Full wwPDB X-ray Structure Validation Report ⓘ

Aug 2, 2023 – 02:11 PM EDT

PDB ID	:	8DLA
Title	:	ClpP2 from Chlamydia trachomatis bound by MAS1-12
Authors	:	Azadmanesh, J.; Struble, L.R.; Seleem, M.A.; Ouellette, S.; Conda-Sheridan, M.; Borgstahl, G.E.O.
Deposited on	:	2022-07-07
Resolution	:	2.66 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

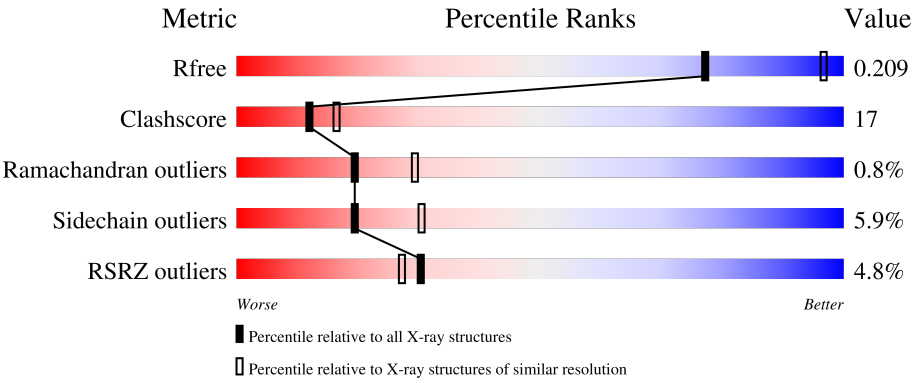
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.66 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	203	6% 61% 36%
1	B	203	5% 72% 25%
1	C	203	5% 73% 25%
1	D	203	3% 66% 32%
1	E	203	4% 70% 26%

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Mol	Chain	Length	Quality of chain
1	F	203	6% 68% 28%
1	G	203	3% 65% 31%
1	H	203	5% 66% 30%
1	I	203	4% 67% 30%
1	J	203	3% 65% 32%
1	K	203	3% 67% 30%
1	L	203	4% 70% 25%
1	M	203	6% 68% 27%
1	N	203	7% 69% 26%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NA	D	302	-	-	-	X

2 Entry composition (i)

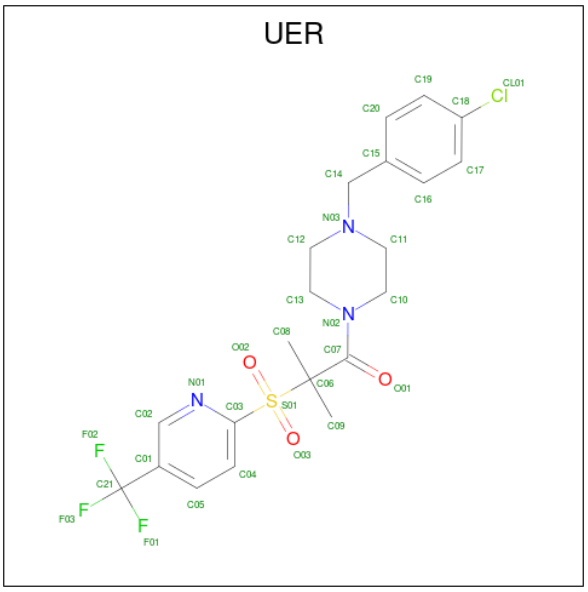
There are 5 unique types of molecules in this entry. The entry contains 22282 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ATP-dependent Clp protease proteolytic subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	0	0	0
			1542	974	256	301	11			
1	B	203	Total	C	N	O	S	0	0	0
			1542	974	256	301	11			
1	C	203	Total	C	N	O	S	0	0	0
			1542	974	256	301	11			
1	D	203	Total	C	N	O	S	0	0	0
			1542	974	256	301	11			
1	E	203	Total	C	N	O	S	0	0	0
			1542	974	256	301	11			
1	F	203	Total	C	N	O	S	0	0	0
			1542	974	256	301	11			
1	G	203	Total	C	N	O	S	0	0	0
			1542	974	256	301	11			
1	H	203	Total	C	N	O	S	0	0	0
			1542	974	256	301	11			
1	I	203	Total	C	N	O	S	0	0	0
			1542	974	256	301	11			
1	J	203	Total	C	N	O	S	0	0	0
			1542	974	256	301	11			
1	K	203	Total	C	N	O	S	0	0	0
			1542	974	256	301	11			
1	L	203	Total	C	N	O	S	0	0	0
			1542	974	256	301	11			
1	M	203	Total	C	N	O	S	0	0	0
			1542	974	256	301	11			
1	N	203	Total	C	N	O	S	0	0	0
			1542	974	256	301	11			

- Molecule 2 is 1-{4-[(4-chlorophenyl)methyl]piperazin-1-yl}-2-methyl-2-[5-(trifluoromethyl)pyridine-2-sulfonyl]propan-1-one (three-letter code: UER) (formula: $C_{21}H_{23}ClF_3N_3O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	S	0	0
			32	21	1	3	3	3	1		
2	A	1	Total	C	Cl	F	N	O	S	0	0
			32	21	1	3	3	3	1		
2	B	1	Total	C	Cl	F	N	O	S	0	0
			32	21	1	3	3	3	1		
2	D	1	Total	C	Cl	F	N	O	S	0	0
			32	21	1	3	3	3	1		
2	G	1	Total	C	Cl	F	N	O	S	0	0
			32	21	1	3	3	3	1		
2	M	1	Total	C	Cl	F	N	O	S	0	0
			32	21	1	3	3	3	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		
3	E	1	Total	Na	0	0
			1	1		
3	F	1	Total	Na	0	0
			1	1		
3	G	1	Total	Na	0	0
			1	1		
3	H	1	Total	Na	0	0
			1	1		

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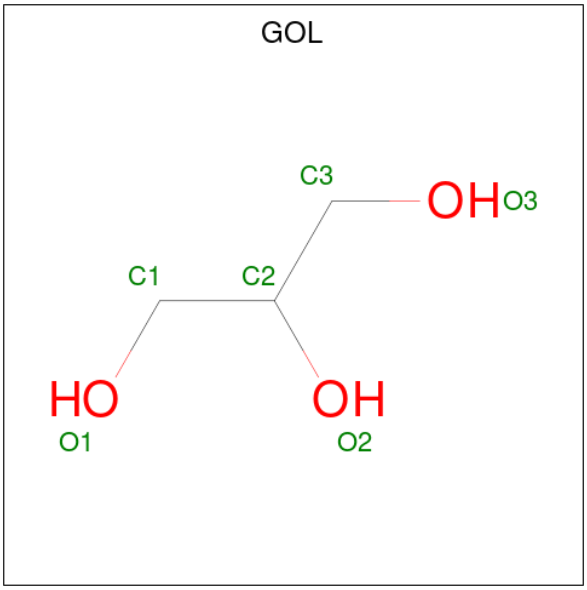
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	L	1	Total Na 1 1	0	0
3	N	1	Total Na 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	G	1	Total C O 6 3 3	0	0
4	N	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	31	Total O 31 31	0	0
5	B	40	Total O 40 40	0	0
5	C	22	Total O 22 22	0	0

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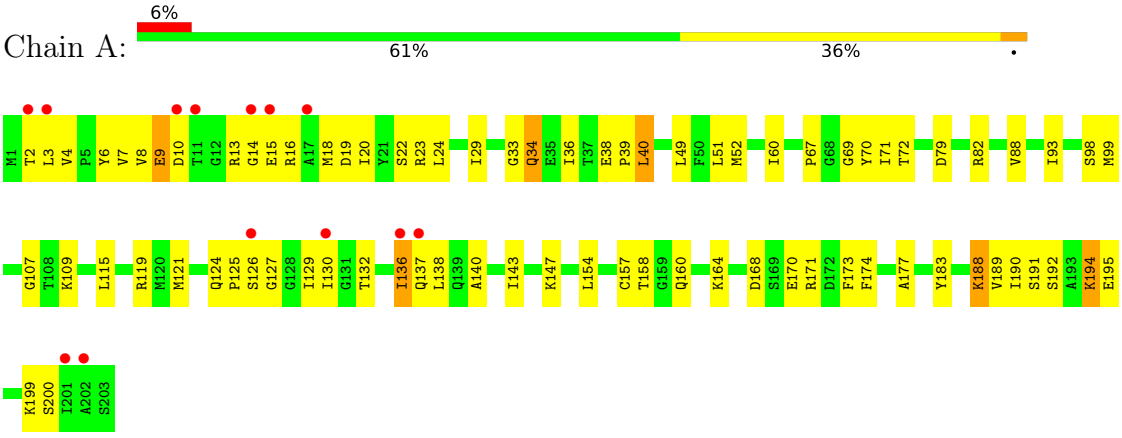
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	34	Total O 34 34	0	0
5	E	37	Total O 37 37	0	0
5	F	49	Total O 49 49	0	0
5	G	31	Total O 31 31	0	0
5	H	30	Total O 30 30	0	0
5	I	31	Total O 31 31	0	0
5	J	30	Total O 30 30	0	0
5	K	43	Total O 43 43	0	0
5	L	29	Total O 29 29	0	0
5	M	36	Total O 36 36	0	0
5	N	27	Total O 27 27	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.

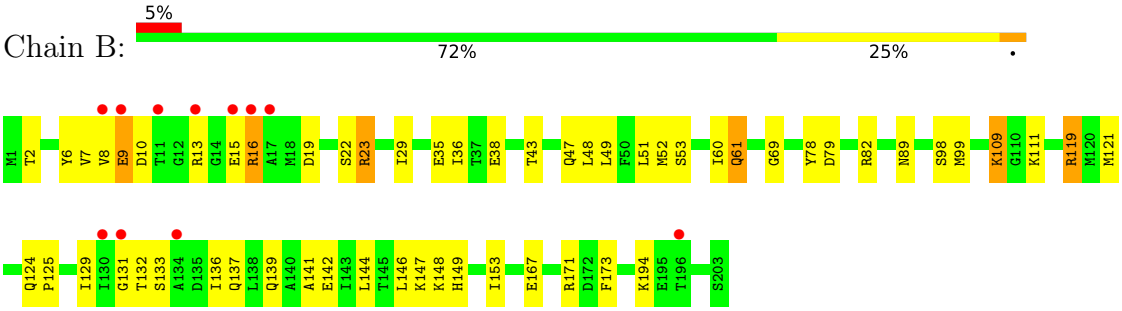
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain A:



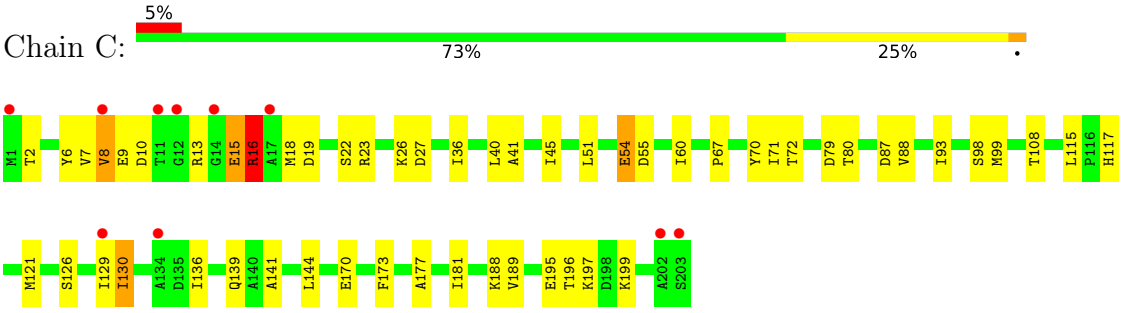
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain B:



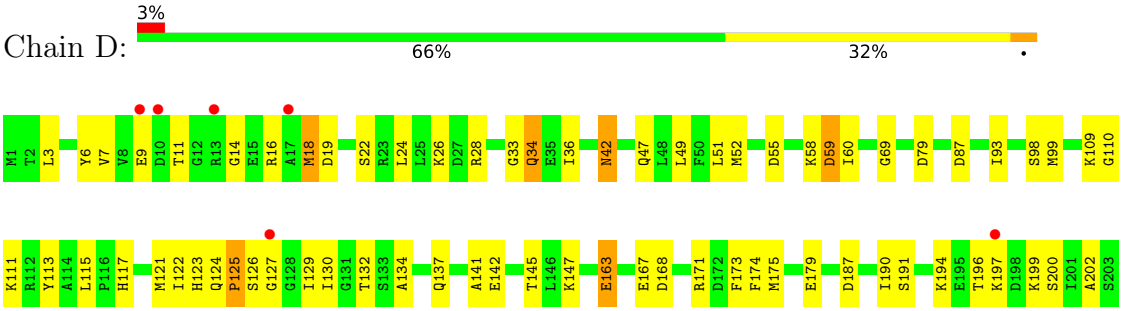
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain C:



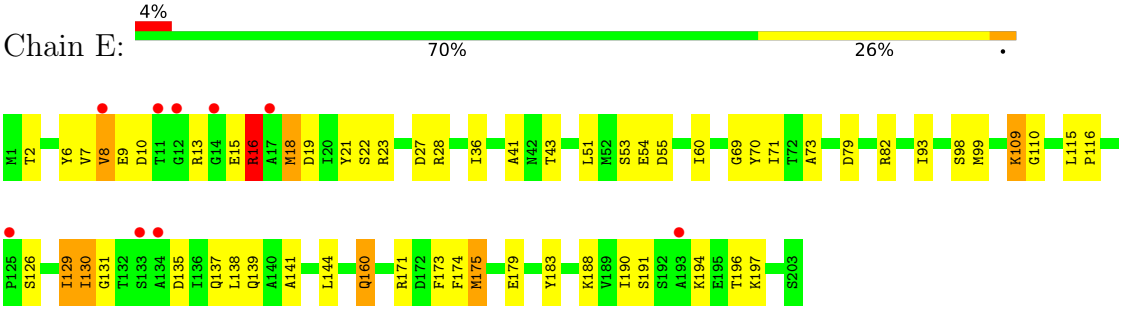
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain D:



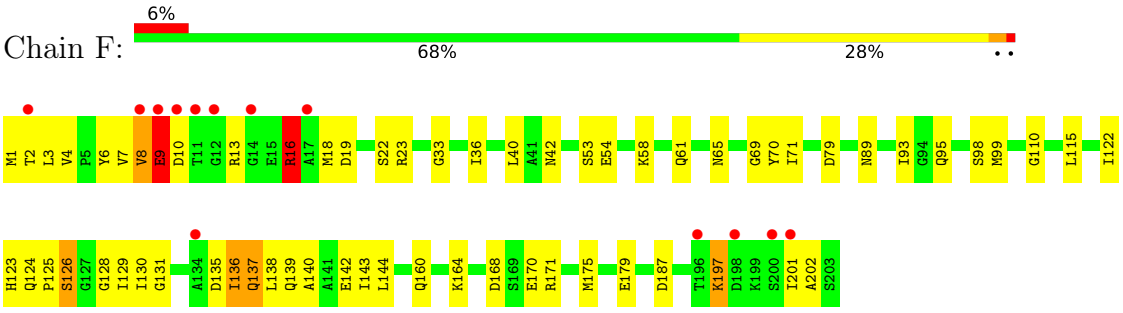
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain E:



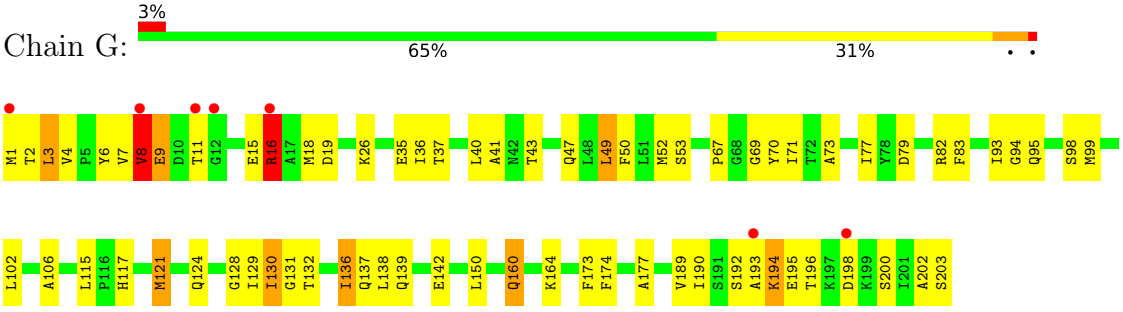
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain F:



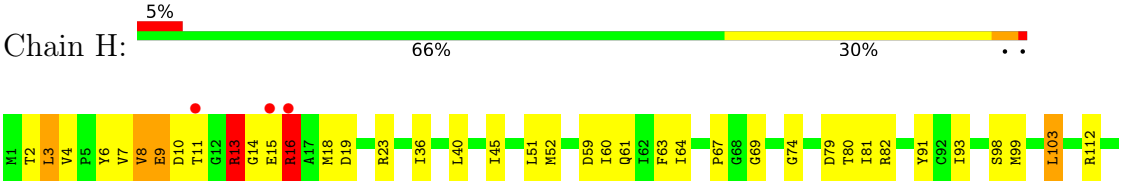
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

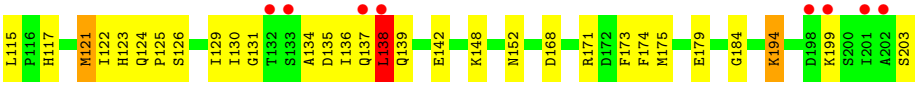
Chain G:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

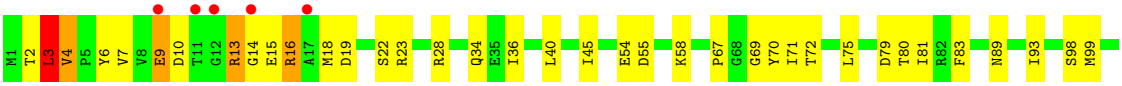
Chain H:

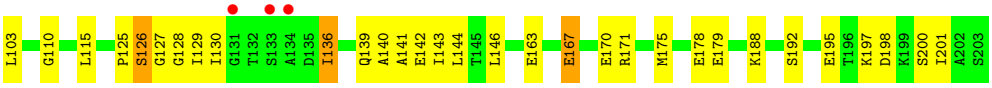




• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

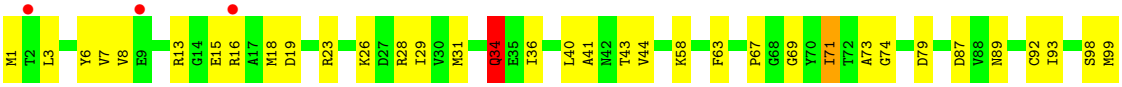
Chain I:

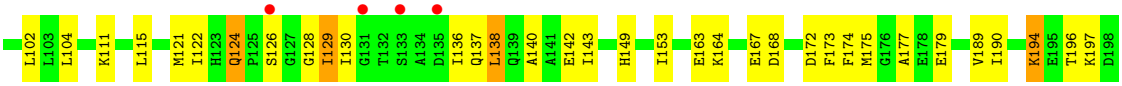




• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

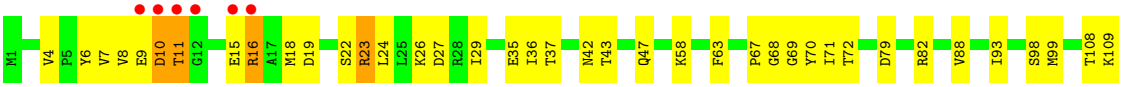
Chain J:

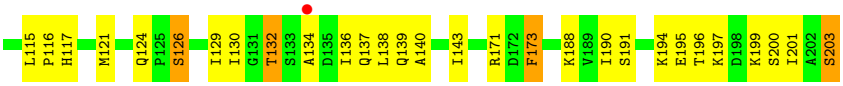




• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

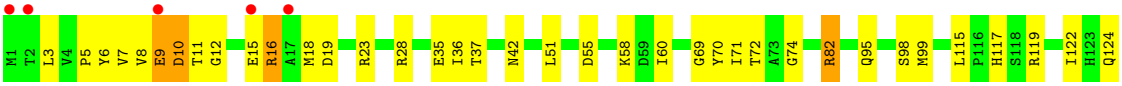
Chain K:





