	1:A:415:GLU:HG3	2.49	0.42
1:D:419:ILE:O	1:D:423:ILE:HG13	2.19	0.42
1:E:241:GLU:OE1	1:E:293:LEU:HD22	2.19	0.42
1:F:138:LYS:H	1:F:138:LYS:HG3	1.62	0.42
1:F:628:ARG:HG2	1:F:649:TRP:CH2	2.53	0.42
1:A:150:GLY:O	1:A:153:ALA:N	2.52	0.42
1:A:241:GLU:HA	1:A:268:LEU:HD22	2.00	0.42
1:A:513:PHE:HE1	1:A:517:ILE:HD11	1.82	0.42
1:B:136:GLU:OE1	1:B:193:ARG:NH2	2.52	0.42
1:C:193:ARG:NH1	1:C:308:VAL:CG2	2.82	0.42
1:C:264:LEU:O	1:C:264:LEU:HD22	2.19	0.42
1:D:195:GLU:O	1:D:196:GLU:C	2.62	0.42
1:E:479:TYR:CE1	1:E:527:LEU:HG	2.54	0.42
1:E:534:TRP:O	1:E:653:ASN:ND2	2.49	0.42
1:A:326:THR:HG23	1:A:433:VAL:HG21	2.02	0.42
1:A:377:THR:HG22	1:A:378:LYS:N	2.34	0.42
1:A:488:GLN:NE2	6:A:815:HOH:O	2.50	0.42
1:A:540:PHE:CE2	1:A:541:GLU:HG3	2.54	0.42
1:B:414:GLY:CA	1:B:416:ASN:N	2.80	0.42
1:D:239:LEU:HD23	1:D:239:LEU:HA	1.77	0.42
1:D:517:ILE:HG13	1:D:518:ALA:N	2.34	0.42
1:D:591:ASP:OD1	1:D:591:ASP:N	2.46	0.42
1:E:161:GLU:HG2	1:E:162:PHE:N	2.34	0.42
1:E:212:VAL:CG2	1:E:299:TYR:CE2	3.02	0.42
1:E:212:VAL:HG22	1:E:299:TYR:CD2	2.55	0.42
1:E:631:VAL:HG23	1:E:631:VAL:O	2.18	0.42
1:F:454:ILE:HG23	1:F:457:GLY:H	1.83	0.42
1:A:485:PRO:HB2	1:A:534:TRP:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:VAL:HA	1:C:147:GLY:HA2	1.57	0.42
1:C:603:ASN:O	1:C:606:LYS:HD2	2.18	0.42
1:D:132:LEU:HD22	1:D:132:LEU:N	2.34	0.42
1:D:160:PRO:CA	1:D:163:LYS:HG3	2.45	0.42
1:D:325:CYS:SG	1:D:394:ILE:HG23	2.60	0.42
1:E:262:ILE:CD1	1:E:265:TRP:HZ3	2.32	0.42
1:A:281:ILE:HD12	1:A:410:GLN:O	2.20	0.42
1:A:447:TRP:C	1:A:448:GLN:CG	2.92	0.42
1:B:390:GLY:C	1:B:391:LEU:HD23	2.45	0.42
1:B:514:MET:HE1	1:B:518:ALA:CB	2.49	0.42
1:C:176:ASN:C	1:C:176:ASN:ND2	2.77	0.42
1:C:631:VAL:O	1:C:631:VAL:HG23	2.18	0.42
1:D:255:LYS:H	1:D:255:LYS:HG3	1.75	0.42
1:E:458:SER:HA	1:E:459:SER:HA	1.81	0.42
1:F:207:LEU:HD12	1:F:319:SER:OG	2.20	0.42
1:F:326:THR:HG23	1:F:433:VAL:HG21	2.01	0.42
1:C:138:LYS:HE3	1:C:138:LYS:HB2	1.86	0.42
1:E:231:ILE:HD12	1:E:265:TRP:CE2	2.55	0.42
1:A:276:ARG:CD	1:A:278:GLU:OE2	2.56	0.42
1:A:341:ILE:HG23	1:B:632:LEU:HA	2.00	0.42
1:A:455:TYR:O	1:A:455:TYR:HD1	2.03	0.42
1:B:403:GLY:HA2	1:B:404:LEU:HA	1.81	0.42
1:D:264:LEU:O	1:D:264:LEU:CD2	2.67	0.42
1:D:574:ASN:HB3	1:D:576:ALA:N	2.34	0.42
1:D:627:ASP:HB3	1:D:636:PHE:CD1	2.54	0.42
1:F:196:GLU:HB3	6:F:837:HOH:O	2.18	0.42
1:A:603:ASN:HA	1:A:606:LYS:HD2	2.01	0.42
1:C:200:TRP:HE1	1:C:379:THR:CG2	2.33	0.42
1:C:532:VAL:HB	1:C:573:ILE:HG23	2.02	0.42
1:D:490:LEU:C	1:D:490:LEU:CD1	2.91	0.42
1:E:326:THR:HG23	1:E:433:VAL:CG2	2.50	0.42
1:E:390:GLY:C	1:E:391:LEU:HD23	2.44	0.42
1:E:632:LEU:HD13	1:E:632:LEU:O	2.16	0.42
1:B:203:ASP:HB3	1:B:205:ASN:H	1.84	0.42
1:B:279:GLY:CA	1:B:411:ILE:HD12	2.50	0.42
1:C:379:THR:HG22	1:C:435:CYS:SG	2.47	0.42
1:C:548:SER:HA	1:C:557:VAL:HG23	2.02	0.42
1:D:534:TRP:O	1:D:653:ASN:ND2	2.51	0.42
1:D:546:ILE:CD1	1:D:626:LEU:HD21	2.49	0.42
1:E:326:THR:HG23	1:E:433:VAL:HG23	2.02	0.42
1:E:445:GLU:H	1:E:445:GLU:HG2	1.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:477:LYS:H	1:E:477:LYS:HG3	1.62	0.42
1:F:414:GLY:HA2	1:F:415:GLU:OE2	2.19	0.42
1:F:620:ILE:N	1:F:621:PRO:HD2	2.35	0.42
1:A:128:ARG:O	1:A:129:PRO:C	2.61	0.42
1:A:152:LYS:O	1:A:153:ALA:HB3	2.20	0.42
1:A:341:ILE:HG21	1:B:632:LEU:HB2	1.95	0.42
1:C:113:LEU:HB2	1:C:504:ASP:O	2.19	0.42
1:C:333:ILE:HB	1:C:441:ILE:HA	2.02	0.42
1:C:539:GLY:CA	1:C:628:ARG:NH2	2.82	0.42
1:C:584:GLN:HG2	1:C:598:THR:C	2.45	0.42
1:D:253:HIS:CD2	1:D:253:HIS:N	2.85	0.42
1:E:576:ALA:O	1:E:577:ASN:HB2	2.20	0.42
1:F:403:GLY:HA2	1:F:404:LEU:HA	1.75	0.42
1:B:220:TRP:CZ3	1:B:257:LYS:HG2	2.54	0.41
1:C:534:TRP:HA	1:C:651:MET:CE	2.49	0.41
1:D:170:ILE:O	1:D:174:GLY:N	2.47	0.41
1:D:172:GLU:CG	1:D:251:LYS:NZ	2.82	0.41
1:D:212:VAL:HG21	1:D:299:TYR:CE2	2.55	0.41
1:F:574:ASN:ND2	1:F:578:GLN:OE1	2.53	0.41
1:A:472:TRP:O	1:A:510:PHE:HB2	2.19	0.41
1:B:276:ARG:HD2	1:B:278:GLU:CD	2.46	0.41
1:D:548:SER:HA	1:D:557:VAL:HG23	2.02	0.41
1:D:626:LEU:HD12	1:D:626:LEU:HA	1.91	0.41
1:F:211:VAL:O	1:F:211:VAL:CG2	2.67	0.41
1:B:143:PRO:HG2	1:B:146:VAL:HG22	2.03	0.41
1:B:553:ASN:HA	1:B:598:THR:HA	2.03	0.41
1:C:196:GLU:OE1	1:C:379:THR:CB	2.62	0.41
1:D:406:ASP:HB2	1:D:498:LEU:CD1	2.49	0.41
1:D:479:TYR:CD1	1:D:528:PRO:HD2	2.56	0.41
1:F:445:GLU:H	1:F:445:GLU:HG2	1.47	0.41
1:A:400:PHE:O	1:A:403:GLY:N	2.54	0.41
1:B:217:ASN:CG	1:B:251:LYS:HG3	2.46	0.41
1:E:187:ARG:O	1:E:187:ARG:HG3	2.20	0.41
1:E:211:VAL:HA	1:E:298:ILE:O	2.21	0.41
1:E:239:LEU:HD13	1:E:268:LEU:HD11	2.02	0.41
1:E:610:TYR:HB2	1:E:617:PHE:CE1	2.56	0.41
1:A:356:TRP:HZ2	1:A:514:MET:CE	2.33	0.41
1:B:187:ARG:HD2	1:B:188:SER:O	2.20	0.41
1:B:513:PHE:CD1	1:B:517:ILE:HG12	2.55	0.41
1:B:539:GLY:CA	1:B:628:ARG:NH2	2.83	0.41
1:C:116:LYS:NZ	1:C:397:GLU:OE1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:620:ILE:N	1:C:621:PRO:HD2	2.36	0.41
1:D:238:TYR:HB3	1:D:311:TYR:CE2	2.56	0.41
1:E:146:VAL:HA	1:E:147:GLY:HA2	1.61	0.41
1:E:632:LEU:HD13	1:E:633:HIS:N	2.34	0.41
1:F:520:ASP:O	1:F:523:SER:HB3	2.20	0.41
