



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 12:13 am BST

PDB ID : 4Z2D  
Title : Quinolone(Levofloxacin)-DNA cleavage complex of gyrase from *S. pneumoniae*  
Authors : Laponogov, I.; Veselkov, D.A.; Pan, X.-S.; Selvarajah, J.; Crevel, I.M.-T.;  
Fisher, L.M.; Sanderson, M.R.  
Deposited on : 2015-03-29  
Resolution : 3.38 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](mailto: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.

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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 : 2.11  
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) : 2.11

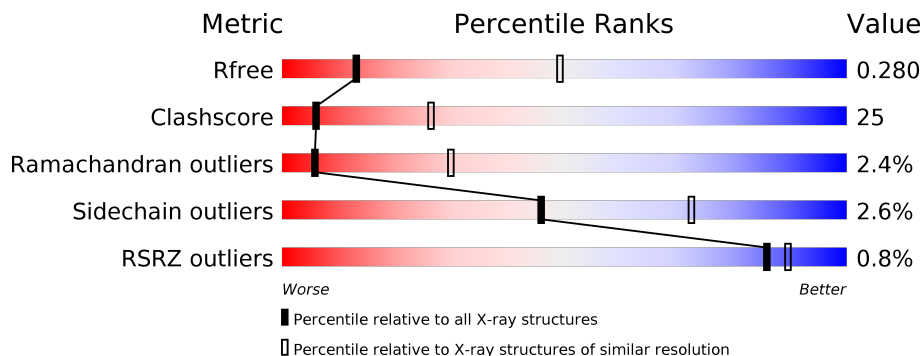
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.38 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	1691 (3.46-3.30)
Clashscore	141614	1762 (3.46-3.30)
Ramachandran outliers	138981	1732 (3.46-3.30)
Sidechain outliers	138945	1731 (3.46-3.30)
RSRZ outliers	127900	1635 (3.46-3.30)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	499	
1	B	499	
2	C	269	
2	D	269	
3	E	15	
3	G	15	

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Mol	Chain	Length	Quality of chain
4	F	19	
4	H	19	

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
5	MG	F	101	-	-	-	X

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 10156 atoms, of which 38 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 gyrase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	485	Total	C	N	O	S	0	0	0
			3479	2182	631	648	18			
1	B	471	Total	C	N	O	S	0	0	0
			3292	2069	592	614	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	494	HIS	-	expression tag	UNP Q9R867
A	495	HIS	-	expression tag	UNP Q9R867
A	496	HIS	-	expression tag	UNP Q9R867
A	497	HIS	-	expression tag	UNP Q9R867
A	498	HIS	-	expression tag	UNP Q9R867
A	499	HIS	-	expression tag	UNP Q9R867
B	494	HIS	-	expression tag	UNP Q9R867
B	495	HIS	-	expression tag	UNP Q9R867
B	496	HIS	-	expression tag	UNP Q9R867
B	497	HIS	-	expression tag	UNP Q9R867
B	498	HIS	-	expression tag	UNP Q9R867
B	499	HIS	-	expression tag	UNP Q9R867

- Molecule 2 is a protein called DNA gyrase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	198	Total	C	N	O	S	0	0	0
			1289	809	232	240	8			
2	D	194	Total	C	N	O	S	0	0	0
			1271	796	227	240	8			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	380	MET	-	initiating methionine	UNP Q59957
C	381	GLY	-	expression tag	UNP Q59957
C	382	HIS	-	expression tag	UNP Q59957
C	383	HIS	-	expression tag	UNP Q59957
C	384	HIS	-	expression tag	UNP Q59957
C	385	HIS	-	expression tag	UNP Q59957
C	386	HIS	-	expression tag	UNP Q59957
C	387	HIS	-	expression tag	UNP Q59957
C	388	HIS	-	expression tag	UNP Q59957
C	389	HIS	-	expression tag	UNP Q59957
C	390	HIS	-	expression tag	UNP Q59957
C	391	HIS	-	expression tag	UNP Q59957
C	392	SER	-	expression tag	UNP Q59957
C	393	SER	-	expression tag	UNP Q59957
C	394	GLY	-	expression tag	UNP Q59957
C	395	HIS	-	expression tag	UNP Q59957
C	396	ILE	-	expression tag	UNP Q59957
C	397	ASP	-	expression tag	UNP Q59957
C	398	ASP	-	expression tag	UNP Q59957
C	399	ASP	-	expression tag	UNP Q59957
C	400	ASP	-	expression tag	UNP Q59957
C	401	LYS	-	expression tag	UNP Q59957
C	402	HIS	-	expression tag	UNP Q59957
C	403	MET	-	expression tag	UNP Q59957
D	380	MET	-	initiating methionine	UNP Q59957
D	381	GLY	-	expression tag	UNP Q59957
D	382	HIS	-	expression tag	UNP Q59957
D	383	HIS	-	expression tag	UNP Q59957
D	384	HIS	-	expression tag	UNP Q59957
D	385	HIS	-	expression tag	UNP Q59957
D	386	HIS	-	expression tag	UNP Q59957
D	387	HIS	-	expression tag	UNP Q59957
D	388	HIS	-	expression tag	UNP Q59957
D	389	HIS	-	expression tag	UNP Q59957
D	390	HIS	-	expression tag	UNP Q59957
D	391	HIS	-	expression tag	UNP Q59957
D	392	SER	-	expression tag	UNP Q59957
D	393	SER	-	expression tag	UNP Q59957
D	394	GLY	-	expression tag	UNP Q59957
D	395	HIS	-	expression tag	UNP Q59957
D	396	ILE	-	expression tag	UNP Q59957
D	397	ASP	-	expression tag	UNP Q59957
D	398	ASP	-	expression tag	UNP Q59957

