Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2023 – 08:41 PM EDT

PDB ID	:	4JUO
Title	:	A low-resolution three-gate structure of topoisomerase IV from Streptococcus pneumoniae in space group H32
Authors	:	Laponogov, I.; Veselkov, D.A.; Pan, X.-S.; Crevel, I.; Fisher, L.M.; Sanderson, M.R.
Deposited on	:	2013-03-25
Resolution	:	6.53 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:

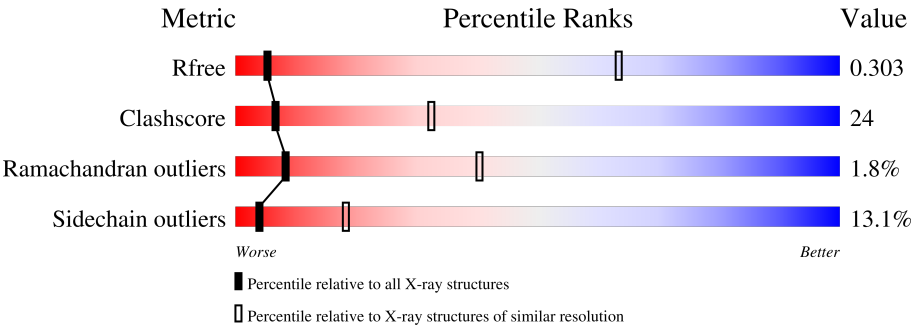
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 6.53 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	1000 (9.00-3.90)
Clashscore	141614	1064 (9.00-3.90)
Ramachandran outliers	138981	1012 (9.00-3.88)
Sidechain outliers	138945	1010 (9.00-3.84)

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%

Mol	Chain	Length	Quality of chain
1	A	496	65% 28%
2	C	670	51% 23% 7% 19%
3	E	11	18% 36% 9% 36%
4	F	15	20% 33% 20% 27%
5	G	11	36% 27% 36%
6	H	15	20% 47% 7% 27%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 8283 atoms, of which 19 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 DNA topoisomerase 4 subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	479	3720	2357	645	705	13	0	1	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	257	THR	ILE	conflict	UNP P72525
A	489	LEU	-	expression tag	UNP P72525
A	490	GLU	-	expression tag	UNP P72525
A	491	HIS	-	expression tag	UNP P72525
A	492	HIS	-	expression tag	UNP P72525
A	493	HIS	-	expression tag	UNP P72525
A	494	HIS	-	expression tag	UNP P72525
A	495	HIS	-	expression tag	UNP P72525
A	496	HIS	-	expression tag	UNP P72525

- Molecule 2 is a protein called DNA topoisomerase 4 subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	546	3786	2407	653	719	7	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-22	MET	-	expression tag	UNP Q59961
C	-21	GLY	-	expression tag	UNP Q59961
C	-20	HIS	-	expression tag	UNP Q59961
C	-19	HIS	-	expression tag	UNP Q59961
C	-18	HIS	-	expression tag	UNP Q59961
C	-17	HIS	-	expression tag	UNP Q59961
C	-16	HIS	-	expression tag	UNP Q59961

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-15	HIS	-	expression tag	UNP Q59961
C	-14	HIS	-	expression tag	UNP Q59961
C	-13	HIS	-	expression tag	UNP Q59961
C	-12	HIS	-	expression tag	UNP Q59961
C	-11	HIS	-	expression tag	UNP Q59961
C	-10	SER	-	expression tag	UNP Q59961
C	-9	SER	-	expression tag	UNP Q59961
C	-8	GLY	-	expression tag	UNP Q59961
C	-7	HIS	-	expression tag	UNP Q59961
C	-6	ILE	-	expression tag	UNP Q59961
C	-5	ASP	-	expression tag	UNP Q59961
C	-4	ASP	-	expression tag	UNP Q59961
C	-3	ASP	-	expression tag	UNP Q59961
C	-2	ASP	-	expression tag	UNP Q59961
C	-1	LYS	-	expression tag	UNP Q59961
C	0	HIS	-	expression tag	UNP Q59961
C	217	ASP	ASN	conflict	UNP Q59961
C	460	ILE	VAL	conflict	UNP Q59961
C	644	ALA	THR	conflict	UNP Q59961

- Molecule 3 is a DNA chain called E-site DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	7	Total	C	N	O	P	0	7	0
			140	69	27	38	6			

- Molecule 4 is a DNA chain called E-site DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	11	Total	C	N	O	P	0	11	0
			225	108	39	67	11			

- Molecule 5 is a DNA chain called E-site DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	7	Total	C	N	O	P	0	7	0
			139	68	25	40	6			

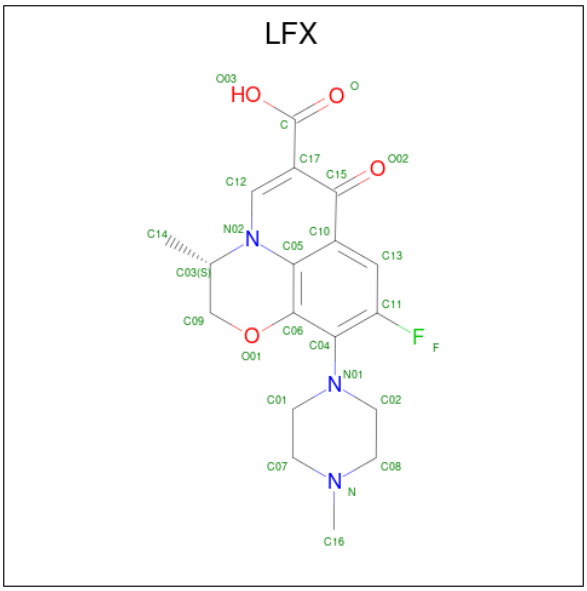
- Molecule 6 is a DNA chain called E-site DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	11	Total	C	N	O	P	0	11	0
			226	107	43	65	11			

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		
7	C	1	Total	Mg	0	0
			1	1		

- Molecule 8 is (3S)-9-fluoro-3-methyl-10-(4-methylpiperazin-1-yl)-7-oxo-2,3-dihydro-7H-[1,4]oxazino[2,3,4-ij]quinoline-6-carboxylic acid (three-letter code: LFX) (formula: $C_{18}H_{20}FN_3O_4$).



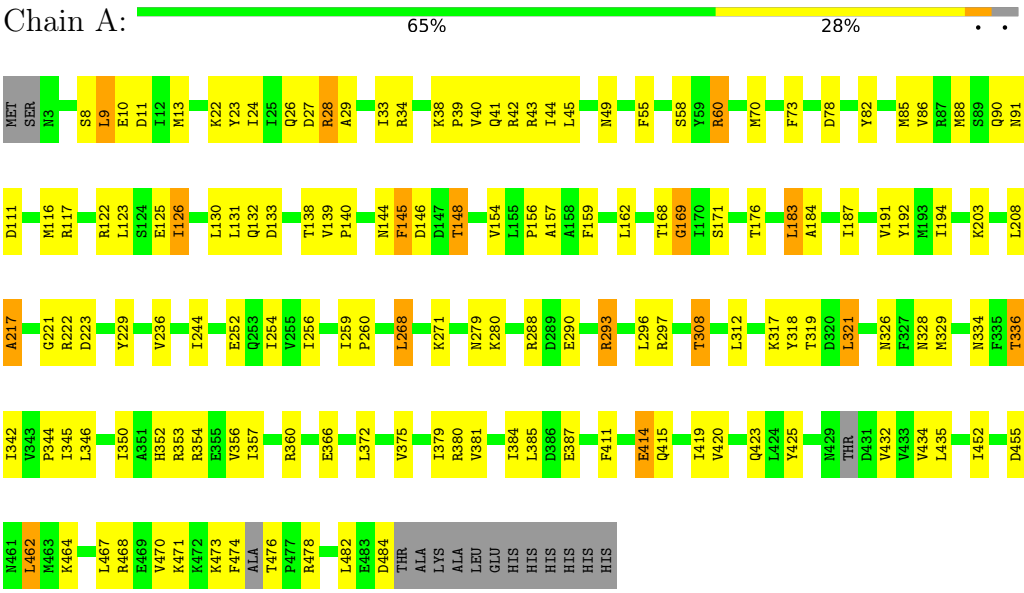
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	F	1	Total	C	F	H	N	O	0	0
			45	18	1	19	3	4		

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. 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. 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.