1:A:190:ASN:C	1:A:190:ASN:ND2	2.76	0.41
1:B:410:GLN:H	1:B:464:ASN:HD21	1.66	0.41
1:C:214:VAL:HG22	1:C:245:ILE:HB	2.03	0.41
1:C:632:LEU:HA	1:D:341:ILE:HG23	2.03	0.41
1:E:211:VAL:CG2	1:E:242:ILE:HG12	2.50	0.41
1:F:584:GLN:HG2	1:F:598:THR:C	2.46	0.41
1:A:176:ASN:C	1:A:176:ASN:ND2	2.77	0.41
1:B:406:ASP:HA	1:B:407:PRO:HD3	1.91	0.41
1:C:377:THR:HG22	1:C:379:THR:N	2.27	0.41
1:C:587:THR:OG1	1:C:588:LYS:N	2.51	0.41
1:D:153:ALA:HB2	1:D:190:ASN:H	1.85	0.41
1:D:306:VAL:CG2	1:D:310:TRP:CD2	3.04	0.41
1:F:454:ILE:CG2	1:F:457:GLY:HA3	2.51	0.41
1:A:276:ARG:HD2	1:A:278:GLU:CD	2.45	0.41
1:A:601:ASN:O	1:A:602:LEU:C	2.64	0.41
1:B:172:GLU:HG3	1:B:251:LYS:HZ3	1.86	0.41
1:B:278:GLU:HG3	1:B:286:ILE:CD1	2.51	0.41
1:B:463:LYS:O	1:B:467:ARG:HG3	2.21	0.41
1:C:136:GLU:O	1:C:137:PRO:C	2.62	0.41
1:C:419:ILE:HG13	1:C:423:ILE:HD11	2.01	0.41
1:C:454:ILE:C	1:C:458:SER:HA	2.33	0.41
1:A:300:LEU:HD12	1:A:300:LEU:HA	1.94	0.41
1:B:115:PHE:HE2	1:B:426:CYS:O	2.04	0.41
1:B:132:LEU:HD21	1:B:199:TYR:CE1	2.52	0.41
1:B:445:GLU:H	1:B:445:GLU:HG2	1.44	0.41
1:C:300:LEU:HD12	1:C:300:LEU:HA	1.92	0.41
1:C:332:VAL:O	1:C:340:ILE:HA	2.21	0.41
1:C:540:PHE:CD2	1:C:541:GLU:HG3	2.56	0.41
1:D:152:LYS:HD3	1:D:152:LYS:N	2.34	0.41
1:D:158:LEU:HD11	1:D:178:VAL:CG2	2.45	0.41
1:D:255:LYS:C	1:D:256:GLU:CG	2.87	0.41
1:D:601:ASN:HB2	1:D:604:GLU:HG3	2.02	0.41
1:E:356:TRP:CZ2	1:E:514:MET:HE1	2.56	0.41
1:E:450:ASN:N	1:E:450:ASN:ND2	2.63	0.41
1:E:628:ARG:CG	1:E:628:ARG:NH1	2.82	0.41
1:F:118:GLN:OE1	1:F:120:PHE:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:128:ARG:O	1:F:129:PRO:C	2.64	0.41
1:F:153:ALA:HB3	1:F:190:ASN:OD1	2.21	0.41
1:F:347:ASP:CB	1:F:351:TYR:O	2.65	0.41
1:F:553:ASN:HA	1:F:598:THR:HA	2.03	0.41
1:F:603:ASN:C	1:F:606:LYS:HD2	2.46	0.41
1:F:632:LEU:HD11	1:F:634:GLN:CG	2.51	0.41
1:B:337:THR:O	1:B:338:TYR:HB2	2.19	0.41
1:C:118:GLN:NE2	1:C:321:ASP:HA	2.36	0.41
1:C:242:ILE:HB	1:C:269:VAL:HG22	2.02	0.41
1:C:457:GLY:CA	1:C:458:SER:C	2.94	0.41
1:D:122:TYR:OH	1:D:203:ASP:O	2.33	0.41
1:D:520:ASP:OD1	1:D:520:ASP:N	2.35	0.41
1:E:169:SER:HB2	1:E:177:MET:HB2	2.03	0.41
1:E:473:TRP:CZ3	1:E:480:PHE:HB2	2.56	0.41
1:F:347:ASP:O	1:F:350:GLY:N	2.41	0.41
1:F:385:PRO:HA	1:F:517:ILE:HD11	2.03	0.41
1:F:534:TRP:CZ2	1:F:653:ASN:HB3	2.56	0.41
1:A:312:ALA:N	1:A:313:PRO:HD2	2.36	0.40
1:B:371:GLU:OE2	1:B:383:ARG:NH2	2.53	0.40
1:B:601:ASN:HB2	1:B:604:GLU:OE1	2.21	0.40
1:C:341:ILE:HG23	1:D:631:VAL:O	2.21	0.40
1:E:380:GLU:HB2	1:E:381:PRO:HD2	2.02	0.40
1:E:584:GLN:HG2	1:E:598:THR:C	2.47	0.40
1:F:224:MET:HA	1:F:224:MET:HE3	2.04	0.40
1:F:422:LYS:HG2	1:F:472:TRP:HZ2	1.84	0.40
1:F:580:MET:HG2	1:F:585:CYS:SG	2.61	0.40
1:B:602:LEU:HD22	1:B:602:LEU:O	2.21	0.40
1:C:255:LYS:O	1:C:257:LYS:N	2.50	0.40
1:C:548:SER:O	1:C:551:LYS:HB2	2.21	0.40
1:E:116:LYS:NZ	1:E:397:GLU:OE1	2.54	0.40
1:E:162:PHE:O	1:E:166:ILE:HG13	2.21	0.40
1:E:242:ILE:HB	1:E:269:VAL:HG22	2.04	0.40
1:E:321:ASP:C	1:E:321:ASP:OD1	2.64	0.40
1:F:212:VAL:O	1:F:212:VAL:HG23	2.21	0.40
1:F:454:ILE:HG12	1:F:457:GLY:HA3	2.04	0.40
1:F:628:ARG:CG	1:F:628:ARG:NH1	2.84	0.40
1:A:131:ILE:O	1:A:199:TYR:HD1	2.05	0.40
1:A:346:GLY:HA3	1:A:366:PRO:CA	2.51	0.40
1:B:194:GLN:O	1:B:197:CYS:HB2	2.21	0.40
1:B:200:TRP:CZ2	1:B:377:THR:HG21	2.55	0.40
1:B:301:ASP:OD2	1:B:303:HIS:NE2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:ARG:HA	1:B:373:ARG:HD2	1.90	0.40
1:B:484:ARG:NE	6:B:803:HOH:O	2.42	0.40
1:C:151:GLU:O	1:C:154:LYS:HB2	2.20	0.40
1:C:173:PHE:CD2	1:C:177:MET:HG3	2.55	0.40
1:D:149:PRO:HG2	1:D:182:MET:O	2.20	0.40
1:D:255:LYS:HA	1:D:273:ARG:NH2	2.36	0.40
1:E:204:GLU:OE1	1:E:204:GLU:N	2.51	0.40
1:E:286:ILE:HG22	1:E:290:LYS:HD2	2.04	0.40
1:F:132:LEU:O	1:F:201:HIS:CE1	2.74	0.40
1:F:411:ILE:CG2	1:F:412:TRP:H	2.25	0.40
1:F:412:TRP:O	1:F:461:THR:CG2	2.69	0.40
1:A:341:ILE:HG12	1:B:633:HIS:CD2	2.56	0.40
1:A:421:TYR:HB3	1:A:425:GLN:NE2	2.37	0.40
1:A:450:ASN:HD22	1:A:450:ASN:H	1.64	0.40
1:A:456:VAL:CG1	1:A:565:MET:HE1	2.48	0.40
1:B:235:PRO:HB2	1:B:238:TYR:CD2	2.57	0.40
1:B:306:VAL:CG2	1:B:310:TRP:CD2	3.04	0.40
1:C:169:SER:HB2	1:C:177:MET:HB2	2.04	0.40
1:C:301:ASP:HB2	1:C:304:CYS:SG	2.61	0.40
1:D:207:LEU:HD11	1:D:319:SER:HA	2.04	0.40
1:D:255:LYS:O	1:D:256:GLU:HG2	2.21	0.40
1:D:537:ILE:HG21	1:D:546:ILE:HD12	2.03	0.40
1:E:301:ASP:OD2	1:E:440:HIS:NE2	2.39	0.40
1:A:300:LEU:HA	1:A:391:LEU:HD22	2.03	0.40
1:A:349:ASP:OD2	1:A:378:LYS:HE3	2.21	0.40
1:C:260:GLU:OE2	1:C:263:LYS:NZ	2.35	0.40
1:C:419:ILE:HD12	1:C:419:ILE:HA	1.93	0.40
1:D:122:TYR:OH	1:D:206:LEU:HD23	2.21	0.40
1:D:586:LEU:CD2	1:D:597:ILE:CG1	2.98	0.40
1:F:620:ILE:H	1:F:621:PRO:HD2	1.86	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	544/597 (91%)	516 (95%)	26 (5%)	2 (0%)	30	51
1	B	544/597 (91%)	520 (96%)	24 (4%)	0	100	100
1	C	544/597 (91%)	515 (95%)	27 (5%)	2 (0%)	30	51
1	D	534/597 (89%)	513 (96%)	20 (4%)	1 (0%)	43	66
1	E	544/597 (91%)	518 (95%)	26 (5%)	0	100	100
1	F	544/597 (91%)	509 (94%)	32 (6%)	3 (1%)	21	42
All	All	3254/3582 (91%)	3091 (95%)	155 (5%)	8 (0%)	43	66