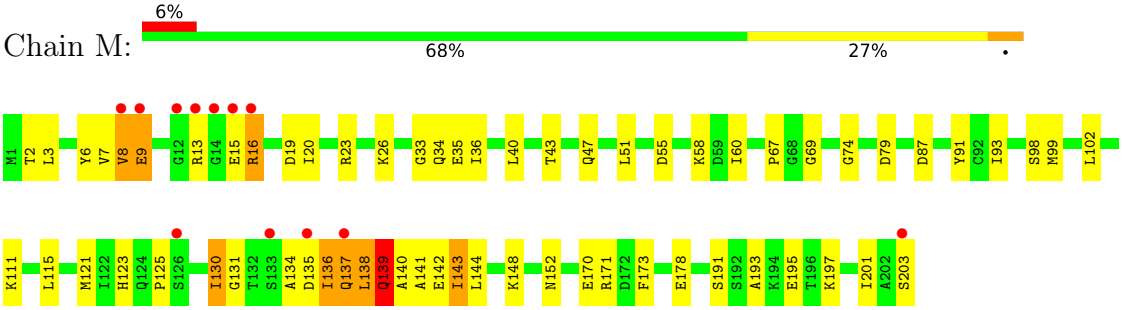
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain L:



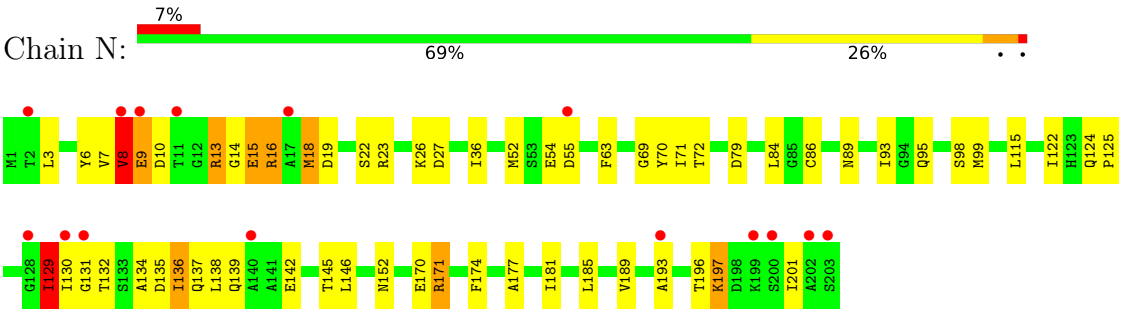
• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain M:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	97.00Å 98.01Å 97.97Å 97.16° 114.15° 114.16°	Depositor
Resolution (Å)	33.09 – 2.66 33.09 – 2.66	Depositor EDS
% Data completeness (in resolution range)	78.2 (33.09-2.66) 78.1 (33.09-2.66)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.173 , 0.210 0.172 , 0.209	Depositor DCC
R_{free} test set	2033 reflections (3.21%)	wwPDB-VP
Wilson B-factor (Å^2)	36.4	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 25.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.449 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	22282	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, GOL, UER

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	0.27	0/1562	0.54	0/2106
1	B	0.29	0/1562	0.53	0/2106
1	C	0.43	3/1562 (0.2%)	0.87	5/2106 (0.2%)
1	D	0.27	0/1562	0.55	0/2106
1	E	0.33	0/1562	0.60	2/2106 (0.1%)
1	F	0.29	0/1562	0.64	3/2106 (0.1%)
1	G	0.52	3/1562 (0.2%)	0.68	3/2106 (0.1%)
1	H	0.38	2/1562 (0.1%)	0.71	4/2106 (0.2%)
1	I	0.36	1/1562 (0.1%)	1.26	10/2106 (0.5%)
1	J	0.35	0/1562	0.64	2/2106 (0.1%)
1	K	0.29	0/1562	0.55	0/2106
1	L	0.28	0/1562	0.56	1/2106 (0.0%)
1	M	0.30	0/1562	0.59	2/2106 (0.1%)
1	N	0.33	0/1562	0.75	7/2106 (0.3%)
All	All	0.34	9/21868 (0.0%)	0.70	39/29484 (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	D	0	2
1	E	0	1
1	F	0	3
1	G	0	1
1	H	0	4
1	I	0	1
1	J	0	1
1	M	0	1
1	N	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	18

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	9	GLU	CD-OE1	-11.66	1.12	1.25
1	C	16	ARG	CB-CG	-6.59	1.34	1.52
1	C	16	ARG	CG-CD	-6.53	1.35	1.51
1	I	9	GLU	CB-CG	5.60	1.62	1.52
1	G	9	GLU	CD-OE2	5.49	1.31	1.25
1	H	16	ARG	CG-CD	-5.42	1.38	1.51
1	H	13	ARG	C-N	5.38	1.42	1.33
1	G	8	VAL	CB-CG1	5.08	1.63	1.52
1	C	15	GLU	CB-CG	5.06	1.61	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	9	GLU	OE1-CD-OE2	-38.23	77.42	123.30
1	C	16	ARG	CG-CD-NE	-25.66	57.92	111.80
1	I	9	GLU	CG-CD-OE1	21.69	161.69	118.30
1	H	3	LEU	CA-CB-CG	13.67	146.73	115.30
1	I	9	GLU	CG-CD-OE2	-13.53	91.24	118.30
1	C	16	ARG	CB-CG-CD	12.79	144.85	111.60
1	F	9	GLU	OE1-CD-OE2	-11.43	109.58	123.30
1	I	9	GLU	CA-CB-CG	11.23	138.11	113.40
1	N	136	ILE	CG1-CB-CG2	-10.14	89.08	111.40
1	N	3	LEU	CB-CG-CD2	-9.55	94.76	111.00
1	F	9	GLU	CG-CD-OE1	8.34	134.97	118.30
1	E	16	ARG	CB-CG-CD	-8.32	89.96	111.60
1	N	129	ILE	CG1-CB-CG2	-8.20	93.35	111.40
1	I	167	GLU	CA-CB-CG	8.13	131.30	113.40
1	I	167	GLU	CG-CD-OE1	7.55	133.40	118.30
1	H	3	LEU	N-CA-CB	-7.41	95.57	110.40
1	F	9	GLU	CG-CD-OE2	-7.21	103.89	118.30
1	J	34	GLN	CA-CB-CG	7.19	129.21	113.40
1	J	138	LEU	CA-CB-CG	7.14	131.73	115.30
1	I	167	GLU	OE1-CD-OE2	-6.89	115.03	123.30
1	G	9	GLU	CG-CD-OE1	6.77	131.85	118.30
1	H	138	LEU	CA-CB-CG	6.65	130.60	115.30
1	I	9	GLU	CB-CG-CD	-6.64	96.28	114.20
1	N	3	LEU	CA-CB-CG	6.55	130.37	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	171	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	H	16	ARG	NE-CZ-NH2	6.33	123.46	120.30
1	G	9	GLU	CG-CD-OE2	-6.22	105.85	118.30
1	C	16	ARG	CD-NE-CZ	6.14	132.20	123.60
1	C	16	ARG	CA-CB-CG	-5.99	100.22	113.40
1	M	139	GLN	N-CA-CB	5.91	121.23	110.60
1	I	9	GLU	CB-CA-C	-5.88	98.64	110.40
1	M	139	GLN	CB-CA-C	-5.84	98.72	110.40
1	C	16	ARG	NE-CZ-NH1	-5.73	117.43	120.30
1	I	3	LEU	CA-CB-CG	5.64	128.27	115.30
1	G	49	LEU	CA-CB-CG	5.62	128.22	115.30
1	L	138	LEU	CA-CB-CG	5.33	127.56	115.30
1	N	171	ARG	CA-CB-CG	-5.22	101.92	113.40
1	N	171	ARG	CG-CD-NE	-5.21	100.86	111.80
1	E	16	ARG	CB-CA-C	-5.06	100.28	110.40

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	125	PRO	Peptide
1	D	127	GLY	Peptide
1	E	16	ARG	Sidechain
1	F	16	ARG	Sidechain
1	F	8	VAL	Peptide
1	F	9	GLU	Sidechain
1	G	16	ARG	Sidechain
1	H	138	LEU	Peptide
1	H	15	GLU	Peptide
1	H	16	ARG	Sidechain
1	H	2	THR	Peptide
1	I	4	VAL	Peptide
1	J	34	GLN	Peptide
1	M	137	GLN	Peptide
1	N	15	GLU	Peptide
1	N	16	ARG	Sidechain
1	N	171	ARG	Sidechain
1	N	8	VAL	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	1542	0	1578	81	0
1	B	1542	0	1578	47	0
1	C	1542	0	1577	64	0
1	D	1542	0	1578	62	0
1	E	1542	0	1578	57	0
1	F	1542	0	1577	70	0
1	G	1542	0	1577	71	0
1	H	1542	0	1578	65	0
1	I	1542	0	1578	63	0
1	J	1542	0	1578	67	0
1	K	1542	0	1578	74	0
1	L	1542	0	1578	47	0
1	M	1542	0	1578	67	0
1	N	1542	0	1578	74	0
2	A	64	0	0	3	0
2	B	32	0	0	0	0
2	D	32	0	0	0	0
2	G	32	0	0	1	0
2	M	32	0	0	1	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	L	1	0	0	0	0
3	N	1	0	0	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	G	6	0	8	3	0
4	N	6	0	8	2	0
5	A	31	0	0	4	0
5	B	40	0	0	1	0
5	C	22	0	0	1	0
5	D	34	0	0	3	0
5	E	37	0	0	2	0
5	F	49	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	31	0	0	1	0
5	H	30	0	0	8	0
5	I	31	0	0	2	0
5	J	30	0	0	0	0
5	K	43	0	0	5	0
5	L	29	0	0	1	0
5	M	36	0	0	2	0
5	N	27	0	0	2	0
All	All	22282	0	22121	754	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 17.

