Full wwPDB X-ray Structure Validation Report (i)

Mar 5, 2024 – 12:49 PM EST

PDB ID	:	2Z86
Title	:	Crystal structure of chondroitin polymerase from Escherichia coli strain K4 (K4CP) complexed with UDP-GlcUA and UDP
Authors	:	Osawa, T.; Sugiura, N.; Shimada, H.; Hirooka, R.; Tsuji, A.; Kimura, M.; Kimata, K.; Kakuta, Y.
Deposited on	:	2007-09-03
Resolution	:	2.40 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 (i) 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 (i)) were used in the production of this report:

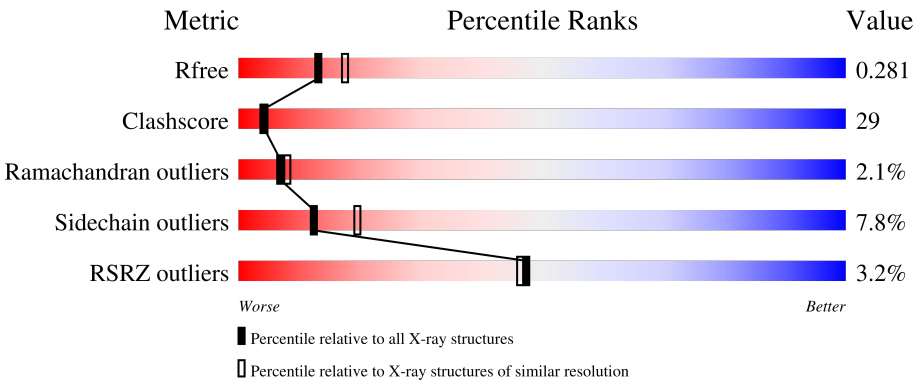
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	625	4%; 44%; 43%; 6%; 7%
1	B	625	2%; 50%; 38%; 8%; •
1	C	625	2%; 53%; 38%; 5%; •
1	D	625	5%; 51%; 39%; 5%; 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UGA	A	684	-	-	X	-

2 Entry composition (i)

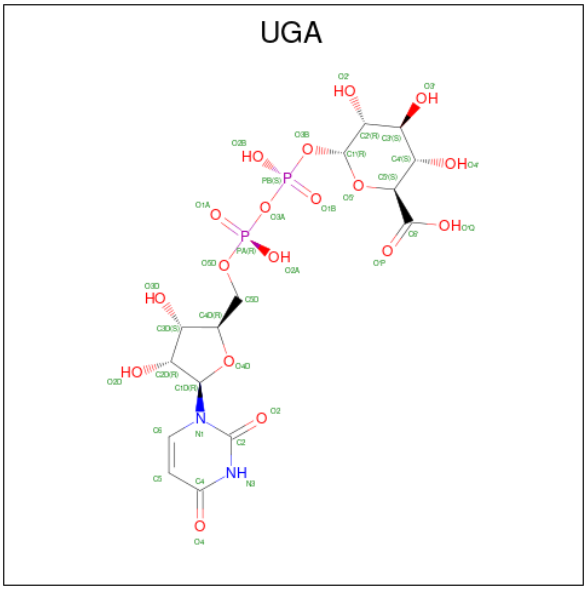
There are 5 unique types of molecules in this entry. The entry contains 20192 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Chondroitin synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	580	4736	3023	805	884	24	24	0	0
1	B	601	4890	3115	835	916	24	25	0	0
1	C	603	4906	3124	835	923	24	25	0	0
1	D	594	4833	3079	824	906	24	25	0	0

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-GLUCURONIC ACID (three-letter code: UGA) (formula: $C_{15}H_{22}N_2O_{18}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	37	15	2	18	2	0	0
2	A	1	37	15	2	18	2	0	0

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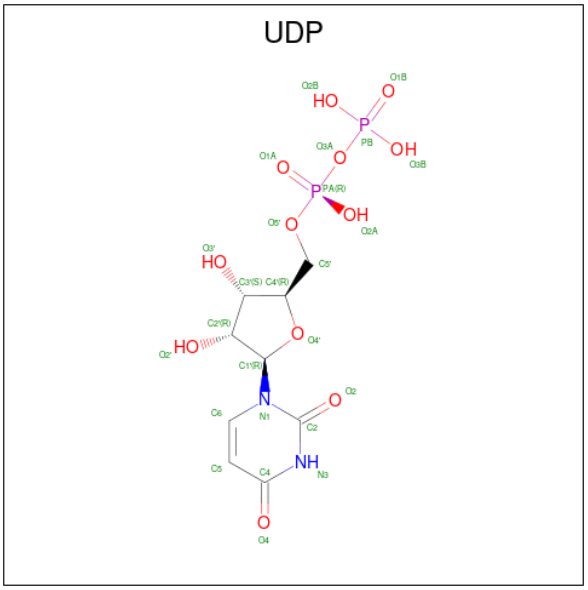
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	B	1	37	15	2	18	2	0	0
			Total	C	N	O	P		
2	C	1	37	15	2	18	2	0	0
			Total	C	N	O	P		
2	D	1	37	15	2	18	2	0	0
			Total	C	N	O	P		
2	D	1	37	15	2	18	2	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
3	A	2	2	2	0	0
			Total	Mn		
3	B	2	2	2	0	0
			Total	Mn		
3	C	2	2	2	0	0
			Total	Mn		
3	D	2	2	2	0	0

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



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

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

- Molecule 5 is water.

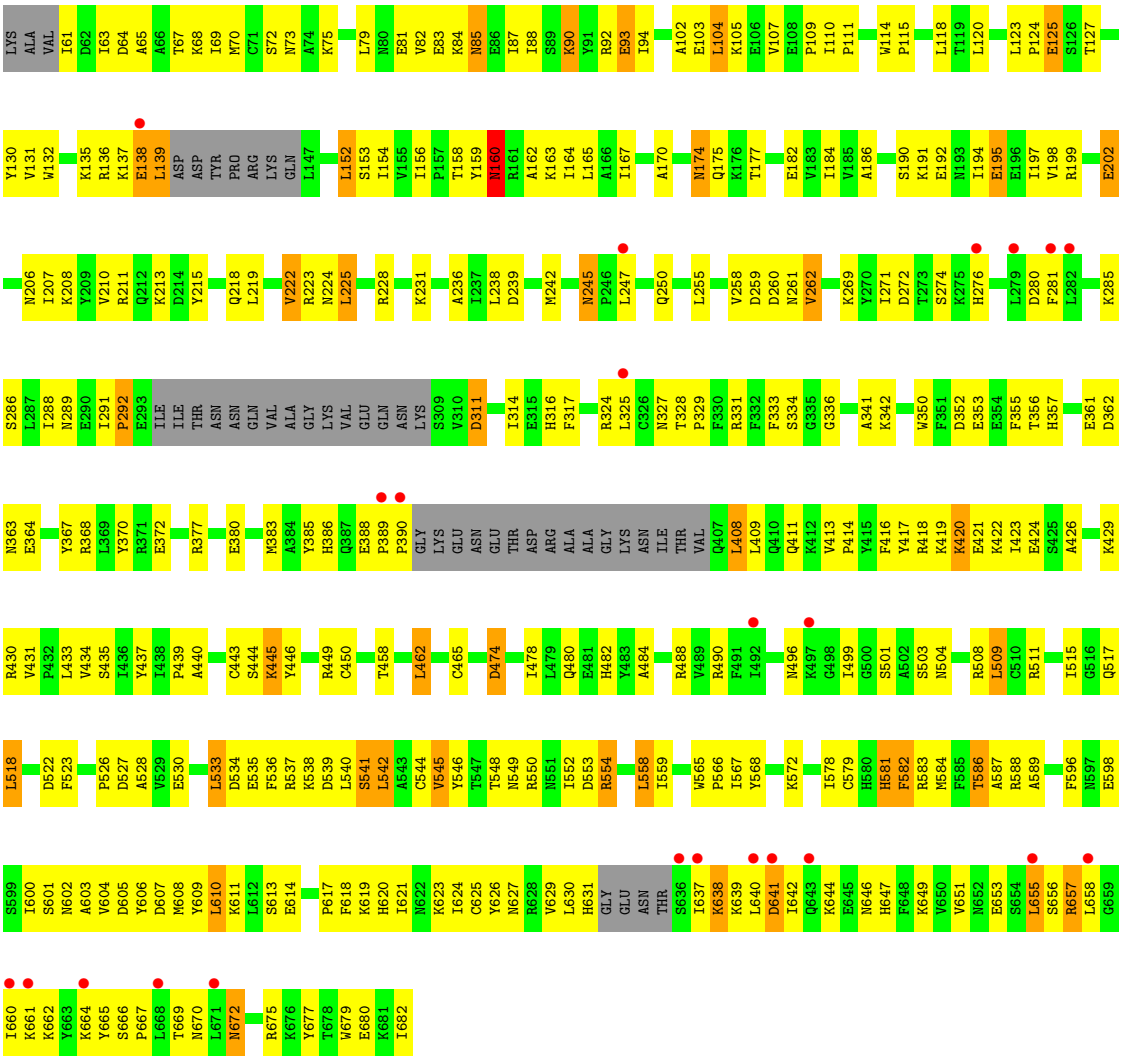
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	107	107	107	0	0
			Total	O		
5	B	140	140	140	0	0
			Total	O		
5	C	177	177	177	0	0
			Total	O		
5	D	123	123	123	0	0

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.

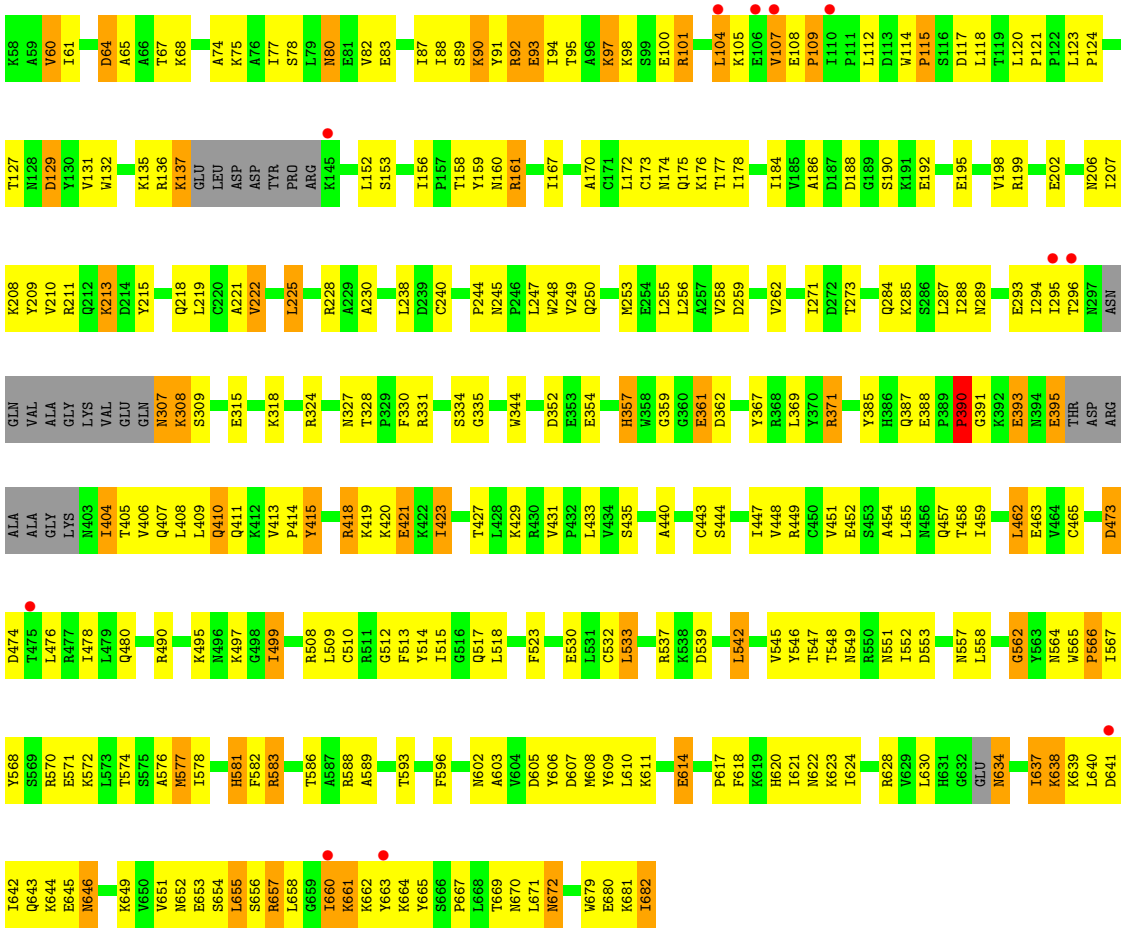
• Molecule 1: Chondroitin synthase

Chain A: 4% 44% 43% 6% 7%



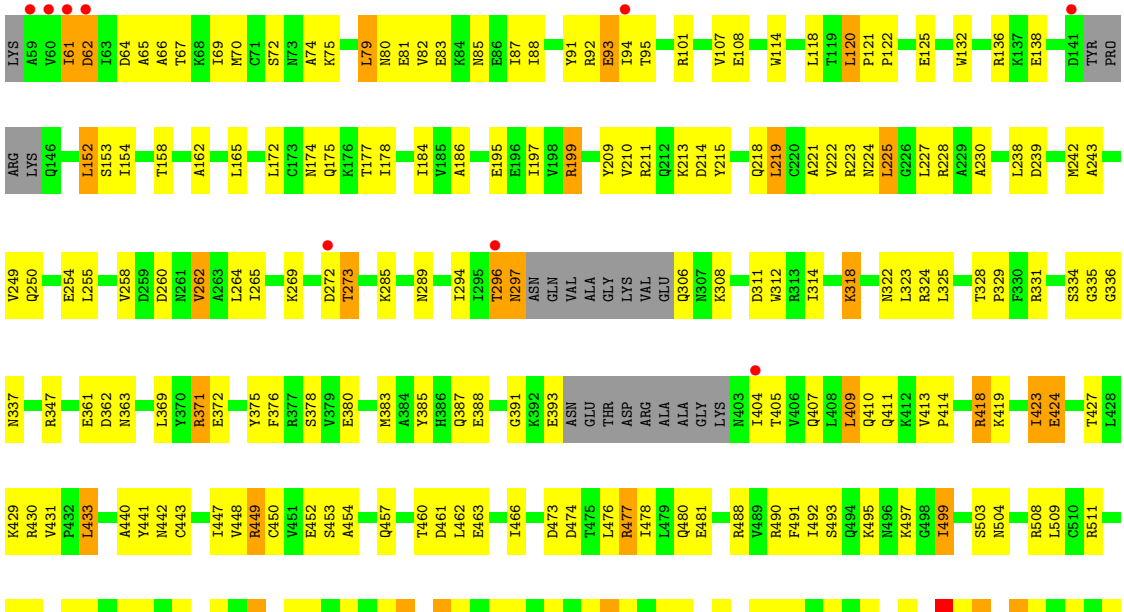
• Molecule 1: Chondroitin synthase

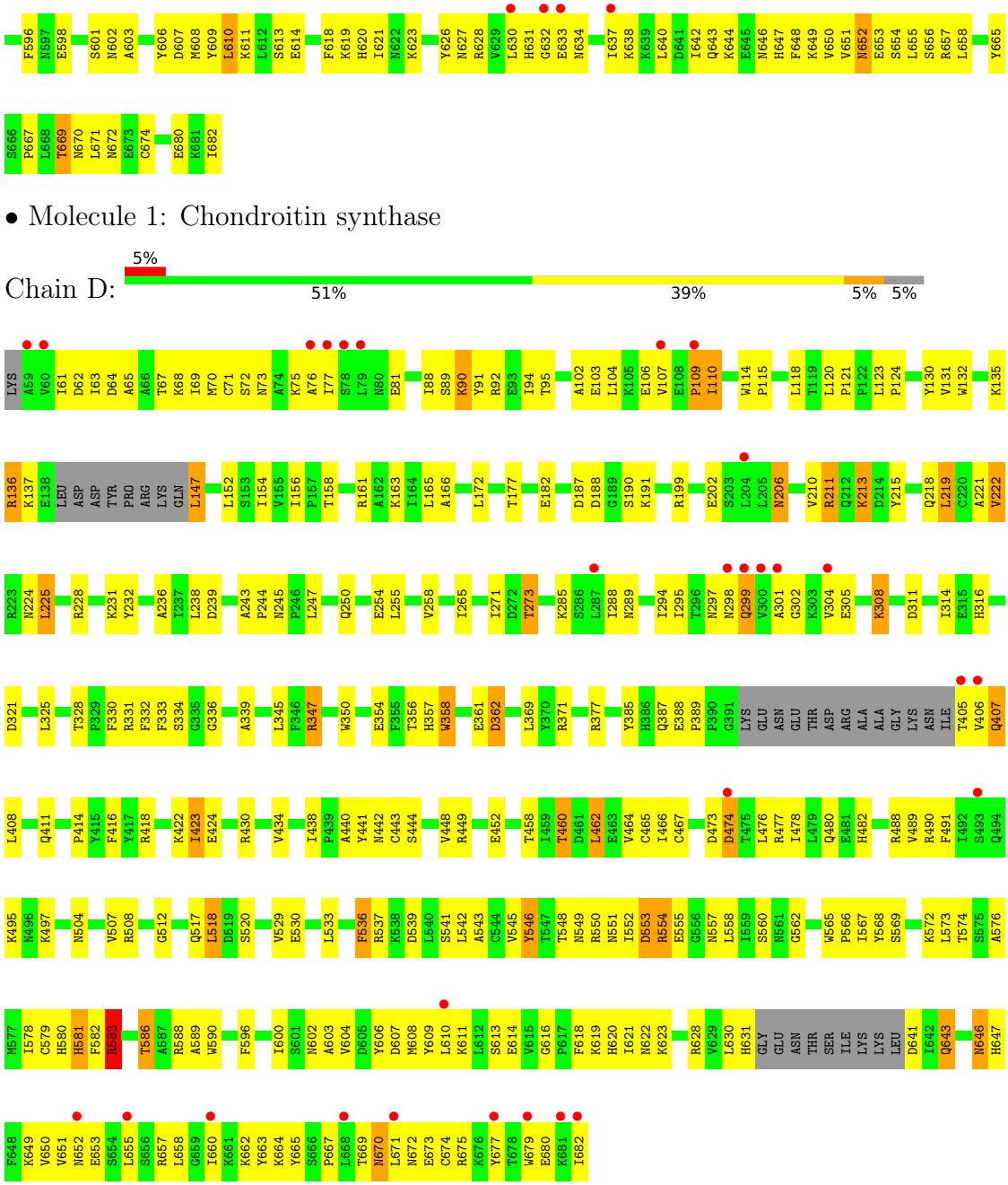
Chain B: 2% 50% 38% 8%



• Molecule 1: Chondroitin synthase

Chain C: 2% 53% 38% 5%





• Molecule 1: Chondroitin synthase

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.09Å 219.83Å 85.86Å 90.00° 103.07° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 42.86 – 2.40	Depositor EDS
% Data completeness (in resolution range)	82.9 (20.00-2.40) 83.0 (42.86-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.286 0.222 , 0.281	Depositor DCC
R_{free} test set	5371 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	35.5	Xtriage
Anisotropy	0.616	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 53.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.023 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	20192	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.57	11/4839 (0.2%)	0.67	5/6543 (0.1%)
1	B	0.65	12/4993 (0.2%)	0.66	1/6751 (0.0%)
1	C	0.62	8/5010 (0.2%)	0.69	2/6777 (0.0%)
1	D	0.61	13/4937 (0.3%)	0.65	4/6680 (0.1%)
All	All	0.62	44/19779 (0.2%)	0.67	12/26751 (0.0%)

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	2
1	B	0	1
1	C	0	2
1	D	0	1
All	All	0	6

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	583	ARG	CZ-NH1	-15.61	1.12	1.33
1	D	583	ARG	CZ-NH1	-14.19	1.14	1.33
1	A	581	HIS	C-O	-13.62	0.97	1.23
1	C	582	PHE	CE2-CZ	-13.18	1.12	1.37
1	B	582	PHE	C-O	-12.59	0.99	1.23
1	C	582	PHE	CD1-CE1	-11.76	1.15	1.39
1	D	583	ARG	CZ-NH2	-11.74	1.17	1.33
1	B	583	ARG	CZ-NH2	-11.66	1.17	1.33
1	C	582	PHE	CE1-CZ	-11.60	1.15	1.37
1	C	582	PHE	CD2-CE2	-11.32	1.16	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	582	PHE	CD2-CE2	-10.79	1.17	1.39
1	D	582	PHE	CE2-CZ	-10.62	1.17	1.37
1	B	582	PHE	CE1-CZ	-10.61	1.17	1.37
1	C	582	PHE	CG-CD1	-10.55	1.23	1.38
1	B	583	ARG	C-O	-10.45	1.03	1.23
1	A	582	PHE	CD1-CE1	-10.29	1.18	1.39
1	A	582	PHE	CE2-CZ	-10.13	1.18	1.37
1	C	582	PHE	CG-CD2	-10.06	1.23	1.38
1	D	581	HIS	C-O	-9.99	1.04	1.23
1	B	582	PHE	CE2-CZ	-9.95	1.18	1.37
1	A	582	PHE	CG-CD2	-9.88	1.24	1.38
1	D	582	PHE	CD2-CE2	-9.83	1.19	1.39
1	C	581	HIS	C-O	-9.75	1.04	1.23
1	A	582	PHE	CE1-CZ	-9.68	1.19	1.37
1	D	582	PHE	CE1-CZ	-9.64	1.19	1.37
1	C	582	PHE	C-O	-9.00	1.06	1.23
1	D	583	ARG	C-O	-8.72	1.06	1.23
1	B	582	PHE	CG-CD1	-8.72	1.25	1.38
1	D	582	PHE	CG-CD1	-8.66	1.25	1.38
1	A	582	PHE	CD2-CE2	-8.55	1.22	1.39
1	B	581	HIS	C-O	-8.46	1.07	1.23
1	A	582	PHE	CG-CD1	-8.20	1.26	1.38
1	A	582	PHE	CB-CG	-8.15	1.37	1.51
1	B	582	PHE	CD1-CE1	-7.40	1.24	1.39
1	D	582	PHE	CD1-CE1	-6.90	1.25	1.39
1	D	582	PHE	C-O	-6.48	1.11	1.23
1	B	582	PHE	CG-CD2	-6.35	1.29	1.38
1	D	582	PHE	CG-CD2	-5.82	1.30	1.38
1	B	583	ARG	NE-CZ	-5.67	1.25	1.33
1	D	583	ARG	NE-CZ	-5.67	1.25	1.33
1	A	582	PHE	C-O	-5.51	1.12	1.23
1	A	582	PHE	N-CA	-5.39	1.35	1.46
1	A	581	HIS	CA-C	-5.31	1.39	1.52
1	D	583	ARG	CG-CD	5.04	1.64	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	581	HIS	CB-CA-C	-10.40	89.61	110.40
1	B	583	ARG	NE-CZ-NH2	7.60	124.10	120.30
1	C	581	HIS	C-N-CA	6.48	137.91	121.70
1	D	583	ARG	NE-CZ-NH2	6.25	123.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	581	HIS	CA-C-N	6.10	130.62	117.20
1	D	582	PHE	N-CA-C	-5.91	95.06	111.00
1	A	409	LEU	N-CA-C	-5.65	95.75	111.00
1	C	582	PHE	N-CA-CB	-5.46	100.78	110.60
1	D	657	ARG	N-CA-C	-5.42	96.37	111.00
1	A	582	PHE	N-CA-CB	-5.07	101.47	110.60
1	A	139	LEU	CA-CB-CG	5.05	126.93	115.30
1	D	581	HIS	CA-C-N	5.05	128.31	117.20

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	581	HIS	Peptide
1	A	609	TYR	Sidechain
1	B	581	HIS	Peptide
1	C	581	HIS	Peptide
1	C	609	TYR	Sidechain
1	D	581	HIS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4736	0	4687	309	0
1	B	4890	0	4844	305	0
1	C	4906	0	4851	271	0
1	D	4833	0	4778	257	0
2	A	74	0	38	9	0
2	B	37	0	19	1	0
2	C	37	0	19	0	0
2	D	74	0	38	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	B	25	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	25	0	11	0	0
5	A	107	0	0	26	0
5	B	140	0	0	13	0
5	C	177	0	0	18	0
5	D	123	0	0	11	0
All	All	20192	0	19296	1135	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 29.