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	459	SER
1	F	411	ILE
1	F	413	GLY
1	D	176	ASN
1	C	453	PRO
1	C	460	PRO
1	F	453	PRO
1	A	592	GLY

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	480/525 (91%)	393 (82%)	87 (18%)	2	3
1	B	480/525 (91%)	383 (80%)	97 (20%)	1	2
1	C	480/525 (91%)	382 (80%)	98 (20%)	1	2
1	D	473/525 (90%)	408 (86%)	65 (14%)	3	7
1	E	480/525 (91%)	394 (82%)	86 (18%)	2	3
1	F	480/525 (91%)	399 (83%)	81 (17%)	2	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2873/3150 (91%)	2359 (82%)	514 (18%)	2 3

All (514) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	THR
1	A	127	LEU
1	A	132	LEU
1	A	138	LYS
1	A	139	GLU
1	A	146	VAL
1	A	151	GLU
1	A	152	LYS
1	A	154	LYS
1	A	156	LEU
1	A	164	GLN
1	A	176	ASN
1	A	178	VAL
1	A	182	MET
1	A	189	VAL
1	A	190	ASN
1	A	193	ARG
1	A	207	LEU
1	A	211	VAL
1	A	212	VAL
1	A	229	SER
1	A	231	ILE
1	A	239	LEU
1	A	250	ASN
1	A	255	LYS
1	A	256	GLU
1	A	258	LEU
1	A	262	ILE
1	A	264	LEU
1	A	268	LEU
1	A	270	LYS
1	A	276	ARG
1	A	293	LEU
1	A	296	VAL
1	A	300	LEU
1	A	301	ASP
1	A	303	HIS

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Mol	Chain	Res	Type
1	A	306	VAL
1	A	308	VAL
1	A	320	LYS
1	A	326	THR
1	A	359	SER
1	A	376	LYS
1	A	379	THR
1	A	394	ILE
1	A	395	GLU
1	A	402	LEU
1	A	409	LEU
1	A	410	GLN
1	A	411	ILE
1	A	415	GLU
1	A	430	LEU
1	A	443	ARG
1	A	445	GLU
1	A	448	GLN
1	A	450	ASN
1	A	454	ILE
1	A	455	TYR
1	A	471	VAL
1	A	490	LEU
1	A	495	ILE
1	A	498	LEU
1	A	506	ASN
1	A	517	ILE
1	A	523	SER
1	A	527	LEU
1	A	542	THR
1	A	547	ASP
1	A	551	LYS
1	A	557	VAL
1	A	579	LEU
1	A	586	LEU
1	A	588	LYS
1	A	591	ASP
1	A	594	LYS
1	A	597	ILE
1	A	598	THR
1	A	602	LEU
1	A	604	GLU

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Mol	Chain	Res	Type
1	A	606	LYS
1	A	614	LEU
1	A	618	THR
1	A	642	SER
1	A	648	LYS
1	A	650	GLU
1	A	655	HIS
1	A	656	SER
1	B	114	THR
1	B	116	LYS
1	B	121	THR
1	B	127	LEU
1	B	132	LEU
1	B	138	LYS
1	B	139	GLU
1	B	151	GLU
1	B	152	LYS
1	B	154	LYS
1	B	156	LEU
1	B	164	GLN
1	B	176	ASN
1	B	178	VAL
1	B	182	MET
1	B	187	ARG
1	B	189	VAL
1	B	190	ASN
1	B	193	ARG
1	B	198	LYS
1	B	203	ASP
1	B	211	VAL
1	B	212	VAL
1	B	229	SER
1	B	231	ILE
1	B	239	LEU
1	B	251	LYS
1	B	255	LYS
1	B	262	ILE
1	B	264	LEU
1	B	268	LEU
1	B	270	LYS
1	B	273	ARG
1	B	276	ARG

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Mol	Chain	Res	Type
1	B	293	LEU
1	B	296	VAL
1	B	300	LEU
1	B	301	ASP
1	B	306	VAL
1	B	308	VAL
1	B	320	LYS
1	B	326	THR
1	B	341	ILE
1	B	359	SER
1	B	376	LYS
1	B	391	LEU
1	B	394	ILE
1	B	395	GLU
1	B	397	GLU
1	B	404	LEU
1	B	406	ASP
1	B	409	LEU
1	B	410	GLN
1	B	411	ILE
1	B	415	GLU
1	B	430	LEU
1	B	443	ARG
1	B	445	GLU
1	B	448	GLN
1	B	450	ASN
1	B	455	TYR
1	B	456	VAL
1	B	461	THR
1	B	462	LEU
1	B	471	VAL
1	B	490	LEU
1	B	495	ILE
1	B	498	LEU
1	B	499	LYS
1	B	506	ASN
1	B	517	ILE
1	B	527	LEU
1	B	541	GLU
1	B	547	ASP
1	B	551	LYS
1	B	557	VAL