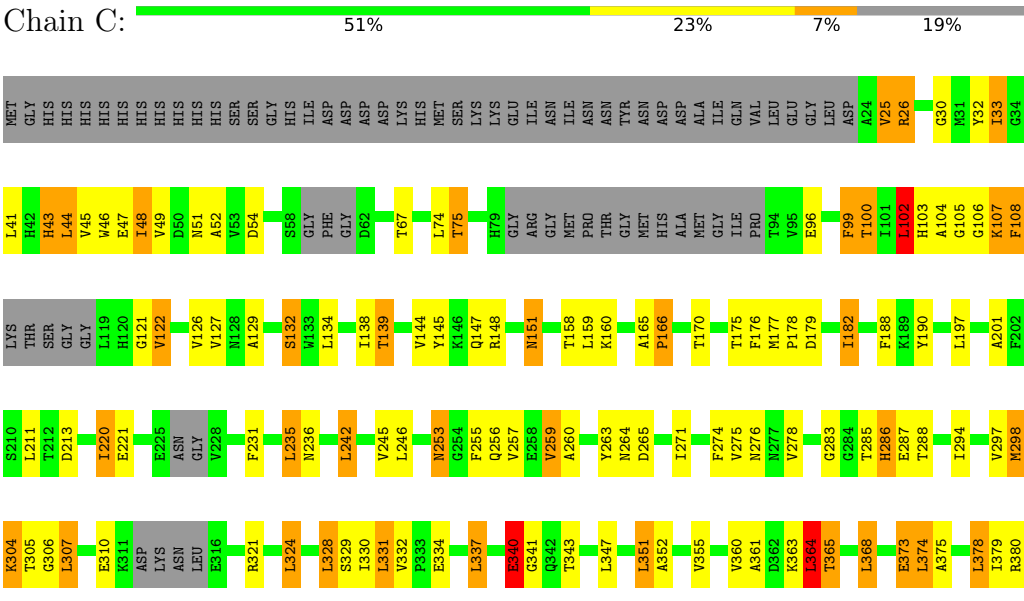
• Molecule 1: DNA topoisomerase 4 subunit A

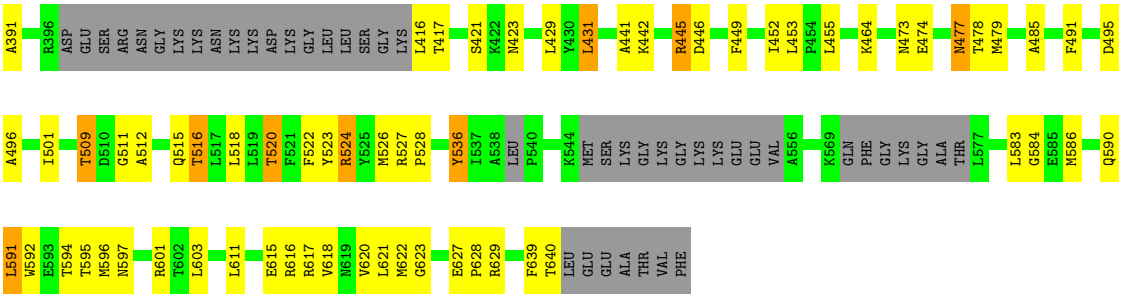
Chain A:



• Molecule 2: DNA topoisomerase 4 subunit B

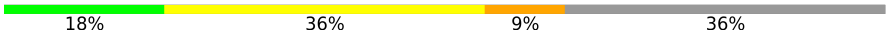
Chain C:

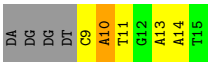




- Molecule 3: E-site DNA

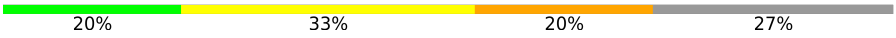
Chain E:





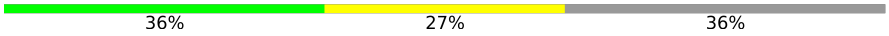
- Molecule 4: E-site DNA

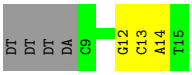
Chain F:



- Molecule 5: E-site DNA

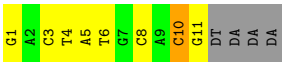
Chain G:





- Molecule 6: E-site DNA

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	213.58Å 213.58Å 211.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.44 – 6.53 53.40 – 6.53	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.44-6.53) 99.3 (53.40-6.53)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.83 (at 6.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.247 , 0.298 0.243 , 0.303	Depositor DCC
R_{free} test set	170 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å^2)	378.8	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 302.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	8283	wwPDB-VP
Average B, all atoms (Å^2)	183.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, LFX

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	0.45	0/3779	0.63	1/5109 (0.0%)
2	C	0.39	0/3845	0.63	2/5251 (0.0%)
3	E	0.88	0/157	1.64	3/241 (1.2%)
4	F	0.83	0/251	1.80	12/385 (3.1%)
5	G	0.76	0/155	1.42	1/238 (0.4%)
6	H	0.75	0/253	1.67	3/388 (0.8%)
All	All	0.47	0/8440	0.81	22/11612 (0.2%)

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
2	C	0	1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	10[B]	DC	O4'-C4'-C3'	-11.97	98.82	106.00
4	F	1[A]	DA	O4'-C1'-N9	10.86	115.60	108.00
3	E	10[A]	DA	O4'-C1'-N9	8.04	113.63	108.00
6	H	1[B]	DG	O4'-C1'-N9	7.95	113.56	108.00
4	F	3[A]	DT	O4'-C4'-C3'	-7.89	101.26	106.00
4	F	6[A]	DT	O4'-C4'-C3'	-6.75	101.80	104.50
4	F	5[A]	DA	O4'-C1'-N9	6.61	112.63	108.00
2	C	102	LEU	CA-CB-CG	6.54	130.34	115.30
3	E	11[A]	DT	C4-C5-C7	6.09	122.65	119.00
4	F	3[A]	DT	O4'-C1'-N1	5.96	112.17	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	183	LEU	CA-CB-CG	5.92	128.92	115.30
5	G	12[B]	DG	O4'-C1'-N9	-5.91	103.86	108.00
4	F	6[A]	DT	C4'-C3'-C2'	-5.80	97.88	103.10
4	F	6[A]	DT	C1'-O4'-C4'	-5.73	104.37	110.10
4	F	8[A]	DC	C1'-O4'-C4'	-5.65	104.45	110.10
4	F	3[A]	DT	C5-C4-O4	-5.51	121.04	124.90
4	F	1[A]	DA	C3'-C2'-C1'	-5.43	95.98	102.50
2	C	364	LEU	CA-CB-CG	5.35	127.61	115.30
3	E	11[A]	DT	C6-C5-C7	-5.13	119.82	122.90
4	F	1[A]	DA	C1'-O4'-C4'	-5.12	104.98	110.10
6	H	10[B]	DC	C1'-O4'-C4'	-5.11	104.99	110.10
4	F	1[A]	DA	O4'-C1'-C2'	-5.11	101.82	105.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	102	LEU	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	3720	0	3629	179	0
2	C	3786	0	3303	181	0
3	E	140	0	71	3	0
4	F	225	0	116	5	0
5	G	139	0	71	1	0
6	H	226	0	115	8	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	F	26	19	19	1	0
All	All	8264	19	7324	368	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 24.