All (754) 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:C:9:GLU:OE2	1:C:23:ARG:NE	1.83	1.12
1:J:34:GLN:HG3	1:J:40:LEU:CD1	1.84	1.07
1:C:129:ILE:HD12	1:H:138:LEU:HD21	1.40	1.01
1:J:34:GLN:HG3	1:J:40:LEU:HD12	1.46	0.96
1:L:124:GLN:HB3	1:M:139:GLN:NE2	1.81	0.94
1:K:7:VAL:HG11	1:K:23:ARG:HG2	1.49	0.94
1:B:8:VAL:HG11	1:L:16:ARG:HD3	1.52	0.91
1:C:139:GLN:NE2	1:H:124:GLN:O	2.05	0.90
1:M:138:LEU:HD11	1:M:143:ILE:HG23	1.54	0.90
1:G:124:GLN:O	1:N:139:GLN:NE2	2.04	0.89
1:C:9:GLU:H	1:C:16:ARG:HH12	1.22	0.87
1:J:34:GLN:HG3	1:J:40:LEU:HD13	1.56	0.87
1:E:8:VAL:O	1:J:26:LYS:NZ	2.08	0.85
1:G:9:GLU:OE1	1:G:16:ARG:NH2	2.09	0.85
1:E:144:LEU:HD21	1:F:144:LEU:HD11	1.57	0.84
1:G:174:PHE:N	1:I:142:GLU:OE2	2.10	0.84
1:E:9:GLU:HB2	1:E:16:ARG:NH2	1.93	0.84
1:G:16:ARG:O	1:G:16:ARG:HG2	1.78	0.84
1:D:168:ASP:OD1	1:D:171:ARG:NH1	2.12	0.83
1:C:9:GLU:N	1:C:16:ARG:HH12	1.77	0.82
1:G:138:LEU:HB3	1:N:129:ILE:HG22	1.60	0.81
1:J:128:GLY:O	1:J:130:ILE:N	2.14	0.81
1:H:79:ASP:HB3	1:J:115:LEU:HD23	1.63	0.80
1:N:129:ILE:CD1	1:N:130:ILE:H	1.96	0.79
1:F:131:GLY:HA2	1:F:135:ASP:HB2	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:136:ILE:HG23	1:M:130:ILE:HD13	1.64	0.79
1:M:87:ASP:OD2	1:M:111:LYS:NZ	2.15	0.79
1:N:9:GLU:OE1	1:N:16:ARG:NH2	2.16	0.78
1:N:70:TYR:HB3	1:N:131:GLY:H	1.48	0.78
1:K:196:THR:HG22	1:K:197:LYS:H	1.48	0.77
1:C:70:TYR:HB3	1:C:130:ILE:HG23	1.65	0.77
1:M:178:GLU:OE2	5:M:401:HOH:O	2.01	0.77
1:A:23:ARG:O	1:A:23:ARG:NH1	2.17	0.76
1:H:59:ASP:OD2	1:H:61:GLN:NE2	2.19	0.76
1:C:9:GLU:H	1:C:16:ARG:NH1	1.82	0.76
1:C:23:ARG:HH12	1:C:26:LYS:HB3	1.52	0.75
1:G:15:GLU:HB3	1:I:16:ARG:HH22	1.51	0.75
1:B:79:ASP:HB3	1:N:115:LEU:HD23	1.68	0.75
1:M:136:ILE:HD12	1:M:137:GLN:H	1.52	0.74
1:F:122:ILE:HD11	1:F:168:ASP:HB3	1.68	0.74
1:D:79:ASP:HB3	1:M:115:LEU:HD23	1.70	0.74
1:G:139:GLN:HB2	1:G:142:GLU:HG2	1.70	0.74
1:A:115:LEU:HD23	1:F:79:ASP:HB3	1.68	0.74
1:E:71:ILE:HG13	1:E:130:ILE:HG12	1.68	0.74
1:N:7:VAL:HG11	1:N:23:ARG:HB2	1.70	0.74
1:J:34:GLN:CG	1:J:40:LEU:HD12	2.17	0.73
1:C:9:GLU:N	1:C:16:ARG:NH1	2.36	0.73
1:L:124:GLN:HB3	1:M:139:GLN:HE22	1.53	0.73
1:D:42:ASN:HD21	1:M:33:GLY:HA3	1.52	0.72
1:G:138:LEU:CB	1:N:129:ILE:HG22	2.19	0.72
1:A:188:LYS:HE3	1:A:194:LYS:HG3	1.72	0.72
1:M:135:ASP:O	1:M:137:GLN:HG2	1.89	0.72
1:E:190:ILE:HD13	1:E:196:THR:HA	1.71	0.72
1:J:7:VAL:HG21	1:J:23:ARG:HB2	1.72	0.72
1:K:10:ASP:OD2	1:K:26:LYS:NZ	2.22	0.72
1:E:6:TYR:HA	1:E:19:ASP:HA	1.72	0.71
1:L:10:ASP:OD1	1:L:10:ASP:N	2.19	0.71
1:C:129:ILE:HD13	1:H:136:ILE:HB	1.72	0.71
1:M:9:GLU:OE2	1:M:23:ARG:NE	2.23	0.71
1:D:130:ILE:HG13	1:D:134:ALA:HA	1.71	0.71
1:H:98:SER:HB2	1:H:124:GLN:HG3	1.73	0.70
1:A:36:ILE:HA	1:A:40:LEU:HD22	1.73	0.70
1:D:115:LEU:HD23	1:G:79:ASP:HB3	1.72	0.70
1:F:126:SER:HA	1:I:126:SER:HA	1.73	0.70
1:M:58:LYS:NZ	1:M:203:SER:OXT	2.23	0.69
1:H:171:ARG:HB2	1:L:171:ARG:HE	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:7:VAL:HG11	1:K:23:ARG:CG	2.21	0.69
1:H:7:VAL:HG12	1:H:16:ARG:HH12	1.58	0.69
1:G:8:VAL:O	1:G:9:GLU:HB2	1.92	0.69
1:C:9:GLU:OE2	1:C:23:ARG:CZ	2.41	0.69
1:N:72:THR:HG23	1:N:130:ILE:HG22	1.75	0.69
1:F:138:LEU:HB2	1:F:143:ILE:HG23	1.75	0.68
1:K:93:ILE:HG23	1:K:115:LEU:HD12	1.75	0.68
1:G:95:GLN:NE2	5:G:401:HOH:O	2.26	0.68
1:K:71:ILE:HG13	1:K:129:ILE:HA	1.74	0.68
1:D:26:LYS:NZ	1:M:8:VAL:O	2.26	0.68
1:H:91:TYR:O	5:H:401:HOH:O	2.11	0.68
1:B:9:GLU:HB3	1:B:23:ARG:HH21	1.57	0.68
1:E:70:TYR:HA	1:E:130:ILE:HG13	1.74	0.68
1:J:34:GLN:CG	1:J:40:LEU:CD1	2.67	0.68
1:E:71:ILE:HB	1:E:130:ILE:HG21	1.75	0.68
1:E:7:VAL:HG11	1:E:23:ARG:HB2	1.75	0.68
1:F:10:ASP:OD1	5:F:401:HOH:O	2.12	0.67
1:L:23:ARG:O	1:L:23:ARG:NH1	2.23	0.67
1:G:9:GLU:OE1	1:G:16:ARG:NE	2.27	0.67
1:B:29:ILE:HD13	1:B:61:GLN:HB2	1.77	0.67
1:K:15:GLU:HG3	1:K:16:ARG:HH12	1.59	0.67
1:G:130:ILE:HD12	1:N:136:ILE:HG21	1.76	0.67
1:D:122:ILE:HD11	1:D:168:ASP:HB2	1.77	0.66
1:K:10:ASP:OD1	1:K:15:GLU:HB2	1.94	0.66
1:L:128:GLY:HA3	1:M:139:GLN:OE1	1.96	0.66
1:A:137:GLN:HG3	1:J:124:GLN:HB2	1.77	0.66
1:B:167:GLU:OE2	1:B:171:ARG:NH2	2.28	0.66
1:I:81:ILE:HD12	1:I:103:LEU:HD12	1.78	0.66
1:M:197:LYS:HG3	1:M:201:ILE:HG13	1.77	0.66
1:B:9:GLU:HG2	1:B:10:ASP:N	2.10	0.66
1:I:110:GLY:O	1:I:188:LYS:NZ	2.29	0.66
1:H:138:LEU:O	5:H:402:HOH:O	2.12	0.65
1:E:15:GLU:H	1:I:15:GLU:HG3	1.60	0.65
1:E:115:LEU:HD23	1:J:79:ASP:HB3	1.77	0.65
1:H:63:PHE:HD1	1:H:93:ILE:HD11	1.61	0.65
1:L:124:GLN:CB	1:M:139:GLN:HE22	2.09	0.65
1:G:3:LEU:HD11	1:I:19:ASP:OD2	1.97	0.64
1:N:129:ILE:HD13	1:N:130:ILE:H	1.63	0.64
1:B:6:TYR:HA	1:B:19:ASP:HA	1.79	0.64
1:B:121:MET:HG3	1:B:173:PHE:O	1.97	0.64
1:H:93:ILE:HD12	5:H:401:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:301:UER:O01	2:A:301:UER:O02	2.13	0.63
1:F:93:ILE:HG23	1:F:115:LEU:HD12	1.80	0.63
1:J:149:HIS:O	1:J:153:ILE:HG13	1.99	0.63
1:C:72:THR:H	1:C:130:ILE:HG21	1.62	0.63
1:M:197:LYS:HE2	1:M:201:ILE:HA	1.79	0.63
1:I:9:GLU:OE1	1:I:14:GLY:N	2.19	0.63
1:F:9:GLU:H	1:F:16:ARG:HH22	1.47	0.63
1:F:16:ARG:H	1:K:16:ARG:NH2	1.96	0.63
1:M:7:VAL:HG11	1:M:23:ARG:HB2	1.80	0.62
1:H:98:SER:OG	1:H:99:MET:N	2.32	0.62
1:C:70:TYR:HA	1:C:130:ILE:HD12	1.81	0.62
1:B:139:GLN:HE22	1:D:124:GLN:HB3	1.65	0.62
1:H:74:GLY:HA3	1:H:99:MET:SD	2.39	0.62
1:J:89:ASN:HD21	1:J:196:THR:HG21	1.65	0.62
1:J:138:LEU:HD12	1:J:143:ILE:HG22	1.81	0.62
1:G:198:ASP:H	1:G:203:SER:HA	1.64	0.62
1:K:98:SER:OG	1:K:99:MET:N	2.33	0.62
1:C:188:LYS:NZ	1:C:195:GLU:O	2.32	0.61
1:J:164:LYS:HE3	1:J:168:ASP:OD2	1.99	0.61
1:C:98:SER:OG	1:C:99:MET:N	2.28	0.61
1:F:9:GLU:N	1:F:16:ARG:HH22	1.98	0.61
1:G:9:GLU:OE1	1:G:16:ARG:CZ	2.48	0.61
1:F:98:SER:OG	1:F:99:MET:N	2.33	0.61
1:K:132:THR:HG22	1:K:134:ALA:H	1.64	0.61
1:N:71:ILE:HB	1:N:130:ILE:HG23	1.83	0.61
1:J:29:ILE:HD11	1:J:197:LYS:HD2	1.81	0.61
1:A:147:LYS:NZ	5:A:401:HOH:O	2.33	0.61
1:J:36:ILE:HB	1:J:69:GLY:HA3	1.83	0.60
1:H:8:VAL:HA	1:H:16:ARG:HH11	1.66	0.60
1:I:130:ILE:HD12	1:K:137:GLN:HB3	1.82	0.60
1:E:135:ASP:OD2	1:I:126:SER:OG	2.19	0.60
1:H:142:GLU:OE2	1:J:174:PHE:HB2	2.01	0.60
1:K:121:MET:HG3	1:K:173:PHE:O	2.02	0.60
1:L:82:ARG:NH1	5:L:401:HOH:O	2.35	0.60
1:H:9:GLU:HG3	1:H:16:ARG:NH2	2.15	0.60
1:H:112:ARG:NH2	5:H:404:HOH:O	2.35	0.60
1:J:34:GLN:HE21	1:J:40:LEU:HB2	1.66	0.60
1:A:129:ILE:HD13	1:J:128:GLY:O	2.01	0.60
1:A:138:LEU:H	1:J:128:GLY:HA2	1.65	0.60
1:K:190:ILE:HG13	1:K:191:SER:H	1.66	0.60
1:M:35:GLU:HG3	1:M:67:PRO:HG2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:TYR:O	1:F:22:SER:OG	2.12	0.60
1:A:98:SER:OG	1:A:99:MET:N	2.34	0.60
1:H:93:ILE:HG23	1:H:115:LEU:HD12	1.82	0.60
1:D:93:ILE:HG23	1:D:115:LEU:HD22	1.84	0.60
1:K:19:ASP:OD2	1:K:22:SER:OG	2.15	0.60
1:K:88:VAL:H	1:K:108:THR:HG23	1.67	0.59
1:E:144:LEU:HD11	1:F:144:LEU:HD21	1.83	0.59
1:F:16:ARG:H	1:K:16:ARG:HH21	1.50	0.59
1:H:129:ILE:HD12	1:H:130:ILE:HG22	1.82	0.59
1:M:171:ARG:HG2	1:M:173:PHE:HD2	1.67	0.59
1:B:149:HIS:O	1:B:153:ILE:HG13	2.02	0.59
1:K:8:VAL:HG21	1:N:16:ARG:CD	2.33	0.59
1:K:8:VAL:HG21	1:N:16:ARG:HD2	1.83	0.59
1:K:115:LEU:HD13	1:N:79:ASP:HB3	1.85	0.59
1:C:15:GLU:HG2	1:L:15:GLU:OE2	2.02	0.59
1:K:8:VAL:HG11	1:N:16:ARG:NE	2.18	0.59
1:D:173:PHE:HB3	1:N:170:GLU:OE2	2.03	0.59
1:F:9:GLU:HG3	1:F:16:ARG:NH1	2.18	0.59
1:I:163:GLU:O	1:I:167:GLU:HB3	2.03	0.59
1:N:98:SER:OG	1:N:99:MET:N	2.36	0.58
1:A:82:ARG:NH1	5:A:402:HOH:O	2.35	0.58
1:C:8:VAL:HA	1:C:16:ARG:HH12	1.68	0.58
1:L:95:GLN:NE2	1:L:119:ARG:HB2	2.18	0.58
1:E:79:ASP:HB3	1:I:115:LEU:HD13	1.85	0.58
1:K:8:VAL:HG21	1:N:16:ARG:CZ	2.33	0.58
1:F:160:GLN:HG2	1:F:164:LYS:HG2	1.85	0.58
1:K:6:TYR:O	1:N:22:SER:HB3	2.02	0.58
1:F:16:ARG:HD3	1:F:16:ARG:N	2.18	0.58
1:N:132:THR:O	1:N:136:ILE:HG23	2.04	0.58
1:D:42:ASN:ND2	1:M:33:GLY:HA3	2.18	0.58
1:N:6:TYR:HA	1:N:19:ASP:HA	1.85	0.58
1:A:170:GLU:OE2	1:E:171:ARG:NH2	2.36	0.58
1:C:36:ILE:HA	1:C:40:LEU:HD23	1.86	0.57
1:B:78:TYR:OH	1:B:82:ARG:NH1	2.36	0.57
1:C:79:ASP:HB3	1:L:115:LEU:HD13	1.85	0.57
1:M:130:ILE:HG12	1:M:131:GLY:N	2.19	0.57
1:F:9:GLU:HG3	1:F:16:ARG:HH12	1.70	0.57
1:G:37:THR:HG22	1:G:70:TYR:HE1	1.69	0.57
1:I:7:VAL:N	1:I:18:MET:O	2.37	0.57
1:J:98:SER:HB2	1:J:124:GLN:HA	1.86	0.57
1:M:131:GLY:HA3	1:M:136:ILE:HG22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:71:ILE:HD12	1:G:132:THR:HG22	1.85	0.57
1:H:6:TYR:HA	1:H:19:ASP:HA	1.85	0.57
1:I:7:VAL:HG11	1:I:23:ARG:HG2	1.85	0.57
1:M:98:SER:OG	1:M:99:MET:N	2.32	0.57
1:B:141:ALA:HA	1:B:144:LEU:HD12	1.87	0.57
1:F:4:VAL:HG22	1:F:19:ASP:HB2	1.87	0.57
1:G:117:HIS:O	4:G:301:GOL:O2	2.13	0.57
1:K:130:ILE:HD13	1:K:138:LEU:HD11	1.87	0.56
1:N:138:LEU:HD13	1:N:142:GLU:HB3	1.88	0.56
1:A:38:GLU:OE2	1:A:130:ILE:HG12	2.04	0.56
1:C:8:VAL:HA	1:C:16:ARG:NH1	2.20	0.56
1:G:6:TYR:HA	1:G:19:ASP:HA	1.88	0.56
1:G:115:LEU:HD13	1:I:79:ASP:HB3	1.86	0.56
1:B:98:SER:OG	1:B:99:MET:N	2.36	0.56
1:G:16:ARG:HD2	1:G:26:LYS:NZ	2.21	0.56
1:L:7:VAL:HG11	1:L:23:ARG:HG2	1.88	0.56
1:M:74:GLY:HA3	1:M:99:MET:SD	2.45	0.56
1:E:137:GLN:HG3	1:E:138:LEU:H	1.69	0.56
1:A:154:LEU:O	1:A:158:THR:OG1	2.23	0.56
1:D:59:ASP:OD1	1:D:87:ASP:HB2	2.06	0.56
1:G:36:ILE:HA	1:G:40:LEU:HD22	1.88	0.56
1:A:15:GLU:HG2	1:C:15:GLU:OE1	2.06	0.56
1:A:132:THR:HB	1:C:67:PRO:HB3	1.88	0.56
1:C:141:ALA:HA	1:C:144:LEU:HD12	1.87	0.56
1:D:16:ARG:NH2	5:D:404:HOH:O	2.38	0.56
1:H:137:GLN:NE2	1:J:172:ASP:OD2	2.38	0.56
1:E:21:TYR:HB2	1:I:4:VAL:HG11	1.87	0.55
1:J:40:LEU:HD23	1:J:41:ALA:N	2.21	0.55
1:E:188:LYS:HD3	1:E:197:LYS:HD2	1.89	0.55
1:J:6:TYR:HA	1:J:19:ASP:HA	1.88	0.55
1:A:16:ARG:HG2	1:C:15:GLU:HA	1.88	0.55
1:J:136:ILE:O	1:J:137:GLN:HG2	2.06	0.55
1:A:36:ILE:HD12	1:A:99:MET:HB3	1.89	0.55
1:A:4:VAL:HG12	1:A:19:ASP:HB2	1.88	0.55
1:D:51:LEU:HD13	1:D:60:ILE:HG12	1.88	0.55
1:K:195:GLU:HG2	1:K:196:THR:OG1	2.07	0.55
1:L:16:ARG:HD2	1:L:18:MET:HE1	1.89	0.55
1:N:93:ILE:HG23	1:N:115:LEU:HD22	1.89	0.55
1:C:7:VAL:HG11	1:C:23:ARG:HD3	1.89	0.55
1:C:170:GLU:HG2	1:H:139:GLN:HE21	1.71	0.55
1:F:129:ILE:HD13	1:F:143:ILE:HB	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:115:LEU:HD13	1:M:79:ASP:HB3	1.88	0.55
1:J:163:GLU:O	1:J:167:GLU:HG3	2.07	0.55
1:D:98:SER:OG	1:D:99:MET:N	2.38	0.55
1:F:115:LEU:HD13	1:K:79:ASP:HB3	1.88	0.55
1:G:129:ILE:HD13	1:N:129:ILE:HG12	1.88	0.55
1:E:98:SER:OG	1:E:99:MET:N	2.38	0.54
1:M:136:ILE:CD1	1:M:137:GLN:H	2.20	0.54
1:E:144:LEU:HD21	1:F:144:LEU:CD1	2.34	0.54
1:K:11:THR:HG21	1:N:13:ARG:H	1.72	0.54
1:L:129:ILE:O	1:L:131:GLY:N	2.35	0.54
1:N:181:ILE:HD11	1:N:189:VAL:HG23	1.88	0.54
1:A:39:PRO:HB2	1:C:2:THR:HG21	1.88	0.54
1:G:11:THR:HA	1:G:15:GLU:HG3	1.89	0.54
1:B:8:VAL:HG21	1:L:16:ARG:HB2	1.89	0.54
1:I:55:ASP:HB3	1:I:58:LYS:HB2	1.89	0.54
1:C:72:THR:H	1:C:130:ILE:CG2	2.21	0.54
1:F:128:GLY:C	1:F:129:ILE:HG13	2.28	0.54
1:C:16:ARG:CZ	1:C:16:ARG:H	2.20	0.54
1:C:41:ALA:O	1:C:45:ILE:HG13	2.08	0.54
1:C:129:ILE:CD1	1:H:136:ILE:HB	2.38	0.54
1:B:7:VAL:HB	1:B:23:ARG:HG3	1.89	0.54
1:L:28:ARG:HH12	1:L:60:ILE:HG13	1.73	0.54
1:M:23:ARG:O	1:M:23:ARG:NH1	2.36	0.54
1:G:43:THR:HG22	1:G:47:GLN:HE21	1.72	0.53
1:L:98:SER:OG	1:L:99:MET:N	2.40	0.53
1:D:11:THR:OG1	1:D:14:GLY:O	2.26	0.53
1:M:191:SER:OG	1:M:195:GLU:OE2	2.26	0.53
1:D:113:TYR:CZ	1:D:196:THR:HG23	2.43	0.53
1:F:6:TYR:HA	1:F:19:ASP:HA	1.90	0.53
1:A:199:LYS:HG2	1:A:200:SER:H	1.73	0.53
1:B:129:ILE:HD12	1:D:137:GLN:HE21	1.74	0.53
1:I:139:GLN:NE2	1:K:124:GLN:O	2.35	0.53
1:M:36:ILE:HA	1:M:40:LEU:HD23	1.89	0.53
1:A:93:ILE:HG23	1:A:115:LEU:HD22	1.91	0.53
1:K:8:VAL:HG21	1:N:16:ARG:NE	2.24	0.53
1:K:36:ILE:HB	1:K:69:GLY:HA3	1.89	0.53
1:L:74:GLY:HA3	1:L:99:MET:SD	2.49	0.53
1:M:93:ILE:HG22	1:M:115:LEU:HD22	1.90	0.53
1:A:129:ILE:HG23	1:J:129:ILE:HG12	1.91	0.53
1:D:132:THR:HG21	1:M:67:PRO:HG3	1.91	0.53
1:A:8:VAL:HG11	1:F:16:ARG:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:SER:HB2	1:A:194:LYS:NZ	2.24	0.53
1:H:11:THR:OG1	1:H:14:GLY:O	2.27	0.53
1:F:9:GLU:HG3	1:F:16:ARG:NH2	2.25	0.52
1:L:138:LEU:CD1	1:L:143:ILE:HG22	2.39	0.52
1:M:43:THR:HG22	1:M:47:GLN:HE21	1.73	0.52
1:J:177:ALA:HB1	1:J:189:VAL:HG22	1.92	0.52
1:A:15:GLU:O	1:A:15:GLU:HG3	2.10	0.52
1:F:16:ARG:HG2	1:F:16:ARG:HH21	1.74	0.52
1:A:33:GLY:O	1:F:42:ASN:ND2	2.41	0.52
1:A:174:PHE:HB2	1:F:142:GLU:OE1	2.10	0.52
1:F:7:VAL:HG11	1:F:23:ARG:HG2	1.90	0.52
1:I:129:ILE:HG21	5:I:304:HOH:O	2.08	0.52
1:K:68:GLY:N	5:K:305:HOH:O	2.41	0.52
1:K:188:LYS:HD2	1:K:196:THR:HG23	1.91	0.52
1:C:196:THR:HG23	1:C:197:LYS:HG2	1.90	0.52
1:F:65:ASN:ND2	1:F:95:GLN:H	2.08	0.52
1:H:13:ARG:HH22	1:M:13:ARG:HB3	1.73	0.52
1:M:123:HIS:CE1	1:M:125:PRO:HA	2.44	0.52
1:D:3:LEU:HD23	1:G:43:THR:HG21	1.91	0.52
1:D:14:GLY:HA3	1:M:15:GLU:HG2	1.91	0.52
1:E:7:VAL:N	1:E:18:MET:O	2.43	0.52
1:J:121:MET:HG3	1:J:173:PHE:O	2.10	0.52
1:N:14:GLY:C	1:N:16:ARG:HH11	2.13	0.52
1:A:121:MET:HE1	1:A:125:PRO:HG3	1.92	0.52
1:J:3:LEU:H	1:J:3:LEU:HD12	1.75	0.52
1:K:8:VAL:HG11	1:N:16:ARG:HE	1.74	0.52
1:L:16:ARG:HD2	1:L:18:MET:CE	2.40	0.52
1:D:55:ASP:OD2	1:D:58:LYS:HE3	2.10	0.51
1:E:9:GLU:HB2	1:E:16:ARG:HH21	1.75	0.51
1:F:7:VAL:HG12	1:F:18:MET:HG2	1.90	0.51
1:K:203:SER:O	1:K:203:SER:OG	2.27	0.51
1:G:35:GLU:HG3	1:G:67:PRO:HG2	1.92	0.51
1:K:27:ASP:HB3	1:K:201:ILE:HG12	1.91	0.51
1:K:139:GLN:NE2	5:K:302:HOH:O	2.26	0.51
1:L:98:SER:HB2	1:L:124:GLN:HA	1.93	0.51
1:L:193:ALA:O	1:L:196:THR:OG1	2.29	0.51
1:N:122:ILE:HD11	1:N:185:LEU:HD21	1.92	0.51
1:B:173:PHE:HB3	1:M:170:GLU:OE2	2.11	0.51
1:E:110:GLY:O	1:E:188:LYS:HE3	2.10	0.51
1:I:28:ARG:NE	1:I:58:LYS:HB3	2.26	0.51
1:A:171:ARG:HE	1:E:171:ARG:HG2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:123:HIS:CE1	1:F:125:PRO:HA	2.46	0.51
1:H:67:PRO:HB3	1:M:134:ALA:HB1	1.92	0.51
1:K:196:THR:HG22	1:K:197:LYS:N	2.22	0.51
1:A:137:GLN:NE2	1:J:129:ILE:H	2.09	0.51
1:E:82:ARG:NH2	5:E:407:HOH:O	2.43	0.51
1:N:130:ILE:HG21	1:N:146:LEU:HD13	1.92	0.51
1:F:71:ILE:HG12	1:F:99:MET:HE3	1.92	0.51
1:F:98:SER:HB2	1:F:124:GLN:NE2	2.25	0.51
1:J:34:GLN:CG	1:J:40:LEU:HD13	2.35	0.51
1:M:136:ILE:HD12	1:M:137:GLN:N	2.22	0.51
1:A:16:ARG:HH21	1:C:16:ARG:HA	1.76	0.51
1:A:190:ILE:HG22	1:A:194:LYS:HG2	1.92	0.51
1:G:93:ILE:HG23	1:G:115:LEU:HD12	1.92	0.51
1:H:124:GLN:NE2	5:H:405:HOH:O	2.36	0.51
1:K:190:ILE:HG22	1:K:196:THR:OG1	2.11	0.51
1:C:6:TYR:HA	1:C:19:ASP:HA	1.93	0.51
1:E:54:GLU:HG3	1:E:55:ASP:H	1.76	0.51
1:G:8:VAL:HG11	1:I:16:ARG:HG3	1.92	0.51
1:D:190:ILE:HD12	1:G:83:PHE:CZ	2.45	0.50
1:G:194:LYS:O	1:G:194:LYS:HD3	2.11	0.50
1:I:141:ALA:HA	1:I:144:LEU:HD23	1.92	0.50
1:J:92:CYS:HB2	1:J:104:LEU:HD22	1.93	0.50
1:E:36:ILE:HB	1:E:69:GLY:HA3	1.93	0.50
1:I:143:ILE:HD12	1:I:144:LEU:N	2.26	0.50
1:C:177:ALA:HB1	1:C:189:VAL:HG22	1.93	0.50
1:D:168:ASP:O	1:D:171:ARG:HB2	2.10	0.50
1:F:8:VAL:HG22	1:K:16:ARG:CZ	2.42	0.50
1:I:71:ILE:HD12	1:I:72:THR:H	1.76	0.50
1:M:6:TYR:HA	1:M:19:ASP:HA	1.93	0.50
1:N:70:TYR:CB	1:N:131:GLY:H	2.20	0.50
1:A:16:ARG:NH2	1:C:16:ARG:HA	2.27	0.50
1:D:123:HIS:O	1:D:125:PRO:HD3	2.12	0.50
1:G:177:ALA:HB1	1:G:189:VAL:HG22	1.94	0.50
1:I:71:ILE:HD12	1:I:72:THR:N	2.27	0.50
1:F:170:GLU:OE1	1:I:171:ARG:NH1	2.45	0.50
1:G:7:VAL:HG12	1:G:9:GLU:OE2	2.12	0.50
1:H:134:ALA:O	1:H:136:ILE:HG23	2.11	0.50
1:M:193:ALA:O	1:M:197:LYS:HB3	2.12	0.50
1:B:8:VAL:HG22	1:B:16:ARG:HB2	1.94	0.50
1:D:36:ILE:HB	1:D:69:GLY:HA3	1.93	0.50
1:I:71:ILE:HD13	1:I:146:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:130:ILE:HG21	1:F:136:ILE:HB	1.94	0.49
1:H:8:VAL:HA	1:H:16:ARG:NH1	2.27	0.49
1:D:141:ALA:O	1:D:145:THR:OG1	2.24	0.49
1:F:36:ILE:HB	1:F:69:GLY:HA3	1.94	0.49
1:H:63:PHE:CD1	1:H:93:ILE:HD11	2.46	0.49
2:M:301:UER:O03	2:M:301:UER:O01	2.29	0.49
1:N:138:LEU:HB2	1:N:142:GLU:CG	2.42	0.49
1:H:137:GLN:NE2	5:H:402:HOH:O	2.35	0.49
1:N:18:MET:HB2	1:N:22:SER:HB2	1.94	0.49
1:D:58:LYS:HA	1:D:202:ALA:HB2	1.94	0.49
1:I:36:ILE:HA	1:I:40:LEU:HD22	1.95	0.49
1:M:15:GLU:O	1:M:16:ARG:HG2	2.12	0.49
1:E:54:GLU:HG3	1:E:55:ASP:N	2.28	0.49
1:D:49:LEU:O	1:D:52:MET:HG2	2.12	0.49
1:L:28:ARG:NH1	1:L:60:ILE:HG13	2.28	0.49
1:A:18:MET:HE2	1:A:23:ARG:HA	1.94	0.49
1:B:146:LEU:HD11	4:N:301:GOL:H2	1.94	0.49
1:H:8:VAL:CA	1:H:16:ARG:NH1	2.76	0.49
1:L:149:HIS:O	1:L:153:ILE:HD12	2.13	0.49
1:D:194:LYS:HA	1:D:199:LYS:HZ1	1.78	0.49
1:E:109:LYS:HD3	1:E:109:LYS:O	2.12	0.49
1:L:6:TYR:HA	1:L:19:ASP:HA	1.95	0.49
1:D:6:TYR:HA	1:D:19:ASP:HA	1.94	0.49
1:D:24:LEU:HD21	1:G:50:PHE:HB2	1.95	0.49
1:E:9:GLU:H	1:E:16:ARG:HE	1.61	0.49
1:E:13:ARG:HG2	1:J:13:ARG:O	2.13	0.49
1:E:190:ILE:CD1	1:E:196:THR:HA	2.42	0.49
1:G:189:VAL:O	1:G:196:THR:HA	2.12	0.49
1:J:58:LYS:NZ	1:J:199:LYS:HG2	2.28	0.49
1:A:6:TYR:HA	1:A:19:ASP:HA	1.95	0.48
1:C:126:SER:O	1:H:137:GLN:HG2	2.13	0.48
1:G:136:ILE:O	1:G:137:GLN:HG2	2.12	0.48