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Mol	Chain	Res	Type
1	B	573	ILE
1	B	579	LEU
1	B	584	GLN
1	B	586	LEU
1	B	588	LYS
1	B	591	ASP
1	B	597	ILE
1	B	598	THR
1	B	600	CYS
1	B	602	LEU
1	B	604	GLU
1	B	614	LEU
1	B	618	THR
1	B	620	ILE
1	B	628	ARG
1	B	632	LEU
1	B	642	SER
1	B	646	THR
1	B	648	LYS
1	B	650	GLU
1	B	656	SER
1	C	114	THR
1	C	116	LYS
1	C	127	LEU
1	C	132	LEU
1	C	138	LYS
1	C	139	GLU
1	C	146	VAL
1	C	151	GLU
1	C	154	LYS
1	C	156	LEU
1	C	163	LYS
1	C	164	GLN
1	C	176	ASN
1	C	178	VAL
1	C	182	MET
1	C	189	VAL
1	C	190	ASN
1	C	193	ARG
1	C	194	GLN
1	C	204	GLU
1	C	205	ASN

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Mol	Chain	Res	Type
1	C	211	VAL
1	C	212	VAL
1	C	229	SER
1	C	239	LEU
1	C	249	SER
1	C	250	ASN
1	C	251	LYS
1	C	252	GLU
1	C	255	LYS
1	C	264	LEU
1	C	268	LEU
1	C	270	LYS
1	C	276	ARG
1	C	277	ARG
1	C	293	LEU
1	C	296	VAL
1	C	300	LEU
1	C	306	VAL
1	C	308	VAL
1	C	320	LYS
1	C	326	THR
1	C	341	ILE
1	C	348	GLU
1	C	376	LYS
1	C	378	LYS
1	C	391	LEU
1	C	394	ILE
1	C	395	GLU
1	C	397	GLU
1	C	404	LEU
1	C	409	LEU
1	C	410	GLN
1	C	415	GLU
1	C	418	GLU
1	C	430	LEU
1	C	443	ARG
1	C	445	GLU
1	C	448	GLN
1	C	450	ASN
1	C	454	ILE
1	C	455	TYR
1	C	459	SER

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Mol	Chain	Res	Type
1	C	461	THR
1	C	462	LEU
1	C	471	VAL
1	C	498	LEU
1	C	499	LYS
1	C	506	ASN
1	C	517	ILE
1	C	523	SER
1	C	527	LEU
1	C	547	ASP
1	C	551	LYS
1	C	557	VAL
1	C	573	ILE
1	C	579	LEU
1	C	586	LEU
1	C	588	LYS
1	C	591	ASP
1	C	597	ILE
1	C	598	THR
1	C	600	CYS
1	C	602	LEU
1	C	604	GLU
1	C	606	LYS
1	C	613	ASN
1	C	614	LEU
1	C	618	THR
1	C	620	ILE
1	C	628	ARG
1	C	629	SER
1	C	632	LEU
1	C	642	SER
1	C	644	LYS
1	C	646	THR
1	C	648	LYS
1	C	656	SER
1	D	116	LYS
1	D	134	ASN
1	D	152	LYS
1	D	178	VAL
1	D	190	ASN
1	D	193	ARG
1	D	206	LEU

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Mol	Chain	Res	Type
1	D	211	VAL
1	D	212	VAL
1	D	229	SER
1	D	231	ILE
1	D	237	LYS
1	D	239	LEU
1	D	249	SER
1	D	250	ASN
1	D	253	HIS
1	D	254	LEU
1	D	255	LYS
1	D	256	GLU
1	D	258	LEU
1	D	264	LEU
1	D	268	LEU
1	D	276	ARG
1	D	280	LEU
1	D	293	LEU
1	D	296	VAL
1	D	300	LEU
1	D	301	ASP
1	D	306	VAL
1	D	308	VAL
1	D	320	LYS
1	D	326	THR
1	D	359	SER
1	D	376	LYS
1	D	391	LEU
1	D	394	ILE
1	D	395	GLU
1	D	397	GLU
1	D	402	LEU
1	D	406	ASP
1	D	409	LEU
1	D	411	ILE
1	D	430	LEU
1	D	462	LEU
1	D	463	LYS
1	D	471	VAL
1	D	475	GLU
1	D	490	LEU
1	D	499	LYS

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Mol	Chain	Res	Type
1	D	517	ILE
1	D	523	SER
1	D	527	LEU
1	D	542	THR
1	D	551	LYS
1	D	557	VAL
1	D	579	LEU
1	D	597	ILE
1	D	600	CYS
1	D	602	LEU
1	D	606	LYS
1	D	614	LEU
1	D	628	ARG
1	D	631	VAL
1	D	648	LYS
1	D	656	SER
1	E	127	LEU
1	E	131	ILE
1	E	132	LEU
1	E	139	GLU
1	E	151	GLU
1	E	152	LYS
1	E	154	LYS
1	E	156	LEU
1	E	164	GLN
1	E	178	VAL
1	E	189	VAL
1	E	190	ASN
1	E	193	ARG
1	E	211	VAL
1	E	212	VAL
1	E	229	SER
1	E	239	LEU
1	E	251	LYS
1	E	255	LYS
1	E	256	GLU
1	E	262	ILE
1	E	264	LEU
1	E	268	LEU
1	E	276	ARG
1	E	293	LEU
1	E	296	VAL

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Mol	Chain	Res	Type
1	E	300	LEU
1	E	306	VAL
1	E	308	VAL
1	E	320	LYS
1	E	326	THR
1	E	341	ILE
1	E	376	LYS
1	E	379	THR
1	E	391	LEU
1	E	394	ILE
1	E	395	GLU
1	E	404	LEU
1	E	411	ILE
1	E	415	GLU
1	E	418	GLU
1	E	430	LEU
1	E	443	ARG
1	E	445	GLU
1	E	448	GLN
1	E	450	ASN
1	E	454	ILE
1	E	456	VAL
1	E	459	SER
1	E	461	THR
1	E	474	ASP
1	E	475	GLU
1	E	477	LYS
1	E	490	LEU
1	E	498	LEU
1	E	499	LYS
1	E	506	ASN
1	E	517	ILE
1	E	523	SER
1	E	527	LEU
1	E	542	THR
1	E	547	ASP
1	E	551	LYS
1	E	557	VAL
1	E	579	LEU
1	E	586	LEU
1	E	588	LYS
1	E	591	ASP

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Mol	Chain	Res	Type
1	E	597	ILE
1	E	598	THR
1	E	600	CYS
1	E	602	LEU
1	E	604	GLU
1	E	606	LYS
1	E	613	ASN
1	E	614	LEU
1	E	618	THR
1	E	620	ILE
1	E	628	ARG
1	E	632	LEU
1	E	638	SER
1	E	644	LYS
1	E	645	THR
1	E	646	THR
1	E	650	GLU
1	E	656	SER
1	F	114	THR
1	F	116	LYS
1	F	127	LEU
1	F	132	LEU
1	F	138	LYS
1	F	139	GLU
1	F	146	VAL
1	F	151	GLU
1	F	154	LYS
1	F	156	LEU
1	F	163	LYS
1	F	164	GLN
1	F	178	VAL
1	F	190	ASN
1	F	211	VAL
1	F	229	SER
1	F	231	ILE
1	F	237	LYS
1	F	239	LEU
1	F	249	SER
1	F	250	ASN
1	F	251	LYS
1	F	255	LYS
1	F	264	LEU

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Mol	Chain	Res	Type
1	F	268	LEU
1	F	270	LYS
1	F	276	ARG
1	F	293	LEU
1	F	296	VAL
1	F	300	LEU
1	F	301	ASP
1	F	306	VAL
1	F	308	VAL
1	F	320	LYS
1	F	341	ILE
1	F	376	LYS
1	F	379	THR
1	F	391	LEU
1	F	394	ILE
1	F	397	GLU
1	F	404	LEU
1	F	415	GLU
1	F	430	LEU
1	F	443	ARG
1	F	445	GLU
1	F	448	GLN
1	F	450	ASN
1	F	454	ILE
1	F	461	THR
1	F	462	LEU
1	F	471	VAL
1	F	490	LEU
1	F	495	ILE
1	F	498	LEU
1	F	499	LYS
1	F	506	ASN
1	F	517	ILE
1	F	520	ASP
1	F	527	LEU
1	F	542	THR
1	F	547	ASP
1	F	551	LYS
1	F	557	VAL
1	F	579	LEU
1	F	586	LEU
1	F	588	LYS