All (1135) 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:132:TRP:HA	1:B:135:LYS:HE2	1.20	1.20
1:C:296:THR:HG22	1:C:297:ASN:H	1.15	1.09
1:D:669:THR:HG22	1:D:670:ASN:H	1.20	1.03
1:D:273:THR:HG21	1:D:387:GLN:HE21	1.22	1.02
1:D:586:THR:HG22	1:D:589:ALA:H	1.20	1.01
1:B:273:THR:HG21	1:B:387:GLN:HE21	1.20	1.00
1:D:423:ILE:H	1:D:423:ILE:HD12	1.22	1.00
1:D:161:ARG:HH11	1:D:389:PRO:HB3	1.26	0.99
1:B:80:ASN:HD21	1:B:83:GLU:H	1.11	0.99
1:C:273:THR:HG21	1:C:387:GLN:HE21	1.28	0.97
1:A:641:ASP:HB2	1:A:672:ASN:HD22	1.26	0.96
1:D:541:SER:HB3	5:D:806:HOH:O	1.66	0.96
1:A:509:LEU:HG	5:A:756:HOH:O	1.64	0.95
1:B:662:LYS:HA	1:B:682:ILE:HD11	1.45	0.95
1:B:553:ASP:HB2	1:B:557:ASN:HB2	1.47	0.94
1:A:245:ASN:ND2	1:A:247:LEU:H	1.64	0.94
1:B:175:GLN:NE2	1:B:249:VAL:H	1.64	0.94
1:C:72:SER:HA	1:C:75:LYS:HE2	1.45	0.94
1:C:586:THR:HG22	1:C:589:ALA:H	1.29	0.94
1:C:405:THR:HA	5:C:820:HOH:O	1.68	0.93
1:B:80:ASN:ND2	1:B:83:GLU:H	1.68	0.91
1:D:643:GLN:H	1:D:643:GLN:NE2	1.68	0.91
1:D:664:LYS:HB2	1:D:682:ILE:HD13	1.51	0.91
1:A:160:ASN:HB3	1:A:190:SER:HB3	1.53	0.90
1:D:583:ARG:HD3	1:D:609:TYR:CE2	2.08	0.89
1:B:328:THR:O	1:B:331:ARG:HG3	1.74	0.87
1:A:423:ILE:HD12	1:A:423:ILE:H	1.37	0.87
1:B:661:LYS:NZ	1:B:661:LYS:HA	1.90	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:ARG:H	1:A:554:ARG:HD3	1.38	0.87
1:B:418:ARG:HH11	1:B:418:ARG:HB2	1.38	0.86
1:B:637:ILE:HD12	1:B:637:ILE:H	1.40	0.86
1:D:405:THR:HG22	1:D:407:GLN:H	1.40	0.86
1:C:371:ARG:HH21	1:C:371:ARG:HG3	1.38	0.86
1:D:548:THR:HG22	1:D:623:LYS:O	1.75	0.85
1:B:637:ILE:HB	1:B:640:LEU:HD13	1.58	0.85
1:C:655:LEU:HD11	5:C:784:HOH:O	1.76	0.85
1:A:637:ILE:HG22	1:A:639:LYS:H	1.40	0.85
1:C:371:ARG:NH2	1:C:587:ALA:HB1	1.91	0.85
1:A:255:LEU:O	1:A:258:VAL:HG22	1.77	0.85
1:C:640:LEU:O	1:C:643:GLN:HG2	1.77	0.84
1:B:553:ASP:CB	1:B:557:ASN:HB2	2.08	0.84
1:D:311:ASP:HB3	1:D:314:ILE:HG13	1.59	0.83
1:C:371:ARG:HH22	1:C:587:ALA:HB1	1.44	0.83
1:C:297:ASN:N	1:C:297:ASN:HD22	1.75	0.83
1:A:641:ASP:HB2	1:A:672:ASN:ND2	1.95	0.82
1:C:614:GLU:OE2	1:C:655:LEU:HD23	1.80	0.81
1:C:646:ASN:O	1:C:650:VAL:HG23	1.79	0.81
1:A:611:LYS:HG2	1:A:657:ARG:NH1	1.96	0.81
1:B:60:VAL:HG22	1:B:61:ILE:H	1.46	0.81
1:D:440:ALA:HB1	1:D:443:CYS:SG	2.21	0.81
1:B:652:ASN:HB3	5:B:775:HOH:O	1.79	0.81
1:A:539:ASP:HB3	1:A:542:LEU:HD22	1.62	0.80
1:D:586:THR:CG2	1:D:589:ALA:H	1.95	0.80
1:B:68:LYS:HD3	1:B:87:ILE:HD13	1.63	0.80
1:B:649:LYS:HG2	1:B:667:PRO:HG3	1.63	0.80
1:B:644:LYS:HD2	5:B:816:HOH:O	1.80	0.80
1:D:583:ARG:HD3	1:D:609:TYR:CZ	2.16	0.80
1:B:78:SER:HA	5:B:786:HOH:O	1.81	0.79
1:C:178:ILE:H	1:C:250:GLN:NE2	1.79	0.79
1:D:131:VAL:HG12	1:D:135:LYS:HE3	1.63	0.79
1:B:421:GLU:HG3	5:B:802:HOH:O	1.82	0.79
1:D:545:VAL:HG12	1:D:619:LYS:HB3	1.62	0.79
1:C:499:ILE:HD13	5:C:811:HOH:O	1.83	0.79
1:D:669:THR:HG21	1:D:671:LEU:HG	1.65	0.79
1:B:547:THR:HG22	1:B:621:ILE:HB	1.65	0.78
1:B:662:LYS:CA	1:B:682:ILE:HD11	2.12	0.78
1:D:273:THR:HG21	1:D:387:GLN:NE2	1.99	0.78
1:C:186:ALA:HA	1:C:210:VAL:HG23	1.65	0.78
1:A:68:LYS:HD2	1:A:87:ILE:HD13	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:ARG:H	1:B:101:ARG:HD3	1.49	0.78
1:A:174:ASN:HD22	1:A:285:LYS:HB3	1.50	0.77
1:B:104:LEU:HD12	1:B:104:LEU:H	1.49	0.77
1:C:404:ILE:HB	5:C:834:HOH:O	1.84	0.77
1:A:637:ILE:HG22	1:A:638:LYS:H	1.50	0.77
1:B:209:TYR:OH	1:B:211:ARG:HD2	1.83	0.77
1:C:72:SER:CA	1:C:75:LYS:HE2	2.15	0.77
1:D:161:ARG:NH1	1:D:389:PRO:HB3	1.99	0.77
1:C:586:THR:HG21	5:C:718:HOH:O	1.84	0.76
1:B:295:ILE:CG2	1:B:308:LYS:HA	2.16	0.76
1:D:669:THR:HG22	1:D:670:ASN:N	2.00	0.76
1:A:462:LEU:HD21	1:A:488:ARG:HH21	1.49	0.76
1:A:656:SER:C	1:A:658:LEU:H	1.87	0.76
1:C:414:PRO:HA	1:C:418:ARG:HB2	1.65	0.76
1:A:174:ASN:HD22	1:A:285:LYS:HE2	1.51	0.76
1:B:60:VAL:HG22	1:B:61:ILE:N	2.00	0.75
1:D:94:ILE:HG23	1:D:95:THR:HG23	1.68	0.75
1:B:295:ILE:HG23	1:B:308:LYS:HA	1.68	0.75
1:C:296:THR:HG22	1:C:297:ASN:N	1.97	0.75
1:D:115:PRO:HB2	1:D:118:LEU:HB2	1.68	0.75
1:A:93:GLU:HG2	5:A:766:HOH:O	1.85	0.75
1:A:462:LEU:CD2	1:A:488:ARG:HH21	1.99	0.75
1:A:440:ALA:HB1	1:A:443:CYS:SG	2.27	0.74
1:B:271:ILE:HG22	1:B:293:GLU:HA	1.68	0.74
1:A:239:ASP:OD1	1:A:336:GLY:HA2	1.87	0.74
1:B:175:GLN:HE21	1:B:249:VAL:H	1.34	0.74
1:B:107:VAL:O	1:B:109:PRO:HD3	1.88	0.74
1:D:213:LYS:HE2	1:D:215:TYR:HB3	1.69	0.74
1:A:199:ARG:HA	1:A:202:GLU:HG3	1.70	0.74
1:B:90:LYS:HE3	1:B:90:LYS:HA	1.69	0.74
1:C:669:THR:HG23	1:C:671:LEU:H	1.51	0.74
1:D:91:TYR:HA	1:D:94:ILE:HG22	1.69	0.73
1:A:215:TYR:CZ	1:A:218:GLN:HG3	2.24	0.73
1:B:118:LEU:HD23	1:B:663:TYR:HD1	1.53	0.73
1:B:583:ARG:HD3	1:B:609:TYR:CZ	2.24	0.73
1:A:224:ASN:O	1:A:228:ARG:HG3	1.89	0.73
1:B:210:VAL:HG11	1:B:225:LEU:HD22	1.69	0.73
1:C:554:ARG:H	1:C:554:ARG:HD3	1.53	0.73
1:B:114:TRP:CZ2	1:B:118:LEU:HD12	2.24	0.72
1:C:80:ASN:HD21	1:C:83:GLU:H	1.36	0.72
1:C:107:VAL:HG11	1:C:565:TRP:CH2	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:ASP:HB3	2:A:684:UGA:H4'1	1.70	0.72
1:B:167:ILE:HB	1:B:387:GLN:HE22	1.54	0.72
1:D:476:LEU:O	1:D:480:GLN:HG3	1.88	0.72
1:D:333:PHE:O	1:D:362:ASP:HB2	1.90	0.72
1:B:115:PRO:HB2	1:B:118:LEU:HB2	1.71	0.71
1:A:288:ILE:HG23	1:A:289:ASN:ND2	2.04	0.71
1:A:420:LYS:HD3	1:A:537:ARG:HH12	1.54	0.71
1:B:124:PRO:HB3	1:B:132:TRP:CE3	2.26	0.71
1:C:410:GLN:NE2	1:C:418:ARG:HA	2.06	0.71
1:C:80:ASN:ND2	1:C:83:GLU:H	1.89	0.71
1:B:418:ARG:HB2	1:B:418:ARG:NH1	2.05	0.71
1:C:296:THR:HG23	1:C:388:GLU:OE1	1.91	0.71
1:D:664:LYS:HB3	1:D:680:GLU:HG2	1.73	0.71
1:A:582:PHE:HA	5:A:772:HOH:O	1.90	0.70
1:D:90:LYS:HE3	1:D:90:LYS:HA	1.73	0.70
1:D:405:THR:CG2	1:D:407:GLN:HB2	2.21	0.70
1:A:614:GLU:HG2	1:A:658:LEU:HD21	1.73	0.70
1:C:178:ILE:H	1:C:250:GLN:HE22	1.36	0.70
1:D:671:LEU:HB2	1:D:674:CYS:HB2	1.73	0.70
1:C:311:ASP:HB3	1:C:314:ILE:HG13	1.74	0.70
1:C:371:ARG:HH21	1:C:371:ARG:CG	2.05	0.69
1:D:653:GLU:OE2	1:D:665:TYR:HB3	1.92	0.69
1:B:656:SER:C	1:B:658:LEU:H	1.95	0.69
5:C:857:HOH:O	1:D:213:LYS:HG2	1.91	0.69
1:D:245:ASN:ND2	1:D:247:LEU:H	1.88	0.69
1:B:137:LYS:N	1:B:137:LYS:HD2	2.08	0.69
1:D:411:GLN:NE2	1:D:430:ARG:H	1.91	0.69
1:D:610:LEU:HD23	1:D:651:VAL:HG12	1.74	0.69
1:D:647:HIS:O	1:D:651:VAL:HG23	1.93	0.69
1:B:167:ILE:HD13	1:B:273:THR:OG1	1.93	0.68
1:D:115:PRO:HB2	1:D:118:LEU:CB	2.24	0.68
1:B:637:ILE:H	1:B:637:ILE:CD1	2.07	0.68
1:A:331:ARG:HD3	1:A:416:PHE:CE2	2.28	0.68
1:D:72:SER:HA	1:D:77:ILE:HG12	1.74	0.68
1:D:606:TYR:O	1:D:610:LEU:HB2	1.94	0.68
1:A:174:ASN:ND2	1:A:285:LYS:HB3	2.08	0.68
1:B:273:THR:HG21	1:B:387:GLN:NE2	2.01	0.68
1:B:586:THR:HG22	1:B:589:ALA:H	1.59	0.68
1:B:255:LEU:O	1:B:258:VAL:HG22	1.94	0.68
1:C:296:THR:C	1:C:297:ASN:HD22	1.96	0.68
1:C:669:THR:CG2	1:C:671:LEU:H	2.06	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:ASP:HA	1:A:644:LYS:HD3	1.75	0.68
1:B:662:LYS:HA	1:B:682:ILE:CD1	2.24	0.67
1:C:648:PHE:HD2	1:C:649:LYS:HD2	1.60	0.67
1:D:422:LYS:HB3	1:D:424:GLU:HG2	1.75	0.67
1:B:199:ARG:HA	1:B:202:GLU:HG3	1.76	0.67
1:C:499:ILE:HD12	1:C:499:ILE:O	1.94	0.67
1:D:114:TRP:CZ2	1:D:118:LEU:HD12	2.30	0.67
1:D:124:PRO:HB3	1:D:132:TRP:CE3	2.30	0.67
1:D:504:ASN:O	1:D:508:ARG:HG3	1.94	0.67
1:B:419:LYS:HE3	1:B:420:LYS:HG2	1.77	0.67
1:B:93:GLU:HG3	1:B:94:ILE:N	2.09	0.67
1:B:404:ILE:HD11	1:B:406:VAL:HB	1.76	0.67
1:D:545:VAL:HA	1:D:619:LYS:O	1.95	0.67
1:C:572:LYS:HG3	1:C:578:ILE:HD13	1.76	0.66
1:C:210:VAL:HG12	1:D:210:VAL:HG22	1.77	0.66
1:C:215:TYR:CE1	1:C:218:GLN:HG3	2.30	0.66
1:D:89:SER:HA	1:D:92:ARG:HG3	1.78	0.66
1:B:176:LYS:HG3	1:B:285:LYS:NZ	2.11	0.66
1:C:223:ARG:NH2	1:C:335:GLY:HA3	2.10	0.66
1:C:554:ARG:H	1:C:554:ARG:CD	2.08	0.66
1:D:88:ILE:O	1:D:92:ARG:HG3	1.95	0.66
1:D:132:TRP:HA	1:D:135:LYS:HD2	1.77	0.66
1:A:499:ILE:HG23	1:A:604:VAL:HG21	1.77	0.66
1:C:643:GLN:HG3	1:C:644:LYS:N	2.11	0.66
1:A:186:ALA:HB1	1:A:222:VAL:HG22	1.78	0.66
1:B:637:ILE:HD12	1:B:637:ILE:N	2.10	0.66
1:A:458:THR:HG21	1:A:530:GLU:CD	2.16	0.66
1:B:160:ASN:OD1	1:B:192:GLU:HG3	1.96	0.66
1:B:596:PHE:CD2	1:B:608:MET:HE2	2.30	0.66
1:C:296:THR:CG2	1:C:297:ASN:H	1.97	0.66
1:D:438:ILE:HG23	1:D:518:LEU:O	1.95	0.66
1:A:657:ARG:HA	5:A:786:HOH:O	1.95	0.66
1:B:661:LYS:HA	1:B:661:LYS:HZ3	1.62	0.65
1:B:245:ASN:ND2	1:B:247:LEU:H	1.94	0.65
1:B:549:ASN:HA	1:B:624:ILE:HG23	1.78	0.65
1:C:186:ALA:HB1	1:C:222:VAL:HG22	1.79	0.65
1:B:114:TRP:CZ2	1:B:571:GLU:HG3	2.31	0.65
1:A:159:TYR:C	1:A:160:ASN:HD22	1.99	0.65
1:A:269:LYS:HG3	1:A:383:MET:HE1	1.79	0.65
1:B:639:LYS:HE2	5:B:817:HOH:O	1.95	0.65
1:A:604:VAL:HB	2:A:684:UGA:O'Q	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:PRO:HB3	1:B:132:TRP:CD2	2.32	0.65
1:B:440:ALA:HB1	1:B:443:CYS:SG	2.36	0.65
1:C:652:ASN:O	1:C:655:LEU:HB3	1.97	0.65
1:D:614:GLU:OE2	1:D:655:LEU:HD22	1.96	0.65
1:D:328:THR:O	1:D:331:ARG:HG3	1.96	0.65
1:A:536:PHE:HE1	1:A:584:MET:HG2	1.62	0.65
1:B:552:ILE:HG22	1:B:553:ASP:O	1.96	0.65
1:C:448:VAL:O	1:C:452:GLU:HG2	1.97	0.65
1:D:546:TYR:CZ	1:D:620:HIS:HB2	2.33	0.64
1:A:637:ILE:HG21	1:A:640:LEU:HD13	1.78	0.64
1:A:288:ILE:HG13	1:A:385:TYR:CD2	2.33	0.64
1:B:661:LYS:HA	1:B:661:LYS:HZ2	1.63	0.64
1:D:586:THR:HG22	1:D:589:ALA:N	2.04	0.64
1:A:423:ILE:HD12	1:A:423:ILE:N	2.11	0.64
1:D:504:ASN:HB3	1:D:508:ARG:NH1	2.12	0.64
1:D:664:LYS:HB2	1:D:682:ILE:CD1	2.26	0.64
1:C:610:LEU:HD23	1:C:651:VAL:HG12	1.80	0.64
1:A:637:ILE:HG22	1:A:638:LYS:N	2.12	0.64
1:D:210:VAL:HG12	1:D:225:LEU:HD13	1.80	0.64
1:A:499:ILE:HD11	2:A:684:UGA:O4'	1.97	0.64
1:A:504:ASN:HB3	1:A:508:ARG:NH1	2.13	0.64
1:C:522:ASP:HB3	1:C:627:ASN:O	1.98	0.64
1:A:474:ASP:O	1:A:478:ILE:HG12	1.98	0.64
1:B:159:TYR:HA	1:B:190:SER:OG	1.98	0.64
1:B:186:ALA:HB1	1:B:222:VAL:HG22	1.79	0.64
1:B:640:LEU:O	1:B:644:LYS:HG3	1.98	0.64
1:D:156:ILE:HG23	1:D:238:LEU:O	1.97	0.64
1:C:551:ASN:OD1	1:C:630:LEU:HD11	1.99	0.63
1:D:210:VAL:HG11	1:D:225:LEU:HD22	1.79	0.63
1:A:586:THR:CG2	1:A:589:ALA:H	2.10	0.63
1:A:311:ASP:HB3	1:A:314:ILE:HG13	1.79	0.63
1:C:138:GLU:HG3	5:C:812:HOH:O	1.97	0.63
1:B:335:GLY:H	1:B:362:ASP:CG	2.01	0.63
1:B:405:THR:O	1:B:409:LEU:HD23	1.99	0.63
1:C:371:ARG:NH2	1:C:587:ALA:CB	2.59	0.63
1:A:554:ARG:HD3	1:A:554:ARG:N	2.12	0.63
1:B:170:ALA:O	1:B:173:CYS:HB2	1.99	0.63
1:B:284:GLN:HG3	1:B:287:LEU:HB2	1.80	0.63
1:A:84:LYS:O	1:A:88:ILE:HG13	1.97	0.62
1:B:444:SER:HB2	1:B:473:ASP:OD1	1.98	0.62
1:B:105:LYS:HG2	1:B:566:PRO:HG2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:VAL:CG2	1:B:324:ARG:HD2	2.29	0.62
1:B:589:ALA:O	1:B:593:THR:HG23	1.98	0.62
1:C:273:THR:HG21	1:C:387:GLN:NE2	2.06	0.62
1:A:210:VAL:HG12	1:A:225:LEU:HD13	1.80	0.62
1:D:423:ILE:H	1:D:423:ILE:CD1	1.95	0.62
1:A:105:LYS:HG3	1:A:107:VAL:HG13	1.82	0.62
1:A:433:LEU:CD1	1:A:434:VAL:HG23	2.29	0.62
1:C:224:ASN:O	1:C:228:ARG:HG3	1.99	0.62
1:D:621:ILE:HG22	1:D:623:LYS:HG2	1.81	0.62
1:A:259:ASP:OD2	1:A:261:ASN:HB2	1.99	0.62
1:A:333:PHE:O	1:A:362:ASP:HB3	1.98	0.62
1:B:404:ILE:HD13	1:B:407:GLN:HG3	1.81	0.62
1:C:655:LEU:HD13	1:C:655:LEU:O	2.00	0.62
1:A:586:THR:HG23	1:A:589:ALA:H	1.62	0.62
1:C:79:LEU:HD21	1:C:83:GLU:HB3	1.80	0.62
1:C:211:ARG:HG2	1:C:211:ARG:HH11	1.65	0.62
1:C:331:ARG:HH11	1:C:331:ARG:HB3	1.65	0.62
1:C:61:ILE:HG23	1:C:62:ASP:N	2.15	0.62
1:B:104:LEU:HD12	1:B:104:LEU:N	2.14	0.62
1:B:551:ASN:HB3	1:B:630:LEU:HD13	1.81	0.62
1:C:527:ASP:OD2	1:C:531:LEU:HD11	2.00	0.62
1:A:638:LYS:O	1:A:642:ILE:HG12	2.00	0.62
1:D:405:THR:HG22	1:D:407:GLN:N	2.14	0.62
1:D:423:ILE:HD12	1:D:423:ILE:N	2.06	0.62
1:A:75:LYS:HB2	1:A:75:LYS:NZ	2.15	0.61
1:A:504:ASN:HB3	1:A:508:ARG:HH12	1.64	0.61
1:B:371:ARG:NH2	1:B:512:GLY:O	2.33	0.61
1:B:656:SER:O	1:B:658:LEU:N	2.34	0.61
1:A:433:LEU:HD13	1:A:434:VAL:HG23	1.81	0.61
1:A:536:PHE:CZ	1:A:545:VAL:HG13	2.35	0.61
1:B:64:ASP:O	1:B:67:THR:HG22	1.99	0.61
1:D:551:ASN:HB3	1:D:630:LEU:HD21	1.81	0.61
1:A:614:GLU:CG	1:A:658:LEU:HD21	2.29	0.61
1:B:423:ILE:HD12	1:B:423:ILE:N	2.15	0.61
1:B:539:ASP:HB3	1:B:542:LEU:HD22	1.81	0.61
1:D:88:ILE:HG22	1:D:92:ARG:HD2	1.82	0.61
1:D:288:ILE:HG13	1:D:385:TYR:CD2	2.34	0.61
1:C:495:LYS:HE3	5:C:707:HOH:O	2.01	0.61
1:D:121:PRO:HG2	1:D:658:LEU:HB3	1.82	0.61
1:A:165:LEU:HD23	1:A:197:ILE:HD11	1.83	0.61
1:C:450:CYS:O	1:C:453:SER:HB3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:495:LYS:O	1:D:497:LYS:HG3	2.00	0.61
1:A:445:LYS:HG3	1:A:446:TYR:CE2	2.35	0.61
1:C:272:ASP:HB2	5:C:803:HOH:O	2.00	0.61
1:C:410:GLN:HE22	1:C:418:ARG:HA	1.65	0.61
1:D:568:TYR:CE2	1:D:618:PHE:HB2	2.36	0.60
1:A:213:LYS:NZ	1:B:206:ASN:HA	2.16	0.60
1:C:215:TYR:CZ	1:C:218:GLN:HG3	2.36	0.60
1:A:653:GLU:O	1:A:656:SER:HB3	2.01	0.60
1:D:546:TYR:CE2	1:D:620:HIS:HB2	2.37	0.60
1:D:669:THR:CG2	1:D:670:ASN:H	2.03	0.60
1:B:97:LYS:HG3	1:B:98:LYS:H	1.67	0.60
1:D:219:LEU:O	1:D:222:VAL:HG12	2.01	0.60
1:A:132:TRP:HA	1:A:135:LYS:HE3	1.82	0.60
1:A:660:ILE:C	1:A:661:LYS:HE2	2.21	0.60
1:D:190:SER:O	1:D:211:ARG:NH2	2.35	0.60
1:A:601:SER:H	1:A:647:HIS:CE1	2.20	0.60
1:B:641:ASP:OD2	1:B:672:ASN:HB3	2.02	0.60
1:D:414:PRO:HB3	1:D:418:ARG:NH2	2.16	0.60
1:A:534:ASP:O	1:A:538:LYS:HG3	2.02	0.60
1:A:605:ASP:CB	2:A:684:UGA:H4'1	2.31	0.60
1:B:462:LEU:HD23	1:B:462:LEU:C	2.22	0.60
1:C:93:GLU:HG3	1:C:94:ILE:N	2.17	0.60
1:A:423:ILE:H	1:A:423:ILE:CD1	2.10	0.59
1:A:499:ILE:HG22	5:A:713:HOH:O	2.02	0.59
1:D:61:ILE:HD11	1:D:482:HIS:HA	1.84	0.59
1:A:413:VAL:HB	1:A:417:TYR:HD2	1.66	0.59
1:B:188:ASP:OD1	1:B:218:GLN:HB2	2.01	0.59
1:C:61:ILE:HG12	1:C:62:ASP:H	1.65	0.59
1:C:572:LYS:CG	1:C:578:ILE:HD13	2.32	0.59
1:A:245:ASN:HD21	1:A:247:LEU:H	1.48	0.59
1:C:418:ARG:HB2	1:C:418:ARG:HH11	1.67	0.59
1:C:553:ASP:HB3	1:C:557:ASN:N	2.17	0.59
1:D:529:VAL:O	1:D:533:LEU:HD13	2.03	0.59
1:A:353:GLU:HG2	5:A:787:HOH:O	2.01	0.59
1:A:411:GLN:NE2	1:A:430:ARG:H	1.99	0.59
1:D:551:ASN:HB3	1:D:630:LEU:CD2	2.33	0.59
1:A:160:ASN:HB2	1:A:192:GLU:HB2	1.85	0.59
1:A:331:ARG:HA	1:A:363:ASN:HD22	1.68	0.59
1:B:474:ASP:O	1:B:478:ILE:HG12	2.02	0.59
1:B:602:ASN:O	1:B:603:ALA:HB3	2.03	0.59
1:B:661:LYS:O	1:B:682:ILE:HD11	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:GLN:C	1:C:308:LYS:H	2.06	0.59
1:C:553:ASP:HB3	1:C:557:ASN:H	1.66	0.59
1:B:458:THR:HG21	1:B:530:GLU:OE1	2.02	0.59
1:C:418:ARG:HB2	1:C:418:ARG:NH1	2.18	0.59
1:B:405:THR:HG23	5:B:792:HOH:O	2.03	0.59
1:A:127:THR:HG23	1:A:327:ASN:OD1	2.02	0.59
1:A:474:ASP:OD1	1:A:474:ASP:N	2.35	0.59
1:B:654:SER:C	1:B:656:SER:H	2.06	0.59
1:D:210:VAL:CG1	1:D:225:LEU:HD13	2.33	0.59
1:D:542:LEU:HD11	1:D:619:LYS:HB2	1.84	0.59
1:A:164:ILE:HD11	1:A:390:PRO:HD3	1.85	0.59
1:B:132:TRP:CH2	1:B:136:ARG:NH1	2.70	0.59
1:C:114:TRP:CZ2	1:C:118:LEU:HD12	2.38	0.59
1:C:388:GLU:OE1	1:C:388:GLU:HA	2.03	0.59
1:D:302:GLY:HA2	5:D:790:HOH:O	2.03	0.59
1:A:64:ASP:HB2	5:A:705:HOH:O	2.02	0.58
1:C:554:ARG:HD3	1:C:554:ARG:N	2.18	0.58
1:B:97:LYS:HG3	1:B:98:LYS:N	2.18	0.58
1:C:503:SER:HB3	1:C:596:PHE:CE1	2.38	0.58
1:D:213:LYS:CE	1:D:215:TYR:HB3	2.32	0.58
1:D:610:LEU:HG	1:D:655:LEU:HD23	1.84	0.58
1:A:124:PRO:HB3	1:A:132:TRP:CE3	2.38	0.58
1:A:682:ILE:HD12	1:A:682:ILE:C	2.24	0.58
1:C:81:GLU:HG3	1:C:85:ASN:HD21	1.68	0.58
1:D:590:TRP:HE1	1:D:608:MET:CE	2.15	0.58
1:B:176:LYS:HG3	1:B:285:LYS:HZ3	1.68	0.58
1:B:404:ILE:HG21	1:B:407:GLN:HE21	1.69	0.58
1:B:542:LEU:HA	1:B:617:PRO:HG2	1.84	0.58
1:A:90:LYS:HE3	1:A:90:LYS:HA	1.86	0.58
1:A:607:ASP:O	1:A:611:LYS:HG3	2.04	0.58
1:A:656:SER:C	1:A:658:LEU:N	2.56	0.58
1:A:548:THR:HG22	1:A:623:LYS:O	2.04	0.58
1:A:610:LEU:HG	1:A:655:LEU:HG	1.86	0.58
1:A:637:ILE:HB	1:A:640:LEU:HB2	1.86	0.58
1:C:611:LYS:HG2	1:C:657:ARG:NH1	2.19	0.58
1:D:250:GLN:HA	1:D:250:GLN:NE2	2.19	0.58
1:D:255:LEU:O	1:D:258:VAL:HG22	2.04	0.58
1:D:554:ARG:NH2	1:D:631:HIS:HA	2.18	0.58
1:D:669:THR:CG2	1:D:671:LEU:HG	2.33	0.58
1:B:104:LEU:H	1:B:104:LEU:CD1	2.16	0.58
1:B:175:GLN:HE21	1:B:249:VAL:HG23	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:GLY:O	1:B:408:LEU:HD13	2.04	0.58
1:B:546:TYR:O	1:B:620:HIS:HD2	1.86	0.58
1:A:87:ILE:HG23	5:A:784:HOH:O	2.04	0.57
1:A:515:ILE:N	1:A:515:ILE:HD12	2.19	0.57
1:B:669:THR:HG21	1:B:671:LEU:HD12	1.86	0.57
1:A:152:LEU:HD13	1:A:154:ILE:HG12	1.85	0.57
1:A:661:LYS:O	1:A:682:ILE:HG12	2.03	0.57
1:B:115:PRO:HB2	1:B:118:LEU:CB	2.33	0.57
1:B:307:ASN:HD22	1:B:308:LYS:N	2.01	0.57
1:B:653:GLU:O	1:B:656:SER:HB3	2.03	0.57
1:D:250:GLN:HA	1:D:250:GLN:HE21	1.69	0.57
1:B:419:LYS:HD2	1:B:420:LYS:H	1.70	0.57
1:A:638:LYS:HA	1:A:641:ASP:OD2	2.05	0.57
1:B:367:TYR:CG	1:B:413:VAL:HG13	2.39	0.57
1:C:653:GLU:O	1:C:656:SER:HB3	2.05	0.57
1:B:664:LYS:HB3	1:B:680:GLU:HG2	1.86	0.57
1:D:70:MET:SD	1:D:460:THR:HG23	2.44	0.57
1:A:603:ALA:N	2:A:684:UGA:O'P	2.28	0.57
1:B:131:VAL:HG23	1:B:324:ARG:HD2	1.86	0.57
1:C:539:ASP:HB3	1:C:542:LEU:HD22	1.87	0.57
1:A:656:SER:O	1:A:658:LEU:N	2.37	0.57
1:D:91:TYR:HA	1:D:94:ILE:CG2	2.35	0.57
1:D:600:ILE:HD12	1:D:602:ASN:O	2.05	0.57