All (368) 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)
2:C:583:LEU:HB3	2:C:586:MET:CE	1.24	1.67
2:C:583:LEU:CB	2:C:586:MET:CE	1.75	1.56
2:C:583:LEU:CB	2:C:586:MET:HE3	1.28	1.53
2:C:583:LEU:HD22	2:C:586:MET:CE	1.56	1.35
2:C:583:LEU:CD2	2:C:586:MET:CE	2.06	1.32
2:C:583:LEU:CG	2:C:586:MET:CE	2.06	1.31
2:C:583:LEU:CD2	2:C:586:MET:HE2	1.65	1.24
1:A:338:ARG:HH12	1:A:344:PRO:CG	1.30	1.20
1:A:354:ARG:NE	1:A:456:GLU:OE1	1.76	1.18
1:A:60:ARG:HH11	1:A:60:ARG:HB2	1.07	1.15
1:A:28:ARG:HG3	1:A:28:ARG:HH11	1.05	1.14
1:A:354:ARG:CD	1:A:456:GLU:OE1	1.96	1.13
1:A:455:ASP:O	1:A:456:GLU:N	1.82	1.12
1:A:184:ALA:HB1	1:A:471:LYS:HE3	1.28	1.12
2:C:583:LEU:HD22	2:C:586:MET:HE1	1.18	1.12
1:A:338:ARG:NH1	1:A:344:PRO:HG2	1.56	1.11
2:C:583:LEU:CB	2:C:586:MET:HE2	1.65	1.11
1:A:357:ILE:CG2	1:A:459:MET:HG2	1.79	1.11
1:A:33:ILE:HD11	1:A:345:ILE:CG1	1.84	1.06
1:A:33:ILE:HD11	1:A:345:ILE:HA	1.37	1.06
1:A:70:MET:HE1	1:A:78:ASP:HB3	1.37	1.06
1:A:354:ARG:HD2	1:A:456:GLU:OE1	1.54	1.06
1:A:33:ILE:HD11	1:A:345:ILE:HG12	1.38	1.05
1:A:455:ASP:C	1:A:456:GLU:N	2.09	1.05
2:C:583:LEU:CA	2:C:586:MET:HE2	1.87	1.05
1:A:354:ARG:HE	1:A:456:GLU:CD	1.62	1.04
2:C:524:ARG:HH11	2:C:524:ARG:HG3	1.13	1.04
2:C:583:LEU:CD2	2:C:586:MET:HE1	1.74	1.03
1:A:357:ILE:HG21	1:A:459:MET:CG	1.89	1.02
2:C:108:PHE:CD1	2:C:276:ASN:HB3	1.94	1.02
1:A:474:PHE:O	1:A:476:THR:HG23	1.61	1.00
1:A:33:ILE:CD1	1:A:345:ILE:HG12	1.95	0.96
1:A:357:ILE:HG21	1:A:459:MET:HG2	0.98	0.96
1:A:338:ARG:HH12	1:A:344:PRO:HG3	1.28	0.96
1:A:144:ASN:HD21	1:A:148:THR:HG23	1.31	0.95
1:A:60:ARG:HH11	1:A:60:ARG:CB	1.80	0.95
2:C:108:PHE:CE1	2:C:276:ASN:HA	1.99	0.95
1:A:33:ILE:CD1	1:A:345:ILE:HA	1.97	0.93
2:C:108:PHE:CE1	2:C:276:ASN:CA	2.46	0.93
1:A:10:GLU:O	2:C:617:ARG:HD2	1.68	0.93
2:C:583:LEU:CG	2:C:586:MET:HE1	1.87	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:583:LEU:CA	2:C:586:MET:CE	2.47	0.91
2:C:524:ARG:HH11	2:C:524:ARG:CG	1.81	0.91
1:A:33:ILE:HD11	1:A:345:ILE:CA	2.01	0.91
1:A:338:ARG:NH1	1:A:344:PRO:CG	1.96	0.91
2:C:583:LEU:HA	2:C:586:MET:HE2	1.53	0.90
1:A:60:ARG:HB2	1:A:60:ARG:NH1	1.86	0.89
1:A:293:ARG:HH11	1:A:293:ARG:HB3	1.36	0.89
1:A:357:ILE:CG2	1:A:459:MET:CG	2.50	0.88
2:C:583:LEU:CD1	2:C:586:MET:HE1	2.05	0.86
1:A:384:ILE:O	1:A:387:GLU:HG2	1.74	0.86
2:C:524:ARG:HG3	2:C:524:ARG:NH1	1.87	0.86
1:A:28:ARG:HG3	1:A:28:ARG:NH1	1.86	0.86
1:A:256:ILE:HD13	1:A:321:LEU:HD21	1.56	0.85
2:C:583:LEU:CG	2:C:586:MET:HE2	1.92	0.84
2:C:516:THR:O	2:C:520:THR:HG23	1.78	0.83
6:H:10[B]:DC:H2"	6:H:11[B]:DG:H5"	1.62	0.81
1:A:44:ILE:HD12	1:A:88:MET:CE	2.10	0.81
2:C:108:PHE:HE1	2:C:276:ASN:HA	1.43	0.81
2:C:583:LEU:HD13	2:C:586:MET:HE1	1.62	0.81
1:A:125:GLU:OE2	1:A:473:LYS:NZ	2.13	0.80
1:A:34:ARG:HD2	1:A:352:HIS:CG	2.17	0.80
2:C:520:THR:HG21	2:C:622:MET:HG3	1.62	0.80
1:A:139:VAL:HG11	1:A:154:VAL:O	1.82	0.79
2:C:203:LEU:HD21	2:C:274:PHE:CD2	2.18	0.79
1:A:38:LYS:H	1:A:41:GLN:NE2	1.83	0.76
1:A:384:ILE:C	1:A:385:LEU:N	2.39	0.76
1:A:33:ILE:HD11	1:A:345:ILE:CB	2.15	0.75
1:A:24:ILE:HG22	1:A:171:SER:HB2	1.70	0.74
1:A:28:ARG:HH11	1:A:28:ARG:CG	1.94	0.74
1:A:187:ILE:HD13	1:A:467:LEU:O	1.86	0.74
1:A:357:ILE:HD12	1:A:459:MET:SD	2.27	0.74
2:C:51:ASN:ND2	2:C:99:PHE:O	2.21	0.74
1:A:169:GLY:HA2	1:A:176:THR:HG22	1.69	0.73
2:C:304:LYS:O	2:C:306:GLY:N	2.21	0.73
1:A:146:ASP:HB3	1:A:148:THR:HG22	1.70	0.73
2:C:301:TYR:HD2	2:C:379:ILE:HD11	1.54	0.73
2:C:583:LEU:CD1	2:C:586:MET:CE	2.64	0.73
3:E:9[A]:DC:H2"	3:E:10[A]:DA:H5"	1.71	0.72
1:A:183:LEU:CD1	1:A:471:LYS:HA	2.19	0.72
2:C:256:GLN:HB3	2:C:331:LEU:HB2	1.71	0.72
2:C:611:LEU:HD13	2:C:611:LEU:C	2.10	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:VAL:HG13	1:A:140:PRO:HD2	1.71	0.72
2:C:203:LEU:CD2	2:C:274:PHE:CD2	2.73	0.72
1:A:317:LYS:HE3	1:A:318:TYR:CE2	2.25	0.71
2:C:259:VAL:HG22	2:C:328:LEU:HD23	1.70	0.71
2:C:584:GLY:CA	2:C:586:MET:N	2.50	0.71
1:A:8:SER:HB3	1:A:11:ASP:OD1	1.90	0.71
2:C:242:LEU:HD22	2:C:423:ASN:ND2	2.05	0.71
2:C:583:LEU:HD23	2:C:586:MET:HE2	1.70	0.71
1:A:184:ALA:HB1	1:A:471:LYS:CE	2.15	0.70
1:A:138:THR:HG22	1:A:360:ARG:HB2	1.73	0.69
2:C:75:THR:HB	2:C:175:THR:HB	1.74	0.69
2:C:108:PHE:CG	2:C:276:ASN:HB3	2.27	0.69
2:C:431:LEU:HD22	2:C:479:MET:HE3	1.73	0.69
2:C:332:VAL:HG12	2:C:334:GLU:H	1.56	0.69
1:A:40:VAL:O	1:A:44:ILE:HG13	1.93	0.69
1:A:244:ILE:HD12	1:A:244:ILE:N	2.08	0.69
2:C:201:ALA:HB2	2:C:209:LEU:HD11	1.75	0.68
2:C:511:GLY:O	2:C:515:GLN:HG3	1.94	0.68
1:A:138:THR:O	1:A:356:VAL:HG22	1.94	0.67
1:A:156:PRO:O	1:A:353:ARG:NH1	2.27	0.67
2:C:67:THR:HB	2:C:75:THR:HG23	1.74	0.67
1:A:138:THR:HB	1:A:356:VAL:HG13	1.75	0.67
2:C:203:LEU:HD21	2:C:274:PHE:CE2	2.29	0.67
1:A:10:GLU:O	2:C:617:ARG:CD	2.43	0.67
1:A:271:LYS:HE3	1:A:319:THR:HB	1.75	0.67
1:A:252:GLU:OE1	1:A:308:THR:HG21	1.95	0.67
1:A:70:MET:CE	1:A:78:ASP:HB3	2.19	0.67
2:C:33:ILE:HD11	2:C:44:LEU:HB3	1.76	0.67
2:C:474:GLU:O	2:C:478:THR:HG23	1.93	0.66
2:C:265:ASP:O	2:C:421:SER:CB	2.44	0.66
1:A:146:ASP:CB	1:A:148:THR:HG22	2.25	0.66
1:A:38:LYS:H	1:A:41:GLN:HE21	1.42	0.66
1:A:146:ASP:CG	1:A:148:THR:HG22	2.16	0.66
8:F:101:LFX:H01	6:H:4[B]:DT:O2	1.95	0.66
6:H:5[B]:DA:H2"	6:H:6[B]:DT:O5'	1.96	0.66
1:A:146:ASP:OD2	1:A:148:THR:HG22	1.96	0.65
2:C:102:LEU:HD21	2:C:127:VAL:HG22	1.79	0.65
2:C:294:ILE:HA	2:C:297:VAL:HG12	1.78	0.65
2:C:203:LEU:CD2	2:C:274:PHE:CE2	2.80	0.65
2:C:104:ALA:O	2:C:106:GLY:N	2.30	0.64
2:C:491:PHE:CE1	2:C:528:PRO:HG2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ILE:HG13	1:A:474:PHE:CD2	2.32	0.64