1:M:137:GLN:O	1:M:138:LEU:HB3	2.13	0.48
1:B:9:GLU:CB	1:B:23:ARG:HH21	2.26	0.48
1:F:9:GLU:HG3	1:F:16:ARG:HH22	1.78	0.48
1:H:138:LEU:N	1:H:138:LEU:HD22	2.27	0.48
1:L:55:ASP:OD2	1:L:58:LYS:HE3	2.14	0.48
1:M:9:GLU:OE1	1:M:9:GLU:HA	2.13	0.48
1:E:141:ALA:HA	1:E:144:LEU:HD23	1.95	0.48
1:F:139:GLN:O	1:F:143:ILE:HG12	2.13	0.48
1:I:175:MET:HB2	1:I:179:GLU:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:87:ASP:OD2	1:J:111:LYS:NZ	2.46	0.48
1:A:34:GLN:NE2	5:A:404:HOH:O	2.46	0.48
1:D:110:GLY:N	1:D:187:ASP:OD2	2.44	0.48
1:H:64:ILE:O	5:H:401:HOH:O	2.20	0.48
1:J:98:SER:OG	1:J:99:MET:N	2.46	0.48
1:C:93:ILE:HG23	1:C:115:LEU:HD12	1.95	0.48
1:C:129:ILE:CD1	1:H:138:LEU:HD21	2.29	0.48
1:G:129:ILE:C	1:G:131:GLY:H	2.17	0.48
1:I:143:ILE:HD11	1:K:143:ILE:HG21	1.95	0.48
1:L:129:ILE:HG13	1:M:130:ILE:HD11	1.95	0.48
1:L:36:ILE:HB	1:L:69:GLY:HA3	1.95	0.48
1:N:124:GLN:OE1	1:N:124:GLN:N	2.46	0.48
1:F:130:ILE:HG23	1:F:137:GLN:H	1.79	0.48
1:G:8:VAL:O	1:G:8:VAL:HG13	2.13	0.48
1:G:129:ILE:HG12	1:N:138:LEU:HG	1.96	0.48
1:M:141:ALA:HB1	1:M:144:LEU:HB3	1.96	0.48
1:E:7:VAL:HG12	1:E:18:MET:HG3	1.95	0.48
1:H:194:LYS:HD3	1:H:194:LYS:H	1.79	0.48
1:E:9:GLU:HB2	1:E:16:ARG:CZ	2.44	0.48
1:I:71:ILE:HD12	1:I:72:THR:HG23	1.96	0.48
1:B:121:MET:HE3	1:B:125:PRO:HG3	1.95	0.48
1:G:129:ILE:CD1	1:N:136:ILE:HG22	2.44	0.48
1:K:9:GLU:OE2	1:N:54:GLU:CD	2.53	0.48
1:J:34:GLN:O	1:J:67:PRO:HD2	2.14	0.47
1:J:140:ALA:O	1:J:143:ILE:HG12	2.14	0.47
1:K:139:GLN:HG3	1:K:140:ALA:H	1.79	0.47
1:D:16:ARG:HG2	1:M:15:GLU:OE1	2.14	0.47
1:D:129:ILE:N	5:D:406:HOH:O	2.40	0.47
1:H:171:ARG:HG2	1:H:173:PHE:CD1	2.49	0.47
1:B:9:GLU:CG	1:B:10:ASP:N	2.77	0.47
1:G:8:VAL:O	1:G:8:VAL:CG1	2.62	0.47
1:G:2:THR:HG23	1:G:3:LEU:H	1.79	0.47
1:G:4:VAL:HG23	1:G:4:VAL:O	2.15	0.47
1:K:171:ARG:HG2	1:K:173:PHE:CD2	2.50	0.47
1:M:58:LYS:HA	1:M:58:LYS:HD3	1.64	0.47
1:D:125:PRO:HD2	1:D:126:SER:HB2	1.97	0.47
1:F:140:ALA:O	1:F:142:GLU:N	2.48	0.47
1:I:178:GLU:H	1:I:178:GLU:CD	2.17	0.47
1:J:40:LEU:HD23	1:J:40:LEU:C	2.35	0.47
1:J:201:ILE:HD12	1:J:201:ILE:HA	1.81	0.47
1:A:160:GLN:NE2	1:A:183:TYR:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:LYS:NZ	5:C:404:HOH:O	2.48	0.47
1:D:117:HIS:HB2	1:G:79:ASP:OD2	2.15	0.47
1:D:121:MET:CE	1:D:125:PRO:HG3	2.44	0.47
1:E:70:TYR:HD1	1:E:130:ILE:HA	1.79	0.47
1:F:36:ILE:HA	1:F:40:LEU:HD22	1.96	0.47
1:F:126:SER:HB2	1:K:136:ILE:HD11	1.97	0.47
1:I:93:ILE:HG23	1:I:115:LEU:HD12	1.95	0.47
1:I:143:ILE:HD12	1:I:144:LEU:HD22	1.96	0.47
1:K:35:GLU:HA	5:K:305:HOH:O	2.15	0.47
1:K:88:VAL:H	1:K:108:THR:CG2	2.27	0.47
1:N:23:ARG:HH11	1:N:26:LYS:HB2	1.80	0.47
1:N:132:THR:HB	1:N:135:ASP:O	2.15	0.47
1:A:79:ASP:HB3	1:C:115:LEU:HD13	1.97	0.47
1:A:137:GLN:HA	1:J:128:GLY:CA	2.44	0.47
1:K:67:PRO:HB3	1:N:137:GLN:HE22	1.80	0.47
1:A:9:GLU:OE1	1:F:54:GLU:OE2	2.33	0.47
1:A:51:LEU:HD13	1:A:60:ILE:HG12	1.97	0.47
1:E:188:LYS:HD3	1:E:197:LYS:CD	2.45	0.47
1:A:194:LYS:HB3	1:A:195:GLU:H	1.60	0.47
1:E:160:GLN:NE2	1:E:183:TYR:O	2.48	0.47
1:K:43:THR:HG22	1:K:47:GLN:HE21	1.80	0.47
1:L:37:THR:HG22	1:L:70:TYR:HE2	1.80	0.47
1:G:3:LEU:HD21	1:I:19:ASP:OD2	2.14	0.46
1:I:18:MET:SD	1:I:23:ARG:HA	2.55	0.46
1:K:116:PRO:HG3	1:K:191:SER:HB3	1.97	0.46
1:H:45:ILE:HG23	1:H:80:THR:HG21	1.96	0.46
1:A:9:GLU:HG2	1:A:10:ASP:H	1.80	0.46
1:G:36:ILE:HB	1:G:69:GLY:HA3	1.97	0.46
1:J:41:ALA:HB2	1:J:73:ALA:HB1	1.97	0.46
1:M:55:ASP:OD1	1:M:58:LYS:HG2	2.15	0.46
1:M:130:ILE:HG12	1:M:131:GLY:H	1.79	0.46
1:M:140:ALA:O	1:M:142:GLU:N	2.45	0.46
1:D:124:GLN:HG3	1:D:126:SER:HB3	1.97	0.46
1:K:194:LYS:HD3	1:K:194:LYS:HA	1.74	0.46
1:C:45:ILE:HG23	1:C:80:THR:HG21	1.98	0.46
1:J:7:VAL:HG21	1:J:23:ARG:CB	2.44	0.46
1:E:131:GLY:HA3	1:E:138:LEU:HD23	1.96	0.46
1:J:40:LEU:O	1:J:44:VAL:HG23	2.16	0.46
1:A:199:LYS:HE2	1:A:199:LYS:HB3	1.68	0.46
1:C:18:MET:HB3	1:C:22:SER:HB2	1.98	0.46
1:E:43:THR:HG23	1:I:3:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:8:VAL:CA	1:H:16:ARG:HH11	2.29	0.46
1:M:36:ILE:HB	1:M:69:GLY:HA3	1.97	0.46
1:F:9:GLU:HG3	1:F:16:ARG:CZ	2.46	0.46
1:A:125:PRO:O	1:E:126:SER:HA	2.15	0.46
1:I:18:MET:HG2	1:I:22:SER:HB2	1.98	0.46
1:I:23:ARG:O	1:I:23:ARG:NH1	2.38	0.46
1:A:124:GLN:NE2	1:A:126:SER:H	2.13	0.46
1:C:23:ARG:O	1:C:23:ARG:NH1	2.49	0.46
1:C:23:ARG:NH1	1:C:26:LYS:HB3	2.27	0.46
1:D:134:ALA:HB3	1:D:137:GLN:HB2	1.98	0.46
1:H:131:GLY:HA3	1:H:135:ASP:OD2	2.16	0.46
1:M:15:GLU:C	1:M:16:ARG:HG2	2.37	0.46
1:A:18:MET:CE	1:A:23:ARG:HA	2.46	0.45
1:C:71:ILE:H	1:C:130:ILE:HD12	1.81	0.45
1:G:128:GLY:O	1:G:132:THR:HG23	2.16	0.45
1:G:198:ASP:OD1	1:G:203:SER:OG	2.31	0.45
1:I:2:THR:OG1	1:I:3:LEU:N	2.50	0.45
1:L:148:LYS:HB3	1:L:148:LYS:HE2	1.66	0.45
1:M:51:LEU:HD13	1:M:60:ILE:HG12	1.97	0.45
1:D:174:PHE:HB2	1:G:142:GLU:OE2	2.16	0.45
1:K:9:GLU:OE1	1:N:54:GLU:HG3	2.16	0.45
1:D:191:SER:O	1:G:83:PHE:HA	2.17	0.45
1:H:7:VAL:HG11	1:H:23:ARG:HG2	1.98	0.45
1:I:128:GLY:HA3	1:K:138:LEU:O	2.17	0.45
1:I:198:ASP:HB3	1:I:200:SER:O	2.16	0.45
1:D:168:ASP:HA	1:D:171:ARG:HH11	1.82	0.45
1:G:98:SER:OG	1:G:99:MET:N	2.38	0.45
1:I:70:TYR:HB3	5:I:304:HOH:O	2.15	0.45
1:K:15:GLU:HA	1:K:16:ARG:NH1	2.30	0.45
1:N:98:SER:HG	1:N:99:MET:H	1.63	0.45
1:A:71:ILE:HD12	1:A:71:ILE:H	1.81	0.45
1:N:71:ILE:HB	1:N:130:ILE:CG2	2.47	0.45
1:B:15:GLU:HG3	1:N:15:GLU:HG2	1.98	0.45
1:I:36:ILE:HB	1:I:69:GLY:HA3	1.98	0.45
1:N:125:PRO:O	5:N:401:HOH:O	2.21	0.45
1:B:142:GLU:OE1	1:N:174:PHE:HB2	2.17	0.45
1:H:51:LEU:HD13	1:H:60:ILE:HG12	1.98	0.45
1:J:175:MET:HB2	1:J:179:GLU:HB3	1.99	0.45
1:B:43:THR:HG22	1:B:47:GLN:HE21	1.82	0.45
1:E:28:ARG:NH1	1:E:54:GLU:OE2	2.47	0.45
1:E:71:ILE:HA	1:E:99:MET:SD	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:PHE:HB2	1:J:142:GLU:OE1	2.17	0.45
1:N:8:VAL:HG12	1:N:16:ARG:O	2.16	0.45
1:N:72:THR:HG23	1:N:130:ILE:CG2	2.45	0.45
1:H:123:HIS:O	1:H:125:PRO:HD3	2.16	0.45
1:I:192:SER:HB2	1:I:197:LYS:H	1.82	0.45
1:J:74:GLY:HA3	1:J:99:MET:HE2	1.99	0.45
1:N:134:ALA:O	1:N:136:ILE:HG13	2.17	0.45
1:A:9:GLU:OE2	1:F:54:GLU:OE2	2.35	0.45
1:B:19:ASP:OD1	1:B:22:SER:OG	2.29	0.45
1:B:109:LYS:H	1:B:109:LYS:CE	2.30	0.45
1:D:22:SER:HB3	1:M:6:TYR:O	2.17	0.45
1:G:129:ILE:HD12	1:G:129:ILE:O	2.16	0.45
1:H:122:ILE:HD11	1:H:168:ASP:HB2	1.98	0.45
1:K:9:GLU:OE2	1:N:54:GLU:OE1	2.35	0.45
1:K:199:LYS:O	1:K:200:SER:HB3	2.17	0.45
1:L:200:SER:O	1:L:201:ILE:HB	2.17	0.45
1:N:129:ILE:HD12	1:N:130:ILE:H	1.80	0.45
1:A:8:VAL:HG11	1:F:16:ARG:CB	2.47	0.44
1:B:119:ARG:CZ	1:L:145:THR:HG21	2.47	0.44
1:D:59:ASP:OD2	1:D:111:LYS:NZ	2.47	0.44
4:G:301:GOL:H12	1:I:75:LEU:HB3	1.99	0.44
1:N:152:ASN:ND2	5:N:406:HOH:O	2.40	0.44
1:A:9:GLU:CD	1:F:54:GLU:OE2	2.55	0.44
1:E:41:ALA:HB2	1:E:73:ALA:HB1	2.00	0.44
1:E:116:PRO:HG3	1:E:191:SER:HB3	2.00	0.44
1:L:163:GLU:H	1:L:163:GLU:HG2	1.60	0.44
1:A:129:ILE:HG23	1:J:129:ILE:CG1	2.47	0.44
1:C:181:ILE:HD11	1:C:189:VAL:HG23	2.00	0.44
1:D:190:ILE:HD12	1:G:83:PHE:HZ	1.82	0.44
1:F:140:ALA:O	1:F:144:LEU:HD22	2.17	0.44
1:H:126:SER:HB2	1:L:126:SER:OG	2.18	0.44
1:L:3:LEU:O	1:L:5:PRO:HD3	2.17	0.44
1:L:71:ILE:HB	1:L:130:ILE:HG23	2.00	0.44
1:N:26:LYS:HE3	1:N:26:LYS:HB3	1.64	0.44
1:A:147:LYS:HD3	1:A:147:LYS:HA	1.81	0.44
1:A:164:LYS:HE3	1:A:168:ASP:OD2	2.17	0.44
1:B:35:GLU:HG2	1:B:69:GLY:HA2	1.98	0.44
1:J:128:GLY:C	1:J:130:ILE:N	2.71	0.44
1:N:193:ALA:O	1:N:196:THR:OG1	2.34	0.44
1:A:8:VAL:HG23	1:A:16:ARG:N	2.33	0.44
1:I:13:ARG:NH1	1:I:15:GLU:HB3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:45:ILE:HG23	1:I:80:THR:HG21	1.99	0.44
1:I:143:ILE:HD12	1:I:144:LEU:H	1.81	0.44
1:A:109:LYS:NZ	1:A:157:CYS:O	2.44	0.44
1:C:87:ASP:HA	1:C:108:THR:HG21	1.99	0.44
1:I:6:TYR:HA	1:I:19:ASP:HA	1.99	0.44
1:C:51:LEU:HD13	1:C:60:ILE:HG12	1.99	0.44
1:D:171:ARG:HD2	1:D:173:PHE:HE2	1.82	0.44
1:F:175:MET:HB2	1:F:179:GLU:HB3	1.98	0.44
1:G:196:THR:HB	1:G:200:SER:OG	2.18	0.44
1:H:36:ILE:HB	1:H:69:GLY:HA3	2.00	0.44
1:H:112:ARG:NH2	1:H:184:GLY:O	2.51	0.44
1:J:8:VAL:HG23	1:J:15:GLU:C	2.37	0.44
1:N:138:LEU:HB2	1:N:142:GLU:HG2	1.99	0.44
1:N:197:LYS:HE2	1:N:197:LYS:HB2	1.76	0.44
1:D:171:ARG:HB3	1:D:173:PHE:CE2	2.53	0.44
1:D:197:LYS:HD2	1:D:200:SER:HB3	2.00	0.44
1:I:55:ASP:OD2	1:I:58:LYS:HD3	2.18	0.44
1:I:195:GLU:HB3	1:I:201:ILE:HG12	2.00	0.44
1:B:22:SER:HB3	1:N:6:TYR:O	2.17	0.44
1:C:88:VAL:H	1:C:108:THR:HG23	1.82	0.44
1:F:98:SER:HB3	1:F:125:PRO:HD3	1.99	0.44
1:G:49:LEU:O	1:G:52:MET:HG2	2.18	0.44
1:I:127:GLY:HA3	1:K:137:GLN:H	1.83	0.44
1:M:144:LEU:O	1:M:148:LYS:HG3	2.18	0.44
1:N:16:ARG:HG3	1:N:18:MET:HE1	2.00	0.44
1:A:8:VAL:HG21	1:F:16:ARG:HB3	2.00	0.43
1:A:140:ALA:O	1:A:143:ILE:HG13	2.18	0.43
1:J:40:LEU:O	1:J:43:THR:HG22	2.18	0.43
1:K:7:VAL:CG1	1:K:23:ARG:HG2	2.34	0.43
1:A:171:ARG:HE	1:E:171:ARG:CG	2.31	0.43
1:N:70:TYR:HB3	1:N:131:GLY:N	2.25	0.43
1:C:79:ASP:OD2	1:L:117:HIS:HB2	2.17	0.43
1:F:70:TYR:CD1	1:F:130:ILE:HA	2.53	0.43
1:F:110:GLY:N	1:F:187:ASP:OD2	2.42	0.43
1:J:71:ILE:H	1:J:71:ILE:HG13	1.46	0.43
1:J:129:ILE:HG21	1:J:143:ILE:HD12	2.00	0.43
1:J:190:ILE:HG22	1:J:194:LYS:HE2	2.00	0.43
1:A:70:TYR:CD2	1:A:130:ILE:HD13	2.53	0.43
1:C:8:VAL:CA	1:C:16:ARG:HH12	2.32	0.43
1:C:136:ILE:HG22	1:H:126:SER:OG	2.19	0.43
1:E:93:ILE:HG23	1:E:115:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:16:ARG:C	1:K:16:ARG:HE	2.22	0.43
1:A:36:ILE:HB	1:A:69:GLY:HA3	2.00	0.43
1:D:28:ARG:HD2	1:D:58:LYS:HD2	1.99	0.43
1:F:10:ASP:OD2	1:F:10:ASP:C	2.55	0.43
1:I:70:TYR:HA	1:I:129:ILE:HD13	2.00	0.43
1:K:124:GLN:O	1:K:126:SER:N	2.50	0.43
1:B:51:LEU:HD13	1:B:60:ILE:HG12	2.00	0.43
1:D:121:MET:HB3	1:D:121:MET:HE2	1.71	0.43
1:G:129:ILE:HG23	1:N:138:LEU:HD11	2.00	0.43
1:J:58:LYS:HZ3	1:J:199:LYS:HE2	1.83	0.43
1:J:129:ILE:HD13	1:J:143:ILE:HD13	2.00	0.43
1:K:9:GLU:O	1:K:10:ASP:OD1	2.36	0.43
1:M:121:MET:HB3	1:M:121:MET:HE2	1.75	0.43
1:A:22:SER:HB3	1:C:6:TYR:H	1.83	0.43
1:A:88:VAL:HG23	1:A:107:GLY:HA2	2.00	0.43
1:B:147:LYS:HE3	5:D:409:HOH:O	2.17	0.43
1:F:197:LYS:HD2	1:F:197:LYS:HA	1.79	0.43
1:G:52:MET:HG3	1:G:53:SER:N	2.33	0.43
1:H:121:MET:HG3	1:H:173:PHE:O	2.19	0.43
1:N:71:ILE:HB	1:N:130:ILE:HG12	2.00	0.43
1:N:95:GLN:HB2	4:N:301:GOL:H11	2.00	0.43
1:D:14:GLY:CA	1:M:15:GLU:HG2	2.49	0.43
1:H:117:HIS:HB2	1:M:79:ASP:OD2	2.19	0.43
1:H:199:LYS:HE3	1:H:199:LYS:HB2	1.94	0.43
1:J:58:LYS:HZ2	1:J:199:LYS:HG2	1.83	0.43
1:A:9:GLU:O	1:A:14:GLY:HA2	2.19	0.43
1:A:124:GLN:HE21	1:A:126:SER:H	1.67	0.43
1:B:7:VAL:CB	1:B:23:ARG:HG3	2.48	0.43
1:E:51:LEU:HB3	1:E:60:ILE:HD11	2.00	0.43
1:E:144:LEU:HD11	1:F:144:LEU:HD11	2.00	0.43
1:F:61:GLN:HG3	1:F:89:ASN:HB2	2.01	0.43
1:J:31:MET:SD	1:J:63:PHE:HB2	2.59	0.43
1:K:24:LEU:HB3	1:K:29:ILE:HB	2.00	0.43
1:L:28:ARG:NH2	1:L:51:LEU:O	2.52	0.43
1:N:71:ILE:HA	1:N:99:MET:SD	2.59	0.43
1:A:177:ALA:HB1	1:A:189:VAL:HG22	2.01	0.42
1:B:49:LEU:O	1:B:52:MET:HG3	2.19	0.42
1:C:121:MET:HG3	1:C:173:PHE:O	2.18	0.42
1:M:135:ASP:O	1:M:136:ILE:HG13	2.19	0.42
1:A:79:ASP:OD2	1:C:117:HIS:HB2	2.19	0.42
1:B:109:LYS:H	1:B:109:LYS:HE2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:MET:HB2	1:D:179:GLU:HB3	2.01	0.42
1:I:98:SER:OG	1:I:99:MET:N	2.51	0.42
1:N:36:ILE:HB	1:N:69:GLY:HA3	2.00	0.42
1:B:148:LYS:HB3	1:B:148:LYS:HE3	1.73	0.42
1:G:192:SER:HB2	1:G:193:ALA:H	1.63	0.42
1:M:171:ARG:HG2	1:M:173:PHE:CD2	2.53	0.42
1:J:7:VAL:CG2	1:J:23:ARG:HB2	2.47	0.42
1:A:23:ARG:HH11	1:A:23:ARG:C	2.18	0.42
1:G:190:ILE:HD12	1:I:83:PHE:CE2	2.54	0.42
1:I:19:ASP:OD1	1:I:22:SER:OG	2.27	0.42
1:N:84:LEU:HD12	1:N:86:CYS:SG	2.59	0.42
1:A:23:ARG:HA	1:A:23:ARG:HD2	1.82	0.42
1:H:23:ARG:HD2	1:H:23:ARG:O	2.19	0.42
1:N:177:ALA:HB1	1:N:189:VAL:HG22	2.01	0.42
1:A:13:ARG:O	1:F:13:ARG:NH2	2.53	0.42
1:A:49:LEU:O	1:A:52:MET:HG2	2.20	0.42
1:A:67:PRO:HG2	5:A:414:HOH:O	2.20	0.42
1:C:54:GLU:HG3	1:C:55:ASP:H	1.84	0.42
1:D:47:GLN:HA	1:M:20:ILE:HD11	2.02	0.42
1:E:7:VAL:HG21	1:E:23:ARG:HG2	2.01	0.42
1:E:51:LEU:HD13	1:E:60:ILE:HG12	2.01	0.42
1:G:195:GLU:OE2	1:G:202:ALA:HB2	2.19	0.42
1:K:15:GLU:CG	1:K:16:ARG:HH12	2.30	0.42
1:A:132:THR:HB	1:C:67:PRO:CB	2.48	0.42
1:H:148:LYS:O	1:H:152:ASN:ND2	2.52	0.42
1:N:63:PHE:HD2	1:N:93:ILE:HD11	1.84	0.42
1:A:20:ILE:O	1:A:23:ARG:HB3	2.20	0.42
1:K:71:ILE:HD12	1:K:129:ILE:HB	2.02	0.42
1:A:72:THR:OG1	1:A:130:ILE:HG21	2.20	0.41
1:D:122:ILE:HD11	1:D:168:ASP:CB	2.48	0.41
1:G:121:MET:HG3	1:G:173:PHE:O	2.20	0.41
1:H:121:MET:SD	1:H:123:HIS:HB3	2.60	0.41
1:A:192:SER:HB2	1:A:194:LYS:HZ3	1.85	0.41
2:A:302:UER:C11	1:C:199:LYS:HG2	2.50	0.41
1:B:36:ILE:HB	1:B:69:GLY:HA3	2.01	0.41
1:H:171:ARG:NE	1:L:170:GLU:OE2	2.48	0.41
1:J:28:ARG:HD3	1:J:58:LYS:HG2	2.02	0.41
1:J:93:ILE:HG23	1:J:115:LEU:HD22	2.01	0.41
1:J:122:ILE:O	1:J:124:GLN:NE2	2.54	0.41
1:J:129:ILE:HB	1:J:143:ILE:HG21	2.01	0.41
1:B:38:GLU:H	1:B:38:GLU:HG2	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:GLU:HG2	5:B:435:HOH:O	2.20	0.41
1:B:48:LEU:O	1:B:52:MET:HG2	2.20	0.41
1:B:89:ASN:OD1	1:B:111:LYS:HD3	2.20	0.41
1:D:33:GLY:H	1:D:34:GLN:NE2	2.18	0.41
1:G:130:ILE:HD11	1:N:129:ILE:HG13	2.03	0.41
1:A:24:LEU:HB3	1:A:29:ILE:HB	2.02	0.41
1:E:144:LEU:CD2	1:F:144:LEU:HD11	2.38	0.41
1:G:82:ARG:NH1	1:G:106:ALA:O	2.51	0.41
1:I:16:ARG:HE	1:I:16:ARG:HB3	1.53	0.41
1:B:137:GLN:NE2	1:D:130:ILE:HD13	2.35	0.41
1:H:81:ILE:HD12	1:H:103:LEU:HD12	2.03	0.41
1:K:37:THR:HG22	1:K:70:TYR:HE2	1.85	0.41
1:L:129:ILE:H	1:L:129:ILE:HG22	1.56	0.41
2:A:302:UER:C19	1:C:27:ASP:HA	2.50	0.41
1:H:64:ILE:N	5:H:401:HOH:O	2.38	0.41
1:K:63:PHE:HD2	1:K:93:ILE:HD11	1.85	0.41
1:K:82:ARG:HG2	5:K:318:HOH:O	2.20	0.41
1:K:129:ILE:N	5:K:308:HOH:O	2.49	0.41
1:A:124:GLN:HE21	1:A:127:GLY:H	1.67	0.41
1:B:119:ARG:HD3	1:L:142:GLU:OE2	2.20	0.41
1:F:201:ILE:HG22	1:F:202:ALA:N	2.35	0.41
1:G:41:ALA:HA	1:G:77:ILE:HD11	2.03	0.41
2:G:302:UER:C02	1:I:83:PHE:CZ	3.04	0.41
1:K:8:VAL:CG2	1:N:16:ARG:HD2	2.49	0.41
1:B:131:GLY:O	1:B:132:THR:HB	2.21	0.41
1:C:9:GLU:OE2	1:C:23:ARG:NH2	2.53	0.41
1:E:19:ASP:OD1	1:E:22:SER:OG	2.30	0.41
1:E:129:ILE:O	1:E:130:ILE:HB	2.20	0.41
1:F:171:ARG:HE	1:I:170:GLU:CD	2.24	0.41
1:G:7:VAL:N	1:G:18:MET:O	2.52	0.41
1:G:41:ALA:HB2	1:G:73:ALA:HB1	2.03	0.41
1:H:139:GLN:HG3	1:J:172:ASP:O	2.21	0.41
1:K:58:LYS:HD2	1:K:58:LYS:HA	1.83	0.41
1:K:117:HIS:HB2	1:N:79:ASP:OD2	2.21	0.41
1:L:8:VAL:C	1:L:9:GLU:HG2	2.41	0.41
1:L:115:LEU:HD23	1:L:115:LEU:HA	1.89	0.41
1:A:171:ARG:HB3	1:A:173:PHE:CD1	2.55	0.41
1:G:94:GLY:HA2	4:G:301:GOL:H11	2.03	0.41
1:G:129:ILE:C	1:G:131:GLY:N	2.75	0.41
1:J:74:GLY:HA3	1:J:99:MET:CE	2.51	0.41
1:K:8:VAL:HG13	1:N:26:LYS:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:89:ASN:OD1	1:N:197:LYS:NZ	2.44	0.41
1:B:2:THR:O	1:B:2:THR:HG22	2.20	0.40
1:B:139:GLN:NE2	1:D:124:GLN:O	2.54	0.40
1:C:51:LEU:HD23	1:C:51:LEU:HA	1.95	0.40
1:C:129:ILE:HD12	1:H:138:LEU:CD2	2.29	0.40
1:F:126:SER:HA	1:I:126:SER:CA	2.47	0.40
1:G:102:LEU:HD13	1:G:150:LEU:HD12	2.03	0.40
1:M:139:GLN:NE2	5:M:408:HOH:O	2.53	0.40
1:F:8:VAL:HG13	1:K:15:GLU:HG2	2.03	0.40
1:F:131:GLY:HA3	1:F:137:GLN:NE2	2.36	0.40
1:G:160:GLN:NE2	1:G:164:LYS:HG2	2.36	0.40
1:H:4:VAL:HG23	1:H:4:VAL:O	2.21	0.40
1:H:175:MET:HB2	1:H:179:GLU:HB3	2.02	0.40
1:M:140:ALA:C	1:M:142:GLU:H	2.23	0.40
1:D:16:ARG:HD3	1:D:16:ARG:HA	1.86	0.40
1:D:163:GLU:OE2	1:D:167:GLU:HG3	2.22	0.40
1:H:174:PHE:HB2	1:M:142:GLU:OE1	2.22	0.40
1:I:140:ALA:O	1:I:142:GLU:N	2.54	0.40
1:A:136:ILE:HG22	1:A:137:GLN:N	2.37	0.40
1:D:7:VAL:N	1:D:18:MET:O	2.49	0.40
1:E:171:ARG:NH1	5:E:402:HOH:O	2.38	0.40
1:E:175:MET:HB2	1:E:179:GLU:HB2	2.03	0.40
1:I:67:PRO:O	1:I:125:PRO:HG2	2.22	0.40
1:L:10:ASP:O	1:L:12:GLY:N	2.54	0.40
1:L:82:ARG:HA	1:L:82:ARG:HD3	1.88	0.40
1:B:131:GLY:C	1:B:133:SER:H	2.25	0.40
1:C:7:VAL:HG12	1:C:18:MET:O	2.22	0.40
1:D:147:LYS:HE2	1:D:147:LYS:HB3	1.80	0.40
1:F:33:GLY:O	1:K:42:ASN:ND2	2.43	0.40
1:K:72:THR:OG1	1:K:130:ILE:HA	2.21	0.40
1:M:26:LYS:N	1:M:26:LYS:HD3	2.37	0.40
1:M:91:TYR:OH	1:M:197:LYS:HD3	2.21	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	201/203 (99%)	185 (92%)	16 (8%)	0	100 100
1	B	201/203 (99%)	182 (90%)	19 (10%)	0	100 100
1	C	201/203 (99%)	180 (90%)	20 (10%)	1 (0%)	29 43
1	D	201/203 (99%)	184 (92%)	17 (8%)	0	100 100
1	E	201/203 (99%)	180 (90%)	18 (9%)	3 (2%)	10 15
1	F	201/203 (99%)	184 (92%)	14 (7%)	3 (2%)	10 15
1	G	201/203 (99%)	184 (92%)	15 (8%)	2 (1%)	15 23
1	H	201/203 (99%)	181 (90%)	19 (10%)	1 (0%)	29 43
1	I	201/203 (99%)	182 (90%)	17 (8%)	2 (1%)	15 23
1	J	201/203 (99%)	179 (89%)	20 (10%)	2 (1%)	15 23
1	K	201/203 (99%)	176 (88%)	24 (12%)	1 (0%)	29 43
1	L	201/203 (99%)	180 (90%)	17 (8%)	4 (2%)	7 10
1	M	201/203 (99%)	182 (90%)	17 (8%)	2 (1%)	15 23
1	N	201/203 (99%)	185 (92%)	15 (8%)	1 (0%)	29 43
All	All	2814/2842 (99%)	2544 (90%)	248 (9%)	22 (1%)	19 29