1:B:388:GLU:OE1	1:B:388:GLU:HA	2.04	0.57
1:C:175:GLN:NE2	1:C:249:VAL:H	2.03	0.57
1:C:262:VAL:HB	1:C:375:TYR:HB2	1.86	0.57
1:C:611:LYS:HG2	1:C:657:ARG:CZ	2.34	0.57
1:D:549:ASN:OD1	1:D:562:GLY:HA3	2.04	0.57
1:A:549:ASN:C	1:A:624:ILE:HG23	2.24	0.57
1:A:682:ILE:HD12	1:A:682:ILE:O	2.05	0.57
1:C:213:LYS:HB3	1:D:202:GLU:HG2	1.87	0.57
1:C:410:GLN:NE2	1:C:419:LYS:H	2.03	0.57
1:D:61:ILE:O	1:D:61:ILE:HG23	2.05	0.57
1:D:316:HIS:HB3	5:D:693:HOH:O	2.04	0.57
1:B:656:SER:C	1:B:658:LEU:N	2.58	0.57
1:C:125:GLU:OE1	1:C:324:ARG:NH2	2.36	0.56
1:A:182:GLU:HB3	1:A:206:ASN:ND2	2.20	0.56
1:B:118:LEU:HD23	1:B:663:TYR:CD1	2.39	0.56
1:C:570:ARG:O	1:C:574:THR:HG23	2.04	0.56
1:D:130:TYR:CE2	1:D:377:ARG:HD2	2.40	0.56
1:A:137:LYS:O	1:A:138:GLU:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:TYR:CE2	1:A:218:GLN:HG3	2.40	0.56
1:A:528:ALA:HB2	1:A:625:CYS:HB3	1.87	0.56
1:B:114:TRP:CE2	1:B:571:GLU:HG3	2.40	0.56
1:B:123:LEU:HD21	1:B:570:ARG:HD2	1.86	0.56
1:B:195:GLU:O	1:B:199:ARG:HG3	2.04	0.56
1:B:262:VAL:HG13	5:B:806:HOH:O	2.05	0.56
1:C:490:ARG:NH2	1:C:511:ARG:CZ	2.68	0.56
1:A:458:THR:HG21	1:A:530:GLU:OE1	2.05	0.56
1:D:107:VAL:HG22	1:D:109:PRO:HD3	1.86	0.56
1:A:123:LEU:HB3	1:A:124:PRO:HD2	1.86	0.56
1:D:434:VAL:HB	1:D:462:LEU:HB2	1.88	0.56
1:B:611:LYS:HG2	1:B:657:ARG:NH1	2.20	0.56
1:D:69:ILE:HD13	1:D:88:ILE:HG13	1.88	0.56
1:D:236:ALA:HA	1:D:339:ALA:HA	1.87	0.56
1:B:64:ASP:OD1	1:B:455:LEU:HD13	2.06	0.56
1:C:70:MET:SD	1:C:460:THR:OG1	2.62	0.56
1:C:178:ILE:HG12	1:C:250:GLN:HE22	1.70	0.56
1:A:184:ILE:N	1:A:184:ILE:HD12	2.20	0.56
1:B:418:ARG:NH2	1:B:431:VAL:O	2.39	0.56
1:A:191:LYS:O	1:A:191:LYS:HD3	2.07	0.55
1:A:602:ASN:O	1:A:603:ALA:HB3	2.06	0.55
1:A:669:THR:HG22	1:A:670:ASN:N	2.21	0.55
1:B:68:LYS:HD3	1:B:87:ILE:CD1	2.35	0.55
1:B:175:GLN:HE22	1:B:249:VAL:H	1.53	0.55
1:A:480:GLN:O	1:A:484:ALA:HB2	2.06	0.55
1:B:293:GLU:OE1	1:B:308:LYS:HE3	2.05	0.55
1:C:61:ILE:O	1:C:62:ASP:HB3	2.06	0.55
1:D:441:TYR:CE1	1:D:442:ASN:ND2	2.75	0.55
1:C:65:ALA:O	1:C:69:ILE:HG13	2.06	0.55
1:C:81:GLU:OE1	1:C:81:GLU:HA	2.07	0.55
1:D:124:PRO:HB3	1:D:132:TRP:CD2	2.41	0.55
1:B:607:ASP:O	1:B:611:LYS:HG3	2.06	0.55
1:A:136:ARG:C	1:A:137:LYS:HG3	2.27	0.55
1:A:367:TYR:CG	1:A:413:VAL:HG13	2.42	0.55
1:A:421:GLU:OE2	1:A:426:ALA:HA	2.06	0.55
1:A:324:ARG:HB3	1:A:325:LEU:HD22	1.89	0.55
1:B:404:ILE:CG2	1:B:407:GLN:HE21	2.19	0.55
1:B:409:LEU:N	1:B:409:LEU:HD22	2.22	0.55
1:C:553:ASP:OD1	1:C:554:ARG:HD3	2.06	0.55
1:D:75:LYS:HB2	5:D:739:HOH:O	2.04	0.55
1:A:195:GLU:O	1:A:199:ARG:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:669:THR:HG23	1:C:671:LEU:HG	1.89	0.55
1:A:138:GLU:O	1:A:139:LEU:HD12	2.06	0.55
1:A:669:THR:HG22	1:A:670:ASN:H	1.72	0.55
1:C:218:GLN:HB3	1:C:221:ALA:HB3	1.88	0.55
1:B:60:VAL:CG2	1:B:61:ILE:H	2.15	0.55
1:A:160:ASN:HA	1:A:194:ILE:HD11	1.88	0.54
1:A:215:TYR:CE1	1:A:218:GLN:HG3	2.42	0.54
1:D:91:TYR:CA	1:D:94:ILE:HG22	2.37	0.54
1:A:269:LYS:HG3	1:A:383:MET:CE	2.36	0.54
1:A:424:GLU:CD	1:A:424:GLU:H	2.10	0.54
1:D:646:ASN:O	1:D:650:VAL:HG23	2.08	0.54
1:D:677:TYR:HE2	1:D:679:TRP:HE1	1.56	0.54
1:B:642:ILE:HD13	1:B:672:ASN:OD1	2.07	0.54
1:A:163:LYS:O	1:A:167:ILE:HG13	2.08	0.54
1:A:637:ILE:HG13	1:A:640:LEU:HD22	1.89	0.54
1:B:60:VAL:CG2	1:B:61:ILE:N	2.70	0.54
1:B:215:TYR:CE1	1:B:218:GLN:HG3	2.42	0.54
1:C:669:THR:HG23	1:C:670:ASN:N	2.23	0.54
1:A:614:GLU:OE2	1:A:655:LEU:CD2	2.56	0.54
1:B:293:GLU:CD	1:B:308:LYS:HE3	2.29	0.54
1:C:433:LEU:HD13	1:C:533:LEU:HD21	1.90	0.54
1:D:177:THR:OG1	1:D:250:GLN:NE2	2.41	0.54
1:D:406:VAL:O	1:D:406:VAL:HG12	2.06	0.54
1:A:450:CYS:SG	1:A:518:LEU:HD13	2.48	0.54
1:B:101:ARG:HA	1:B:623:LYS:HA	1.88	0.54
1:B:210:VAL:HG12	1:B:225:LEU:HD13	1.90	0.54
1:B:583:ARG:HD3	1:B:609:TYR:CE2	2.43	0.54
1:C:64:ASP:O	1:C:67:THR:HG22	2.08	0.54
1:C:474:ASP:O	1:C:478:ILE:HG12	2.07	0.54
1:D:273:THR:CG2	1:D:387:GLN:HE21	2.09	0.54
1:A:653:GLU:HG2	5:A:746:HOH:O	2.08	0.54
1:D:163:LYS:O	1:D:166:ALA:HB3	2.08	0.54
1:A:75:LYS:HB2	1:A:75:LYS:HZ3	1.71	0.53
1:C:648:PHE:CD2	1:C:649:LYS:HD2	2.42	0.53
1:D:649:LYS:HG2	1:D:667:PRO:HG3	1.89	0.53
1:C:107:VAL:HG11	1:C:565:TRP:CZ3	2.42	0.53
1:A:164:ILE:HA	1:A:167:ILE:HD12	1.89	0.53
1:A:250:GLN:HA	1:A:250:GLN:NE2	2.23	0.53
1:A:269:LYS:HD2	1:A:385:TYR:HE1	1.72	0.53
1:B:94:ILE:HG23	1:B:95:THR:HG23	1.90	0.53
1:C:558:LEU:HD13	1:C:558:LEU:C	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:LYS:HA	1:A:682:ILE:HD11	1.89	0.53
1:B:423:ILE:HD12	1:B:423:ILE:H	1.73	0.53
1:C:184:ILE:HD11	1:C:230:ALA:HA	1.89	0.53
1:C:325:LEU:N	1:C:325:LEU:HD22	2.23	0.53
1:C:631:HIS:CD2	1:C:632:GLY:N	2.76	0.53
1:A:568:TYR:CE2	1:A:618:PHE:HB2	2.44	0.53
1:A:610:LEU:CD2	1:A:651:VAL:HG12	2.39	0.53
1:C:107:VAL:HG12	1:C:108:GLU:N	2.23	0.53
1:C:602:ASN:O	1:C:603:ALA:HB3	2.07	0.53
1:A:63:ILE:HD12	1:A:67:THR:HG23	1.91	0.53
1:A:614:GLU:OE2	1:A:655:LEU:HD22	2.08	0.53
1:A:680:GLU:HB3	5:A:747:HOH:O	2.08	0.53
1:D:607:ASP:O	1:D:611:LYS:HG3	2.08	0.53
1:D:224:ASN:O	1:D:228:ARG:HG3	2.08	0.53
1:D:311:ASP:HB3	1:D:314:ILE:CG1	2.34	0.53
1:B:653:GLU:OE2	1:B:665:TYR:HB3	2.09	0.53
1:D:507:VAL:HG21	1:D:596:PHE:HE1	1.73	0.53
1:A:118:LEU:HD21	1:A:660:ILE:HG21	1.91	0.53
1:D:121:PRO:HD2	1:D:658:LEU:HD13	1.91	0.53
1:A:549:ASN:HB3	1:A:626:TYR:HB3	1.89	0.53
1:A:586:THR:HG22	1:A:589:ALA:CB	2.39	0.52
1:B:596:PHE:CG	1:B:608:MET:HE2	2.44	0.52
1:A:115:PRO:HB2	1:A:118:LEU:HB3	1.91	0.52
1:A:610:LEU:HB3	1:A:655:LEU:HD23	1.91	0.52
1:B:295:ILE:HG22	1:B:308:LYS:HA	1.89	0.52
1:B:352:ASP:OD1	1:B:354:GLU:HB2	2.08	0.52
1:C:545:VAL:HA	1:C:619:LYS:O	2.09	0.52
1:D:152:LEU:HD12	1:D:154:ILE:HG12	1.92	0.52
1:D:302:GLY:CA	5:D:790:HOH:O	2.57	0.52
1:A:408:LEU:CD1	1:A:408:LEU:N	2.71	0.52
1:D:405:THR:HG22	1:D:406:VAL:N	2.25	0.52
1:D:548:THR:HG22	1:D:623:LYS:C	2.30	0.52
1:A:61:ILE:HD12	1:A:61:ILE:O	2.10	0.52
1:D:655:LEU:O	1:D:655:LEU:HD13	2.09	0.52
1:B:423:ILE:H	1:B:423:ILE:CD1	2.21	0.52
1:B:586:THR:CG2	1:B:588:ARG:HB3	2.39	0.52
1:B:628:ARG:HG2	1:B:628:ARG:HH11	1.75	0.52
1:C:642:ILE:HD13	1:C:672:ASN:OD1	2.10	0.52
1:A:419:LYS:HZ2	1:A:420:LYS:HE3	1.75	0.52
1:A:655:LEU:O	1:A:658:LEU:HG	2.09	0.52
1:B:80:ASN:HD21	1:B:83:GLU:N	1.94	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ILE:HB	5:B:743:HOH:O	2.09	0.52
1:C:462:LEU:HD23	1:C:463:GLU:N	2.25	0.52
1:C:549:ASN:HB3	1:C:626:TYR:HB3	1.92	0.52
1:A:210:VAL:CG1	1:A:225:LEU:HD13	2.40	0.52
1:A:522:ASP:HB3	1:A:627:ASN:O	2.09	0.52
1:B:610:LEU:CD2	1:B:651:VAL:HG12	2.40	0.52
1:C:91:TYR:O	1:C:94:ILE:HG22	2.10	0.52
1:C:553:ASP:OD1	1:C:555:GLU:N	2.36	0.52
1:C:601:SER:HB2	1:C:647:HIS:HE1	1.74	0.52
1:A:132:TRP:HA	1:A:135:LYS:CE	2.39	0.51
1:A:370:TYR:CE2	1:A:588:ARG:HD2	2.45	0.51
1:A:649:LYS:HG2	1:A:667:PRO:HG3	1.92	0.51
1:B:642:ILE:O	1:B:645:GLU:HB3	2.10	0.51
1:D:405:THR:HG22	1:D:407:GLN:HB2	1.93	0.51
1:A:675:ARG:HH11	1:A:675:ARG:HG2	1.74	0.51
1:D:136:ARG:HG2	1:D:136:ARG:HH11	1.75	0.51
1:D:554:ARG:H	1:D:554:ARG:HD2	1.75	0.51
1:C:548:THR:HG22	1:C:623:LYS:O	2.11	0.51
1:C:654:SER:C	1:C:656:SER:H	2.13	0.51
1:B:152:LEU:HB2	1:B:253:MET:SD	2.51	0.51
1:B:414:PRO:HA	1:B:418:ARG:NH1	2.25	0.51
1:C:114:TRP:CZ2	1:C:118:LEU:CD1	2.93	0.51
1:A:291:ILE:CG2	1:A:292:PRO:HD2	2.41	0.51
1:A:552:ILE:HG22	1:A:553:ASP:O	2.11	0.51
1:C:285:LYS:HB2	1:C:285:LYS:NZ	2.24	0.51
1:D:152:LEU:CD1	1:D:154:ILE:HG12	2.40	0.51
1:D:568:TYR:CZ	1:D:618:PHE:HB2	2.46	0.51
1:B:449:ARG:HD3	1:B:523:PHE:CD2	2.45	0.51
1:D:121:PRO:HD3	1:D:660:ILE:HD11	1.92	0.51
1:A:262:VAL:HG13	5:A:685:HOH:O	2.10	0.51
1:A:325:LEU:HD22	1:A:325:LEU:N	2.26	0.51
1:A:414:PRO:HB2	1:A:433:LEU:HD23	1.93	0.51
1:B:607:ASP:HA	1:B:651:VAL:HG13	1.92	0.51
1:C:209:TYR:OH	1:C:211:ARG:HD2	2.11	0.51
1:C:294:ILE:HD11	1:C:388:GLU:CG	2.41	0.51
1:D:643:GLN:H	1:D:643:GLN:CD	2.14	0.51
1:A:82:VAL:O	1:A:85:ASN:ND2	2.43	0.51
1:B:634:ASN:OD1	1:B:634:ASN:N	2.44	0.51
1:C:74:ALA:HB2	1:C:427:THR:OG1	2.10	0.51
1:C:158:THR:HG21	1:C:165:LEU:HD22	1.91	0.51
1:C:405:THR:CA	5:C:820:HOH:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:GLU:CD	1:A:658:LEU:HD21	2.31	0.51
1:B:129:ASP:OD1	1:B:132:TRP:N	2.25	0.51
1:B:390:PRO:HD2	1:B:393:GLU:OE2	2.10	0.51
1:B:454:ALA:O	1:B:457:GLN:HG2	2.11	0.51
1:D:539:ASP:O	1:D:542:LEU:HB2	2.11	0.51
1:A:198:VAL:HG13	1:A:207:ILE:HD13	1.93	0.50
1:A:269:LYS:HB2	1:A:385:TYR:CD1	2.46	0.50
1:A:271:ILE:HG22	1:A:272:ASP:N	2.25	0.50
1:B:65:ALA:HB1	1:B:87:ILE:HG22	1.92	0.50
1:B:101:ARG:H	1:B:101:ARG:CD	2.22	0.50
1:C:334:SER:HA	1:C:362:ASP:OD1	2.11	0.50
1:C:536:PHE:CZ	1:C:545:VAL:HG13	2.47	0.50
1:A:239:ASP:HB2	1:A:242:MET:HG2	1.92	0.50
1:A:372:GLU:HB3	5:A:737:HOH:O	2.11	0.50
1:A:605:ASP:CG	2:A:684:UGA:H4'1	2.31	0.50
1:B:294:ILE:HD12	1:B:294:ILE:C	2.32	0.50
1:C:587:ALA:O	1:C:591:ASN:ND2	2.45	0.50
1:A:558:LEU:HD22	1:A:559:ILE:N	2.27	0.50
1:B:245:ASN:HD21	1:B:247:LEU:HB2	1.77	0.50
1:D:123:LEU:HB3	1:D:124:PRO:HD2	1.92	0.50
1:D:224:ASN:OD1	1:D:350:TRP:HB3	2.11	0.50
1:D:610:LEU:CD2	1:D:651:VAL:HG12	2.40	0.50
1:B:178:ILE:H	1:B:250:GLN:NE2	2.10	0.50
1:C:433:LEU:HB2	1:C:461:ASP:CG	2.31	0.50
1:B:124:PRO:HD3	1:B:132:TRP:CE2	2.47	0.50
1:C:503:SER:HB3	1:C:596:PHE:CD1	2.47	0.50
1:C:586:THR:CG2	1:C:589:ALA:H	2.13	0.50
1:D:295:ILE:HA	1:D:308:LYS:HA	1.92	0.50
1:B:649:LYS:CG	1:B:667:PRO:HG3	2.40	0.50
1:A:64:ASP:CG	1:A:67:THR:HG22	2.32	0.50
1:A:535:GLU:HG2	1:A:621:ILE:HD11	1.94	0.50
1:B:238:LEU:HD13	1:B:248:TRP:CZ2	2.47	0.50
1:C:539:ASP:OD2	1:C:541:SER:HB2	2.12	0.50
1:D:546:TYR:CE1	1:D:579:CYS:HA	2.47	0.50
1:A:68:LYS:HD2	1:A:87:ILE:CD1	2.37	0.50
1:A:114:TRP:CZ2	1:A:118:LEU:HD12	2.46	0.50
1:A:388:GLU:OE1	1:A:388:GLU:HA	2.12	0.50
1:A:458:THR:HB	5:A:759:HOH:O	2.12	0.50
1:C:64:ASP:OD1	1:C:67:THR:CG2	2.60	0.50
1:D:308:LYS:O	1:D:308:LYS:HG3	2.10	0.50
1:D:553:ASP:HB3	1:D:557:ASN:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:VAL:HG13	1:B:207:ILE:CD1	2.41	0.49
1:A:131:VAL:CG2	1:A:324:ARG:HD2	2.42	0.49
1:A:276:HIS:HA	1:A:280:ASP:OD1	2.12	0.49
1:B:558:LEU:C	1:B:558:LEU:HD13	2.32	0.49
1:C:553:ASP:CB	1:C:557:ASN:HB2	2.42	0.49
1:C:674:CYS:SG	5:C:836:HOH:O	2.60	0.49
1:A:115:PRO:HB2	1:A:118:LEU:CB	2.42	0.49
1:A:213:LYS:HZ3	1:B:206:ASN:HA	1.77	0.49
1:A:660:ILE:O	1:A:661:LYS:HE2	2.11	0.49
1:B:80:ASN:HD22	1:B:82:VAL:N	2.09	0.49
1:B:115:PRO:HD3	1:B:679:TRP:CD1	2.47	0.49
1:B:137:LYS:HD2	1:B:137:LYS:H	1.77	0.49
1:B:662:LYS:C	1:B:682:ILE:HD11	2.31	0.49
1:D:465:CYS:HA	1:D:490:ARG:O	2.11	0.49
1:C:79:LEU:CD2	1:C:83:GLU:HB3	2.42	0.49
1:C:238:LEU:HA	1:C:336:GLY:O	2.13	0.49
1:C:265:ILE:O	1:C:378:SER:HA	2.13	0.49
1:D:107:VAL:HG23	1:D:567:ILE:CD1	2.42	0.49
1:C:152:LEU:HD13	1:C:154:ILE:CG1	2.43	0.49
1:C:297:ASN:N	1:C:297:ASN:ND2	2.47	0.49
1:C:423:ILE:HD12	1:C:424:GLU:H	1.78	0.49
1:D:147:LEU:N	1:D:147:LEU:HD23	2.28	0.49
1:D:187:ASP:HB3	1:D:211:ARG:HB2	1.95	0.49
1:D:254:GLU:O	1:D:258:VAL:HG13	2.11	0.49
1:D:596:PHE:CE2	1:D:608:MET:HG2	2.47	0.49
1:A:130:TYR:CE2	1:A:377:ARG:HD2	2.47	0.49
1:A:211:ARG:NH1	1:B:202:GLU:OE2	2.45	0.49
1:B:551:ASN:OD1	1:B:630:LEU:HD11	2.12	0.49
1:B:628:ARG:HG2	1:B:628:ARG:NH1	2.28	0.49
1:D:158:THR:HG21	1:D:165:LEU:HD22	1.93	0.49
1:B:118:LEU:HA	5:B:811:HOH:O	2.11	0.49
1:B:296:THR:HG22	1:B:309:SER:CB	2.43	0.49
1:B:308:LYS:H	1:B:308:LYS:HD2	1.78	0.49
1:C:669:THR:CG2	1:C:670:ASN:N	2.76	0.49
1:B:586:THR:HG22	1:B:588:ARG:N	2.28	0.49
1:C:94:ILE:HG23	1:C:95:THR:HG23	1.93	0.49
1:D:115:PRO:HB3	1:D:663:TYR:CZ	2.47	0.49
1:D:568:TYR:CG	1:D:569:SER:N	2.80	0.49
1:B:614:GLU:OE2	1:B:655:LEU:HD22	2.13	0.49
1:D:590:TRP:HE1	1:D:608:MET:HE3	1.78	0.49
1:D:630:LEU:HD22	1:D:630:LEU:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:VAL:HB	1:A:462:LEU:HB2	1.95	0.49
1:B:135:LYS:O	1:B:136:ARG:HB2	2.12	0.49
1:D:65:ALA:O	1:D:68:LYS:HB3	2.12	0.49
1:D:550:ARG:HA	1:D:562:GLY:H	1.78	0.49
1:A:411:GLN:HE22	1:A:430:ARG:H	1.60	0.48
1:A:552:ILE:CG2	1:A:553:ASP:N	2.75	0.48
1:B:404:ILE:CD1	1:B:407:GLN:HG3	2.43	0.48
1:B:419:LYS:CE	1:B:420:LYS:HG2	2.41	0.48
1:C:80:ASN:ND2	1:C:82:VAL:HB	2.27	0.48
1:D:298:ASN:ND2	1:D:299:GLN:HG3	2.28	0.48
1:A:167:ILE:HG23	1:A:281:PHE:CD2	2.49	0.48
1:A:607:ASP:OD2	1:A:611:LYS:HE3	2.13	0.48
1:B:199:ARG:HA	1:B:202:GLU:CG	2.42	0.48
1:B:654:SER:C	1:B:656:SER:N	2.67	0.48
1:C:621:ILE:HG22	1:C:623:LYS:HG2	1.94	0.48
1:D:213:LYS:CD	1:D:215:TYR:HB3	2.43	0.48
1:A:87:ILE:HG12	5:A:784:HOH:O	2.12	0.48
1:A:434:VAL:HB	1:A:462:LEU:CB	2.44	0.48
1:B:115:PRO:HD3	1:B:679:TRP:NE1	2.29	0.48
1:C:440:ALA:HB1	1:C:443:CYS:SG	2.54	0.48
1:C:447:ILE:HG23	1:C:448:VAL:N	2.28	0.48
1:C:453:SER:OG	1:C:524:LEU:N	2.41	0.48
1:D:552:ILE:HD13	1:D:558:LEU:HA	1.95	0.48
1:D:649:LYS:O	1:D:653:GLU:HG2	2.14	0.48
1:A:462:LEU:HD21	1:A:488:ARG:NH2	2.25	0.48
1:C:568:TYR:CZ	1:C:618:PHE:HB2	2.48	0.48
1:C:656:SER:C	1:C:658:LEU:H	2.17	0.48
1:D:673:GLU:HA	1:D:675:ARG:HH12	1.79	0.48
1:B:127:THR:HG23	1:B:327:ASN:OD1	2.14	0.48
1:B:435:SER:HB3	1:B:510:CYS:SG	2.54	0.48
1:B:640:LEU:O	1:B:643:GLN:HG2	2.14	0.48
1:C:521:ASP:OD1	1:C:631:HIS:HE1	1.97	0.48
1:C:568:TYR:CE2	1:C:618:PHE:HB2	2.49	0.48
1:B:328:THR:HG23	5:B:749:HOH:O	2.14	0.48
1:B:465:CYS:HA	1:B:490:ARG:O	2.13	0.48
1:B:564:ASN:OD1	1:B:620:HIS:HE1	1.95	0.48
1:D:71:CYS:O	1:D:76:ALA:HB3	2.14	0.48
1:D:152:LEU:HD12	1:D:154:ILE:CG1	2.44	0.48
1:A:664:LYS:HD3	1:A:666:SER:OG	2.13	0.48
1:B:178:ILE:H	1:B:250:GLN:HE22	1.61	0.48
1:B:447:ILE:HG23	1:B:448:VAL:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:568:TYR:CE2	1:B:618:PHE:HB2	2.48	0.48
1:C:492:ILE:HG12	1:C:493:SER:N	2.28	0.48
1:C:680:GLU:O	1:C:680:GLU:HG3	2.14	0.48
1:D:652:ASN:O	1:D:655:LEU:HB3	2.14	0.48
1:B:411:GLN:HE22	1:B:429:LYS:HA	1.79	0.48
1:A:434:VAL:O	1:A:462:LEU:HA	2.14	0.47
1:A:639:LYS:O	1:A:642:ILE:HB	2.13	0.47
1:C:371:ARG:NH2	1:C:371:ARG:CG	2.70	0.47
1:D:325:LEU:N	1:D:325:LEU:HD22	2.29	0.47
1:B:90:LYS:HE3	1:B:90:LYS:CA	2.42	0.47
1:B:517:GLN:NE2	1:B:609:TYR:OH	2.47	0.47
1:B:605:ASP:O	1:B:609:TYR:HD2	1.97	0.47
1:C:517:GLN:NE2	1:C:583:ARG:HH11	2.12	0.47
1:D:517:GLN:HE22	1:D:583:ARG:HH11	1.61	0.47
1:A:210:VAL:HG11	1:A:225:LEU:HD22	1.96	0.47
1:B:177:THR:OG1	1:B:250:GLN:NE2	2.46	0.47
1:D:330:PHE:C	1:D:332:PHE:H	2.17	0.47
1:A:368:ARG:O	1:A:372:GLU:HG2	2.14	0.47
1:B:508:ARG:HG3	1:B:508:ARG:HH11	1.79	0.47
1:C:211:ARG:HG2	1:C:211:ARG:NH1	2.29	0.47
1:A:536:PHE:CE1	1:A:584:MET:HG2	2.47	0.47
1:B:610:LEU:HG	1:B:655:LEU:HG	1.96	0.47
1:D:321:ASP:HB3	1:D:325:LEU:CD2	2.44	0.47
1:D:449:ARG:HD2	5:D:718:HOH:O	2.13	0.47
1:D:551:ASN:CB	1:D:630:LEU:HD21	2.43	0.47
1:A:272:ASP:OD2	1:A:274:SER:HB2	2.13	0.47
1:B:391:GLY:C	1:B:393:GLU:N	2.67	0.47
1:C:525:GLU:HB3	5:C:785:HOH:O	2.14	0.47
1:C:596:PHE:CG	1:C:608:MET:HE3	2.50	0.47
1:D:115:PRO:HD3	5:D:804:HOH:O	2.13	0.47
1:D:199:ARG:O	1:D:202:GLU:HB2	2.15	0.47
1:D:301:ALA:HB1	5:D:798:HOH:O	2.15	0.47
1:D:331:ARG:HH21	1:D:332:PHE:HZ	1.62	0.47
1:A:182:GLU:OE1	1:A:231:LYS:HG2	2.15	0.47
1:A:637:ILE:CG2	1:A:638:LYS:H	2.25	0.47
1:C:83:GLU:O	1:C:87:ILE:HG13	2.15	0.47
1:C:596:PHE:CD2	1:C:608:MET:HE3	2.49	0.47
1:C:649:LYS:HG2	1:C:667:PRO:HG3	1.95	0.47
1:D:188:ASP:HB2	1:D:222:VAL:HG21	1.97	0.47
1:A:342:LYS:HD3	5:A:720:HOH:O	2.13	0.47
1:A:600:ILE:HD11	1:A:604:VAL:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:TYR:CD1	1:A:677:TYR:N	2.82	0.47
1:B:551:ASN:HD21	1:B:562:GLY:HA2	1.80	0.47
1:B:607:ASP:OD2	1:B:611:LYS:HE3	2.15	0.47
1:B:610:LEU:HD22	1:B:651:VAL:HG12	1.97	0.47
1:C:586:THR:HG22	1:C:589:ALA:N	2.12	0.47
1:D:610:LEU:HG	1:D:655:LEU:CD2	2.45	0.47
1:D:63:ILE:HD11	1:D:68:LYS:HA	1.96	0.46
1:D:464:VAL:HB	1:D:489:VAL:HG22	1.97	0.46
1:D:543:ALA:HB2	1:D:616:GLY:HA3	1.97	0.46
1:D:628:ARG:NH1	1:D:628:ARG:HG2	2.31	0.46
1:A:69:ILE:HG22	1:A:73:ASN:HD21	1.80	0.46
1:A:210:VAL:HG22	1:B:210:VAL:HG13	1.97	0.46
1:A:288:ILE:HG23	1:A:289:ASN:HD22	1.79	0.46
1:A:637:ILE:CG2	1:A:640:LEU:H	2.28	0.46
1:B:661:LYS:O	1:B:682:ILE:CD1	2.62	0.46
1:C:363:ASN:CB	1:C:409:LEU:HD21	2.45	0.46
1:D:265:ILE:HD11	1:D:333:PHE:HD2	1.80	0.46
1:A:539:ASP:C	1:A:541:SER:H	2.19	0.46
1:B:462:LEU:HD23	1:B:463:GLU:N	2.30	0.46
1:C:132:TRP:CH2	1:C:136:ARG:HD2	2.50	0.46
1:C:371:ARG:HG2	1:C:372:GLU:OE1	2.15	0.46
1:C:433:LEU:HB2	1:C:461:ASP:OD1	2.15	0.46
1:A:271:ILE:CG2	1:A:272:ASP:N	2.79	0.46
1:C:255:LEU:HB2	1:C:264:LEU:HD11	1.98	0.46
1:C:449:ARG:O	1:C:449:ARG:HG2	2.15	0.46
1:D:206:ASN:ND2	5:D:715:HOH:O	2.49	0.46
1:D:458:THR:HG21	1:D:530:GLU:CD	2.35	0.46
1:A:156:ILE:HG23	1:A:238:LEU:O	2.16	0.46
1:A:356:THR:HG23	1:A:357:HIS:N	2.30	0.46
1:A:437:TYR:CE1	1:A:517:GLN:HB2	2.50	0.46
1:C:631:HIS:C	1:C:633:GLU:H	2.19	0.46
1:C:643:GLN:CG	1:C:644:LYS:N	2.78	0.46
1:D:191:LYS:HD2	1:D:191:LYS:O	2.15	0.46
1:A:160:ASN:HD22	1:A:160:ASN:N	2.14	0.46
1:A:535:GLU:CG	1:A:621:ILE:HD11	2.46	0.46