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Mol	Chain	Res	Type
1	F	591	ASP
1	F	597	ILE
1	F	598	THR
1	F	602	LEU
1	F	604	GLU
1	F	618	THR
1	F	620	ILE
1	F	628	ARG
1	F	632	LEU
1	F	645	THR
1	F	646	THR
1	F	648	LYS
1	F	650	GLU
1	F	651	MET
1	F	656	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	176	ASN
1	A	190	ASN
1	A	194	GLN
1	A	201	HIS
1	A	253	HIS
1	A	266	ASN
1	A	343	GLN
1	A	425	GLN
1	A	450	ASN
1	A	531	ASN
1	A	568	ASN
1	A	574	ASN
1	A	578	GLN
1	A	634	GLN
1	A	647	GLN
1	A	652	ASN
1	A	653	ASN
1	B	118	GLN
1	B	176	ASN
1	B	190	ASN
1	B	201	HIS
1	B	253	HIS

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Mol	Chain	Res	Type
1	B	266	ASN
1	B	450	ASN
1	B	568	ASN
1	B	574	ASN
1	B	577	ASN
1	B	578	GLN
1	B	615	HIS
1	B	647	GLN
1	B	652	ASN
1	B	653	ASN
1	C	118	GLN
1	C	176	ASN
1	C	190	ASN
1	C	201	HIS
1	C	216	HIS
1	C	250	ASN
1	C	253	HIS
1	C	266	ASN
1	C	289	GLN
1	C	425	GLN
1	C	450	ASN
1	C	574	ASN
1	C	578	GLN
1	C	599	HIS
1	C	603	ASN
1	C	634	GLN
1	C	647	GLN
1	C	653	ASN
1	D	118	GLN
1	D	176	ASN
1	D	201	HIS
1	D	205	ASN
1	D	266	ASN
1	D	289	GLN
1	D	410	GLN
1	D	488	GLN
1	D	506	ASN
1	D	568	ASN
1	D	574	ASN
1	D	599	HIS
1	D	603	ASN
1	D	613	ASN

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Mol	Chain	Res	Type
1	D	647	GLN
1	D	652	ASN
1	E	118	GLN
1	E	164	GLN
1	E	176	ASN
1	E	190	ASN
1	E	253	HIS
1	E	266	ASN
1	E	289	GLN
1	E	343	GLN
1	E	425	GLN
1	E	450	ASN
1	E	464	ASN
1	E	568	ASN
1	E	574	ASN
1	E	577	ASN
1	E	578	GLN
1	E	599	HIS
1	E	647	GLN
1	E	653	ASN
1	F	118	GLN
1	F	176	ASN
1	F	190	ASN
1	F	201	HIS
1	F	289	GLN
1	F	343	GLN
1	F	450	ASN
1	F	464	ASN
1	F	531	ASN
1	F	568	ASN
1	F	574	ASN
1	F	577	ASN
1	F	578	GLN
1	F	647	GLN
1	F	653	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	NAG	D	701	-	15,15,15	1.59	2 (13%)	21,21,21	1.04	2 (9%)
4	UDP	D	702	2	25,26,26	3.14	5 (20%)	38,40,40	0.60	0
5	UD2	D	704	-	40,41,41	3.90	22 (55%)	59,62,62	2.14	17 (28%)

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	NAG	D	701	-	-	1/6/26/26	0/1/1/1
4	UDP	D	702	2	-	9/16/32/32	0/2/2/2
5	UD2	D	704	-	-	2/26/63/63	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	704	UD2	PA-O3A	14.80	1.75	1.59
4	D	702	UDP	PA-O3A	14.28	1.74	1.59
5	D	704	UD2	PB-O1'	9.32	1.87	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	704	UD2	O4B-C4B	5.94	1.58	1.45
5	D	704	UD2	PB-O3A	5.51	1.65	1.59
5	D	704	UD2	C2-N3	5.41	1.47	1.38
5	D	704	UD2	C4-N3	5.06	1.47	1.38
5	D	704	UD2	O5'-C1'	4.73	1.54	1.41
3	D	701	NAG	O5-C1	4.71	1.54	1.42
5	D	704	UD2	O4B-C1B	3.78	1.50	1.42
5	D	704	UD2	C6-N1	3.68	1.46	1.38
5	D	704	UD2	O3B-C3B	3.54	1.51	1.43
5	D	704	UD2	C3'-C2'	3.29	1.59	1.53
4	D	702	UDP	PB-O2B	3.25	1.66	1.54
5	D	704	UD2	O4'-C4'	3.19	1.50	1.43
5	D	704	UD2	C6-C5	3.04	1.42	1.35
5	D	704	UD2	PA-O5B	3.03	1.71	1.59
5	D	704	UD2	O5'-C5'	2.95	1.51	1.44
5	D	704	UD2	O2'-C2B	2.92	1.50	1.43
5	D	704	UD2	C8'-C7'	2.87	1.56	1.50
5	D	704	UD2	O3'-C3'	2.86	1.50	1.43
4	D	702	UDP	PB-O1B	2.73	1.59	1.50
5	D	704	UD2	C2'-N2'	2.68	1.50	1.45
4	D	702	UDP	C2-N1	2.42	1.42	1.38
5	D	704	UD2	C3B-C2B	2.35	1.59	1.53
5	D	704	UD2	PA-O2A	2.34	1.58	1.50
3	D	701	NAG	C3-C2	2.25	1.57	1.53
4	D	702	UDP	O4-C4	2.11	1.28	1.24
5	D	704	UD2	C2-N1	-2.09	1.35	1.38

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	704	UD2	O1'-PB-O2B	-9.39	79.79	109.81
5	D	704	UD2	O4B-C1B-C2B	-4.21	97.60	106.62
5	D	704	UD2	O1B-PB-O1'	-4.15	89.79	106.70
5	D	704	UD2	C4-N3-C2	-3.90	121.77	126.61
5	D	704	UD2	O4-C4-C5	-3.27	119.52	125.16
5	D	704	UD2	O1B-PB-O2B	2.98	126.30	112.44
5	D	704	UD2	C5-C4-N3	2.95	118.94	114.80
5	D	704	UD2	O4B-C1B-N1	-2.86	101.87	108.36
5	D	704	UD2	C4B-O4B-C1B	-2.77	103.36	109.47
5	D	704	UD2	N3-C2-N1	2.63	118.32	114.89
3	D	701	NAG	C1-O5-C5	-2.47	108.88	113.65
5	D	704	UD2	C1B-N1-C2	2.46	122.01	117.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	704	UD2	O1B-PB-O3A	2.46	113.92	107.27
5	D	704	UD2	C1'-O5'-C5'	-2.42	108.99	113.72
5	D	704	UD2	O5'-C1'-O1'	-2.31	108.34	111.36
5	D	704	UD2	O3A-PB-O2B	2.17	117.24	110.70
3	D	701	NAG	O3-C3-C2	2.03	113.62	109.58
5	D	704	UD2	PB-O1'-C1'	-2.01	113.03	121.21
5	D	704	UD2	O5B-PA-O2A	2.01	116.89	108.94

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	702	UDP	C5'-O5'-PA-O1A
5	D	704	UD2	C5B-O5B-PA-O3A
3	D	701	NAG	O5-C5-C6-O6
4	D	702	UDP	C2'-C1'-N1-C6
4	D	702	UDP	C5'-O5'-PA-O2A
4	D	702	UDP	C5'-O5'-PA-O3A
5	D	704	UD2	C5B-O5B-PA-O2A
4	D	702	UDP	O4'-C1'-N1-C6
4	D	702	UDP	PB-O3A-PA-O2A
4	D	702	UDP	O4'-C4'-C5'-O5'
4	D	702	UDP	O4'-C1'-N1-C2
4	D	702	UDP	PB-O3A-PA-O1A