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	129	ILE
1	M	130	ILE
1	C	130	ILE
1	F	136	ILE
1	G	130	ILE
1	J	16	ARG
1	L	136	ILE
1	L	198	ASP
1	L	201	ILE
1	N	201	ILE
1	E	130	ILE
1	F	137	GLN
1	H	3	LEU
1	E	16	ARG
1	G	136	ILE

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Mol	Chain	Res	Type
1	I	126	SER
1	I	136	ILE
1	M	136	ILE
1	F	126	SER
1	K	132	THR
1	L	199	LYS
1	E	139	GLN

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	167/167 (100%)	156 (93%)	11 (7%)	16	25
1	B	167/167 (100%)	156 (93%)	11 (7%)	16	25
1	C	167/167 (100%)	162 (97%)	5 (3%)	41	59
1	D	167/167 (100%)	159 (95%)	8 (5%)	25	39
1	E	167/167 (100%)	154 (92%)	13 (8%)	12	20
1	F	167/167 (100%)	159 (95%)	8 (5%)	25	39
1	G	167/167 (100%)	160 (96%)	7 (4%)	30	45
1	H	167/167 (100%)	153 (92%)	14 (8%)	11	16
1	I	167/167 (100%)	159 (95%)	8 (5%)	25	39
1	J	167/167 (100%)	159 (95%)	8 (5%)	25	39
1	K	167/167 (100%)	157 (94%)	10 (6%)	19	30
1	L	167/167 (100%)	153 (92%)	14 (8%)	11	16
1	M	167/167 (100%)	156 (93%)	11 (7%)	16	25
1	N	167/167 (100%)	156 (93%)	11 (7%)	16	25
All	All	2338/2338 (100%)	2199 (94%)	139 (6%)	19	30

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	3	LEU
1	A	7	VAL
1	A	9	GLU
1	A	34	GLN
1	A	40	LEU
1	A	119	ARG
1	A	136	ILE
1	A	188	LYS
1	A	191	SER
1	A	194	LYS
1	B	9	GLU
1	B	13	ARG
1	B	16	ARG
1	B	23	ARG
1	B	53	SER
1	B	61	GLN
1	B	109	LYS
1	B	119	ARG
1	B	124	GLN
1	B	136	ILE
1	B	194	LYS
1	C	8	VAL
1	C	10	ASP
1	C	13	ARG
1	C	16	ARG
1	C	54	GLU
1	D	9	GLU
1	D	18	MET
1	D	34	GLN
1	D	42	ASN
1	D	59	ASP
1	D	109	LYS
1	D	142	GLU
1	D	163	GLU
1	E	2	THR
1	E	8	VAL
1	E	10	ASP
1	E	16	ARG
1	E	18	MET
1	E	27	ASP
1	E	53	SER
1	E	109	LYS

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Mol	Chain	Res	Type
1	E	129	ILE
1	E	160	GLN
1	E	173	PHE
1	E	175	MET
1	E	194	LYS
1	F	1	MET
1	F	2	THR
1	F	3	LEU
1	F	9	GLU
1	F	16	ARG
1	F	53	SER
1	F	58	LYS
1	F	197	LYS
1	G	1	MET
1	G	3	LEU
1	G	8	VAL
1	G	16	ARG
1	G	121	MET
1	G	160	GLN
1	G	194	LYS
1	H	8	VAL
1	H	9	GLU
1	H	10	ASP
1	H	13	ARG
1	H	16	ARG
1	H	18	MET
1	H	40	LEU
1	H	52	MET
1	H	82	ARG
1	H	103	LEU
1	H	121	MET
1	H	138	LEU
1	H	194	LYS
1	H	203	SER
1	I	3	LEU
1	I	10	ASP
1	I	13	ARG
1	I	16	ARG
1	I	34	GLN
1	I	54	GLU
1	I	89	ASN
1	I	136	ILE

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Mol	Chain	Res	Type
1	J	1	MET
1	J	18	MET
1	J	71	ILE
1	J	102	LEU
1	J	124	GLN
1	J	126	SER
1	J	194	LYS
1	J	199	LYS
1	K	4	VAL
1	K	10	ASP
1	K	11	THR
1	K	16	ARG
1	K	18	MET
1	K	23	ARG
1	K	109	LYS
1	K	126	SER
1	K	173	PHE
1	K	203	SER
1	L	9	GLU
1	L	10	ASP
1	L	11	THR
1	L	16	ARG
1	L	35	GLU
1	L	42	ASN
1	L	72	THR
1	L	82	ARG
1	L	122	ILE
1	L	126	SER
1	L	138	LEU
1	L	144	LEU
1	L	196	THR
1	L	198	ASP
1	M	2	THR
1	M	3	LEU
1	M	8	VAL
1	M	9	GLU
1	M	16	ARG
1	M	34	GLN
1	M	102	LEU
1	M	138	LEU
1	M	139	GLN
1	M	143	ILE

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Mol	Chain	Res	Type
1	M	152	ASN
1	N	8	VAL
1	N	9	GLU
1	N	10	ASP
1	N	13	ARG
1	N	18	MET
1	N	27	ASP
1	N	52	MET
1	N	55	ASP
1	N	129	ILE
1	N	145	THR
1	N	197	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	42	ASN
1	A	124	GLN
1	A	139	GLN
1	A	152	ASN
1	B	95	GLN
1	B	124	GLN
1	B	137	GLN
1	B	139	GLN
1	C	42	ASN
1	C	61	GLN
1	D	34	GLN
1	D	42	ASN
1	D	137	GLN
1	E	139	GLN
1	F	47	GLN
1	F	65	ASN
1	F	123	HIS
1	F	124	GLN
1	G	34	GLN
1	G	117	HIS
1	G	124	GLN
1	G	137	GLN
1	H	95	GLN
1	H	137	GLN
1	H	139	GLN

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Mol	Chain	Res	Type
1	H	152	ASN
1	I	95	GLN
1	J	34	GLN
1	J	123	HIS
1	J	137	GLN
1	J	149	HIS
1	L	42	ASN
1	L	95	GLN
1	L	137	GLN
1	M	47	GLN
1	M	139	GLN
1	N	95	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
2	UER	A	301	-	32,34,34	6.84	11 (34%)	45,52,52	3.39	19 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	UER	B	301	-	32,34,34	6.88	10 (31%)	45,52,52	2.81	16 (35%)
2	UER	G	302	-	32,34,34	6.86	11 (34%)	45,52,52	3.27	16 (35%)
4	GOL	G	301	-	5,5,5	0.91	0	5,5,5	0.95	0
4	GOL	N	301	-	5,5,5	0.94	0	5,5,5	0.97	0
2	UER	A	302	-	32,34,34	6.86	10 (31%)	45,52,52	3.10	17 (37%)
4	GOL	C	301	-	5,5,5	0.89	0	5,5,5	0.96	0
2	UER	M	301	-	32,34,34	6.87	11 (34%)	45,52,52	3.19	17 (37%)
2	UER	D	301	-	32,34,34	6.87	11 (34%)	45,52,52	3.06	16 (35%)
4	GOL	B	303	-	5,5,5	0.92	0	5,5,5	0.97	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UER	A	301	-	-	15/31/45/45	0/3/3/3
2	UER	B	301	-	-	7/31/45/45	0/3/3/3
2	UER	G	302	-	-	17/31/45/45	0/3/3/3
4	GOL	G	301	-	-	0/4/4/4	-
4	GOL	N	301	-	-	2/4/4/4	-
2	UER	A	302	-	-	11/31/45/45	0/3/3/3
4	GOL	C	301	-	-	0/4/4/4	-
2	UER	M	301	-	-	18/31/45/45	0/3/3/3
2	UER	D	301	-	-	5/31/45/45	0/3/3/3
4	GOL	B	303	-	-	0/4/4/4	-