1:C:66:ALA:O	1:C:70:MET:HG3	2.16	0.46
1:C:162:ALA:HB1	1:C:197:ILE:HD11	1.97	0.46
1:C:322:ASN:O	1:C:323:LEU:HB2	2.15	0.46
1:C:596:PHE:CG	1:C:608:MET:CE	2.98	0.46
1:C:631:HIS:HD2	1:C:632:GLY:N	2.14	0.46
1:D:289:ASN:ND2	1:D:385:TYR:OH	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:474:ASP:HB2	1:D:477:ARG:HB3	1.97	0.46
1:A:70:MET:HA	1:A:73:ASN:HD22	1.81	0.46
1:A:175:GLN:NE2	5:A:761:HOH:O	2.48	0.46
1:A:198:VAL:HG13	1:A:207:ILE:CD1	2.46	0.46
1:B:90:LYS:HA	1:B:90:LYS:CE	2.41	0.46
1:B:175:GLN:NE2	1:B:249:VAL:HG23	2.31	0.46
1:C:427:THR:HG22	1:C:429:LYS:HZ1	1.81	0.46
1:D:91:TYR:O	1:D:94:ILE:HG22	2.16	0.46
1:A:158:THR:HG21	1:A:165:LEU:HD22	1.98	0.46
1:B:606:TYR:O	1:B:610:LEU:HB2	2.16	0.46
1:B:669:THR:HG22	1:B:670:ASN:N	2.31	0.46
1:D:238:LEU:HA	1:D:336:GLY:O	2.16	0.46
1:D:462:LEU:HD23	1:D:462:LEU:C	2.37	0.46
1:A:170:ALA:O	1:A:174:ASN:OD1	2.34	0.46
1:C:613:SER:HA	1:C:618:PHE:CE1	2.51	0.46
1:C:631:HIS:CD2	1:C:631:HIS:C	2.90	0.46
1:D:88:ILE:O	1:D:92:ARG:CG	2.61	0.46
1:D:89:SER:CA	1:D:92:ARG:HG3	2.43	0.46
1:C:409:LEU:HB3	1:C:413:VAL:HB	1.98	0.45
1:C:447:ILE:O	1:C:450:CYS:HB3	2.15	0.45
1:D:88:ILE:CG2	1:D:92:ARG:HD2	2.45	0.45
1:A:465:CYS:HA	1:A:490:ARG:O	2.16	0.45
1:A:542:LEU:HD12	1:A:617:PRO:O	2.16	0.45
1:B:160:ASN:C	1:B:161:ARG:HG2	2.37	0.45
1:B:184:ILE:N	1:B:184:ILE:HD12	2.31	0.45
1:B:419:LYS:HE3	1:B:420:LYS:CG	2.44	0.45
1:C:174:ASN:CG	1:C:285:LYS:HG2	2.36	0.45
1:C:255:LEU:O	1:C:258:VAL:HG22	2.16	0.45
1:C:296:THR:HG23	1:C:388:GLU:CD	2.36	0.45
1:C:306:GLN:C	1:C:308:LYS:N	2.69	0.45
1:D:551:ASN:N	1:D:560:SER:O	2.40	0.45
1:D:553:ASP:OD2	1:D:555:GLU:HB3	2.15	0.45
1:A:115:PRO:HD3	1:A:679:TRP:CD1	2.52	0.45
1:A:356:THR:HG23	1:A:357:HIS:H	1.82	0.45
1:A:364:GLU:CD	1:A:368:ARG:HE	2.19	0.45
1:A:501:SER:HA	1:A:598:GLU:OE1	2.17	0.45
1:C:669:THR:CG2	1:C:671:LEU:HG	2.47	0.45
1:D:643:GLN:HA	1:D:646:ASN:HB3	1.99	0.45
1:A:515:ILE:HD11	1:A:587:ALA:HB2	1.99	0.45
1:B:549:ASN:CA	1:B:624:ILE:HG23	2.45	0.45
1:B:639:LYS:O	1:B:642:ILE:HB	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:GLN:NE2	1:C:430:ARG:H	2.14	0.45
1:C:427:THR:HG22	1:C:429:LYS:NZ	2.31	0.45
1:C:466:ILE:O	1:C:491:PHE:HA	2.16	0.45
1:C:596:PHE:CE2	1:C:608:MET:HE3	2.52	0.45
1:D:602:ASN:O	1:D:603:ALA:HB3	2.16	0.45
1:A:316:HIS:HB3	5:A:692:HOH:O	2.17	0.45
1:B:80:ASN:ND2	1:B:83:GLU:N	2.51	0.45
1:B:606:TYR:HE2	1:B:652:ASN:OD1	1.99	0.45
1:C:410:GLN:O	1:C:418:ARG:NH1	2.50	0.45
1:D:250:GLN:HE21	1:D:250:GLN:CA	2.27	0.45
1:A:238:LEU:HA	1:A:336:GLY:O	2.16	0.45
1:B:532:CYS:HB3	1:B:545:VAL:HG21	1.98	0.45
1:A:420:LYS:HD3	1:A:537:ARG:NH1	2.27	0.45
1:A:511:ARG:NH1	5:A:751:HOH:O	2.48	0.45
1:C:477:ARG:NH2	1:C:481:GLU:OE2	2.50	0.45
1:C:648:PHE:HE2	1:C:665:TYR:HH	1.60	0.45
1:D:328:THR:HG21	1:D:416:PHE:CD1	2.51	0.45
1:D:443:CYS:SG	1:D:520:SER:HB2	2.57	0.45
1:D:662:LYS:HG3	1:D:663:TYR:HD1	1.82	0.45
1:A:94:ILE:HG12	1:A:94:ILE:O	2.17	0.45
1:B:174:ASN:CG	1:B:285:LYS:HB3	2.38	0.45
1:B:361:GLU:HG2	5:B:794:HOH:O	2.16	0.45
1:C:454:ALA:O	1:C:457:GLN:HG2	2.16	0.45
1:D:172:LEU:HG	1:D:244:PRO:HG3	1.99	0.45
1:D:474:ASP:O	1:D:478:ILE:HG12	2.17	0.45
1:A:367:TYR:CD1	1:A:413:VAL:HG13	2.52	0.45
1:B:548:THR:O	1:B:624:ILE:HA	2.17	0.45
1:B:577:MET:O	1:B:577:MET:HG3	2.17	0.45
1:C:347:ARG:HD3	5:C:762:HOH:O	2.17	0.45
1:C:418:ARG:NH2	1:C:431:VAL:O	2.49	0.45
1:C:611:LYS:CG	1:C:657:ARG:NH1	2.80	0.45
1:D:422:LYS:CB	1:D:424:GLU:HG2	2.42	0.45
1:A:363:ASN:HB3	1:A:417:TYR:OH	2.16	0.45
1:A:572:LYS:HG3	1:A:578:ILE:HG21	1.99	0.45
1:B:663:TYR:CE2	1:B:681:LYS:HG3	2.52	0.45
1:C:596:PHE:HA	1:C:608:MET:HE2	1.99	0.45
1:D:590:TRP:HE1	1:D:608:MET:HE1	1.81	0.45
1:B:344:TRP:HB3	1:B:369:LEU:HD11	1.99	0.44
1:D:63:ILE:HD12	1:D:67:THR:HG22	1.99	0.44
1:C:607:ASP:HA	1:C:651:VAL:HG13	1.99	0.44
1:D:104:LEU:N	1:D:104:LEU:HD22	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:ASP:O	1:B:662:LYS:HE3	2.17	0.44
1:B:448:VAL:O	1:B:452:GLU:HG2	2.17	0.44
1:C:210:VAL:HB	1:C:225:LEU:HD13	1.99	0.44
1:C:254:GLU:HG2	5:C:694:HOH:O	2.18	0.44
1:C:606:TYR:O	1:C:610:LEU:HB2	2.17	0.44
1:C:643:GLN:O	1:C:646:ASN:HB3	2.16	0.44
1:A:552:ILE:HD13	1:A:552:ILE:HA	1.78	0.44
1:D:572:LYS:HG3	1:D:578:ILE:HG21	1.99	0.44
1:B:91:TYR:HA	1:B:94:ILE:HG22	1.98	0.44
1:B:357:HIS:CD2	1:B:357:HIS:C	2.91	0.44
1:B:606:TYR:CE2	1:B:652:ASN:OD1	2.71	0.44
1:D:243:ALA:HA	1:D:244:PRO:HD2	1.89	0.44
1:D:613:SER:HA	1:D:618:PHE:CE1	2.53	0.44
1:A:602:ASN:O	1:A:603:ALA:CB	2.64	0.44
1:B:645:GLU:OE2	1:B:645:GLU:HA	2.18	0.44
1:C:239:ASP:HB2	1:C:242:MET:CG	2.47	0.44
1:C:312:TRP:HA	5:C:752:HOH:O	2.16	0.44
1:C:328:THR:N	1:C:329:PRO:CD	2.81	0.44
1:C:565:TRP:CE2	1:C:572:LYS:HE2	2.53	0.44
1:D:679:TRP:CG	5:D:804:HOH:O	2.68	0.44
1:A:85:ASN:C	1:A:85:ASN:HD22	2.21	0.44
1:B:447:ILE:O	1:B:451:VAL:HG23	2.18	0.44
1:B:602:ASN:O	1:B:603:ALA:CB	2.66	0.44
1:C:64:ASP:CG	1:C:67:THR:HG22	2.37	0.44
1:D:131:VAL:HG12	1:D:135:LYS:CE	2.40	0.44
1:D:298:ASN:CG	1:D:299:GLN:H	2.20	0.44
1:A:536:PHE:HZ	1:A:584:MET:O	2.01	0.44
1:A:655:LEU:CD2	1:A:657:ARG:NH1	2.81	0.44
1:C:391:GLY:C	1:C:393:GLU:H	2.20	0.44
1:A:65:ALA:HA	5:A:784:HOH:O	2.17	0.44
1:A:350:TRP:CD1	1:A:350:TRP:N	2.86	0.44
1:A:566:PRO:C	1:A:567:ILE:HD13	2.38	0.44
1:B:80:ASN:ND2	1:B:82:VAL:HB	2.32	0.44
1:B:334:SER:HB2	5:B:789:HOH:O	2.17	0.44
1:C:568:TYR:CG	1:C:569:SER:N	2.86	0.44
1:D:660:ILE:HD12	1:D:660:ILE:N	2.32	0.44
1:A:177:THR:OG1	1:A:250:GLN:NE2	2.50	0.43
1:A:328:THR:N	1:A:329:PRO:CD	2.81	0.43
1:A:613:SER:HA	1:A:618:PHE:CE1	2.53	0.43
1:B:495:LYS:O	1:B:497:LYS:HG3	2.18	0.43
1:C:410:GLN:HE22	1:C:419:LYS:H	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:517:GLN:HE22	1:C:583:ARG:HH11	1.66	0.43
1:C:565:TRP:CD2	1:C:572:LYS:HE2	2.53	0.43
1:A:124:PRO:HB3	1:A:132:TRP:CD2	2.53	0.43
1:A:501:SER:N	1:A:598:GLU:HG2	2.32	0.43
1:C:363:ASN:HB2	1:C:409:LEU:HD21	2.01	0.43
1:C:596:PHE:CD1	1:C:608:MET:HE3	2.53	0.43
1:D:356:THR:HG23	1:D:357:HIS:N	2.33	0.43
1:D:371:ARG:NH2	1:D:512:GLY:O	2.51	0.43
1:D:600:ILE:HD11	1:D:604:VAL:HA	2.01	0.43
1:A:79:LEU:HD22	1:A:83:GLU:HG2	1.99	0.43
1:B:156:ILE:HG23	1:B:238:LEU:O	2.17	0.43
1:B:404:ILE:CD1	1:B:406:VAL:HB	2.45	0.43
1:C:107:VAL:HG12	1:C:108:GLU:H	1.83	0.43
1:C:172:LEU:HD23	1:C:172:LEU:HA	1.86	0.43
1:C:177:THR:OG1	1:C:250:GLN:NE2	2.50	0.43
1:C:607:ASP:OD2	1:C:611:LYS:HE3	2.17	0.43
1:A:167:ILE:HG23	1:A:281:PHE:CE2	2.53	0.43
1:A:291:ILE:HG23	1:A:292:PRO:HD2	2.00	0.43
1:B:549:ASN:C	1:B:624:ILE:HG23	2.38	0.43
1:B:611:LYS:O	1:B:614:GLU:HG3	2.18	0.43
1:C:335:GLY:H	1:C:362:ASP:CG	2.22	0.43
1:C:499:ILE:HD12	1:C:499:ILE:C	2.38	0.43
1:D:444:SER:HB2	1:D:473:ASP:OD1	2.18	0.43
1:A:503:SER:HB3	1:A:596:PHE:CE1	2.54	0.43
1:B:271:ILE:C	1:B:271:ILE:HD12	2.38	0.43
1:B:476:LEU:O	1:B:480:GLN:HG3	2.18	0.43
1:C:61:ILE:O	1:C:62:ASP:CB	2.66	0.43
1:C:239:ASP:HB2	1:C:242:MET:HG2	2.00	0.43
1:C:318:LYS:HB2	1:C:318:LYS:NZ	2.33	0.43
1:C:441:TYR:CZ	1:C:442:ASN:ND2	2.86	0.43
1:A:499:ILE:CD1	2:A:684:UGA:H5A1	2.48	0.43
1:B:213:LYS:HD2	1:B:215:TYR:CD1	2.54	0.43
1:B:395:GLU:OE2	1:B:395:GLU:C	2.57	0.43
1:B:655:LEU:HD22	1:B:655:LEU:HA	1.85	0.43
1:C:219:LEU:O	1:C:222:VAL:HG12	2.19	0.43
1:C:596:PHE:N	1:C:608:MET:HE1	2.33	0.43
1:D:546:TYR:N	1:D:546:TYR:CD2	2.87	0.43
1:A:565:TRP:CD2	1:A:572:LYS:HE2	2.54	0.43
1:A:629:VAL:C	1:A:630:LEU:HD12	2.39	0.43
1:B:331:ARG:HH11	1:B:331:ARG:HB3	1.84	0.43
1:D:358:TRP:CD1	1:D:408:LEU:HD22	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:LEU:O	1:A:509:LEU:HD13	2.18	0.43
1:B:100:GLU:CD	1:B:624:ILE:HD12	2.39	0.43
1:B:682:ILE:HD12	1:B:682:ILE:H	1.83	0.43
1:C:227:LEU:HD23	1:C:227:LEU:HA	1.91	0.43
1:A:79:LEU:HD22	1:A:83:GLU:CG	2.48	0.43
1:A:607:ASP:HA	1:A:651:VAL:HG13	2.01	0.43
1:A:630:LEU:HD12	1:A:630:LEU:N	2.33	0.43
1:B:238:LEU:HD21	1:B:244:PRO:HD3	1.99	0.43
1:B:288:ILE:HG23	1:B:289:ASN:ND2	2.34	0.43
1:B:577:MET:SD	1:B:606:TYR:CD1	3.12	0.43
1:C:114:TRP:CZ2	1:C:120:LEU:HD13	2.54	0.43
1:D:109:PRO:O	1:D:110:ILE:C	2.58	0.43
1:A:72:SER:HB2	1:A:79:LEU:HD12	1.99	0.43
1:A:499:ILE:HD12	2:A:684:UGA:H5A1	2.01	0.43
1:C:79:LEU:HD21	1:C:83:GLU:CB	2.48	0.43
1:D:136:ARG:HG2	1:D:136:ARG:NH1	2.34	0.43
1:D:271:ILE:HA	1:D:294:ILE:HG23	2.01	0.43
1:A:550:ARG:HB3	1:A:624:ILE:HG21	1.99	0.42
1:A:619:LYS:HD2	1:A:620:HIS:N	2.34	0.42
1:A:653:GLU:OE1	1:A:665:TYR:O	2.37	0.42
1:B:80:ASN:HD22	1:B:80:ASN:C	2.22	0.42
1:B:288:ILE:HG13	1:B:385:TYR:CD2	2.54	0.42
1:C:242:MET:HE2	1:C:337:ASN:HB2	2.01	0.42
1:C:490:ARG:NH2	1:C:511:ARG:NE	2.67	0.42
1:C:490:ARG:HH12	1:C:511:ARG:HD2	1.82	0.42
1:D:67:THR:OG1	1:D:488:ARG:HD3	2.18	0.42
1:D:565:TRP:HA	1:D:566:PRO:HD2	1.81	0.42
1:A:110:ILE:HG22	1:A:111:PRO:O	2.20	0.42
1:A:152:LEU:HD22	1:A:153:SER:N	2.35	0.42
1:A:260:ASP:HB2	1:A:341:ALA:HB2	2.00	0.42
1:A:637:ILE:CB	1:A:640:LEU:HB2	2.49	0.42
1:B:107:VAL:O	1:B:107:VAL:HG13	2.18	0.42
1:B:195:GLU:HG2	1:B:199:ARG:HD2	2.01	0.42
1:C:476:LEU:O	1:C:480:GLN:HG3	2.19	0.42
1:C:570:ARG:HD3	5:C:764:HOH:O	2.19	0.42
1:C:610:LEU:CD2	1:C:651:VAL:HG12	2.49	0.42
1:D:542:LEU:HD21	1:D:619:LYS:CB	2.49	0.42
1:A:314:ILE:HA	1:A:317:PHE:HD2	1.84	0.42
1:B:108:GLU:OE1	1:B:112:LEU:HD13	2.19	0.42
1:B:576:ALA:O	1:B:578:ILE:N	2.51	0.42
1:C:654:SER:C	1:C:656:SER:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:545:VAL:HG23	1:D:545:VAL:O	2.19	0.42
1:A:389:PRO:HA	1:A:390:PRO:HD2	1.92	0.42
1:B:124:PRO:HD3	1:B:132:TRP:CZ2	2.54	0.42
1:D:94:ILE:HG12	1:D:94:ILE:O	2.18	0.42
1:A:655:LEU:HD22	1:A:655:LEU:HA	1.81	0.42
1:A:675:ARG:HG2	1:A:675:ARG:NH1	2.34	0.42
1:B:218:GLN:HB3	1:B:221:ALA:HB3	2.01	0.42
1:C:121:PRO:HA	1:C:122:PRO:HD3	1.73	0.42
1:C:462:LEU:HD23	1:C:462:LEU:C	2.39	0.42
1:C:504:ASN:HB3	1:C:508:ARG:CZ	2.49	0.42
1:D:102:ALA:O	1:D:104:LEU:HD22	2.20	0.42
1:D:354:GLU:CD	1:D:430:ARG:HH22	2.22	0.42
1:B:256:LEU:HA	1:B:256:LEU:HD23	1.79	0.42
1:B:409:LEU:N	1:B:409:LEU:CD2	2.82	0.42
1:B:459:ILE:HG12	1:B:530:GLU:HB2	2.01	0.42
1:B:513:PHE:CZ	1:B:586:THR:HG23	2.55	0.42
1:C:533:LEU:HD12	1:C:533:LEU:HA	1.77	0.42
1:C:614:GLU:OE2	1:C:655:LEU:CD2	2.59	0.42
1:D:356:THR:HG23	1:D:357:HIS:H	1.83	0.42
1:D:458:THR:HG21	1:D:530:GLU:OE1	2.19	0.42
1:A:488:ARG:NH2	5:A:706:HOH:O	2.53	0.42
1:A:69:ILE:HD11	1:A:88:ILE:HA	2.01	0.42
1:A:125:GLU:HG2	1:A:325:LEU:HD11	2.01	0.42
1:A:228:ARG:HB3	1:B:228:ARG:O	2.20	0.42
1:A:606:TYR:O	1:A:610:LEU:HB2	2.20	0.42
1:B:418:ARG:HE	1:B:429:LYS:HG3	1.84	0.42
1:B:429:LYS:HA	1:B:429:LYS:HD3	1.93	0.42
1:B:533:LEU:HA	1:B:533:LEU:HD12	1.86	0.42
1:B:649:LYS:HE3	1:B:667:PRO:HG3	2.01	0.42
1:C:596:PHE:CD2	1:C:608:MET:CE	3.03	0.42
1:D:466:ILE:HB	1:D:491:PHE:HB3	2.01	0.42
1:D:517:GLN:NE2	1:D:583:ARG:HH11	2.18	0.42
1:A:160:ASN:CB	1:A:190:SER:HB3	2.38	0.42
1:A:429:LYS:HD3	1:A:429:LYS:HA	1.87	0.42
1:B:120:LEU:HD21	1:B:574:THR:HG21	2.02	0.42
1:C:64:ASP:HB2	5:C:706:HOH:O	2.19	0.42
1:C:177:THR:HA	1:C:250:GLN:HE21	1.84	0.42
1:C:596:PHE:CZ	1:C:608:MET:HE3	2.55	0.42
1:D:63:ILE:HD12	1:D:67:THR:CG2	2.49	0.42
1:A:331:ARG:NH1	5:A:760:HOH:O	2.53	0.42
1:A:449:ARG:HD3	1:A:523:PHE:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:LEU:HB3	5:A:748:HOH:O	2.20	0.42
1:A:537:ARG:NH1	5:A:748:HOH:O	2.52	0.42
1:A:544:CYS:O	1:A:618:PHE:HA	2.20	0.42
1:B:174:ASN:HB3	1:B:285:LYS:HB2	2.02	0.42
1:C:289:ASN:ND2	1:C:385:TYR:OH	2.52	0.42
1:C:490:ARG:NH1	1:C:511:ARG:CD	2.83	0.42
1:D:411:GLN:HE21	1:D:430:ARG:H	1.65	0.42
1:A:372:GLU:HA	1:A:372:GLU:OE2	2.20	0.41
1:A:548:THR:HG22	1:A:623:LYS:C	2.39	0.41
1:B:89:SER:HA	1:B:92:ARG:HB2	2.02	0.41
1:B:499:ILE:HD13	2:B:683:UGA:O4D	2.20	0.41
1:B:565:TRP:CZ2	1:B:572:LYS:HE2	2.55	0.41
1:C:504:ASN:ND2	1:C:598:GLU:OE1	2.44	0.41
1:A:420:LYS:CE	1:A:420:LYS:H	2.32	0.41
1:A:501:SER:CA	1:A:598:GLU:HG2	2.50	0.41
1:A:546:TYR:CE1	1:A:579:CYS:HA	2.55	0.41
1:A:565:TRP:NE1	1:A:572:LYS:HG2	2.35	0.41
1:B:91:TYR:CD2	1:B:423:ILE:HG21	2.55	0.41
1:B:123:LEU:HB3	1:B:124:PRO:HD2	2.02	0.41
1:C:269:LYS:HG3	1:C:383:MET:SD	2.60	0.41
1:C:404:ILE:HG13	1:C:407:GLN:HE21	1.86	0.41
1:D:115:PRO:HB2	1:D:118:LEU:HB3	1.99	0.41
1:D:334:SER:HB3	5:D:787:HOH:O	2.19	0.41
1:B:120:LEU:HD12	1:B:660:ILE:HD11	2.02	0.41
1:C:492:ILE:HG12	1:C:493:SER:H	1.85	0.41
1:D:73:ASN:C	1:D:75:LYS:H	2.23	0.41
1:D:114:TRP:O	1:D:115:PRO:C	2.57	0.41
1:D:448:VAL:O	1:D:452:GLU:HG2	2.20	0.41
1:D:607:ASP:OD1	1:D:611:LYS:HE3	2.20	0.41
1:A:462:LEU:HD21	5:A:706:HOH:O	2.20	0.41
1:B:105:LYS:HG2	1:B:566:PRO:CG	2.49	0.41
1:B:121:PRO:HG2	1:B:658:LEU:O	2.20	0.41
1:B:622:ASN:O	1:B:623:LYS:HG3	2.20	0.41
1:C:596:PHE:CE1	1:C:608:MET:HE3	2.56	0.41
1:D:218:GLN:HB3	1:D:221:ALA:HB3	2.03	0.41
1:D:231:LYS:HE3	1:D:232:TYR:CZ	2.55	0.41
1:D:358:TRP:CD1	1:D:358:TRP:N	2.85	0.41
1:A:90:LYS:O	1:A:94:ILE:HG22	2.20	0.41
1:A:152:LEU:HD21	1:A:236:ALA:HB2	2.00	0.41
1:B:367:TYR:CD1	1:B:413:VAL:HG13	2.55	0.41
1:C:108:GLU:O	1:C:108:GLU:CD	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:ASP:C	1:C:214:ASP:OD1	2.59	0.41
1:D:345:LEU:C	1:D:347:ARG:H	2.24	0.41
1:D:476:LEU:O	1:D:476:LEU:HD12	2.20	0.41
1:D:574:THR:O	1:D:652:ASN:ND2	2.52	0.41
1:A:160:ASN:N	1:A:160:ASN:ND2	2.68	0.41
1:B:153:SER:CB	1:B:230:ALA:HB1	2.50	0.41
1:B:158:THR:OG1	1:B:240:CYS:HB3	2.20	0.41
1:C:442:ASN:HA	1:C:473:ASP:OD1	2.19	0.41
1:A:418:ARG:NH2	1:A:431:VAL:O	2.50	0.41
1:A:435:SER:O	1:A:515:ILE:HA	2.21	0.41
1:B:114:TRP:HZ3	1:B:574:THR:OG1	2.04	0.41
1:C:195:GLU:OE2	1:C:199:ARG:NH1	2.54	0.41
1:C:621:ILE:HG22	1:C:623:LYS:CG	2.51	0.41
1:C:642:ILE:CD1	1:C:672:ASN:OD1	2.69	0.41
1:D:107:VAL:HG13	1:D:107:VAL:O	2.21	0.41
1:D:671:LEU:O	1:D:673:GLU:N	2.54	0.41
1:A:222:VAL:CG1	1:A:223:ARG:N	2.84	0.41
1:A:653:GLU:O	1:A:656:SER:CB	2.68	0.41
1:B:390:PRO:HD2	1:B:393:GLU:CD	2.41	0.41
1:B:433:LEU:HD21	1:B:514:TYR:HD2	1.86	0.41
1:B:596:PHE:HA	1:B:608:MET:HE1	2.03	0.41
1:C:64:ASP:HA	5:C:743:HOH:O	2.21	0.41
1:C:153:SER:CB	1:C:230:ALA:HB1	2.51	0.41
1:C:680:GLU:HG3	1:C:682:ILE:HG23	2.02	0.41
1:D:63:ILE:HD12	1:D:67:THR:HB	2.02	0.41
1:D:72:SER:CA	1:D:77:ILE:HG12	2.48	0.41
1:A:103:GLU:OE1	1:A:104:LEU:N	2.42	0.41
1:A:228:ARG:O	1:B:228:ARG:HB3	2.21	0.41
1:A:242:MET:SD	1:A:386:HIS:HD2	2.44	0.41
1:A:269:LYS:HD2	1:A:385:TYR:CE1	2.53	0.41
1:A:334:SER:HB3	5:A:735:HOH:O	2.21	0.41
1:A:352:ASP:HB3	1:A:355:PHE:HD2	1.84	0.41
1:A:527:ASP:HB3	5:A:723:HOH:O	2.21	0.41
1:B:74:ALA:O	1:B:75:LYS:HB2	2.20	0.41
1:B:123:LEU:HA	5:B:705:HOH:O	2.20	0.41
1:B:210:VAL:HG12	1:B:225:LEU:CD1	2.51	0.41
1:B:565:TRP:CH2	1:B:572:LYS:HE2	2.56	0.41
1:C:70:MET:CE	1:C:488:ARG:HD2	2.51	0.41
1:C:120:LEU:HD21	1:C:574:THR:HG21	2.02	0.41
1:C:376:PHE:CD2	1:C:376:PHE:N	2.88	0.41
1:C:411:GLN:HE21	1:C:430:ARG:H	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:PRO:HB2	1:C:433:LEU:HD23	2.03	0.41
1:C:581:HIS:HD2	1:C:628:ARG:NH1	2.19	0.41
1:D:304:VAL:HG12	1:D:305:GLU:N	2.34	0.41
1:A:132:TRP:CD1	1:A:135:LYS:HE3	2.56	0.41
1:A:271:ILE:HD13	1:A:291:ILE:HB	2.03	0.41
1:B:172:LEU:CD2	1:B:244:PRO:HG3	2.51	0.41
1:A:69:ILE:HG22	1:A:73:ASN:ND2	2.36	0.40
1:A:250:GLN:HA	1:A:250:GLN:HE21	1.86	0.40
1:B:410:GLN:O	1:B:418:ARG:NH1	2.53	0.40
1:B:545:VAL:O	1:B:545:VAL:HG23	2.21	0.40
1:C:219:LEU:HD22	1:C:223:ARG:NE	2.36	0.40
1:D:610:LEU:HD12	1:D:610:LEU:HA	1.83	0.40
1:A:102:ALA:HB2	1:A:548:THR:HG21	2.04	0.40
1:A:596:PHE:CE1	1:A:608:MET:HE3	2.57	0.40
1:B:114:TRP:HZ3	1:B:574:THR:HG1	1.63	0.40
1:B:330:PHE:CZ	1:B:415:TYR:HD2	2.39	0.40
1:B:552:ILE:HG22	1:B:553:ASP:N	2.36	0.40
1:C:88:ILE:O	1:C:91:TYR:HB3	2.21	0.40
1:C:602:ASN:O	1:C:603:ALA:CB	2.69	0.40
1:D:273:THR:O	1:D:273:THR:HG23	2.21	0.40
1:D:466:ILE:HG22	1:D:467:CYS:N	2.36	0.40
1:D:588:ARG:HH11	1:D:588:ARG:HG3	1.85	0.40
1:A:662:LYS:HA	1:A:682:ILE:CD1	2.52	0.40
1:D:182:GLU:OE1	1:D:231:LYS:HG2	2.20	0.40
1:D:536:PHE:CE1	1:D:545:VAL:HG22	2.56	0.40
1:D:607:ASP:CG	1:D:611:LYS:HE3	2.41	0.40
1:A:528:ALA:CB	1:A:625:CYS:HB3	2.50	0.40
1:B:259:ASP:O	1:B:262:VAL:HG12	2.22	0.40
1:B:669:THR:HG21	1:B:671:LEU:CD1	2.49	0.40
1:C:243:ALA:O	1:C:385:TYR:N	2.33	0.40
1:C:546:TYR:CZ	1:C:620:HIS:HB2	2.56	0.40
1:D:550:ARG:O	1:D:550:ARG:HG3	2.20	0.40
2:A:684:UGA:O1A	2:A:684:UGA:O1B	2.39	0.40
1:B:262:VAL:HG13	1:B:262:VAL:O	2.22	0.40
1:B:532:CYS:HB3	1:B:545:VAL:CG2	2.52	0.40
1:B:565:TRP:HD1	1:B:567:ILE:O	2.05	0.40
1:B:640:LEU:HD12	1:B:640:LEU:N	2.36	0.40
1:D:504:ASN:HB3	1:D:508:ARG:HH12	1.85	0.40
1:D:568:TYR:CD2	1:D:618:PHE:HB2	2.55	0.40
1:D:573:LEU:HA	1:D:576:ALA:O	2.22	0.40
1:D:620:HIS:HE1	1:D:622:ASN:OD1	2.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	570/625 (91%)	508 (89%)	47 (8%)	15 (3%)	5 5
1	B	591/625 (95%)	527 (89%)	45 (8%)	19 (3%)	4 3
1	C	595/625 (95%)	546 (92%)	44 (7%)	5 (1%)	19 29
1	D	586/625 (94%)	526 (90%)	50 (8%)	10 (2%)	9 11
All	All	2342/2500 (94%)	2107 (90%)	186 (8%)	49 (2%)	7 8