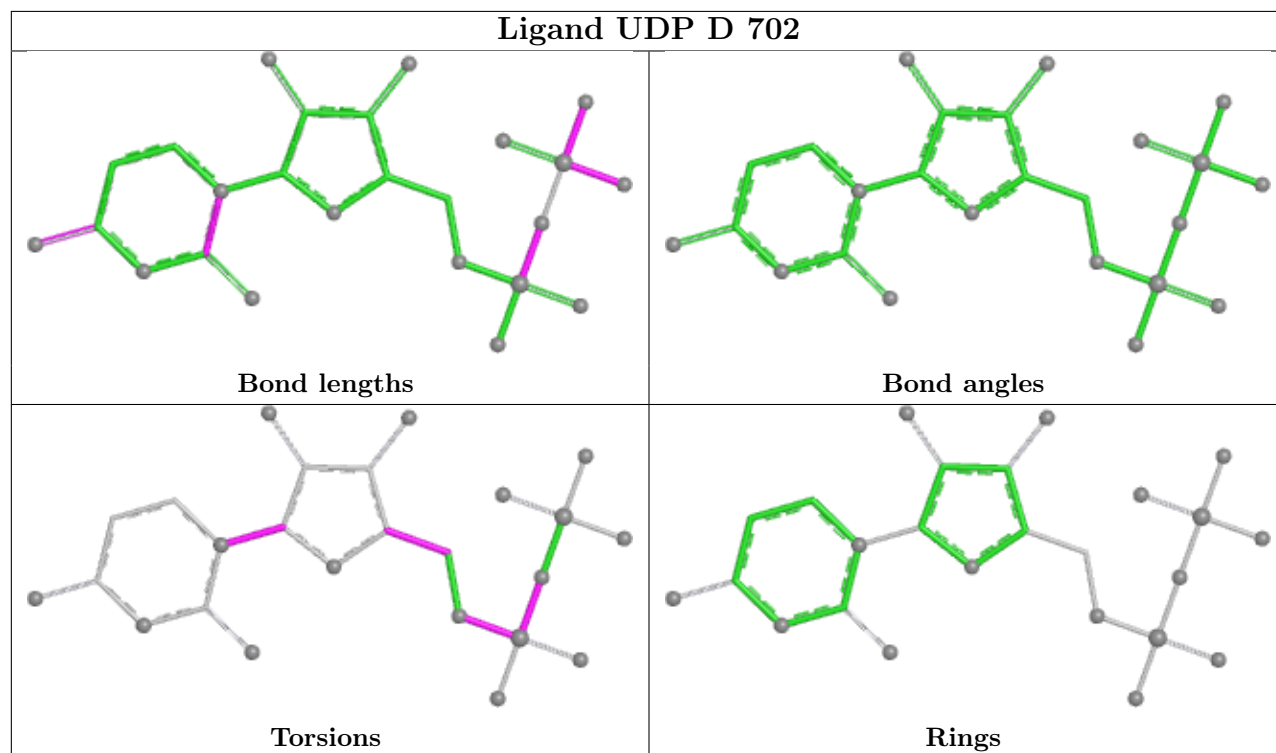
There are no ring outliers.

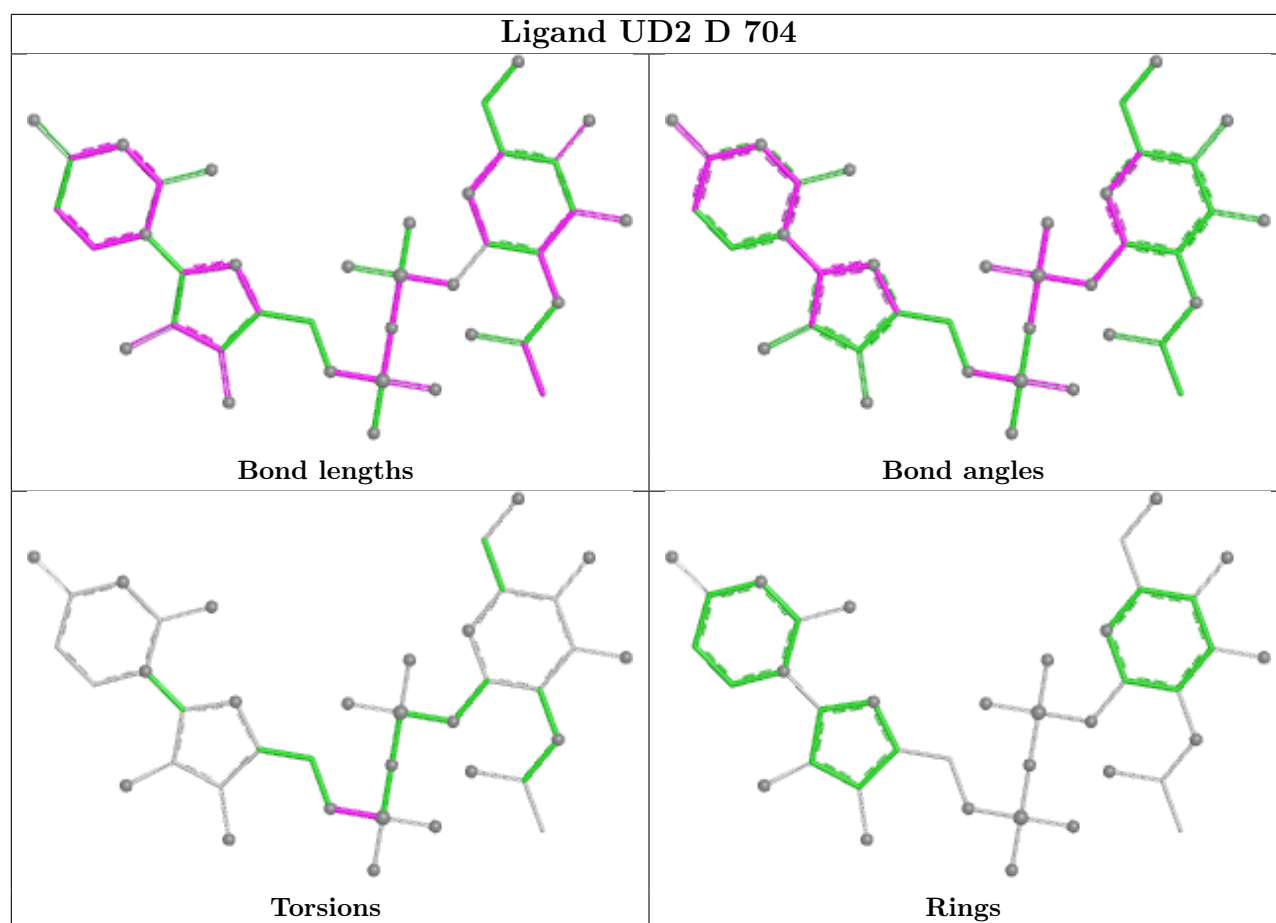
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	701	NAG	1	0
4	D	702	UDP	2	0
5	D	704	UD2	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	546/597 (91%)	0.01	35 (6%)	25 20	23, 33, 59, 111	0
1	B	546/597 (91%)	0.15	42 (7%)	19 15	26, 37, 64, 116	0
1	C	546/597 (91%)	0.49	70 (12%)	7 6	24, 42, 82, 138	0
1	D	538/597 (90%)	0.48	44 (8%)	17 14	29, 47, 75, 92	0
1	E	546/597 (91%)	0.55	57 (10%)	11 9	26, 46, 83, 154	0
1	F	546/597 (91%)	0.99	93 (17%)	4 3	34, 59, 86, 136	0
All	All	3268/3582 (91%)	0.45	341 (10%)	11 9	23, 43, 79, 154	0

All (341) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	454	ILE	10.0
1	A	458	SER	8.9
1	C	456	VAL	8.5
1	F	452	PRO	7.9
1	C	657	VAL	7.7
1	F	451	PRO	7.6
1	B	458	SER	7.3
1	E	456	VAL	7.2
1	E	454	ILE	7.1
1	A	454	ILE	7.0
1	E	457	GLY	7.0
1	C	451	PRO	7.0
1	E	657	VAL	7.0
1	C	453	PRO	6.9
1	A	403	GLY	6.8
1	C	452	PRO	6.5
1	B	112	TYR	6.2
1	E	656	SER	6.2
1	F	446	GLY	6.1