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Chain	Residue	Modelled	Actual	Comment	Reference
D	399	ASP	-	expression tag	UNP Q59957
D	400	ASP	-	expression tag	UNP Q59957
D	401	LYS	-	expression tag	UNP Q59957
D	402	HIS	-	expression tag	UNP Q59957
D	403	MET	-	expression tag	UNP Q59957

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
3	E	7	Total	C	N	O	P	0	0	0
			142	70	23	43	6			
3	G	7	Total	C	N	O	P	0	0	0
			141	70	23	42	6			

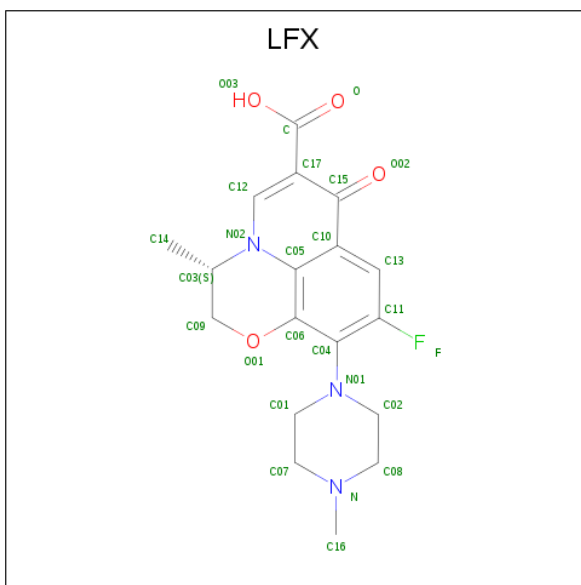
- Molecule 4 is a DNA chain called Symmetrized E-site DNA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
4	F	11	Total	C	N	O	P	0	0	0
			221	107	43	61	10			
4	H	11	Total	C	N	O	P	0	0	0
			221	107	43	61	10			

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	1	Total	Mg	0	0
			1	1		
5	E	1	Total	Mg	0	0
			1	1		

- Molecule 6 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<sub>18</sub>H<sub>20</sub>FN<sub>3</sub>O<sub>4</sub>).



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

- Molecule 7 is water.

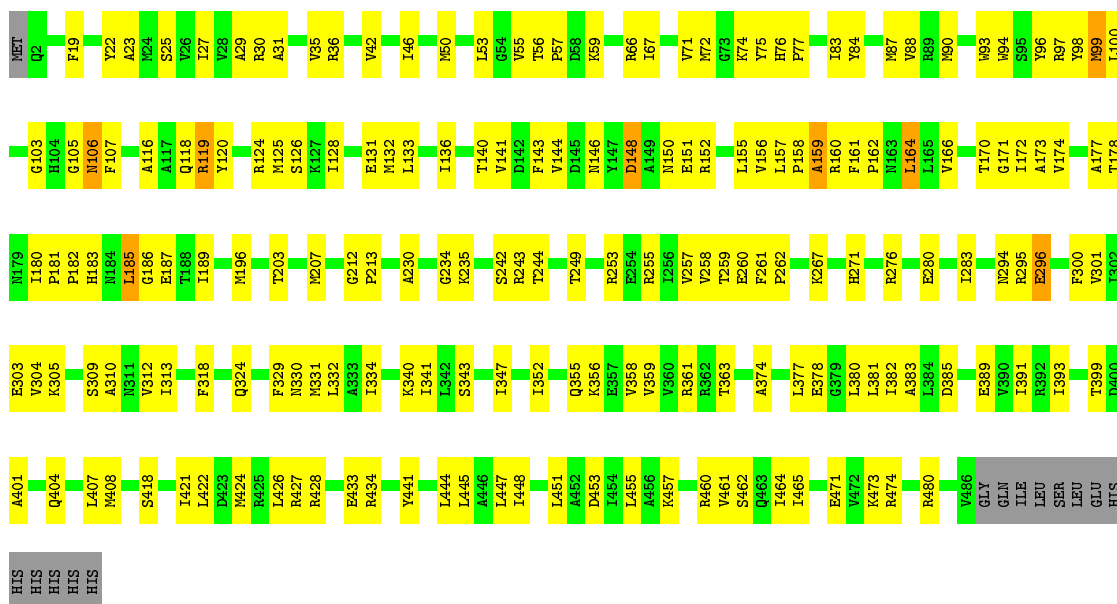
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	5	Total 5 O	0	0
7	B	3	Total 3 O	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