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	GLU
1	A	292	PRO
1	A	657	ARG
1	B	638	LYS
1	C	638	LYS
1	D	109	PRO
1	D	285	LYS
1	D	299	GLN
1	A	160	ASN
1	A	162	ALA
1	A	286	SER
1	B	60	VAL
1	B	64	ASP
1	B	129	ASP
1	B	577	MET
1	B	637	ILE
1	B	657	ARG
1	C	62	ASP
1	C	296	THR
1	D	81	GLU

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Mol	Chain	Res	Type
1	D	407	GLN
1	A	540	LEU
1	B	97	LYS
1	B	562	GLY
1	B	646	ASN
1	C	634	ASN
1	D	672	ASN
1	A	109	PRO
1	A	202	GLU
1	A	672	ASN
1	B	115	PRO
1	B	473	ASP
1	B	672	ASN
1	D	106	GLU
1	A	81	GLU
1	A	311	ASP
1	A	439	PRO
1	A	496	ASN
1	B	415	TYR
1	D	239	ASP
1	A	526	PRO
1	B	390	PRO
1	D	580	HIS
1	B	660	ILE
1	D	110	ILE
1	B	107	VAL
1	B	566	PRO
1	C	61	ILE
1	B	109	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	521/558 (93%)	478 (92%)	43 (8%)	11 17
1	B	538/558 (96%)	493 (92%)	45 (8%)	11 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	540/558 (97%)	500 (93%)	40 (7%)	13	22
1	D	531/558 (95%)	492 (93%)	39 (7%)	14	22
All	All	2130/2232 (95%)	1963 (92%)	167 (8%)	12	19