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Mol	Chain	Res	Type	RSRZ
1	F	455	TYR	6.0
1	E	452	PRO	6.0
1	F	454	ILE	6.0
1	E	453	PRO	6.0
1	F	112	TYR	5.9
1	E	451	PRO	5.9
1	C	656	SER	5.8
1	A	456	VAL	5.8
1	C	147	GLY	5.7
1	F	449	GLY	5.7
1	B	457	GLY	5.4
1	B	456	VAL	5.4
1	B	147	GLY	5.4
1	B	452	PRO	5.2
1	A	457	GLY	5.2
1	A	452	PRO	5.1
1	E	590	ALA	5.1
1	E	147	GLY	5.1
1	C	631	VAL	5.0
1	B	346	GLY	5.0
1	C	455	TYR	4.9
1	F	456	VAL	4.9
1	A	112	TYR	4.9
1	E	112	TYR	4.8
1	B	451	PRO	4.8
1	F	450	ASN	4.8
1	A	455	TYR	4.8
1	C	112	TYR	4.8
1	A	592	GLY	4.7
1	A	449	GLY	4.7
1	E	458	SER	4.6
1	D	112	TYR	4.6
1	A	147	GLY	4.6
1	F	147	GLY	4.6
1	C	458	SER	4.6
1	E	556	PHE	4.5
1	B	592	GLY	4.5
1	B	631	VAL	4.5
1	B	632	LEU	4.4
1	F	138	LYS	4.4
1	C	450	ASN	4.3
1	E	455	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	411	ILE	4.3
1	B	454	ILE	4.3
1	E	602	LEU	4.2
1	F	196	GLU	4.2
1	F	447	TRP	4.2
1	F	164	GLN	4.2
1	F	453	PRO	4.1
1	C	590	ALA	4.1
1	F	657	VAL	4.1
1	C	373	ARG	4.1
1	C	449	GLY	4.0
1	F	193	ARG	4.0
1	B	159	GLY	3.9
1	B	449	GLY	3.9
1	A	591	ASP	3.9
1	E	346	GLY	3.9
1	C	459	SER	3.9
1	B	148	GLY	3.9
1	C	403	GLY	3.9
1	E	449	GLY	3.9
1	E	450	ASN	3.8
1	F	631	VAL	3.8
1	C	632	LEU	3.8
1	F	346	GLY	3.7
1	F	448	GLN	3.7
1	D	656	SER	3.7
1	F	146	VAL	3.7
1	D	139	GLU	3.7
1	F	592	GLY	3.7
1	A	451	PRO	3.7
1	F	123	HIS	3.6
1	D	153	ALA	3.6
1	F	159	GLY	3.6
1	B	414	GLY	3.6
1	D	457	GLY	3.6
1	C	644	LYS	3.6
1	C	133	GLY	3.5
1	D	448	GLN	3.5
1	E	655	HIS	3.5
1	E	598	THR	3.5
1	C	556	PHE	3.5
1	C	611	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	632	LEU	3.5
1	F	167	GLN	3.5
1	F	148	GLY	3.4
1	E	159	GLY	3.4
1	B	455	TYR	3.4
1	F	131	ILE	3.3
1	F	656	SER	3.3
1	E	348	GLU	3.3
1	F	345	GLY	3.3
1	B	450	ASN	3.3
1	A	657	VAL	3.3
1	E	148	GLY	3.3
1	E	592	GLY	3.3
1	A	138	LYS	3.3
1	E	459	SER	3.3
1	A	453	PRO	3.3
1	F	632	LEU	3.3
1	B	373	ARG	3.3
1	F	373	ARG	3.3
1	C	552	THR	3.3
1	D	345	GLY	3.3
1	E	133	GLY	3.3
1	D	138	LYS	3.2
1	C	148	GLY	3.2
1	D	592	GLY	3.2
1	F	591	ASP	3.2
1	F	121	THR	3.2
1	C	592	GLY	3.2
1	E	414	GLY	3.2
1	D	657	VAL	3.2
1	C	159	GLY	3.2
1	D	403	GLY	3.2
1	F	160	PRO	3.2
1	F	152	LYS	3.1
1	F	614	LEU	3.1
1	E	593	SER	3.1
1	F	593	SER	3.1
1	A	194	GLN	3.1
1	B	133	GLY	3.1
1	C	613	ASN	3.1
1	D	205	ASN	3.1
1	D	121	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	612	LYS	3.1
1	C	404	LEU	3.1
1	A	590	ALA	3.1
1	C	594	LYS	3.1
1	D	251	LYS	3.1
1	E	591	ASP	3.0
1	D	602	LEU	3.0
1	B	599	HIS	3.0
1	C	448	GLN	3.0
1	A	411	ILE	3.0
1	E	345	GLY	3.0
1	D	346	GLY	3.0
1	F	378	LYS	3.0
1	C	598	THR	2.9
1	E	631	VAL	2.9
1	F	611	PHE	2.9
1	F	458	SER	2.9
1	C	410	GLN	2.9
1	F	266	ASN	2.9
1	A	656	SER	2.9
1	C	574	ASN	2.9
1	C	645	THR	2.9
1	F	590	ALA	2.9
1	F	145	VAL	2.9
1	F	139	GLU	2.8
1	A	133	GLY	2.8
1	A	345	GLY	2.8
1	F	171	LYS	2.8
1	D	377	THR	2.8
1	E	196	GLU	2.8
1	F	443	ARG	2.8
1	B	657	VAL	2.8
1	D	167	GLN	2.8
1	B	412	TRP	2.8
1	D	159	GLY	2.8
1	B	453	PRO	2.8
1	A	148	GLY	2.8
1	D	127	LEU	2.8
1	A	413	GLY	2.7
1	D	120	PHE	2.7
1	D	164	GLN	2.7
1	C	414	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	457	GLY	2.7
1	F	414	GLY	2.7
1	D	173	PHE	2.7
1	F	120	PHE	2.7
1	D	171	LYS	2.7
1	E	448	GLN	2.7
1	D	199	TYR	2.7
1	F	582	TYR	2.7
1	D	132	LEU	2.7
1	F	132	LEU	2.7
1	F	602	LEU	2.7
1	F	457	GLY	2.7
1	F	205	ASN	2.7
1	E	605	PHE	2.7
1	F	214	VAL	2.7
1	F	201	HIS	2.6
1	A	346	GLY	2.6
1	A	450	ASN	2.6
1	F	236	ARG	2.6
1	D	152	LYS	2.6
1	D	163	LYS	2.6
1	A	461	THR	2.6
1	F	162	PHE	2.6
1	B	442	TYR	2.6
1	F	133	GLY	2.6
1	F	179	ALA	2.6
1	F	445	GLU	2.6
1	C	591	ASP	2.5
1	E	583	ASP	2.5
1	B	590	ALA	2.5
1	C	648	LYS	2.5
1	C	621	PRO	2.5
1	F	173	PHE	2.5
1	C	640	CYS	2.5
1	E	589	GLY	2.5
1	D	146	VAL	2.5
1	F	153	ALA	2.5
1	E	530	LYS	2.5
1	F	203	ASP	2.5
1	E	599	HIS	2.5
1	F	348	GLU	2.5
1	C	597	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	412	TRP	2.4
1	C	138	LYS	2.4
1	A	601	ASN	2.4
1	F	194	GLN	2.4
1	C	411	ILE	2.4
1	B	656	SER	2.4
1	B	348	GLU	2.4
1	C	445	GLU	2.4
1	C	588	LYS	2.4
1	A	159	GLY	2.4
1	B	345	GLY	2.4
1	F	276	ARG	2.4
1	D	123	HIS	2.4
1	C	348	GLU	2.4
1	E	412	TRP	2.4
1	E	594	LYS	2.4
1	F	556	PHE	2.4
1	C	490	LEU	2.3
1	C	544	TYR	2.3
1	D	582	TYR	2.3
1	E	490	LEU	2.3
1	E	645	THR	2.3
1	F	601	ASN	2.3
1	F	195	GLU	2.3
1	C	349	ASP	2.3
1	F	137	PRO	2.3
1	E	120	PHE	2.3
1	C	655	HIS	2.3
1	B	203	ASP	2.3
1	A	448	GLN	2.3
1	B	410	GLN	2.3
1	C	495	ILE	2.3
1	D	154	LYS	2.3
1	F	163	LYS	2.3
1	F	277	ARG	2.3
1	E	554	GLY	2.3
1	B	556	PHE	2.3
1	E	163	LYS	2.3
1	F	217	ASN	2.3
1	B	591	ASP	2.3
1	E	496	SER	2.3
1	D	118	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	341	ILE	2.2
1	E	373	ARG	2.2
1	F	140	PRO	2.2
1	C	609	GLN	2.2
1	F	623	GLY	2.2
1	E	597	ILE	2.2
1	F	168	ALA	2.2
1	A	348	GLU	2.2
1	F	125	PRO	2.2
1	C	623	GLY	2.2
1	F	583	ASP	2.2
1	B	614	LEU	2.2
1	B	138	LYS	2.2
1	C	557	VAL	2.2
1	F	636	PHE	2.2
1	B	640	CYS	2.2
1	E	121	THR	2.2
1	F	189	VAL	2.2
1	C	377	THR	2.2
1	C	442	TYR	2.2
1	D	238	TYR	2.2
1	E	574	ASN	2.2
1	F	376	LYS	2.2
1	F	149	PRO	2.1
1	F	442	TYR	2.1
1	E	498	LEU	2.1
1	C	566	GLY	2.1
1	D	341	ILE	2.1
1	E	619	HIS	2.1
1	F	517	ILE	2.1
1	F	655	HIS	2.1
1	D	165	ALA	2.1
1	D	260	GLU	2.1
1	B	613	ASN	2.1
1	C	345	GLY	2.1
1	D	148	GLY	2.1
1	C	599	HIS	2.1
1	A	583	ASP	2.1
1	C	605	PHE	2.1
1	D	114	THR	2.1
1	E	646	THR	2.1
1	F	158	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	601	ASN	2.1
1	B	413	GLY	2.1
1	F	130	GLY	2.1
1	D	175	PHE	2.1
1	A	139	GLU	2.1
1	E	461	THR	2.1
1	B	488	GLN	2.1
1	D	194	GLN	2.1
1	F	250	ASN	2.1
1	D	446	GLY	2.1
1	C	595	VAL	2.1
1	C	540	PHE	2.1
1	F	115	PHE	2.1
1	D	236	ARG	2.0
1	B	114	THR	2.0
1	E	584	GLN	2.0
1	F	280	LEU	2.0
1	C	615	HIS	2.0
1	A	120	PHE	2.0
1	C	236	ARG	2.0
1	C	636	PHE	2.0
1	F	136	GLU	2.0
1	C	463	LYS	2.0
1	F	113	LEU	2.0
1	B	344	GLY	2.0
1	C	589	GLY	2.0
1	D	394	ILE	2.0
1	C	564	ARG	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.