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	302	UER	O02-S01	24.96	1.65	1.44
2	B	301	UER	O03-S01	24.94	1.65	1.44
2	A	301	UER	O02-S01	24.93	1.65	1.44
2	D	301	UER	O02-S01	24.91	1.65	1.44
2	B	301	UER	O02-S01	24.90	1.65	1.44
2	A	302	UER	O03-S01	24.90	1.65	1.44
2	M	301	UER	O02-S01	24.89	1.65	1.44
2	D	301	UER	O03-S01	24.89	1.65	1.44
2	M	301	UER	O03-S01	24.82	1.65	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	302	UER	O03-S01	24.81	1.65	1.44
2	A	302	UER	O02-S01	24.78	1.65	1.44
2	A	301	UER	O03-S01	24.58	1.65	1.44
2	M	301	UER	C13-N02	-8.03	1.32	1.47
2	D	301	UER	C13-N02	-8.01	1.32	1.47
2	G	302	UER	C13-N02	-7.93	1.32	1.47
2	A	302	UER	C10-N02	-7.91	1.33	1.47
2	B	301	UER	C13-N02	-7.89	1.33	1.47
2	A	301	UER	C13-N02	-7.86	1.33	1.47
2	B	301	UER	C07-N02	7.72	1.48	1.35
2	A	301	UER	C10-N02	-7.70	1.33	1.47
2	A	302	UER	C13-N02	-7.70	1.33	1.47
2	G	302	UER	C10-N02	-7.65	1.33	1.47
2	M	301	UER	C07-N02	7.65	1.48	1.35
2	D	301	UER	C07-N02	7.62	1.48	1.35
2	A	301	UER	C07-N02	7.60	1.48	1.35
2	B	301	UER	C10-N02	-7.58	1.33	1.47
2	M	301	UER	C10-N02	-7.56	1.33	1.47
2	A	302	UER	C07-N02	7.53	1.48	1.35
2	D	301	UER	C10-N02	-7.45	1.33	1.47
2	G	302	UER	C07-N02	7.40	1.47	1.35
2	A	302	UER	C11-N03	-5.21	1.32	1.46
2	A	301	UER	C11-N03	-5.19	1.32	1.46
2	G	302	UER	C11-N03	-5.16	1.32	1.46
2	M	301	UER	C12-N03	-5.14	1.32	1.46
2	B	301	UER	C12-N03	-5.11	1.32	1.46
2	D	301	UER	C11-N03	-5.10	1.32	1.46
2	M	301	UER	C11-N03	-5.08	1.32	1.46
2	B	301	UER	C11-N03	-5.05	1.33	1.46
2	D	301	UER	C12-N03	-5.02	1.33	1.46
2	G	302	UER	C12-N03	-5.00	1.33	1.46
2	A	301	UER	C12-N03	-4.99	1.33	1.46
2	A	302	UER	C12-N03	-4.82	1.33	1.46
2	A	302	UER	C11-C10	-3.23	1.39	1.51
2	M	301	UER	C13-C12	-3.23	1.39	1.51
2	A	301	UER	C11-C10	-3.21	1.39	1.51
2	B	301	UER	C13-C12	-3.19	1.39	1.51
2	G	302	UER	C11-C10	-3.14	1.39	1.51
2	D	301	UER	C13-C12	-3.10	1.39	1.51
2	G	302	UER	C13-C12	-3.10	1.39	1.51
2	D	301	UER	C11-C10	-3.06	1.39	1.51
2	A	301	UER	C13-C12	-3.06	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	UER	C11-C10	-3.04	1.39	1.51
2	M	301	UER	C11-C10	-3.03	1.39	1.51
2	A	302	UER	C13-C12	-2.91	1.40	1.51
2	D	301	UER	C18-CL01	2.13	1.79	1.74
2	A	301	UER	O01-C07	-2.11	1.18	1.22
2	D	301	UER	O01-C07	-2.10	1.18	1.22
2	A	301	UER	C18-CL01	2.09	1.79	1.74
2	G	302	UER	C18-CL01	2.09	1.79	1.74
2	M	301	UER	C18-CL01	2.08	1.79	1.74
2	B	301	UER	C18-CL01	2.08	1.79	1.74
2	A	302	UER	C18-CL01	2.07	1.79	1.74
2	M	301	UER	O01-C07	-2.03	1.18	1.22
2	G	302	UER	O01-C07	-2.01	1.19	1.22

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	301	UER	O03-S01-O02	-10.01	107.98	118.98
2	A	301	UER	C06-C07-N02	9.81	130.13	120.90
2	G	302	UER	O03-S01-O02	-9.67	108.35	118.98
2	D	301	UER	O03-S01-O02	-9.55	108.49	118.98
2	A	302	UER	O03-S01-O02	-9.05	109.04	118.98
2	A	301	UER	O03-S01-O02	-8.40	109.75	118.98
2	M	301	UER	C06-S01-C03	8.36	118.21	106.26
2	B	301	UER	O03-S01-O02	-8.18	109.99	118.98
2	A	301	UER	C06-S01-C03	7.72	117.28	106.26
2	G	302	UER	C06-S01-C03	7.10	116.40	106.26
2	A	302	UER	C14-N03-C12	6.76	126.11	111.06
2	G	302	UER	C09-C06-C08	-6.71	105.59	111.33
2	D	301	UER	C02-N01-C03	6.30	122.61	115.91
2	D	301	UER	C06-C07-N02	6.07	126.61	120.90
2	G	302	UER	C06-C07-N02	5.81	126.36	120.90
2	G	302	UER	C02-N01-C03	5.67	121.94	115.91
2	A	302	UER	C06-C07-N02	5.58	126.15	120.90
2	M	301	UER	C06-C07-N02	5.50	126.08	120.90
2	A	302	UER	C10-C11-N03	5.46	121.85	110.64
2	A	302	UER	C02-N01-C03	5.40	121.65	115.91
2	M	301	UER	C13-C12-N03	5.32	121.55	110.64
2	A	301	UER	C02-N01-C03	5.27	121.52	115.91
2	B	301	UER	C14-N03-C11	5.27	122.79	111.06
2	M	301	UER	C02-N01-C03	5.23	121.47	115.91
2	D	301	UER	C13-C12-N03	5.23	121.36	110.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	302	UER	C13-C12-N03	5.23	121.36	110.64
2	G	302	UER	C13-C12-N03	5.21	121.34	110.64
2	B	301	UER	C13-C12-N03	5.20	121.30	110.64
2	A	301	UER	C13-C12-N03	5.18	121.28	110.64
2	B	301	UER	C02-N01-C03	5.02	121.25	115.91
2	B	301	UER	C10-C11-N03	5.00	120.90	110.64
2	D	301	UER	C10-C11-N03	5.00	120.90	110.64
2	A	301	UER	C10-C11-N03	4.98	120.85	110.64
2	A	301	UER	C11-C10-N02	4.96	121.07	110.44
2	M	301	UER	C10-C11-N03	4.94	120.77	110.64
2	D	301	UER	C06-S01-C03	4.92	113.28	106.26
2	M	301	UER	C14-N03-C11	4.90	121.97	111.06
2	G	302	UER	C10-C11-N03	4.89	120.67	110.64
2	M	301	UER	C11-C10-N02	4.83	120.79	110.44
2	B	301	UER	C12-C13-N02	4.81	120.75	110.44
2	G	302	UER	C11-C10-N02	4.81	120.74	110.44
2	A	302	UER	C11-C10-N02	4.79	120.70	110.44
2	B	301	UER	C11-C10-N02	4.78	120.67	110.44
2	D	301	UER	C11-C10-N02	4.77	120.66	110.44
2	M	301	UER	C12-C13-N02	4.77	120.66	110.44
2	D	301	UER	C12-C13-N02	4.69	120.48	110.44
2	D	301	UER	C14-N03-C11	4.64	121.39	111.06
2	A	302	UER	C09-C06-C08	-4.63	107.37	111.33
2	A	301	UER	C12-C13-N02	4.59	120.28	110.44
2	A	301	UER	C14-N03-C12	4.56	121.20	111.06
2	A	302	UER	C12-C13-N02	4.55	120.19	110.44
2	G	302	UER	C04-C03-N01	-4.49	120.35	125.28
2	A	302	UER	C06-S01-C03	4.47	112.64	106.26
2	G	302	UER	C14-N03-C12	4.46	121.00	111.06
2	G	302	UER	C12-C13-N02	4.46	120.00	110.44
2	A	301	UER	C14-N03-C11	4.30	120.62	111.06
2	G	302	UER	C14-N03-C11	4.29	120.61	111.06
2	B	301	UER	C06-C07-N02	4.29	124.94	120.90
2	G	302	UER	C12-N03-C11	4.25	118.39	108.83
2	D	301	UER	C14-N03-C12	4.22	120.46	111.06
2	A	301	UER	C12-N03-C11	4.15	118.18	108.83
2	D	301	UER	C12-N03-C11	4.13	118.13	108.83
2	B	301	UER	C12-N03-C11	4.13	118.12	108.83
2	D	301	UER	C04-C03-N01	-4.12	120.75	125.28
2	M	301	UER	C12-N03-C11	4.08	118.02	108.83
2	M	301	UER	C14-N03-C12	4.02	120.01	111.06
2	A	302	UER	C15-C14-N03	3.87	120.64	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	302	UER	C12-N03-C11	3.80	117.39	108.83
2	M	301	UER	C04-C03-N01	-3.63	121.29	125.28
2	B	301	UER	C14-N03-C12	3.61	119.08	111.06
2	A	302	UER	C04-C03-N01	-3.60	121.32	125.28
2	A	301	UER	O01-C07-N02	-3.52	114.13	121.91
2	B	301	UER	O02-S01-C06	3.50	110.18	107.72
2	A	301	UER	C09-C06-C08	-3.49	108.34	111.33
2	A	301	UER	O03-S01-C06	-3.36	105.35	107.72
2	B	301	UER	O03-S01-C06	3.33	110.06	107.72
2	B	301	UER	C01-C02-N01	-3.32	120.17	123.34
2	A	301	UER	C01-C02-N01	-3.27	120.22	123.34
2	G	302	UER	C13-N02-C10	3.24	118.85	112.62
2	D	301	UER	C01-C02-N01	-3.15	120.33	123.34
2	M	301	UER	C01-C02-N01	-3.13	120.36	123.34
2	A	302	UER	C13-N02-C10	3.06	118.51	112.62
2	D	301	UER	C13-N02-C10	3.03	118.46	112.62
2	A	301	UER	C04-C03-N01	-2.99	121.99	125.28
2	A	301	UER	C13-N02-C10	2.97	118.34	112.62
2	B	301	UER	C13-N02-C10	2.92	118.25	112.62
2	B	301	UER	C04-C03-N01	-2.90	122.09	125.28
2	M	301	UER	C13-N02-C10	2.90	118.21	112.62
2	M	301	UER	C09-C06-C08	-2.86	108.89	111.33
2	A	302	UER	C01-C02-N01	-2.65	120.81	123.34
2	A	302	UER	C14-N03-C11	2.45	116.50	111.06
2	G	302	UER	O01-C07-N02	-2.43	116.53	121.91
2	D	301	UER	O03-S01-C06	2.43	109.42	107.72
2	D	301	UER	O01-C07-N02	-2.36	116.69	121.91
2	A	302	UER	O01-C07-N02	-2.32	116.78	121.91
2	G	302	UER	C01-C02-N01	-2.32	121.13	123.34
2	A	301	UER	O02-S01-C06	2.32	109.35	107.72
2	M	301	UER	C04-C05-C01	-2.28	118.17	121.22
2	M	301	UER	O01-C07-N02	-2.26	116.91	121.91
2	A	301	UER	C08-C06-C07	2.10	115.88	109.92
2	B	301	UER	C04-C05-C01	-2.01	118.53	121.22

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	UER	C04-C03-S01-O02
2	A	301	UER	N01-C03-S01-O02
2	A	301	UER	C08-C06-C07-O01

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Mol	Chain	Res	Type	Atoms
2	A	301	UER	C09-C06-C07-N02
2	A	301	UER	C07-C06-S01-O02
2	A	301	UER	C07-C06-S01-O03
2	A	301	UER	C08-C06-S01-C03
2	A	301	UER	C08-C06-S01-O02
2	A	301	UER	C08-C06-S01-O03
2	A	301	UER	C09-C06-S01-C03
2	A	301	UER	C09-C06-S01-O02
2	A	301	UER	C09-C06-S01-O03
2	A	302	UER	C04-C03-S01-O02
2	A	302	UER	N01-C03-S01-O02
2	A	302	UER	C07-C06-S01-O02
2	A	302	UER	C07-C06-S01-O03
2	A	302	UER	C08-C06-S01-C03
2	A	302	UER	C08-C06-S01-O02
2	A	302	UER	C08-C06-S01-O03
2	A	302	UER	C09-C06-S01-C03
2	A	302	UER	C09-C06-S01-O02
2	A	302	UER	C09-C06-S01-O03
2	B	301	UER	C07-C06-S01-O03
2	B	301	UER	C08-C06-S01-C03
2	B	301	UER	C08-C06-S01-O02
2	B	301	UER	C08-C06-S01-O03
2	D	301	UER	C04-C03-S01-O03
2	D	301	UER	N01-C03-S01-O03
2	G	302	UER	C04-C03-S01-O03
2	G	302	UER	N01-C03-S01-O03
2	G	302	UER	C07-C06-S01-O02
2	G	302	UER	C07-C06-S01-O03
2	G	302	UER	C08-C06-S01-C03
2	G	302	UER	C08-C06-S01-O02
2	G	302	UER	C08-C06-S01-O03
2	G	302	UER	C09-C06-S01-C03
2	G	302	UER	C09-C06-S01-O02
2	G	302	UER	C09-C06-S01-O03
2	M	301	UER	C04-C03-S01-C06
2	M	301	UER	C04-C03-S01-O02
2	M	301	UER	C04-C03-S01-O03
2	M	301	UER	N01-C03-S01-O02
2	M	301	UER	N01-C03-S01-O03
2	M	301	UER	C07-C06-S01-O02
2	M	301	UER	C07-C06-S01-O03

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Mol	Chain	Res	Type	Atoms
2	M	301	UER	C08-C06-S01-C03
2	M	301	UER	C08-C06-S01-O02
2	M	301	UER	C08-C06-S01-O03
2	M	301	UER	C09-C06-S01-C03
2	M	301	UER	C09-C06-S01-O02
2	M	301	UER	C09-C06-S01-O03
2	A	302	UER	C15-C14-N03-C12
2	G	302	UER	C15-C14-N03-C11
2	B	301	UER	C15-C14-N03-C11
2	D	301	UER	C15-C14-N03-C12
2	A	301	UER	C15-C14-N03-C11
2	G	302	UER	C04-C03-S01-C06
4	N	301	GOL	O1-C1-C2-O2
4	N	301	GOL	O1-C1-C2-C3
2	M	301	UER	C15-C14-N03-C11
2	B	301	UER	C09-C06-S01-C03
2	G	302	UER	C04-C03-S01-O02
2	G	302	UER	N01-C03-S01-O02
2	A	301	UER	C08-C06-C07-N02
2	B	301	UER	C09-C06-S01-O03
2	G	302	UER	C02-C01-C21-F03
2	M	301	UER	C02-C01-C21-F01
2	A	301	UER	C15-C14-N03-C12
2	G	302	UER	C02-C01-C21-F02
2	M	301	UER	C02-C01-C21-F02
2	M	301	UER	C02-C01-C21-F03
2	G	302	UER	C02-C01-C21-F01
2	M	301	UER	C15-C14-N03-C12
2	D	301	UER	C04-C03-S01-O02
2	D	301	UER	N01-C03-S01-O02

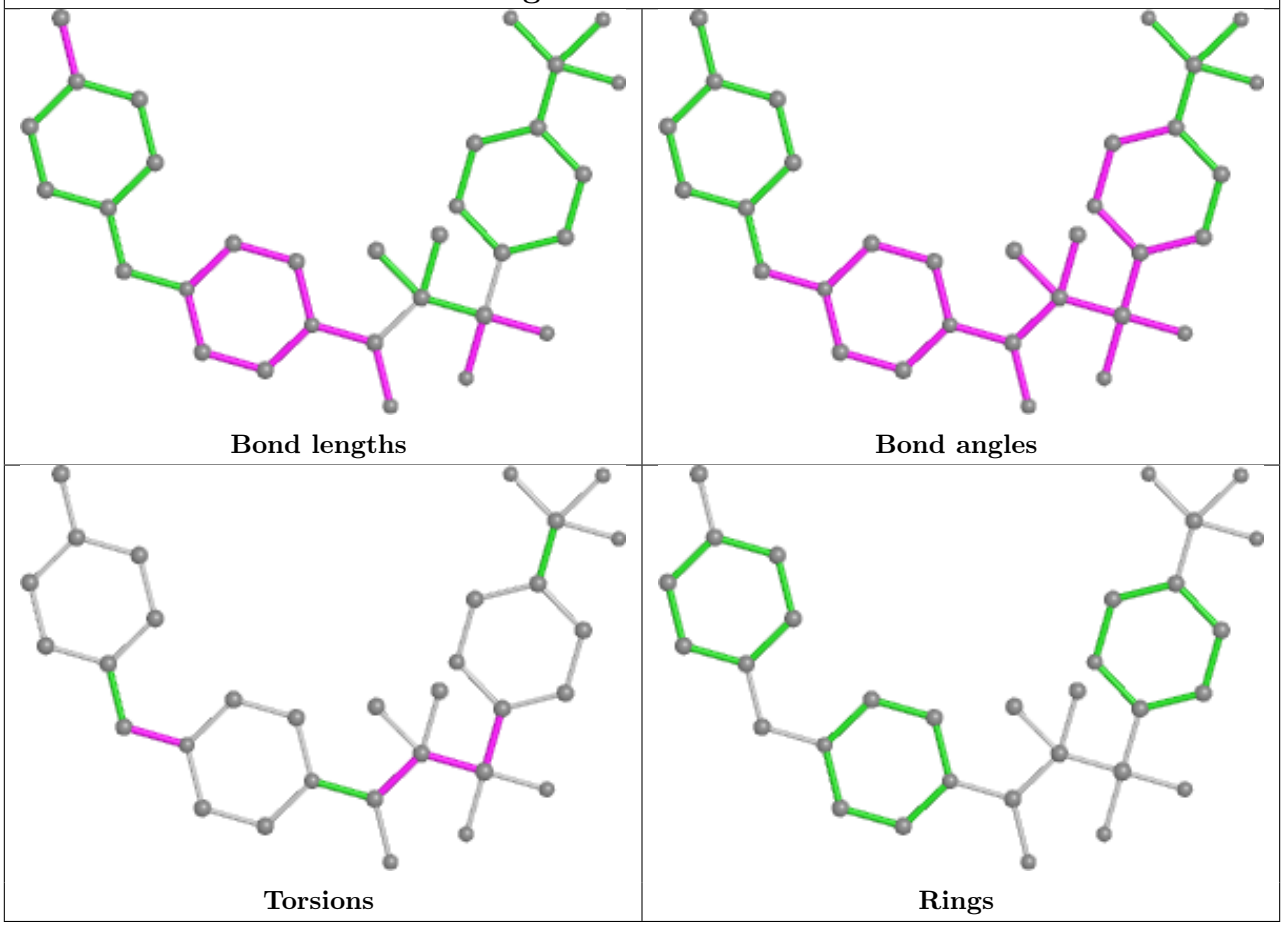
There are no ring outliers.