1:A:222:ARG:HD3	1:A:484:ASP:HA	1.78	0.64
1:A:70:MET:HE1	1:A:78:ASP:CB	2.20	0.64
1:A:209:PRO:HB2	1:A:482:LEU:CD1	2.26	0.64
1:A:169:GLY:CA	1:A:176:THR:HG22	2.27	0.64
1:A:60:ARG:HH11	1:A:60:ARG:CG	2.11	0.64
2:C:527:ARG:N	2:C:528:PRO:HD2	2.13	0.63
2:C:583:LEU:HB3	2:C:586:MET:HB2	1.80	0.63
2:C:441:ALA:HB1	2:C:452:ILE:HD12	1.80	0.63
2:C:473:ASN:O	2:C:477:ASN:HB2	1.98	0.63
1:A:288:ARG:HD2	1:A:290:GLU:OE2	1.99	0.63
4:F:3[A]:DT:H4'	4:F:4[A]:DC:OP1	1.99	0.62
2:C:102:LEU:HD23	2:C:126:VAL:HG22	1.81	0.62
2:C:583:LEU:HA	2:C:586:MET:CE	2.21	0.62
1:A:211:PRO:O	1:A:478:ARG:NH2	2.30	0.62
1:A:259:ILE:HB	1:A:260:PRO:CD	2.30	0.62
2:C:583:LEU:HD13	2:C:586:MET:CE	2.30	0.62
2:C:132:SER:O	2:C:151:ASN:N	2.25	0.61
1:A:194:ILE:CD1	1:A:464:LYS:HG3	2.31	0.61
1:A:381:VAL:HG23	1:A:411:PHE:CZ	2.36	0.61
2:C:301:TYR:CD2	2:C:379:ILE:HD11	2.37	0.60
1:A:338:ARG:HH12	1:A:344:PRO:HG2	1.19	0.60
1:A:22:LYS:O	1:A:26:GLN:HG3	2.01	0.60
1:A:23:TYR:HD1	1:A:24:ILE:HD13	1.66	0.60
6:H:3[B]:DC:H2'	6:H:4[B]:DT:C6	2.37	0.60
2:C:431:LEU:HD22	2:C:479:MET:CE	2.32	0.60
1:A:381:VAL:CG2	1:A:411:PHE:CZ	2.85	0.59
2:C:139:THR:HG23	2:C:144:VAL:HB	1.84	0.59
1:A:145:PHE:CE1	1:A:146:ASP:HB2	2.38	0.59
1:A:146:ASP:OD2	1:A:148:THR:CG2	2.50	0.59
1:A:354:ARG:NE	1:A:456:GLU:CD	2.37	0.59
1:A:381:VAL:HG23	1:A:411:PHE:CE1	2.37	0.59
2:C:583:LEU:CB	2:C:586:MET:HB2	2.32	0.59
1:A:33:ILE:CD1	1:A:345:ILE:CG1	2.64	0.58
2:C:271:ILE:HD11	2:C:324:LEU:HD13	1.85	0.58
1:A:184:ALA:CB	1:A:471:LYS:HE3	2.19	0.58
1:A:183:LEU:HD11	1:A:470:VAL:HG12	1.86	0.58
2:C:134:LEU:HD12	2:C:176:PHE:HB3	1.86	0.58
1:A:317:LYS:HE3	1:A:318:TYR:CZ	2.38	0.57
2:C:446:ASP:OD1	2:C:449:PHE:CE1	2.58	0.57
2:C:51:ASN:HD21	2:C:99:PHE:HA	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:TYR:CZ	1:A:203:LYS:HE2	2.39	0.57
2:C:616:ARG:O	2:C:620:VAL:HG23	2.04	0.57
2:C:416:LEU:HG	2:C:417:THR:N	2.20	0.57
2:C:583:LEU:CA	2:C:586:MET:HB2	2.32	0.57
2:C:48:ILE:HD11	2:C:127:VAL:HG11	1.85	0.57
1:A:259:ILE:HB	1:A:260:PRO:HD2	1.86	0.56
1:A:288:ARG:NH1	1:A:290:GLU:OE2	2.30	0.56
2:C:584:GLY:HA2	2:C:586:MET:N	2.21	0.55
2:C:584:GLY:C	2:C:586:MET:N	2.59	0.55
2:C:190:TYR:CD2	2:C:213:ASP:HB2	2.42	0.55
2:C:48:ILE:HD11	2:C:127:VAL:HG21	1.87	0.55
1:A:210:GLY:HA2	1:A:229:TYR:OH	2.07	0.55
6:H:11[B]:DG:H5'	6:H:11[B]:DG:C8	2.42	0.55
1:A:139:VAL:HG13	1:A:140:PRO:CD	2.36	0.55
2:C:257:VAL:HB	2:C:330:ILE:HG22	1.88	0.54
2:C:197:LEU:HD22	2:C:209:LEU:HD22	1.90	0.54
1:A:184:ALA:HA	1:A:471:LYS:HD2	1.90	0.54
2:C:253:ASN:O	2:C:253:ASN:ND2	2.36	0.54
1:A:13:MET:O	2:C:621:LEU:CD1	2.56	0.54
2:C:380:ARG:HD3	2:C:495:ASP:HA	1.89	0.54
2:C:491:PHE:HE1	2:C:528:PRO:HG2	1.71	0.54
2:C:431:LEU:HD11	2:C:501:ILE:CG2	2.39	0.53
1:A:117[A]:ARG:HH22	4:F:1[A]:DA:H8	1.56	0.53
2:C:442:LYS:O	2:C:445:ARG:HD3	2.08	0.53
1:A:290:GLU:HB2	1:A:297:ARG:HG2	1.90	0.53
2:C:285:THR:HG23	2:C:347:LEU:O	2.09	0.53
2:C:479:MET:HE1	2:C:522:PHE:CZ	2.44	0.53
1:A:293:ARG:HB3	1:A:293:ARG:NH1	2.15	0.53
1:A:326:ASN:ND2	4:F:11[A]:DG:H4'	2.24	0.53
2:C:52:ALA:HB2	2:C:99:PHE:CE1	2.44	0.53
1:A:146:ASP:CG	1:A:148:THR:CG2	2.78	0.52
2:C:373:GLU:C	2:C:375:ALA:H	2.11	0.52
1:A:192:TYR:OH	1:A:203:LYS:HE2	2.09	0.52
1:A:194:ILE:HD13	1:A:464:LYS:HG3	1.91	0.52
2:C:591:LEU:HD22	2:C:596:MET:HG3	1.91	0.52
1:A:216:GLY:O	1:A:217:ALA:HB3	2.08	0.52
1:A:452:ILE:HG12	1:A:458:THR:CG2	2.40	0.52
1:A:357:ILE:CD1	1:A:459:MET:SD	2.97	0.52
1:A:33:ILE:HD13	1:A:345:ILE:HA	1.89	0.51
1:A:126:ILE:HG13	1:A:474:PHE:CE2	2.44	0.51
2:C:139:THR:O	2:C:170:THR:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:96:GLU:HG2	2:C:138:ILE:HD11	1.91	0.51
2:C:373:GLU:O	2:C:375:ALA:N	2.43	0.51
1:A:434:VAL:HG13	1:A:435:LEU:N	2.25	0.51
1:A:256:ILE:CD1	1:A:321:LEU:HD21	2.33	0.51
2:C:590:GLN:O	2:C:594:THR:HG23	2.11	0.51
2:C:54:ASP:OD1	2:C:107:LYS:HA	2.11	0.50
2:C:479:MET:CE	2:C:522:PHE:CZ	2.94	0.50
2:C:611:LEU:HD13	2:C:611:LEU:O	2.10	0.50
2:C:132:SER:N	2:C:177:MET:O	2.42	0.50
2:C:321:ARG:HG2	2:C:324:LEU:HD12	1.92	0.50
2:C:43:HIS:O	2:C:47:GLU:HG2	2.12	0.49
2:C:464:LYS:HD2	6:H:8[B]:DC:OP2	2.12	0.49
1:A:350:ILE:HG23	1:A:460:TYR:CE1	2.48	0.49
1:A:159:PHE:HB3	1:A:470:VAL:HG11	1.94	0.49
1:A:194:ILE:HG21	1:A:464:LYS:CD	2.42	0.49
6:H:3[B]:DC:H4'	6:H:4[B]:DT:OP1	2.12	0.49
1:A:357:ILE:CG2	1:A:459:MET:HG3	2.40	0.49
2:C:360:VAL:O	2:C:364:LEU:HD12	2.13	0.49
1:A:38:LYS:N	1:A:41:GLN:HE21	2.07	0.48
1:A:354:ARG:NE	1:A:456:GLU:OE2	2.40	0.48
2:C:263:TYR:CE2	2:C:378:LEU:HD21	2.47	0.48
2:C:592:TRP:CE2	2:C:597:ASN:HB2	2.47	0.48
1:A:452:ILE:HG12	1:A:458:THR:HG22	1.96	0.48
2:C:351:LEU:HD22	2:C:355:VAL:HG13	1.95	0.48
2:C:516:THR:O	2:C:520:THR:CG2	2.57	0.48
1:A:194:ILE:HD12	1:A:464:LYS:CG	2.43	0.48
2:C:203:LEU:HD23	2:C:274:PHE:CD2	2.46	0.48
1:A:360:ARG:HH12	1:A:462:LEU:HD13	1.79	0.47
1:A:381:VAL:HG22	1:A:411:PHE:CZ	2.49	0.47
2:C:246:LEU:O	2:C:260:ALA:HA	2.15	0.47
2:C:242:LEU:CD2	2:C:423:ASN:ND2	2.76	0.47
2:C:361:ALA:O	2:C:365:THR:OG1	2.32	0.47
2:C:179:ASP:OD1	2:C:182:ILE:HG23	2.15	0.47
2:C:190:TYR:HD2	2:C:213:ASP:HB2	1.79	0.47
1:A:96:GLU:HG2	1:A:126:ILE:HD12	1.95	0.47
1:A:130:LEU:HD23	1:A:157:ALA:HA	1.96	0.47
1:A:268:LEU:HD11	1:A:321:LEU:HD23	1.97	0.47
1:A:334:ASN:O	1:A:336:THR:HG23	2.15	0.47
1:A:44:ILE:HD13	1:A:85:MET:HB2	1.96	0.47
1:A:360:ARG:HH12	1:A:462:LEU:CD1	2.28	0.47
2:C:524:ARG:CG	2:C:524:ARG:NH1	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ILE:HD12	1:A:88:MET:HE1	1.96	0.46