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	90	LYS
1	A	92	ARG
1	A	93	GLU
1	A	104	LEU
1	A	120	LEU
1	A	125	GLU
1	A	152	LEU
1	A	160	ASN
1	A	174	ASN
1	A	195	GLU
1	A	208	LYS
1	A	219	LEU
1	A	222	VAL
1	A	225	LEU
1	A	245	ASN
1	A	262	VAL
1	A	361	GLU
1	A	380	GLU
1	A	408	LEU
1	A	420	LYS
1	A	422	LYS
1	A	444	SER
1	A	445	LYS
1	A	462	LEU
1	A	474	ASP
1	A	482	HIS
1	A	509	LEU
1	A	518	LEU
1	A	533	LEU
1	A	541	SER
1	A	542	LEU
1	A	545	VAL
1	A	554	ARG

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Mol	Chain	Res	Type
1	A	558	LEU
1	A	583	ARG
1	A	586	THR
1	A	610	LEU
1	A	631	HIS
1	A	638	LYS
1	A	641	ASP
1	A	646	ASN
1	A	655	LEU
1	B	77	ILE
1	B	80	ASN
1	B	90	LYS
1	B	92	ARG
1	B	93	GLU
1	B	101	ARG
1	B	104	LEU
1	B	137	LYS
1	B	161	ARG
1	B	208	LYS
1	B	213	LYS
1	B	219	LEU
1	B	222	VAL
1	B	225	LEU
1	B	307	ASN
1	B	308	LYS
1	B	315	GLU
1	B	318	LYS
1	B	357	HIS
1	B	361	GLU
1	B	371	ARG
1	B	390	PRO
1	B	393	GLU
1	B	395	GLU
1	B	404	ILE
1	B	410	GLN
1	B	418	ARG
1	B	421	GLU
1	B	423	ILE
1	B	427	THR
1	B	462	LEU
1	B	499	ILE
1	B	509	LEU

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Mol	Chain	Res	Type
1	B	515	ILE
1	B	518	LEU
1	B	533	LEU
1	B	537	ARG
1	B	542	LEU
1	B	614	GLU
1	B	634	ASN
1	B	638	LYS
1	B	646	ASN
1	B	655	LEU
1	B	661	LYS
1	B	682	ILE
1	C	79	LEU
1	C	92	ARG
1	C	93	GLU
1	C	101	ARG
1	C	120	LEU
1	C	152	LEU
1	C	199	ARG
1	C	219	LEU
1	C	225	LEU
1	C	260	ASP
1	C	262	VAL
1	C	273	THR
1	C	297	ASN
1	C	318	LYS
1	C	361	GLU
1	C	369	LEU
1	C	371	ARG
1	C	380	GLU
1	C	409	LEU
1	C	418	ARG
1	C	423	ILE
1	C	424	GLU
1	C	433	LEU
1	C	449	ARG
1	C	477	ARG
1	C	497	LYS
1	C	499	ILE
1	C	509	LEU
1	C	518	LEU
1	C	533	LEU

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Mol	Chain	Res	Type
1	C	537	ARG
1	C	542	LEU
1	C	545	VAL
1	C	554	ARG
1	C	583	ARG
1	C	586	THR
1	C	610	LEU
1	C	637	ILE
1	C	652	ASN
1	C	669	THR
1	D	62	ASP
1	D	64	ASP
1	D	90	LYS
1	D	103	GLU
1	D	120	LEU
1	D	136	ARG
1	D	137	LYS
1	D	147	LEU
1	D	206	ASN
1	D	211	ARG
1	D	213	LYS
1	D	219	LEU
1	D	222	VAL
1	D	225	LEU
1	D	273	THR
1	D	297	ASN
1	D	308	LYS
1	D	347	ARG
1	D	358	TRP
1	D	361	GLU
1	D	362	ASP
1	D	369	LEU
1	D	388	GLU
1	D	423	ILE
1	D	460	THR
1	D	462	LEU
1	D	474	ASP
1	D	518	LEU
1	D	536	PHE
1	D	537	ARG
1	D	546	TYR
1	D	553	ASP

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Mol	Chain	Res	Type
1	D	554	ARG
1	D	583	ARG
1	D	586	THR
1	D	641	ASP
1	D	643	GLN
1	D	646	ASN
1	D	670	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	174	ASN
1	A	175	GLN
1	A	245	ASN
1	A	250	GLN
1	A	284	GLN
1	A	289	ASN
1	A	387	GLN
1	A	411	GLN
1	A	517	GLN
1	A	557	ASN
1	A	620	HIS
1	A	643	GLN
1	A	646	ASN
1	A	647	HIS
1	B	80	ASN
1	B	174	ASN
1	B	175	GLN
1	B	212	GLN
1	B	245	ASN
1	B	250	GLN
1	B	289	ASN
1	B	307	ASN
1	B	387	GLN
1	B	407	GLN
1	B	410	GLN
1	B	411	GLN
1	B	517	GLN
1	B	557	ASN
1	B	620	HIS
1	B	643	GLN

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Mol	Chain	Res	Type
1	B	646	ASN
1	B	670	ASN
1	C	80	ASN
1	C	85	ASN
1	C	174	ASN
1	C	175	GLN
1	C	212	GLN
1	C	245	ASN
1	C	250	GLN
1	C	289	ASN
1	C	297	ASN
1	C	363	ASN
1	C	387	GLN
1	C	407	GLN
1	C	410	GLN
1	C	411	GLN
1	C	517	GLN
1	C	557	ASN
1	C	620	HIS
1	C	631	HIS
1	D	73	ASN
1	D	174	ASN
1	D	175	GLN
1	D	206	ASN
1	D	212	GLN
1	D	245	ASN
1	D	250	GLN
1	D	289	ASN
1	D	298	ASN
1	D	299	GLN
1	D	306	GLN
1	D	387	GLN
1	D	410	GLN
1	D	411	GLN
1	D	517	GLN
1	D	557	ASN
1	D	620	HIS
1	D	643	GLN
1	D	646	ASN
1	D	670	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
4	UDP	C	1	3	24,26,26	0.97	2 (8%)	37,40,40	1.67	6 (16%)
2	UGA	A	683	3	32,39,39	1.47	1 (3%)	42,60,60	1.16	5 (11%)
2	UGA	D	684	3	32,39,39	1.45	2 (6%)	42,60,60	1.30	7 (16%)
4	UDP	B	1	3	24,26,26	0.83	0	37,40,40	1.52	6 (16%)
2	UGA	B	683	3	32,39,39	1.43	1 (3%)	42,60,60	1.17	3 (7%)
2	UGA	C	683	3	32,39,39	1.47	1 (3%)	42,60,60	1.27	7 (16%)
2	UGA	A	684	3	32,39,39	1.41	1 (3%)	42,60,60	1.26	6 (14%)
2	UGA	D	683	3	32,39,39	1.45	1 (3%)	42,60,60	1.02	3 (7%)

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
4	UDP	C	1	3	-	3/16/32/32	0/2/2/2
2	UGA	A	683	3	-	5/23/61/61	0/3/3/3
2	UGA	D	684	3	-	7/23/61/61	0/3/3/3
4	UDP	B	1	3	-	1/16/32/32	0/2/2/2
2	UGA	B	683	3	-	6/23/61/61	0/3/3/3
2	UGA	C	683	3	-	6/23/61/61	0/3/3/3
2	UGA	A	684	3	-	6/23/61/61	0/3/3/3
2	UGA	D	683	3	-	5/23/61/61	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	683	UGA	O'P-C6'	7.03	1.43	1.22
2	D	683	UGA	O'P-C6'	7.02	1.43	1.22
2	A	683	UGA	O'P-C6'	7.01	1.43	1.22
2	D	684	UGA	O'P-C6'	7.00	1.43	1.22
2	C	683	UGA	O'P-C6'	6.89	1.43	1.22
2	A	684	UGA	O'P-C6'	6.58	1.42	1.22
4	C	1	UDP	C2-N1	2.81	1.42	1.38
4	C	1	UDP	C5-C4	-2.03	1.39	1.43
2	D	684	UGA	O4D-C1D	2.02	1.43	1.41

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1	UDP	C4-N3-C2	-4.85	120.19	126.58
4	B	1	UDP	C4-N3-C2	-4.37	120.82	126.58
4	C	1	UDP	O4-C4-C5	-4.25	117.69	125.16
4	B	1	UDP	N3-C2-N1	3.60	119.67	114.89
4	C	1	UDP	N3-C2-N1	3.48	119.50	114.89
4	C	1	UDP	C5-C4-N3	3.43	119.97	114.84
2	D	684	UGA	C1'-O5'-C5'	3.42	117.84	112.20
4	B	1	UDP	C5-C4-N3	3.39	119.91	114.84
2	D	683	UGA	O4D-C1D-C2D	-3.17	102.30	106.93
4	B	1	UDP	O4-C4-C5	-3.06	119.78	125.16
2	A	683	UGA	C1'-O5'-C5'	2.97	117.09	112.20
2	C	683	UGA	PA-O3A-PB	-2.83	123.12	132.83
2	A	684	UGA	PA-O3A-PB	-2.82	123.14	132.83
4	B	1	UDP	PA-O3A-PB	-2.56	124.05	132.83
2	A	683	UGA	O'Q-C6'-O'P	-2.48	118.45	124.09
2	B	683	UGA	O4D-C1D-C2D	-2.45	103.35	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	683	UGA	O5'-C1'-O3B	-2.42	108.20	111.36
2	A	684	UGA	O5'-C1'-O3B	-2.40	108.23	111.36
2	A	683	UGA	O5'-C5'-C6'	2.40	112.33	105.88
2	B	683	UGA	C3D-C2D-C1D	2.40	104.58	100.98
2	A	684	UGA	O2B-PB-O1B	2.37	123.96	112.24
2	C	683	UGA	O2B-PB-O1B	2.36	123.92	112.24
2	A	684	UGA	O5'-C1'-C2'	-2.35	105.38	110.35
2	A	683	UGA	O'Q-C6'-C5'	2.35	122.24	113.65
2	C	683	UGA	O5'-C1'-C2'	-2.33	105.42	110.35
2	D	684	UGA	PA-O3A-PB	-2.29	124.97	132.83
2	C	683	UGA	O5'-C5'-C6'	2.28	112.00	105.88
2	A	684	UGA	O5'-C5'-C6'	2.27	111.99	105.88
2	B	683	UGA	O'Q-C6'-O'P	-2.26	118.97	124.09
2	D	683	UGA	O'Q-C6'-O'P	-2.25	118.97	124.09
2	D	684	UGA	C3'-C4'-C5'	2.21	113.02	109.25
2	D	684	UGA	O'Q-C6'-O'P	-2.19	119.11	124.09
2	A	684	UGA	O'Q-C6'-C5'	2.18	121.63	113.65
2	C	683	UGA	O'Q-C6'-C5'	2.15	121.53	113.65
2	D	684	UGA	O5'-C1'-O3B	-2.08	108.64	111.36
2	D	684	UGA	O4D-C1D-C2D	-2.07	103.90	106.93
4	C	1	UDP	O4-C4-N3	2.07	122.34	119.31
2	D	684	UGA	O'Q-C6'-C5'	2.06	121.18	113.65
4	C	1	UDP	PA-O3A-PB	-2.05	125.79	132.83
2	D	683	UGA	O'Q-C6'-C5'	2.04	121.12	113.65
2	C	683	UGA	O'Q-C6'-O'P	-2.02	119.49	124.09
2	A	683	UGA	C5-C4-N3	-2.02	118.86	123.31
4	B	1	UDP	O3B-PB-O2B	2.01	115.33	107.64

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	683	UGA	O4D-C1D-N1-C6
2	A	683	UGA	C2D-C1D-N1-C6
2	A	684	UGA	O4D-C1D-N1-C6
2	A	684	UGA	C2D-C1D-N1-C6
2	B	683	UGA	O4D-C1D-N1-C6
2	B	683	UGA	C2D-C1D-N1-C6
2	C	683	UGA	O4D-C1D-N1-C6
2	C	683	UGA	C2D-C1D-N1-C6
2	D	683	UGA	O4D-C1D-N1-C6
2	D	683	UGA	C2D-C1D-N1-C6

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Mol	Chain	Res	Type	Atoms
2	D	684	UGA	O4D-C1D-N1-C6
2	D	684	UGA	C2D-C1D-N1-C6
2	A	684	UGA	C1'-O3B-PB-O3A
2	B	683	UGA	C1'-O3B-PB-O3A
2	C	683	UGA	C1'-O3B-PB-O3A
2	D	683	UGA	C1'-O3B-PB-O3A
2	D	684	UGA	C1'-O3B-PB-O3A
2	A	683	UGA	C2'-C1'-O3B-PB
2	D	683	UGA	C2'-C1'-O3B-PB
4	C	1	UDP	PA-O3A-PB-O1B
2	A	684	UGA	C5D-O5D-PA-O3A
2	C	683	UGA	C5D-O5D-PA-O3A
2	D	684	UGA	C5D-O5D-PA-O3A
4	B	1	UDP	C5'-O5'-PA-O3A
2	A	683	UGA	PB-O3A-PA-O1A
2	A	684	UGA	C1'-O3B-PB-O1B
2	C	683	UGA	C1'-O3B-PB-O1B
2	D	684	UGA	C1'-O3B-PB-O1B
2	D	684	UGA	C1'-O3B-PB-O2B
2	D	684	UGA	C4D-C5D-O5D-PA
2	B	683	UGA	PB-O3A-PA-O1A
2	D	683	UGA	PB-O3A-PA-O1A
2	A	684	UGA	C4D-C5D-O5D-PA
2	C	683	UGA	C4D-C5D-O5D-PA
4	C	1	UDP	PA-O3A-PB-O2B
4	C	1	UDP	PA-O3A-PB-O3B
2	A	683	UGA	PB-O3A-PA-O2A
2	B	683	UGA	C1'-O3B-PB-O1B
2	B	683	UGA	PB-O3A-PA-O2A

There are no ring outliers.