6 monomers are involved in 10 short contacts:

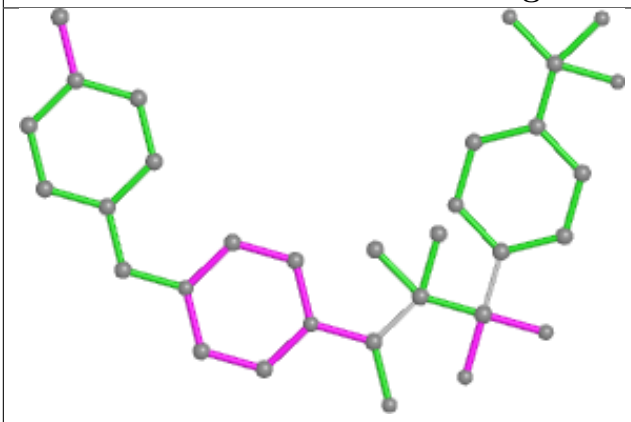
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	UER	1	0
2	G	302	UER	1	0
4	G	301	GOL	3	0
4	N	301	GOL	2	0
2	A	302	UER	2	0
2	M	301	UER	1	0

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

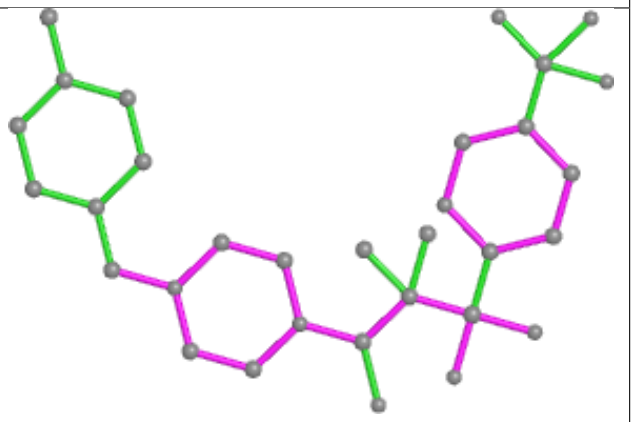
Ligand UER A 301



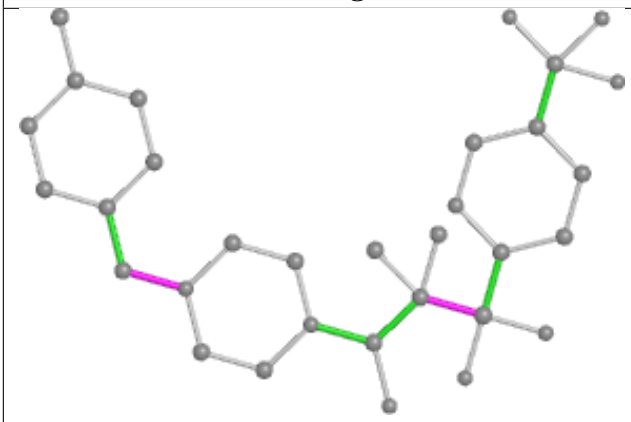
Ligand UER B 301



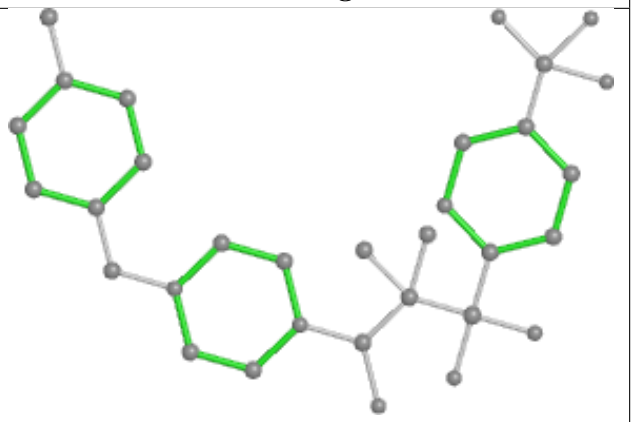
Bond lengths



Bond angles

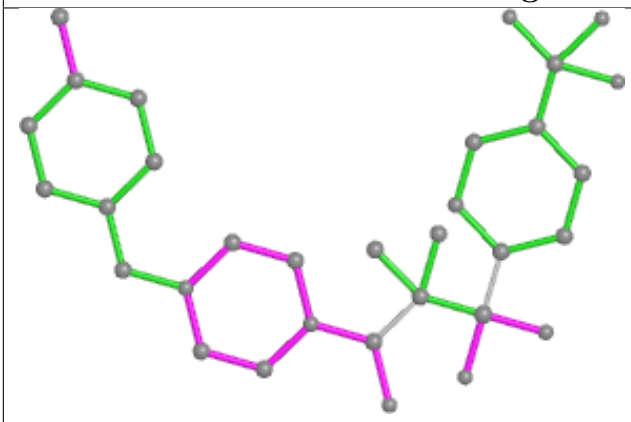


Torsions

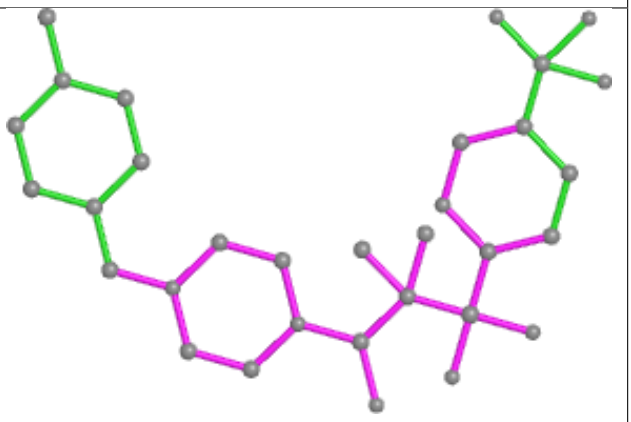


Rings

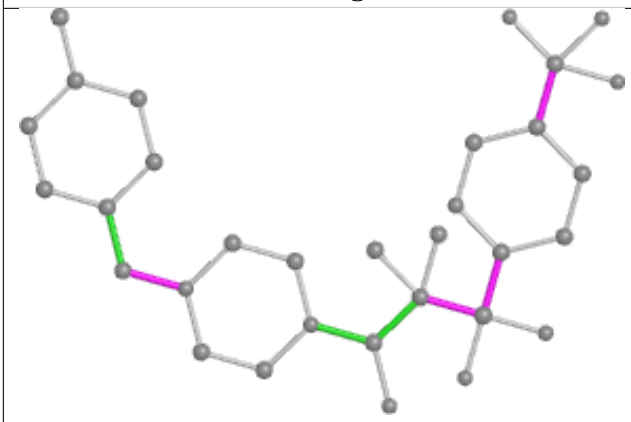
Ligand UER G 302



Bond lengths



Bond angles



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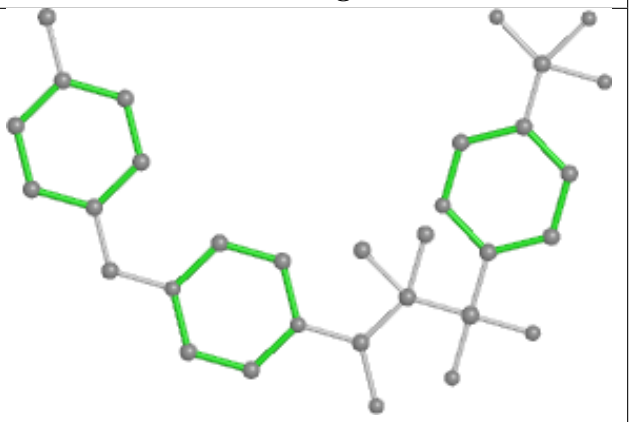
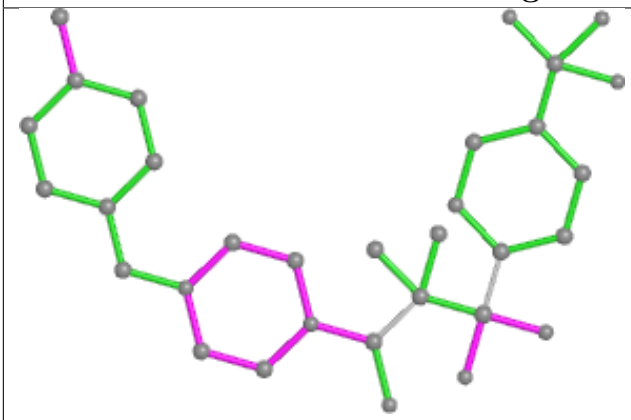
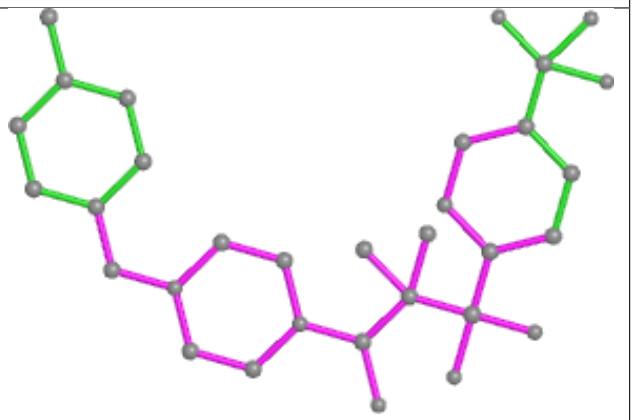


Rings

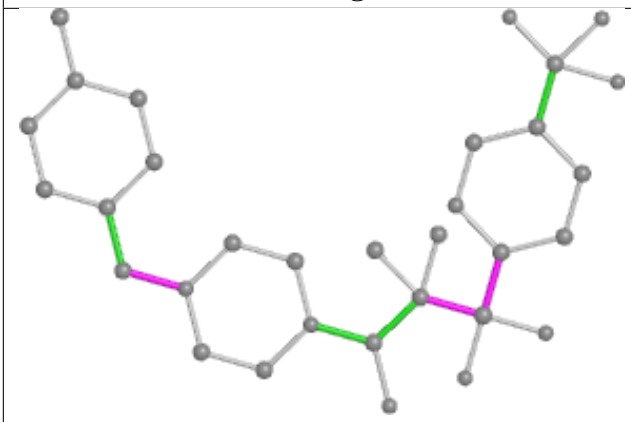
Ligand UER A 302



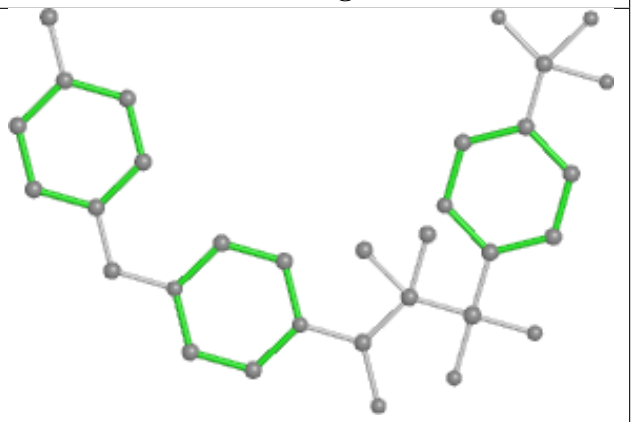
Bond lengths



Bond angles

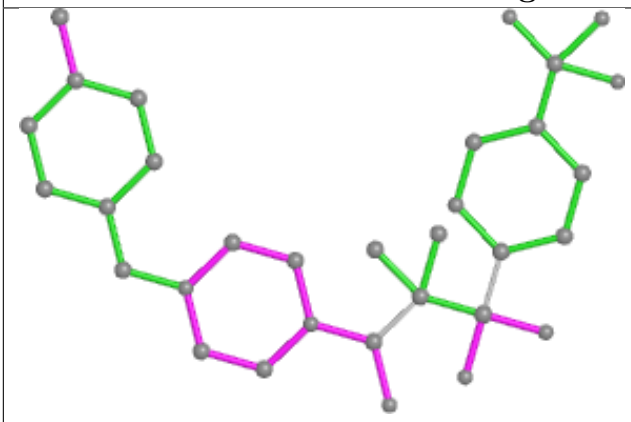


Torsions

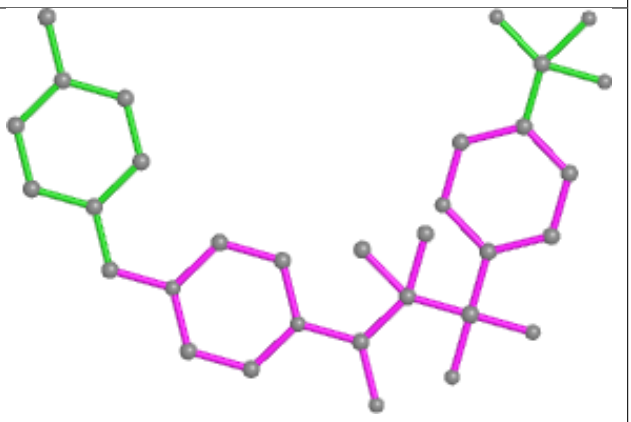


Rings

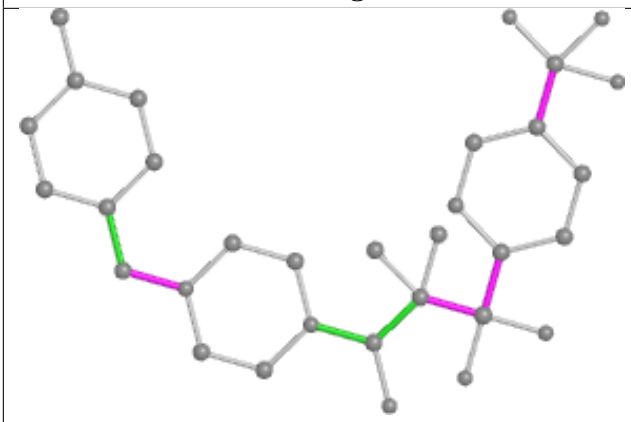
Ligand UER M 301



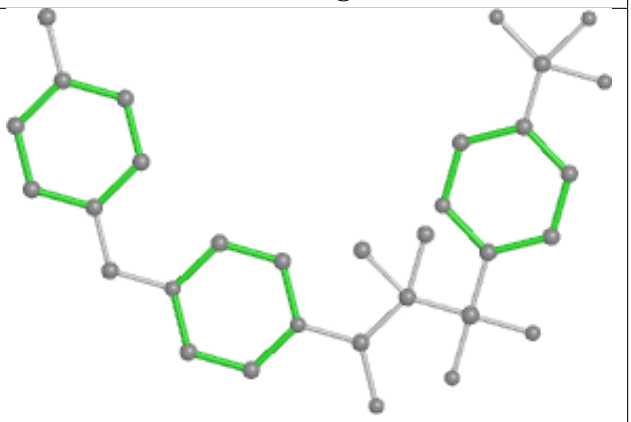
Bond lengths



Bond angles

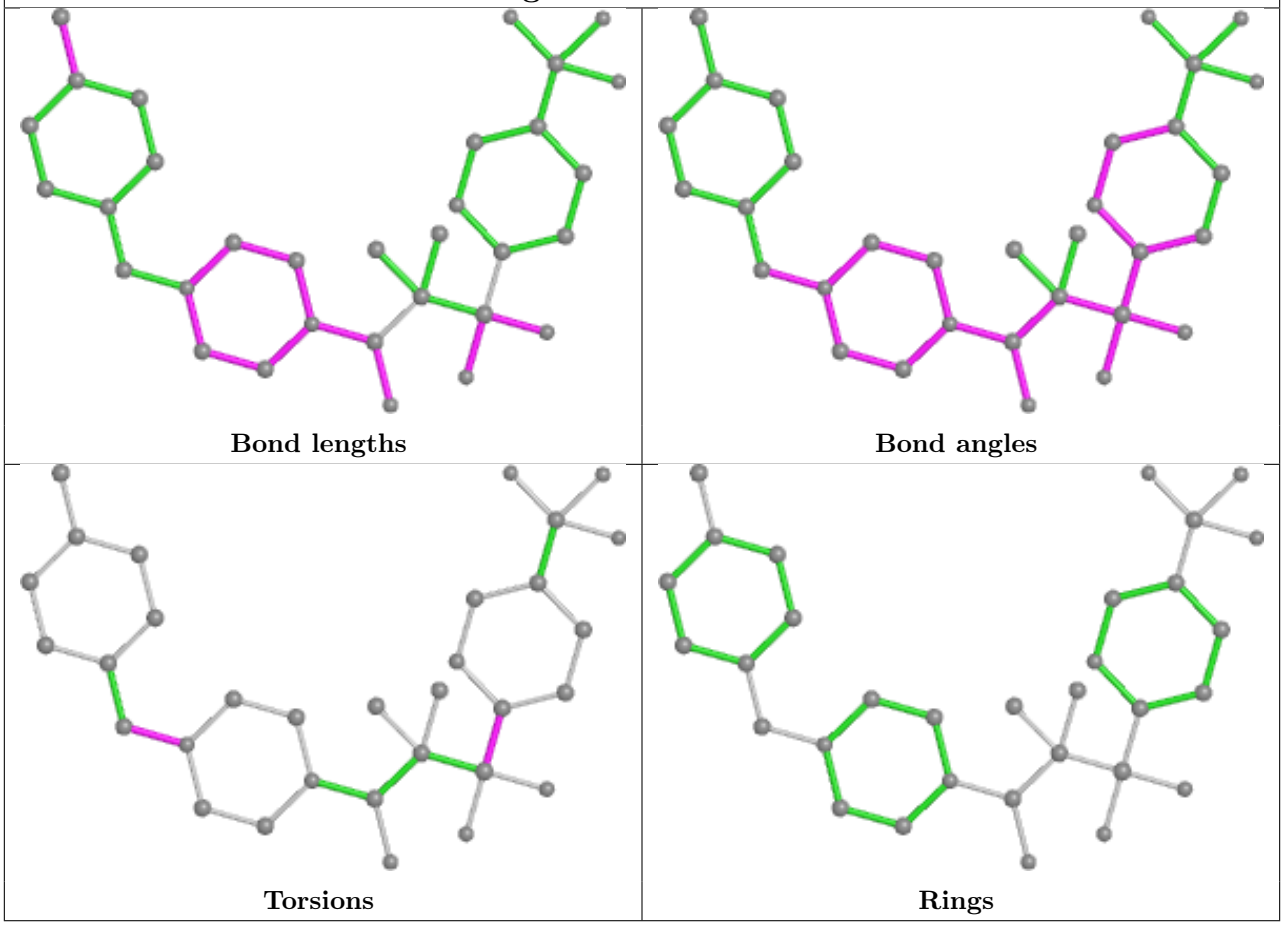


Torsions



Rings

Ligand UER D 301



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, 95^{th} 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	203/203 (100%)	-0.29	13 (6%)	19	16	21, 37, 101, 132	0
1	B	203/203 (100%)	-0.39	11 (5%)	25	23	17, 34, 103, 132	0
1	C	203/203 (100%)	-0.33	10 (4%)	29	26	21, 38, 100, 136	0
1	D	203/203 (100%)	-0.43	6 (2%)	50	47	18, 34, 93, 120	0
1	E	203/203 (100%)	-0.29	9 (4%)	34	31	17, 32, 95, 131	0
1	F	203/203 (100%)	-0.34	13 (6%)	19	16	22, 33, 103, 132	0
1	G	203/203 (100%)	-0.45	7 (3%)	45	41	16, 33, 93, 129	0
1	H	203/203 (100%)	-0.37	11 (5%)	25	23	19, 36, 109, 131	0
1	I	203/203 (100%)	-0.31	8 (3%)	39	35	20, 34, 99, 135	0
1	J	203/203 (100%)	-0.42	7 (3%)	45	41	21, 37, 99, 114	0
1	K	203/203 (100%)	-0.39	7 (3%)	45	41	20, 34, 97, 137	0
1	L	203/203 (100%)	-0.35	8 (3%)	39	35	21, 32, 94, 134	0
1	M	203/203 (100%)	-0.38	12 (5%)	22	19	14, 30, 96, 138	0
1	N	203/203 (100%)	-0.25	15 (7%)	14	12	20, 35, 108, 133	0
All	All	2842/2842 (100%)	-0.36	137 (4%)	30	27	14, 35, 103, 138	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	14	GLY	10.4
1	B	134	ALA	7.9
1	C	202	ALA	7.3
1	M	203	SER	7.2
1	H	201	ILE	6.3
1	M	12	GLY	6.1
1	E	11	THR	5.8
1	F	10	ASP	5.4