2:C:303:ARG:NH1	2:C:310:GLU:HA	2.30	0.46
1:A:146:ASP:OD2	1:A:146:ASP:O	2.33	0.46
2:C:255:PHE:CE2	2:C:332:VAL:HG22	2.50	0.46
1:A:49:ASN:HB2	1:A:131:LEU:HD13	1.97	0.46
1:A:194:ILE:HD12	1:A:464:LYS:HG3	1.97	0.46
2:C:41:LEU:HD11	2:C:178:PRO:HG3	1.98	0.46
2:C:304:LYS:C	2:C:306:GLY:H	2.18	0.46
2:C:374:LEU:O	2:C:378:LEU:HB2	2.16	0.46
1:A:338:ARG:HB3	1:A:340:VAL:HG13	1.98	0.46
1:A:229:TYR:O	1:A:342:ILE:HB	2.15	0.46
2:C:263:TYR:CZ	2:C:378:LEU:HD21	2.50	0.46
2:C:455:LEU:CD1	2:C:518:LEU:HD11	2.46	0.46
1:A:24:ILE:HD13	1:A:24:ILE:N	2.29	0.45
2:C:611:LEU:C	2:C:611:LEU:CD1	2.81	0.45
1:A:33:ILE:CG1	1:A:345:ILE:HG12	2.44	0.45
1:A:86:VAL:O	1:A:90:GLN:HG3	2.16	0.45
2:C:526:MET:C	2:C:528:PRO:HD2	2.36	0.45
2:C:623:GLY:O	2:C:629:ARG:NH2	2.38	0.45
2:C:75:THR:HB	2:C:175:THR:CB	2.43	0.45
2:C:25:VAL:HB	2:C:32:TYR:CZ	2.51	0.45
2:C:242:LEU:CD2	2:C:423:ASN:HD22	2.30	0.45
2:C:523:TYR:OH	2:C:615:GLU:HB2	2.16	0.45
2:C:100:THR:O	2:C:102:LEU:HD13	2.17	0.45
2:C:265:ASP:HB2	2:C:421:SER:CB	2.47	0.45
1:A:187:ILE:HG12	1:A:467:LEU:HD22	1.99	0.45
2:C:334:GLU:HA	2:C:337:LEU:HB2	1.98	0.45
1:A:44:ILE:HG21	1:A:88:MET:HE3	1.99	0.45
1:A:82:TYR:CD1	1:A:116:MET:HB3	2.51	0.45
2:C:307:LEU:HD13	2:C:307:LEU:N	2.32	0.45
2:C:509:THR:O	2:C:512:ALA:HB3	2.16	0.44
1:A:296:LEU:C	1:A:296:LEU:HD23	2.38	0.44
1:A:42:ARG:NE	1:A:154:VAL:HA	2.32	0.44
1:A:45:LEU:HD22	1:A:123:LEU:HD22	1.98	0.44
1:A:194:ILE:HG21	1:A:464:LYS:HD2	2.00	0.44
1:A:415:GLN:O	1:A:419:ILE:HG13	2.18	0.44
1:A:169:GLY:HA3	1:A:176:THR:O	2.18	0.44
3:E:13[A]:DA:H2"	3:E:14[A]:DA:O5'	2.17	0.44
1:A:132:GLN:O	1:A:133:ASP:HB2	2.18	0.44
2:C:30:GLY:HA2	2:C:35:SER:H	1.83	0.44
2:C:108:PHE:CD1	2:C:276:ASN:CB	2.69	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ASN:HD21	1:A:148:THR:CG2	2.14	0.43
2:C:26:ARG:HD2	2:C:129:ALA:O	2.18	0.43
1:A:43:ARG:HG2	1:A:73:PHE:HB3	2.01	0.43
1:A:326:ASN:CG	4:F:11[A]:DG:H4'	2.39	0.43
2:C:352:ALA:HA	2:C:355:VAL:HG22	2.00	0.43
1:A:29:ALA:O	1:A:38:LYS:HE2	2.19	0.43
2:C:203:LEU:HD21	2:C:274:PHE:CG	2.53	0.43
2:C:388:ALA:HA	2:C:391:ALA:HB3	2.00	0.43
2:C:285:THR:OG1	2:C:352:ALA:HB3	2.18	0.43
2:C:298:MET:SD	2:C:368:LEU:HD21	2.58	0.43
1:A:55:PHE:HA	1:A:122:ARG:HD2	2.00	0.43
2:C:431:LEU:CD2	2:C:479:MET:CE	2.96	0.43
2:C:341:GLY:O	2:C:343:THR:N	2.44	0.43
2:C:524:ARG:HH11	2:C:524:ARG:CB	2.32	0.43
6:H:10[B]:DC:H2"	6:H:11[B]:DG:C5'	2.40	0.43
1:A:169:GLY:CA	1:A:176:THR:CG2	2.95	0.43
2:C:283:GLY:HA2	2:C:287:GLU:OE1	2.19	0.42
1:A:423:GLN:NE2	1:A:425:TYR:HE1	2.17	0.42
2:C:328:LEU:HD22	2:C:329:SER:N	2.34	0.42
5:G:13[B]:DC:H2"	5:G:14[B]:DA:O5'	2.19	0.42
1:A:191:VAL:HG22	1:A:464:LYS:HG2	2.00	0.42
1:A:194:ILE:CG2	1:A:464:LYS:HD2	2.49	0.42
1:A:312:LEU:HA	1:A:312:LEU:HD12	1.80	0.42
1:A:375:VAL:O	1:A:379:ILE:HG13	2.19	0.42
2:C:639:PHE:O	2:C:640:THR:CB	2.67	0.42
1:A:184:ALA:HB2	1:A:471:LYS:HG3	2.00	0.42
1:A:414:GLU:CD	1:A:414:GLU:H	2.22	0.42
2:C:37:ASP:HA	2:C:38:GLY:HA2	1.71	0.42
2:C:197:LEU:HD23	2:C:197:LEU:HA	1.87	0.42
2:C:536:TYR:N	2:C:536:TYR:CD2	2.87	0.42
1:A:191:VAL:HG11	1:A:468:ARG:NH2	2.35	0.42
1:A:346:LEU:HD23	1:A:346:LEU:HA	1.84	0.42
2:C:297:VAL:HG11	2:C:364:LEU:HD11	2.01	0.42
2:C:431:LEU:HD11	2:C:501:ILE:HG22	2.02	0.42
4:F:6[A]:DT:H2"	4:F:7[A]:DT:H5'	2.02	0.42
1:A:146:ASP:OD2	1:A:148:THR:HB	2.20	0.42
2:C:380:ARG:CD	2:C:495:ASP:HA	2.49	0.42
1:A:13:MET:CE	2:C:618:VAL:HA	2.49	0.42
1:A:184:ALA:CB	1:A:471:LYS:HG3	2.50	0.42
1:A:280:LYS:HB3	1:A:280:LYS:HE3	1.79	0.42
2:C:297:VAL:HG11	2:C:364:LEU:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:441:ALA:O	2:C:445:ARG:HB3	2.20	0.42
1:A:385:LEU:HA	1:A:385:LEU:HD23	1.86	0.41
2:C:102:LEU:HB2	2:C:103:HIS:H	1.71	0.41
2:C:601:ARG:CZ	2:C:603:LEU:HD11	2.50	0.41
1:A:23:TYR:CD1	1:A:24:ILE:HD13	2.52	0.41
2:C:99:PHE:C	2:C:99:PHE:CD1	2.93	0.41
1:A:334:ASN:O	1:A:336:THR:CG2	2.69	0.41
2:C:96:GLU:O	2:C:99:PHE:HB3	2.19	0.41
2:C:145:TYR:HA	2:C:160:LYS:O	2.19	0.41
2:C:485:ALA:HB3	2:C:491:PHE:CE2	2.56	0.41
1:A:169:GLY:HA2	1:A:176:THR:CG2	2.46	0.41
1:A:357:ILE:CB	1:A:459:MET:CG	2.99	0.41
2:C:165:ALA:HA	2:C:166:PRO:HD3	1.90	0.41
1:A:244:ILE:N	1:A:244:ILE:CD1	2.79	0.41
2:C:74:LEU:HB2	2:C:188:PHE:CE2	2.55	0.41
2:C:446:ASP:OD1	2:C:449:PHE:HE1	2.00	0.41
1:A:184:ALA:HA	1:A:471:LYS:CD	2.50	0.41
2:C:523:TYR:HH	2:C:615:GLU:HB2	1.86	0.41
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.89	0.41
2:C:220:ILE:HG22	2:C:221:GLU:H	1.86	0.41
1:A:27:ASP:HA	1:A:39:PRO:HG2	2.03	0.41
1:A:44:ILE:HD12	1:A:88:MET:HE3	1.99	0.41
2:C:337:LEU:HD23	2:C:337:LEU:HA	1.81	0.41
2:C:627:GLU:N	2:C:628:PRO:CD	2.84	0.41
1:A:340:VAL:HB	1:A:345:ILE:HG13	1.85	0.41
2:C:147:GLN:HB2	2:C:159:LEU:HA	2.03	0.41
1:A:29:ALA:HB3	1:A:171:SER:HB3	2.02	0.40
3:E:9[A]:DC:C2'	3:E:10[A]:DA:H5"	2.48	0.40
1:A:28:ARG:NH1	1:A:28:ARG:CG	2.64	0.40
2:C:383:ILE:H	2:C:383:ILE:HG13	1.62	0.40
1:A:254:ILE:HD13	1:A:312:LEU:HD13	2.04	0.40
2:C:41:LEU:O	2:C:44:LEU:HD12	2.21	0.40
2:C:235:LEU:HD12	2:C:235:LEU:HA	1.88	0.40
2:C:340:GLU:HB3	2:C:341:GLY:H	1.50	0.40
2:C:520:THR:CG2	2:C:622:MET:HG3	2.44	0.40
1:A:13:MET:O	2:C:621:LEU:HD13	2.21	0.40
2:C:236:ASN:ND2	2:C:264:ASN:HD22	2.20	0.40
1:A:9:LEU:O	1:A:9:LEU:CD2	2.69	0.40
2:C:236:ASN:HD21	2:C:264:ASN:HD22	1.69	0.40
2:C:283:GLY:O	2:C:286:HIS:HE1	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	468/496 (94%)	443 (95%)	20 (4%)	5 (1%)	14 52
2	C	524/670 (78%)	455 (87%)	56 (11%)	13 (2%)	5 32
All	All	992/1166 (85%)	898 (90%)	76 (8%)	18 (2%)	8 40