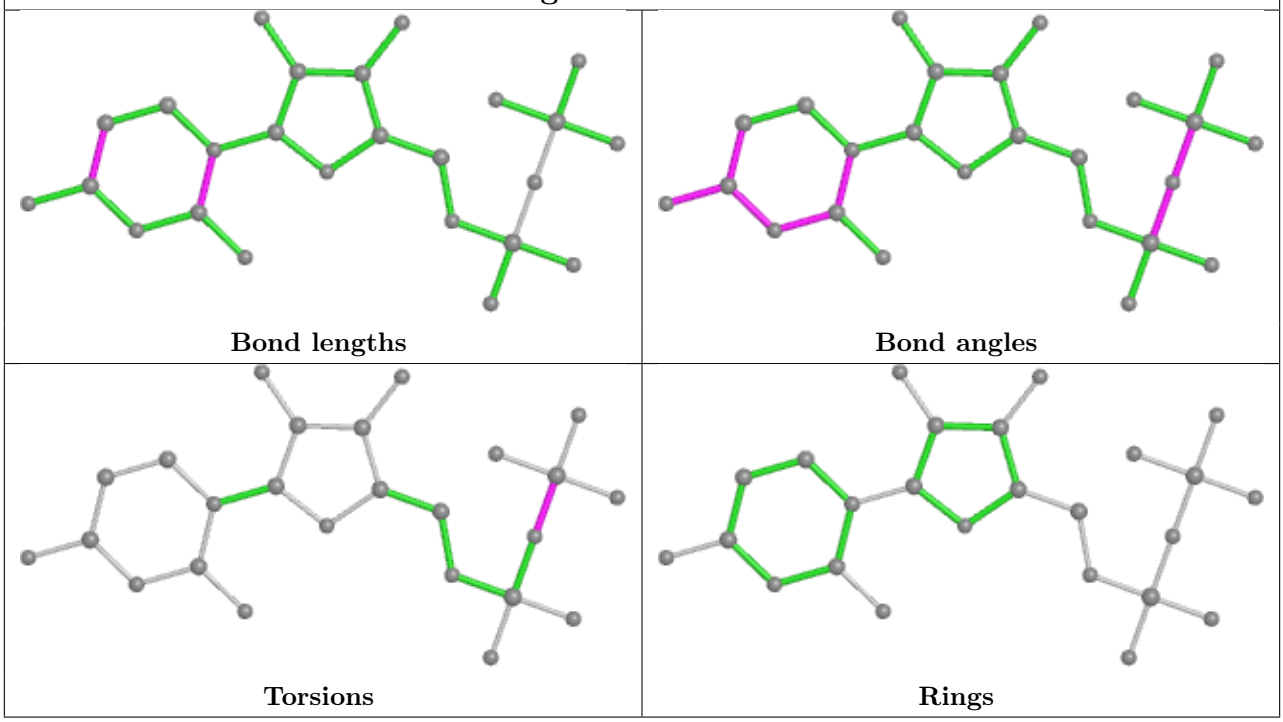
2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	683	UGA	1	0
2	A	684	UGA	9	0

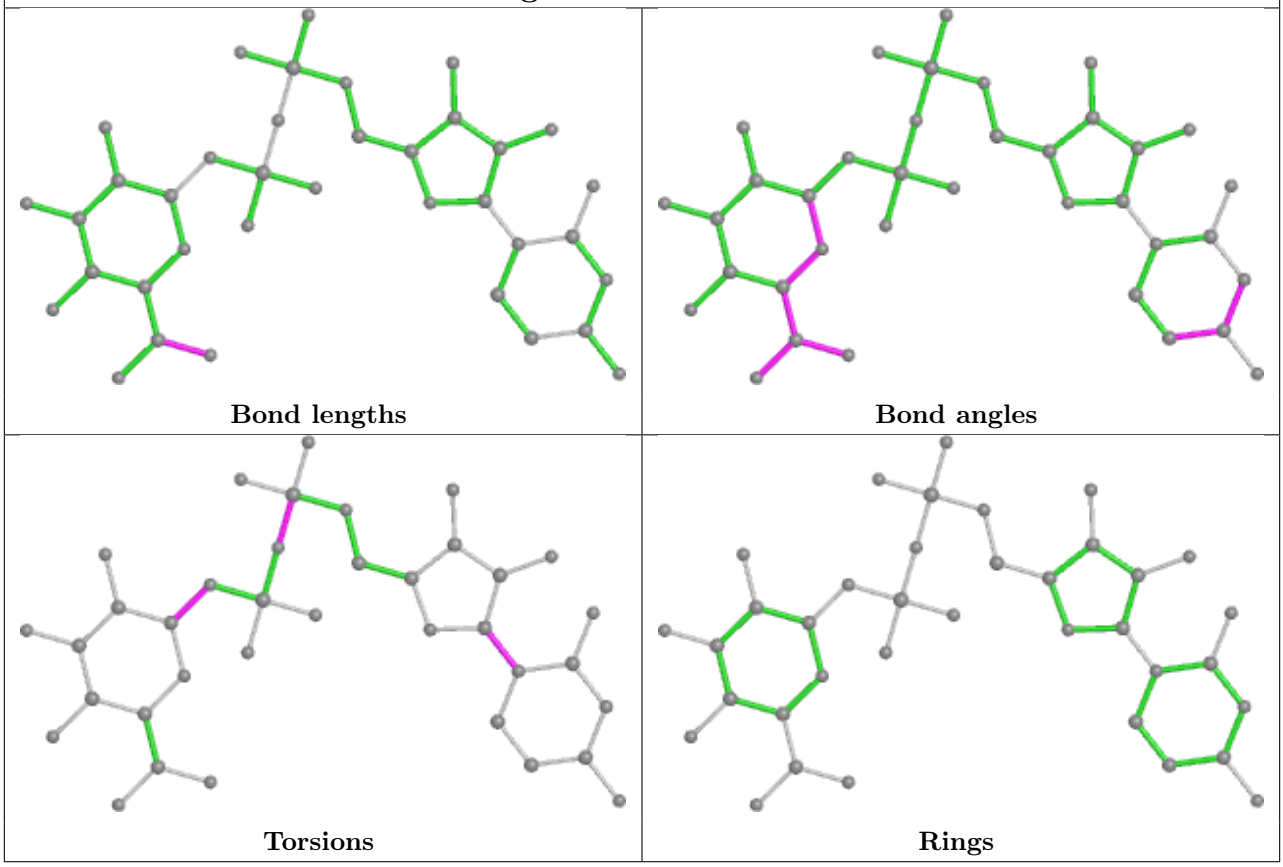
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