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Mol	Chain	Res	Type	RSRZ
1	E	8	VAL	5.4
1	C	12	GLY	5.3
1	E	12	GLY	5.2
1	N	202	ALA	5.2
1	L	9	GLU	5.2
1	M	14	GLY	5.0
1	J	9	GLU	4.9
1	K	11	THR	4.8
1	A	14	GLY	4.8
1	L	134	ALA	4.7
1	B	11	THR	4.6
1	I	133	SER	4.6
1	H	199	LYS	4.6
1	A	11	THR	4.5
1	A	2	THR	4.5
1	G	193	ALA	4.4
1	N	200	SER	4.3
1	N	130	ILE	4.2
1	N	9	GLU	4.2
1	M	137	GLN	4.2
1	I	11	THR	4.2
1	I	17	ALA	4.1
1	B	17	ALA	4.1
1	A	126	SER	4.0
1	F	9	GLU	4.0
1	B	8	VAL	3.9
1	I	134	ALA	3.9
1	E	17	ALA	3.8
1	H	133	SER	3.8
1	L	2	THR	3.8
1	B	196	THR	3.7
1	C	203	SER	3.7
1	I	131	GLY	3.6
1	L	138	LEU	3.6
1	F	14	GLY	3.6
1	H	202	ALA	3.5
1	L	17	ALA	3.5
1	C	14	GLY	3.5
1	D	127	GLY	3.5
1	F	2	THR	3.5
1	N	2	THR	3.4
1	B	16	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	198	ASP	3.4
1	G	8	VAL	3.4
1	K	10	ASP	3.3
1	N	193	ALA	3.3
1	G	11	THR	3.3
1	B	131	GLY	3.3
1	C	11	THR	3.3
1	I	12	GLY	3.3
1	D	10	ASP	3.2
1	C	134	ALA	3.2
1	E	193	ALA	3.2
1	H	138	LEU	3.2
1	E	133	SER	3.2
1	J	2	THR	3.2
1	N	140	ALA	3.2
1	N	8	VAL	3.1
1	B	9	GLU	3.1
1	D	9	GLU	3.1
1	N	203	SER	3.1
1	E	125	PRO	3.1
1	L	199	LYS	3.0
1	J	126	SER	3.0
1	H	11	THR	3.0
1	F	196	THR	3.0
1	M	16	ARG	3.0
1	N	128	GLY	2.9
1	F	201	ILE	2.9
1	B	13	ARG	2.9
1	F	12	GLY	2.9
1	F	198	ASP	2.9
1	C	17	ALA	2.9
1	A	136	ILE	2.9
1	M	126	SER	2.8
1	C	8	VAL	2.8
1	N	17	ALA	2.8
1	A	130	ILE	2.8
1	A	202	ALA	2.7
1	G	1	MET	2.7
1	A	15	GLU	2.7
1	J	16	ARG	2.7
1	F	8	VAL	2.7
1	N	199	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	M	8	VAL	2.6
1	M	9	GLU	2.6
1	L	1	MET	2.6
1	F	11	THR	2.6
1	G	12	GLY	2.6
1	I	14	GLY	2.6
1	D	17	ALA	2.5
1	M	15	GLU	2.5
1	C	1	MET	2.5
1	F	17	ALA	2.5
1	G	16	ARG	2.5
1	D	13	ARG	2.5
1	K	12	GLY	2.5
1	A	17	ALA	2.5
1	N	131	GLY	2.4
1	A	10	ASP	2.4
1	K	16	ARG	2.4
1	K	9	GLU	2.4
1	F	200	SER	2.4
1	M	13	ARG	2.4
1	I	9	GLU	2.4
1	J	133	SER	2.3
1	K	134	ALA	2.3
1	F	134	ALA	2.3
1	N	55	ASP	2.3
1	A	137	GLN	2.2
1	J	131	GLY	2.2
1	H	132	THR	2.2
1	N	11	THR	2.2
1	C	129	ILE	2.2
1	H	16	ARG	2.2
1	B	15	GLU	2.2
1	L	15	GLU	2.2
1	H	198	ASP	2.2
1	H	137	GLN	2.1
1	E	134	ALA	2.1
1	B	130	ILE	2.1
1	H	15	GLU	2.1
1	M	135	ASP	2.1
1	M	133	SER	2.1
1	A	3	LEU	2.1
1	A	201	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	135	ASP	2.1
1	K	15	GLU	2.1
1	D	197	LYS	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

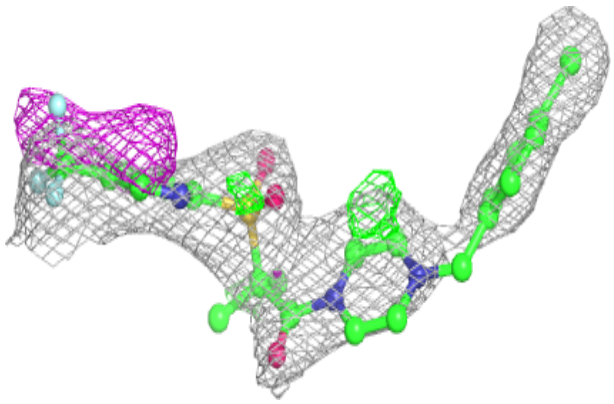
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NA	D	302	1/1	0.37	1.11	64,64,64,64	0
3	NA	B	302	1/1	0.77	0.13	41,41,41,41	0
2	UER	A	302	32/32	0.84	0.25	65,80,93,94	0
2	UER	G	302	32/32	0.85	0.32	74,96,104,106	0
2	UER	D	301	32/32	0.86	0.25	59,74,88,91	0
2	UER	M	301	32/32	0.89	0.19	51,89,108,113	0
2	UER	A	301	32/32	0.90	0.23	75,122,133,135	0
2	UER	B	301	32/32	0.91	0.21	43,97,121,130	0
3	NA	L	301	1/1	0.92	0.08	38,38,38,38	0
4	GOL	B	303	6/6	0.92	0.08	38,48,52,60	0
4	GOL	N	301	6/6	0.92	0.18	24,28,30,35	0
3	NA	F	301	1/1	0.93	0.08	19,19,19,19	0
4	GOL	G	301	6/6	0.95	0.26	27,29,35,46	0
4	GOL	C	301	6/6	0.96	0.15	37,39,42,46	0
3	NA	E	301	1/1	0.96	0.06	20,20,20,20	0
3	NA	H	301	1/1	0.96	0.08	21,21,21,21	0
3	NA	G	303	1/1	0.97	0.10	32,32,32,32	0
3	NA	N	302	1/1	0.98	0.06	15,15,15,15	0

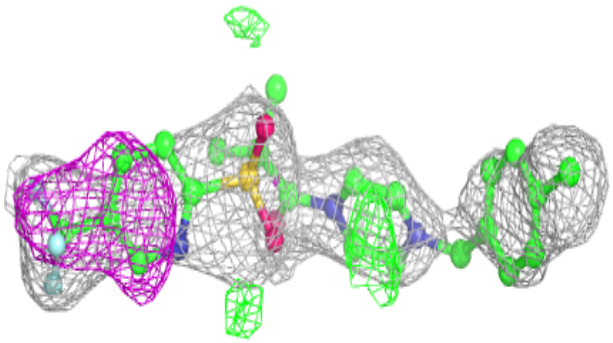
The following is a graphical depiction of the model fit to experimental electron density of all

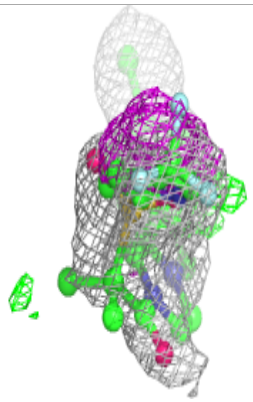
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around UER A 302:

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

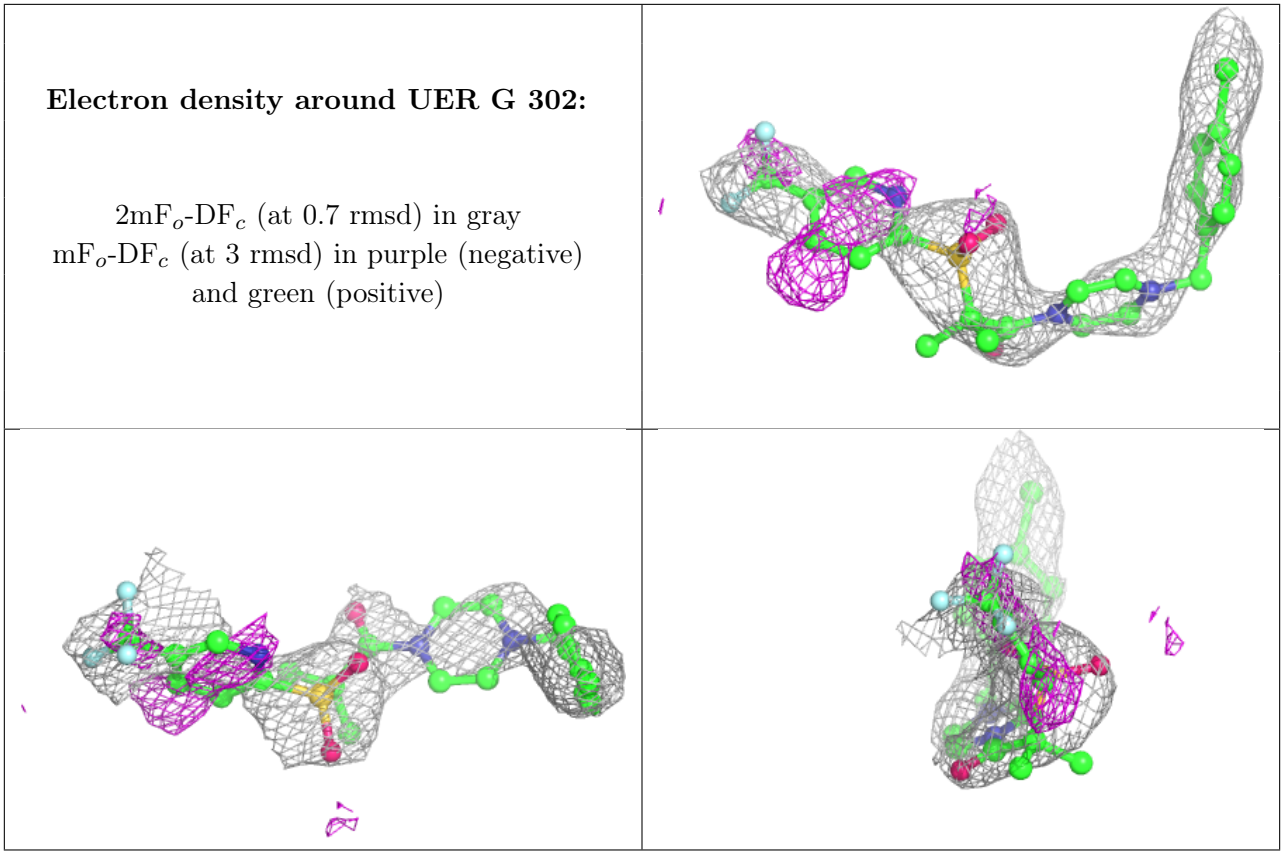






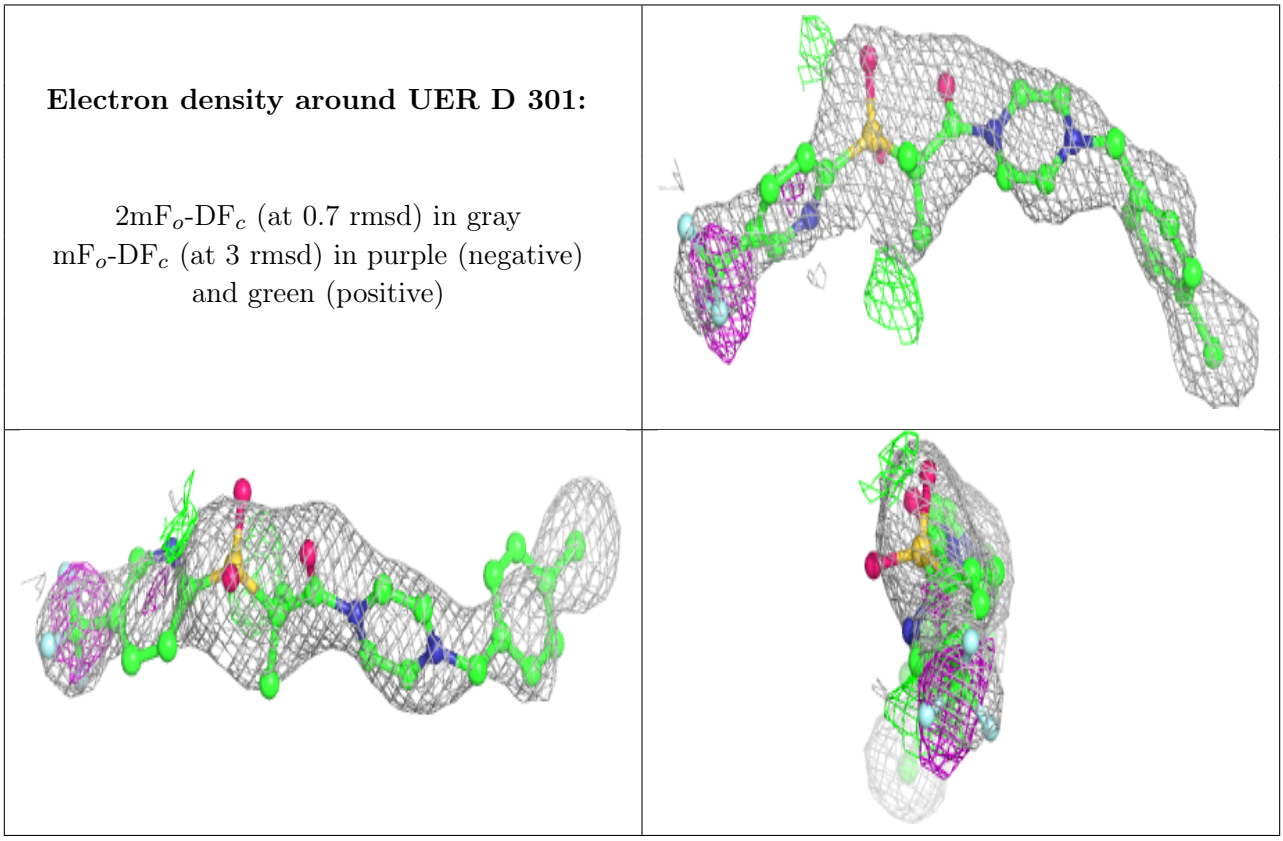
Electron density around UER G 302:

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



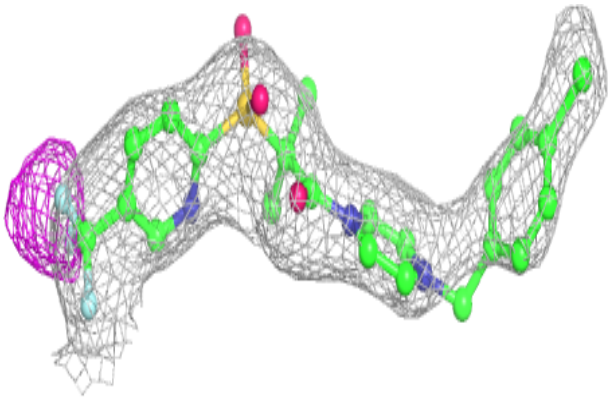
Electron density around UER D 301:

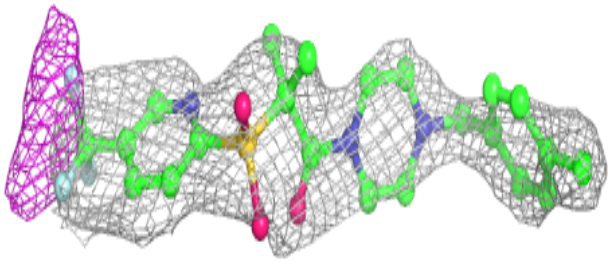
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

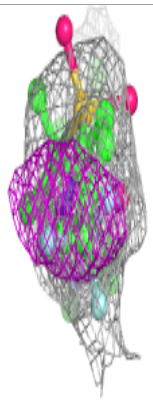


Electron density around UER M 301:

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

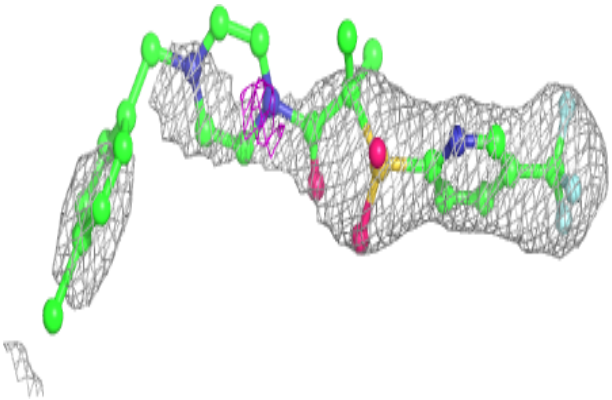


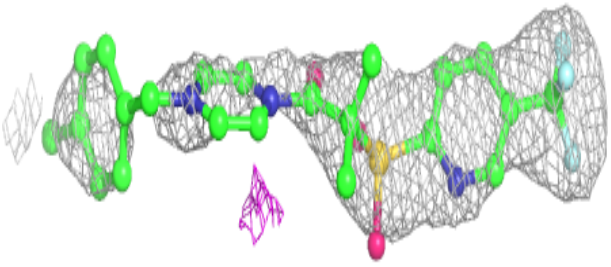


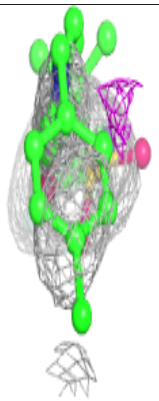


Electron density around UER A 301:

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

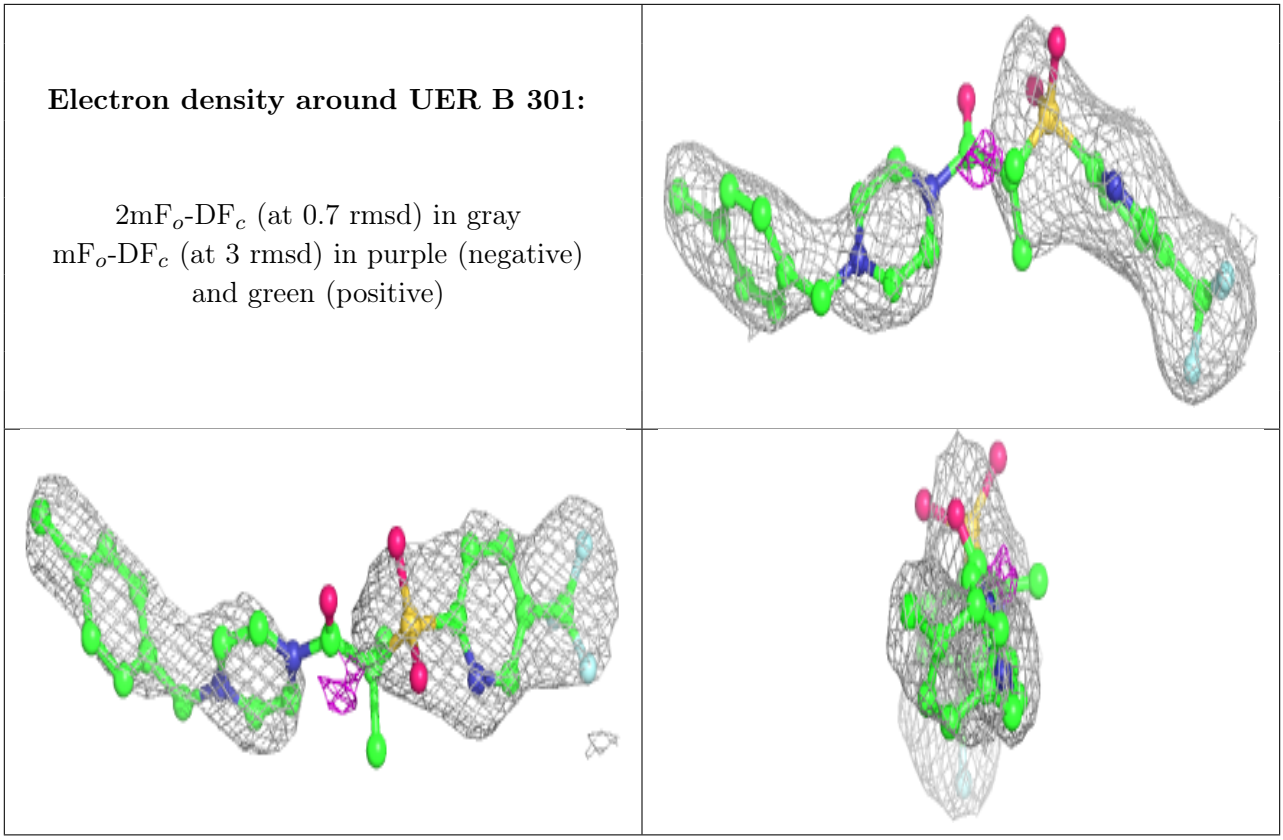






Electron density around UER B 301:

$2mF_o$-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.