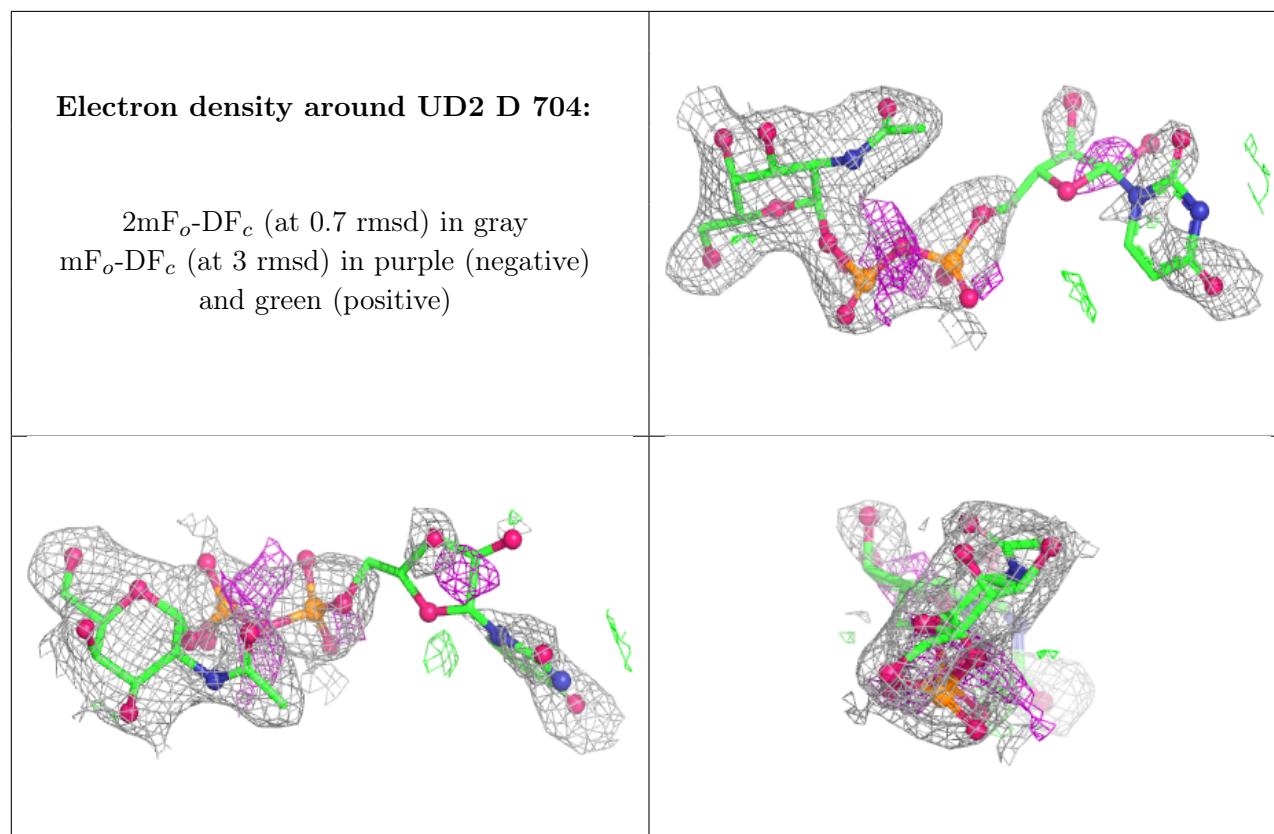
6.4 Ligands [i](#)

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.

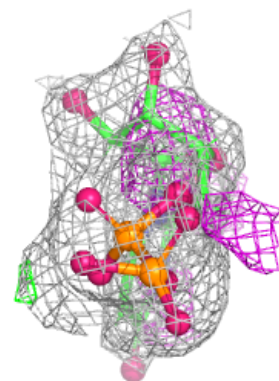
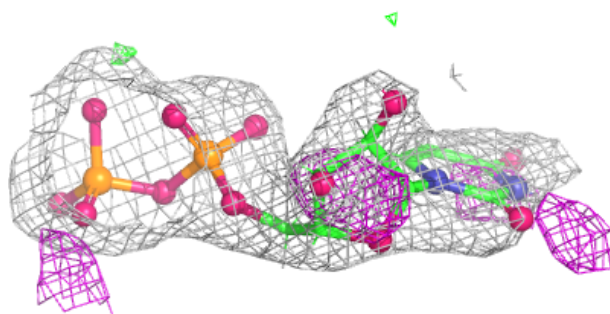
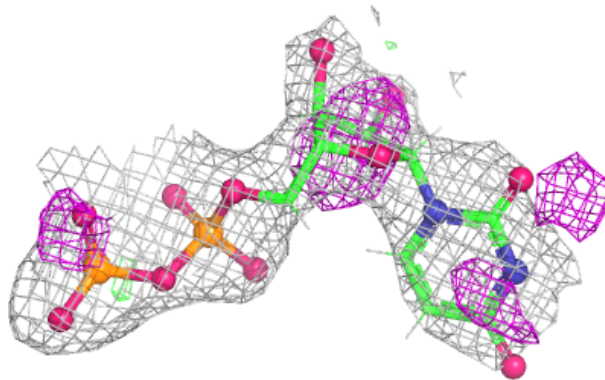
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MN	A	701	1/1	0.49	0.33	100,100,100,100	0
2	MN	F	701	1/1	0.62	0.32	91,91,91,91	0
2	MN	C	701	1/1	0.72	0.18	93,93,93,93	0
2	MN	B	701	1/1	0.72	0.20	87,87,87,87	0
3	NAG	D	701	15/15	0.79	0.15	52,68,79,82	0
5	UD2	D	704	39/39	0.79	0.17	36,81,113,113	0
2	MN	E	701	1/1	0.80	0.15	82,82,82,82	0
4	UDP	D	702	25/25	0.86	0.12	55,69,81,82	0
2	MN	D	703	1/1	0.98	0.04	56,56,56,56	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 D 702:

$2mF_o-DF_c$ (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.