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	305	THR
2	C	373	GLU
1	A	145	PHE
1	A	329	MET
2	C	105	GLY
2	C	122	VAL
2	C	304	LYS
2	C	340	GLU
2	C	496	ALA
2	C	107	LYS
2	C	151	ASN
2	C	374	LEU
1	A	169	GLY
2	C	132	SER
1	A	217	ALA
1	A	221	GLY
2	C	121	GLY
2	C	166	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	377/431 (88%)	348 (92%)	29 (8%)	13 37
2	C	313/558 (56%)	252 (80%)	61 (20%)	1 8
All	All	690/989 (70%)	600 (87%)	90 (13%)	4 18

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	28	ARG
1	A	58	SER
1	A	60	ARG
1	A	91	ASN
1	A	102	HIS
1	A	111	ASP
1	A	126	ILE
1	A	148	THR
1	A	162	LEU
1	A	168	THR
1	A	208	LEU
1	A	223	ASP
1	A	236	VAL
1	A	268	LEU
1	A	279	ASN
1	A	293	ARG
1	A	308	THR
1	A	321	LEU
1	A	328	ASN
1	A	336	THR
1	A	338	ARG
1	A	366	GLU
1	A	372	LEU
1	A	380	ARG
1	A	414	GLU
1	A	420	VAL
1	A	432	VAL
1	A	462	LEU
2	C	25	VAL
2	C	26	ARG
2	C	33	ILE
2	C	43	HIS