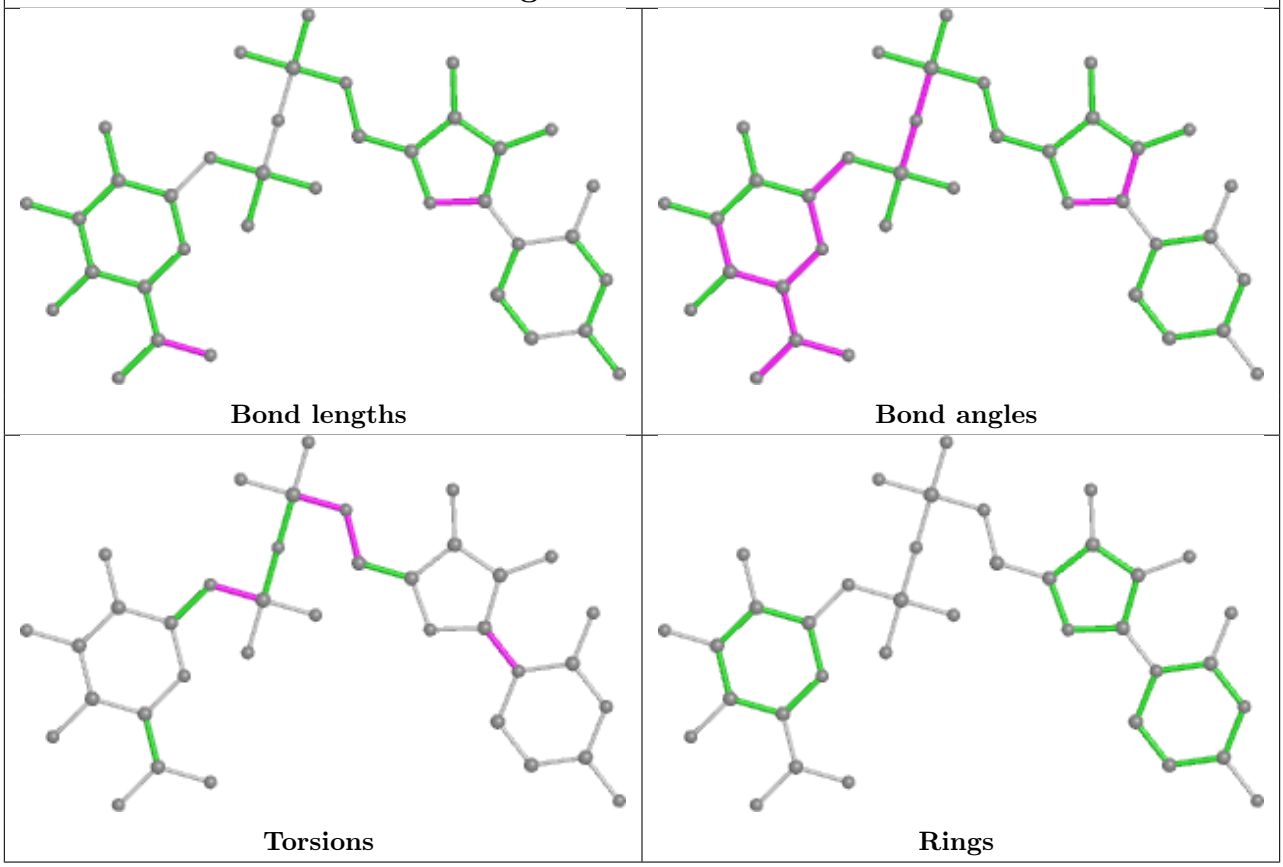
Ligand UDP C 1



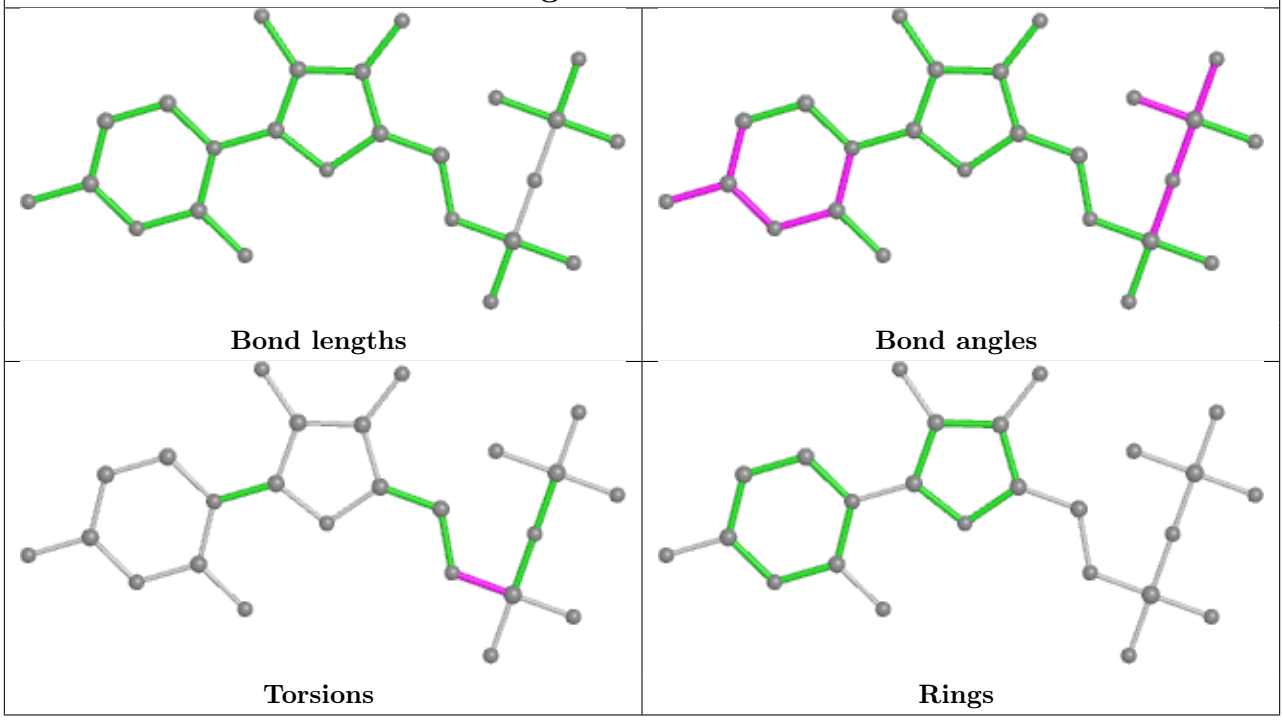
Ligand UGA A 683



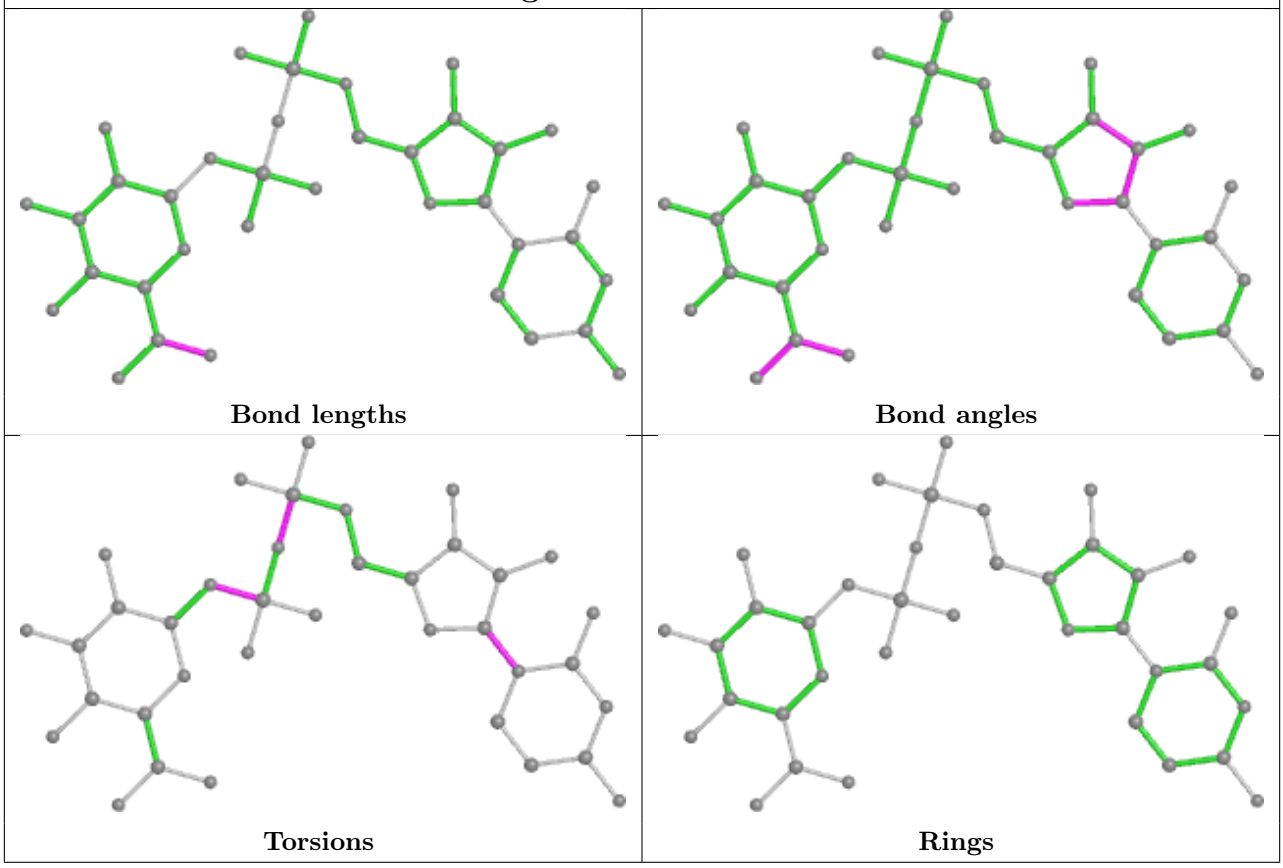
Ligand UGA D 684



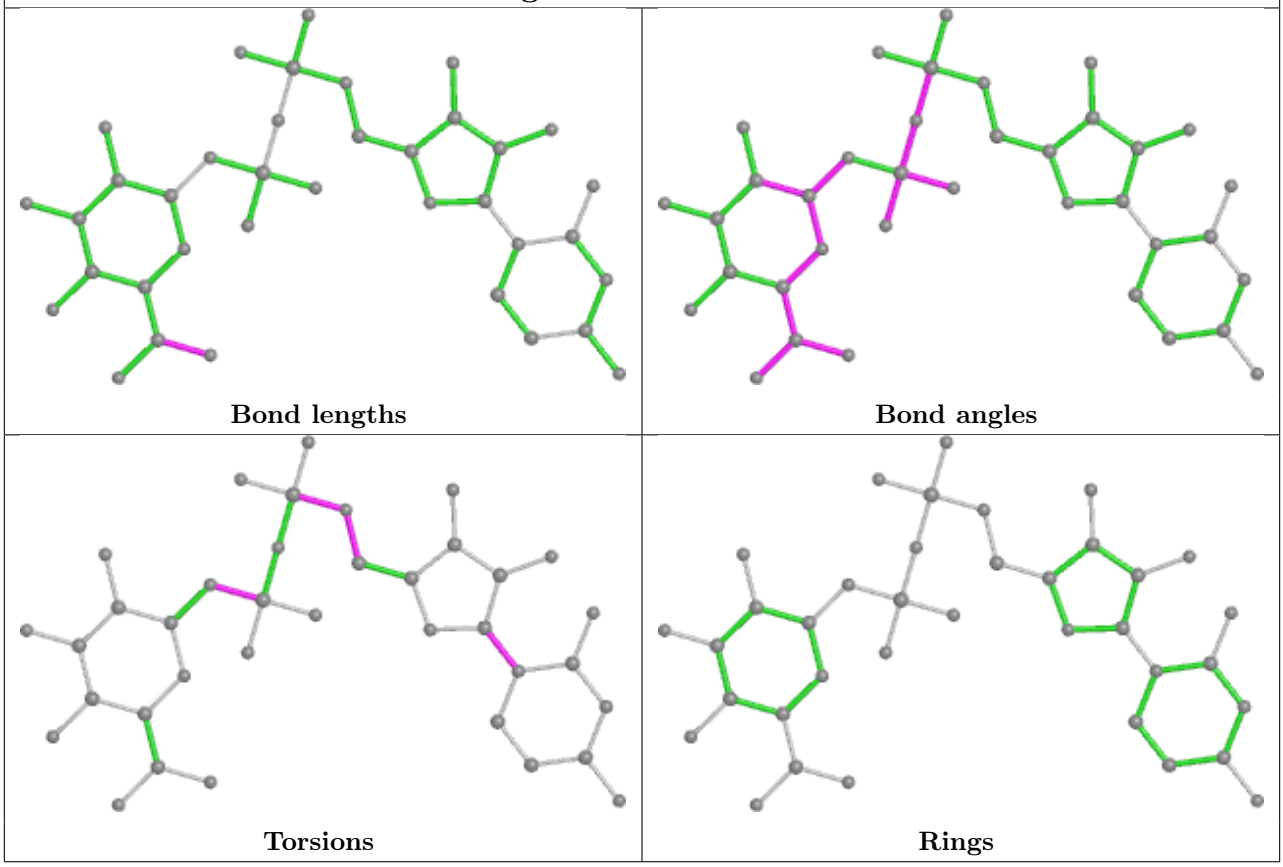
Ligand UDP B 1



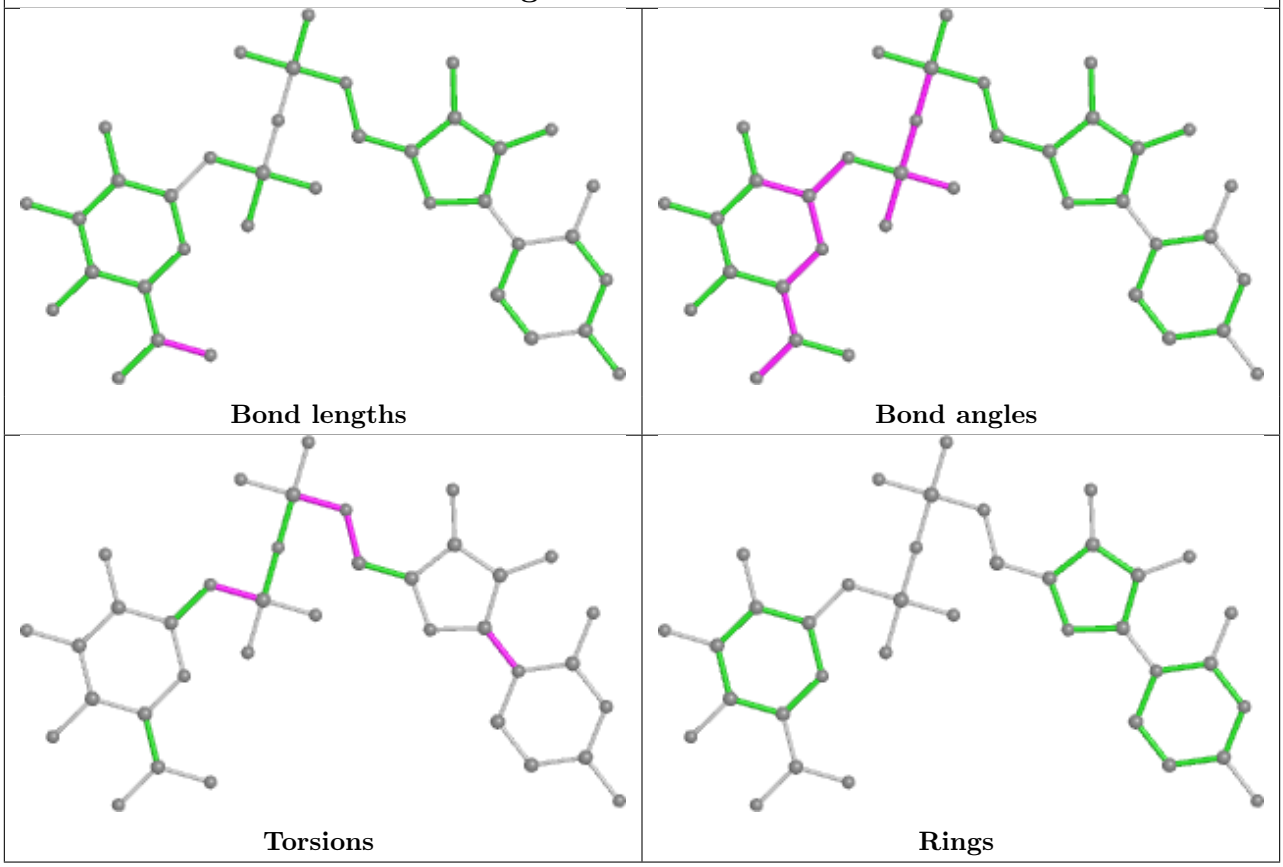
Ligand UGA B 683

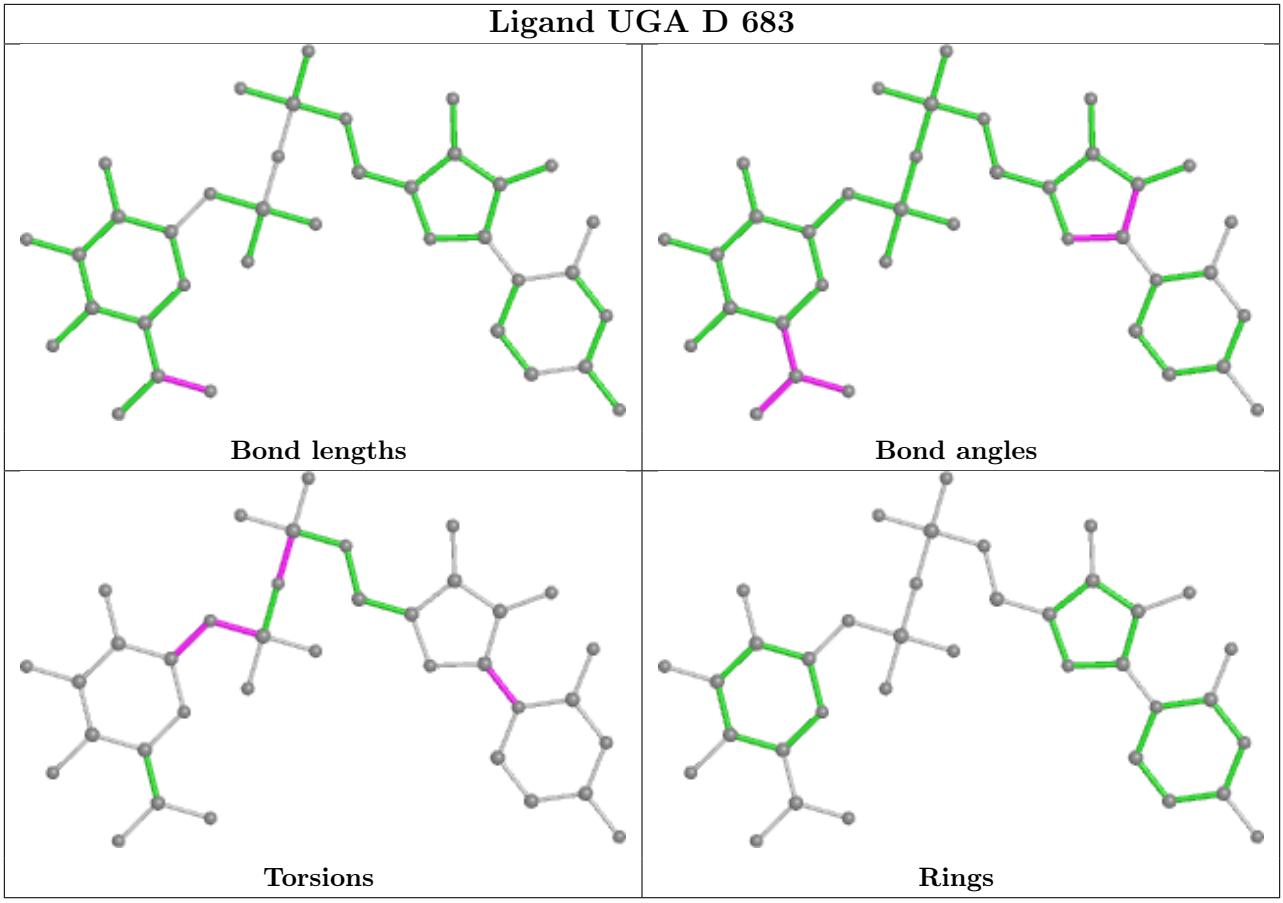


Ligand UGA C 683



Ligand UGA A 684





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	580/625 (92%)	0.24	23 (3%)	38	37	34, 54, 83, 105	20 (3%)
1	B	601/625 (96%)	0.09	11 (1%)	68	66	30, 48, 80, 99	22 (3%)
1	C	603/625 (96%)	-0.01	13 (2%)	62	60	21, 40, 69, 99	22 (3%)
1	D	594/625 (95%)	0.23	29 (4%)	29	28	29, 52, 92, 107	21 (3%)
All	All	2378/2500 (95%)	0.13	76 (3%)	47	46	21, 49, 83, 107	85 (3%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	77	ILE	8.3
1	D	60	VAL	6.7
1	D	300	VAL	6.5
1	C	296	THR	4.5
1	B	107	VAL	4.4
1	A	668	LEU	4.3
1	D	79	LEU	4.2
1	D	78	SER	4.1
1	A	390	PRO	4.0
1	C	632	GLY	4.0
1	D	299	GLN	4.0
1	C	60	VAL	3.9
1	A	655	LEU	3.6
1	D	301	ALA	3.6
1	C	637	ILE	3.5
1	D	682	ILE	3.4
1	D	59	ALA	3.4
1	A	640	LEU	3.3
1	A	389	PRO	3.2
1	A	660	ILE	3.2
1	A	281	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	630	LEU	3.1
1	A	279	LEU	3.1
1	D	405	THR	3.1
1	A	282	LEU	2.9
1	A	492	ILE	2.9
1	C	404	ILE	2.9
1	A	661	LYS	2.8
1	D	655	LEU	2.8
1	D	660	ILE	2.8
1	D	298	ASN	2.8
1	A	664	LYS	2.7
1	D	681	LYS	2.7
1	D	76	ALA	2.7
1	B	296	THR	2.7
1	D	204	LEU	2.6
1	D	107	VAL	2.6
1	A	247	LEU	2.6
1	D	652	ASN	2.6
1	B	295	ILE	2.5
1	D	304	VAL	2.5
1	D	610	LEU	2.5
1	D	671	LEU	2.5
1	D	493	SER	2.4
1	A	276	HIS	2.4
1	C	62	ASP	2.4
1	B	663	TYR	2.4
1	D	406	VAL	2.4
1	B	660	ILE	2.4
1	B	104	LEU	2.4
1	B	475	THR	2.4
1	D	109	PRO	2.3
1	B	106	GLU	2.3
1	A	637	ILE	2.3
1	A	636	SER	2.3
1	C	59	ALA	2.3
1	B	145	LYS	2.2
1	C	633	GLU	2.2
1	D	677	TYR	2.2
1	B	110	ILE	2.2
1	D	679	TRP	2.2
1	C	61	ILE	2.2
1	C	141	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	671	LEU	2.2
1	C	94	ILE	2.2
1	D	668	LEU	2.1
1	A	658	LEU	2.1
1	D	287	LEU	2.1
1	C	272	ASP	2.1
1	D	474	ASP	2.1
1	A	138	GLU	2.1
1	B	641	ASP	2.1
1	A	643	GLN	2.1
1	A	641	ASP	2.0
1	A	497	LYS	2.0
1	A	325	LEU	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 monosaccharides 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	UGA	A	684	37/37	0.90	0.17	52,64,71,76	0
2	UGA	A	683	37/37	0.95	0.14	49,56,72,76	0
2	UGA	B	683	37/37	0.95	0.15	46,52,58,61	0
2	UGA	D	683	37/37	0.95	0.15	44,53,66,68	0
2	UGA	C	683	37/37	0.96	0.14	37,43,50,52	0
2	UGA	D	684	37/37	0.96	0.12	47,52,60,60	0
4	UDP	B	1	25/25	0.96	0.15	37,42,58,60	0
3	MN	B	4	1/1	0.97	0.11	62,62,62,62	0
4	UDP	C	1	25/25	0.97	0.14	33,39,49,53	0
3	MN	D	7	1/1	0.98	0.14	46,46,46,46	0

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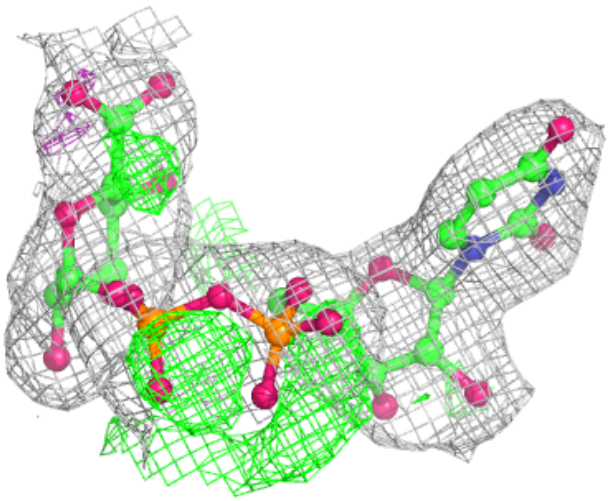
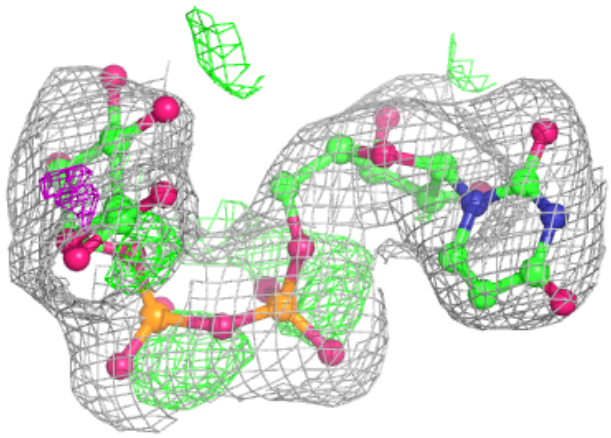
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MN	B	3	1/1	0.98	0.13	47,47,47,47	0
3	MN	A	2	1/1	0.98	0.15	60,60,60,60	0
3	MN	A	1	1/1	0.99	0.17	58,58,58,58	0
3	MN	D	8	1/1	0.99	0.12	64,64,64,64	0
3	MN	C	5	1/1	0.99	0.15	44,44,44,44	0
3	MN	C	6	1/1	0.99	0.15	49,49,49,49	0

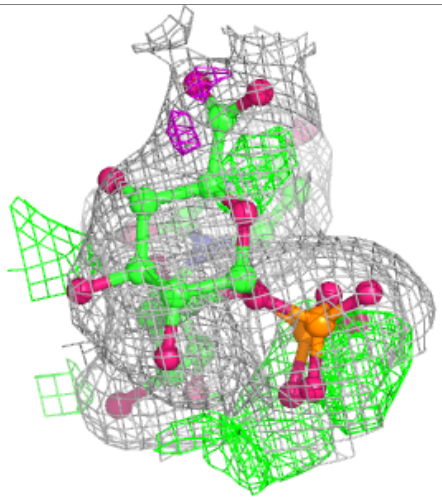
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UGA A 684:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

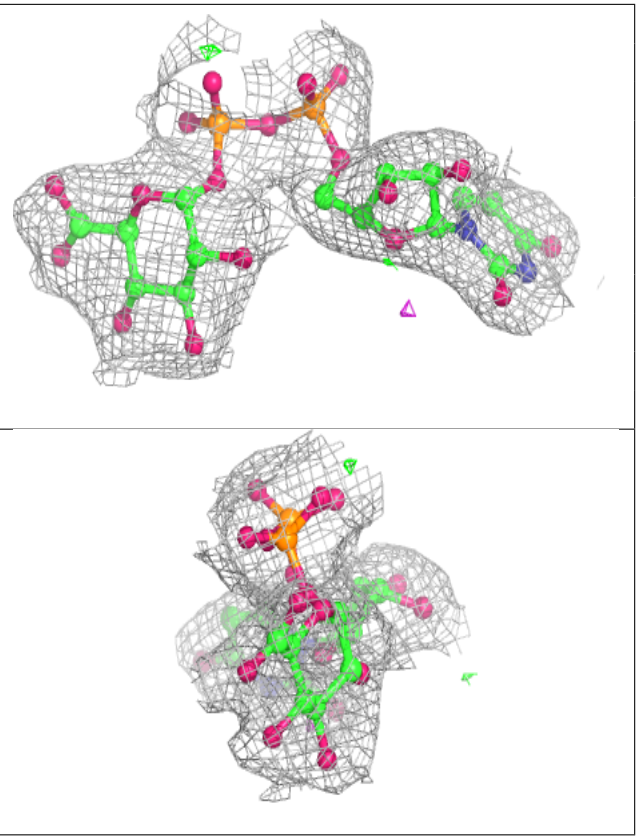






Electron density around UGA A 683:

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



Electron density around UGA B 683:

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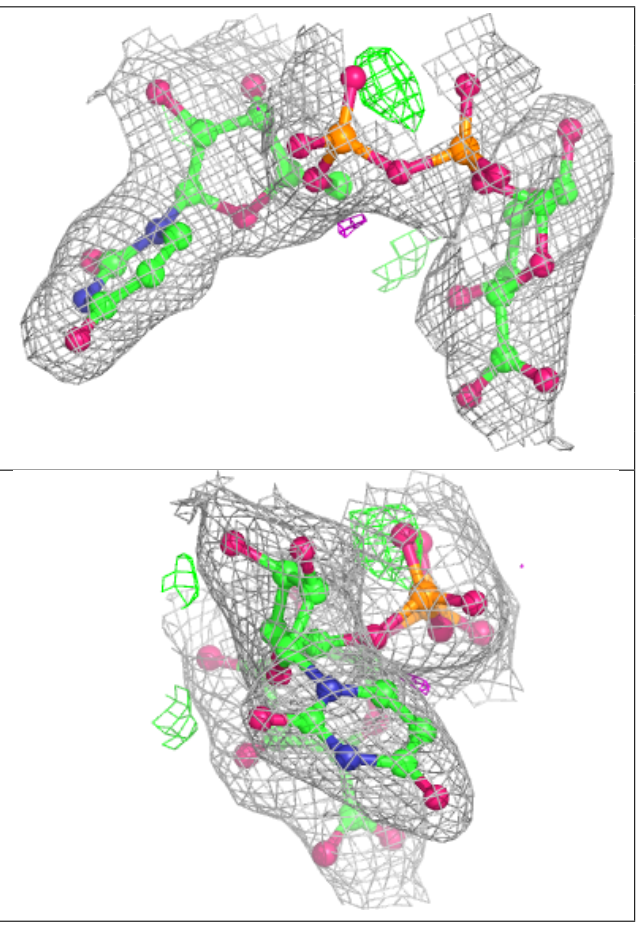
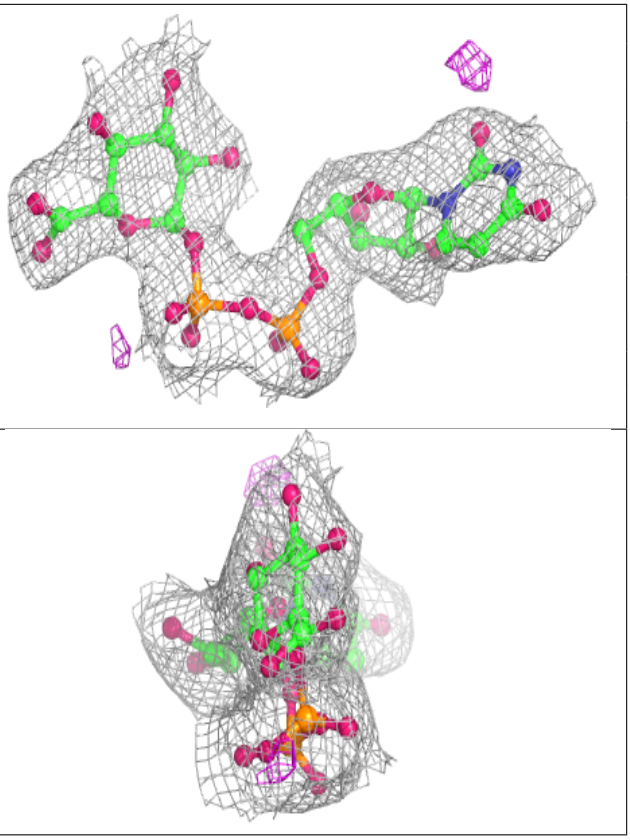
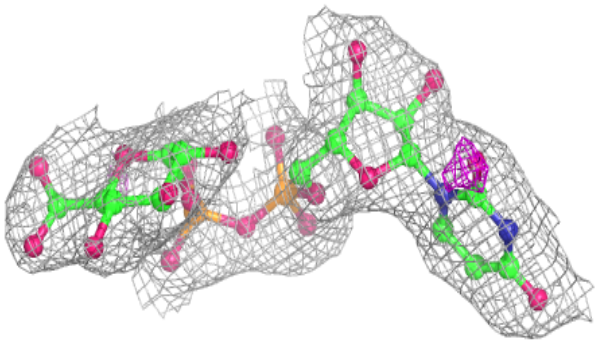
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around UGA D 683:

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





Electron density around UGA C 683:

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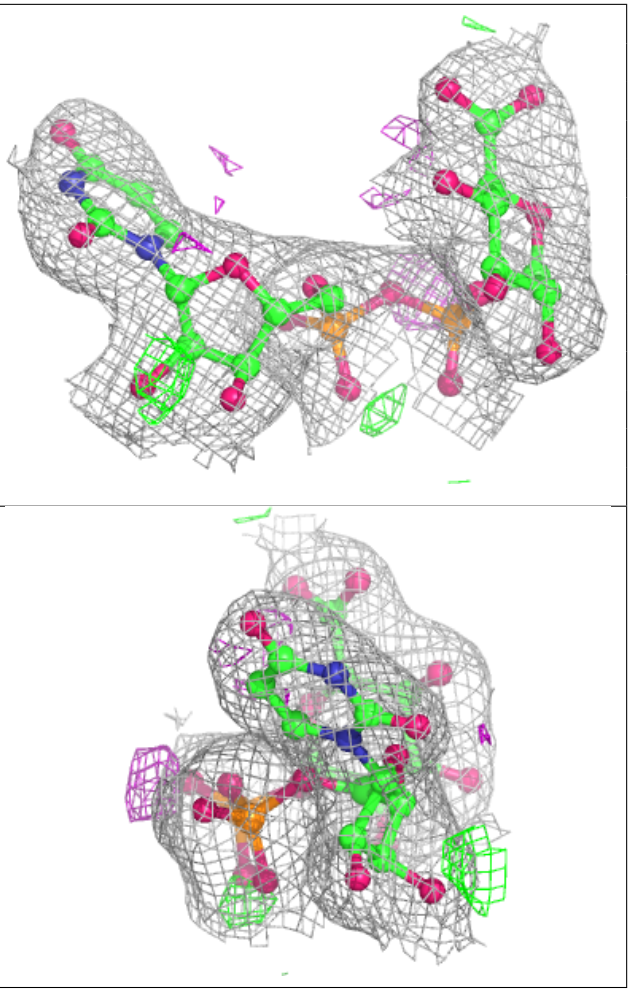
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around UGA D 684:

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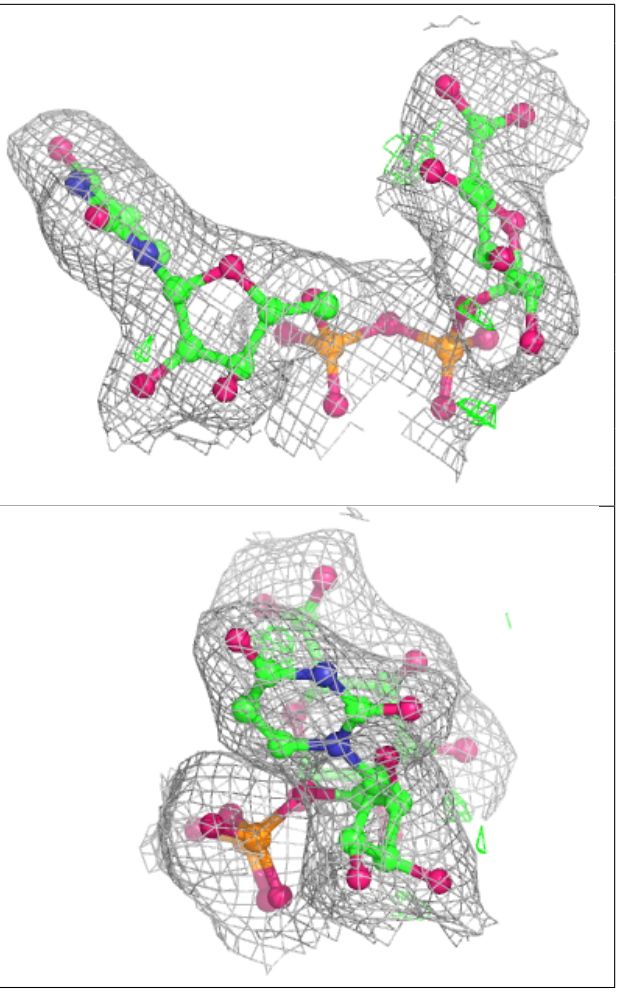
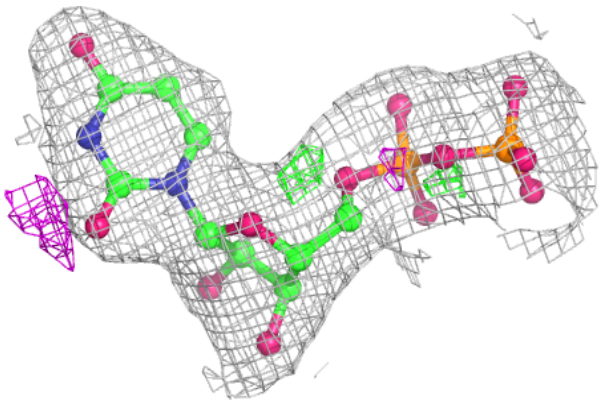
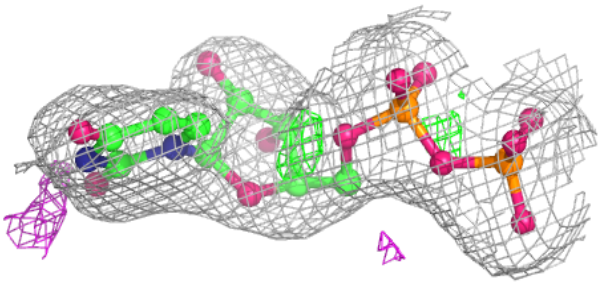
and green (positive)

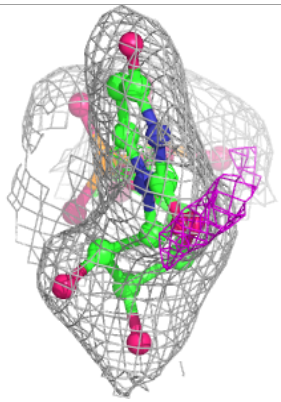


Electron density around UDP B 1:

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

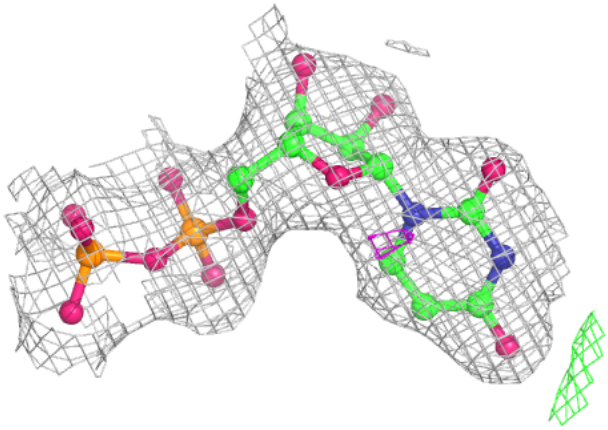


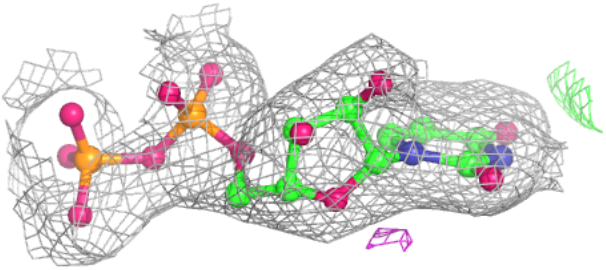


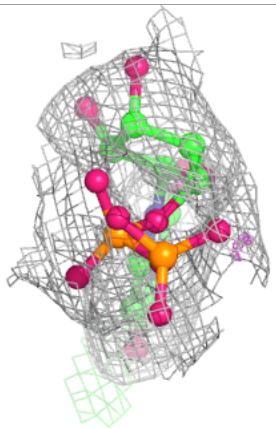


Electron density around UDP C 1:

$2mF_o$-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.