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Mol	Chain	Res	Type
2	C	44	LEU
2	C	45	VAL
2	C	46	TRP
2	C	48	ILE
2	C	49	VAL
2	C	75	THR
2	C	99	PHE
2	C	100	THR
2	C	102	LEU
2	C	108	PHE
2	C	122	VAL
2	C	139	THR
2	C	148	ARG
2	C	158	THR
2	C	182	ILE
2	C	203	LEU
2	C	204	LEU
2	C	208	THR
2	C	209	LEU
2	C	211	LEU
2	C	220	ILE
2	C	231	PHE
2	C	235	LEU
2	C	242	LEU
2	C	245	VAL
2	C	253	ASN
2	C	259	VAL
2	C	275	VAL
2	C	278	VAL
2	C	286	HIS
2	C	288	THR
2	C	298	MET
2	C	299	ASN
2	C	307	LEU
2	C	324	LEU
2	C	328	LEU
2	C	331	LEU
2	C	337	LEU
2	C	340	GLU
2	C	351	LEU
2	C	363	LYS
2	C	364	LEU

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Mol	Chain	Res	Type
2	C	365	THR
2	C	368	LEU
2	C	378	LEU
2	C	429	LEU
2	C	431	LEU
2	C	445	ARG
2	C	453	LEU
2	C	477	ASN
2	C	509	THR
2	C	516	THR
2	C	520	THR
2	C	524	ARG
2	C	536	TYR
2	C	591	LEU
2	C	595	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	91	ASN
1	A	267	ASN
1	A	328	ASN
1	A	423	GLN
2	C	51	ASN
2	C	264	ASN
2	C	477	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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
8	LFX	F	101	7	29,29,29	0.83	1 (3%)	44,44,44	1.58	11 (25%)

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
8	LFX	F	101	7	-	0/8/27/27	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	101	LFX	O02-C15	3.07	1.29	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	F	101	LFX	O-C-C17	-3.50	114.78	122.46
8	F	101	LFX	C06-C05-N02	-3.37	117.79	119.89
8	F	101	LFX	C06-C04-C11	-2.52	113.89	116.02
8	F	101	LFX	O01-C06-C04	-2.49	115.37	117.90
8	F	101	LFX	C14-C03-C09	-2.40	105.16	112.58
8	F	101	LFX	C13-C11-C04	2.38	126.67	123.22
8	F	101	LFX	C10-C05-C06	2.38	122.73	120.07
8	F	101	LFX	C10-C15-C17	-2.33	112.63	115.59
8	F	101	LFX	F-C11-C04	-2.33	114.99	118.36
8	F	101	LFX	C02-N01-C01	2.31	116.62	111.52
8	F	101	LFX	C13-C10-C05	-2.17	116.00	118.84

There are no chirality outliers.

There are no torsion outliers.

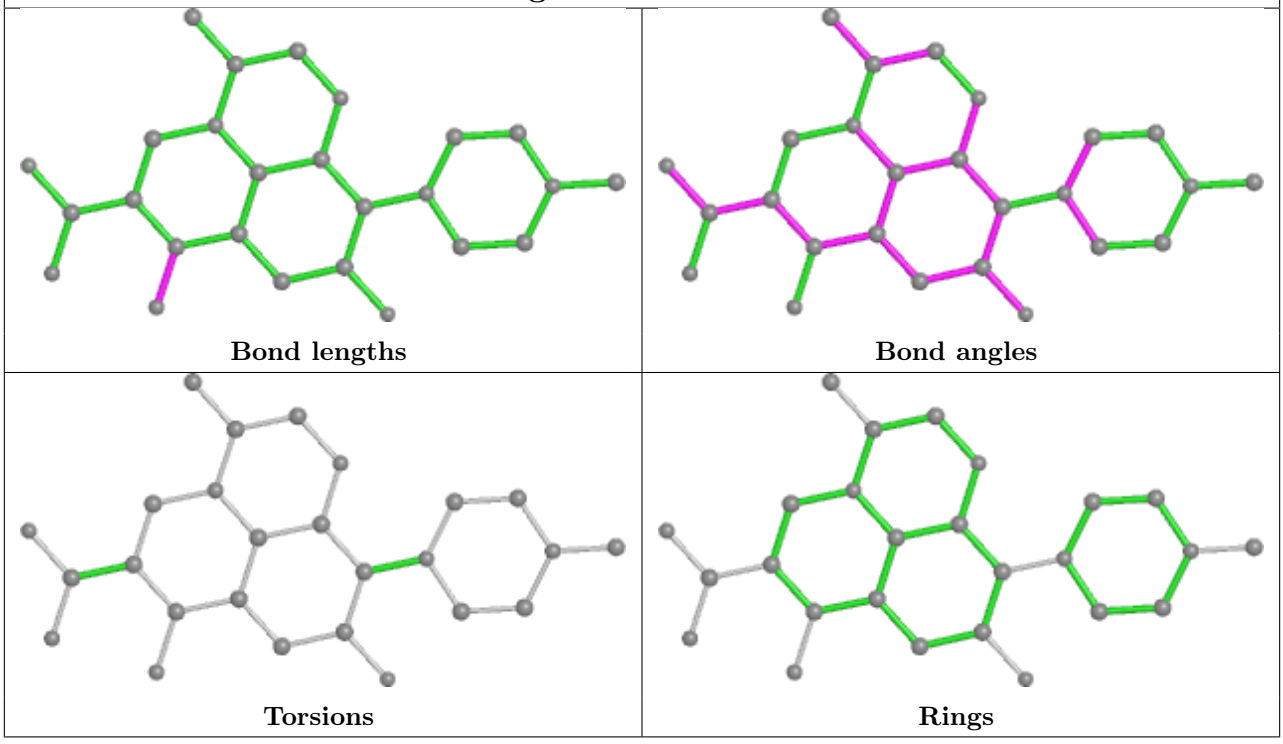
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	101	LFX	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 LFX F 101



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
2	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	585:GLU	C	586:MET	N	3.85
1	A	384:ILE	C	385:LEU	N	2.39
1	A	455:ASP	C	456:GLU	N	2.09

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

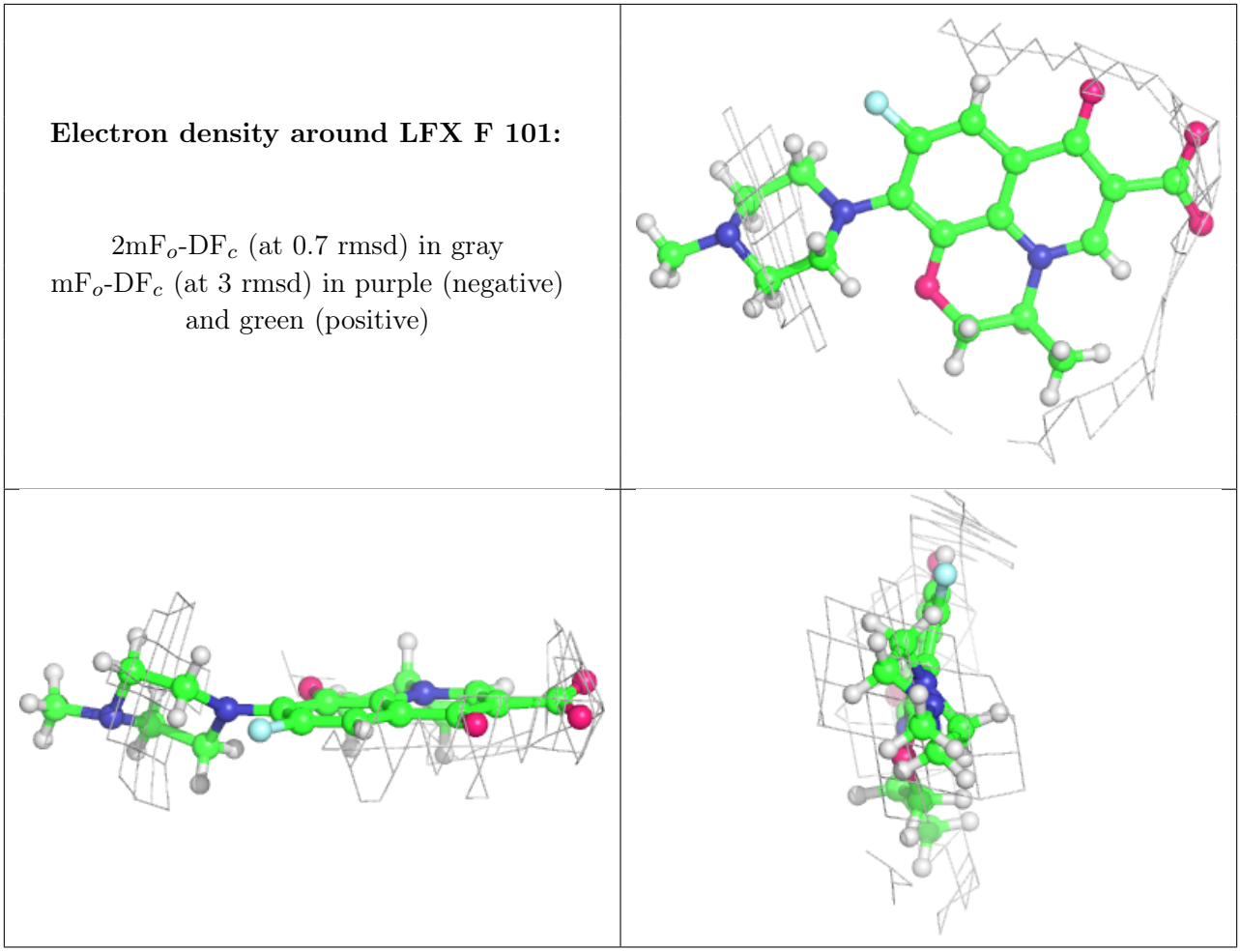
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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 LFX F 101:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.