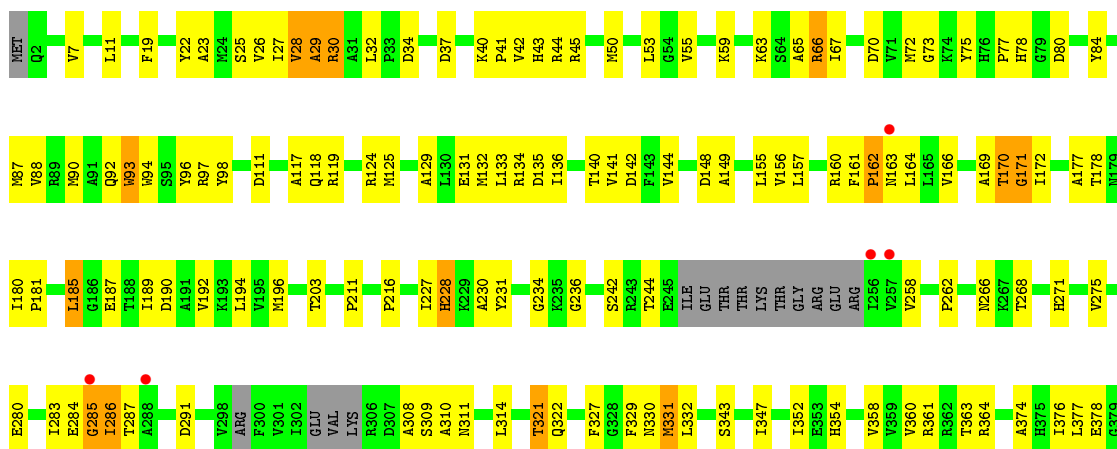
- Molecule 1: DNA gyrase subunit A

Chain A:



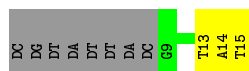
- Molecule 1: DNA gyrase subunit A

Chain B:

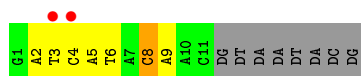
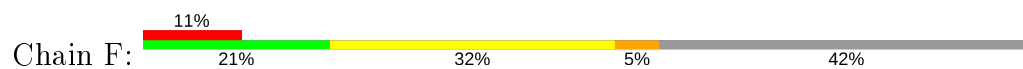




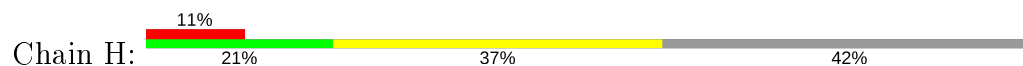




- Molecule 4: Symmetrized E-site DNA



- Molecule 4: Symmetrized E-site DNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.13Å 95.88Å 275.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.54 – 3.38 31.54 – 3.32	Depositor EDS
% Data completeness (in resolution range)	99.8 (31.54-3.38) 95.0 (31.54-3.32)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 3.31Å)	Xtrriage
Refinement program	PHENIX 1.8_1069	Depositor
R, $R_{free}$	0.229 , 0.280 0.230 , 0.280	Depositor DCC
$R_{free}$ test set	1763 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	99.7	Xtrriage
Anisotropy	0.554	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 82.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.024 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	10156	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	108.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.22	0/3534	0.39	0/4812
1	B	0.21	0/3343	0.38	0/4561
2	C	0.20	0/1309	0.37	0/1792
2	D	0.22	0/1292	0.37	0/1763
3	E	0.50	0/158	1.16	0/243
3	G	0.46	0/157	1.16	0/242
4	F	0.51	0/248	1.13	2/380 (0.5%)
4	H	0.49	0/248	0.96	0/380
All	All	0.25	0/10289	0.49	2/14173 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	F	8	DC	O4'-C4'-C3'	-6.61	101.86	104.50
4	F	8	DC	C1'-O4'-C4'	-6.44	103.66	110.10

There are no chirality outliers.

There are no planarity outliers.

### 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	3479	0	3141	159	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3292	0	2890	173	0
2	C	1289	0	1053	69	0
2	D	1271	0	1002	68	0
3	E	142	0	83	4	0
3	G	141	0	80	7	0
4	F	221	0	125	9	0
4	H	221	0	125	10	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	F	26	19	19	0	0
6	H	26	19	19	0	0
7	A	5	0	0	0	0
7	B	3	0	0	0	0
All	All	10118	38	8537	461	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 25.

All (461) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:THR:HB	1:B:358:VAL:HG13	1.27	1.07
1:B:144:VAL:HG11	1:B:155:LEU:HD21	1.40	1.04
2:D:520:THR:HG21	2:D:626:MET:HG3	1.37	1.04
1:B:30:ARG:NH1	3:G:14:DA:H4'	1.82	0.94
1:A:99:MET:H	1:A:99:MET:CE	1.83	0.91
1:B:189:ILE:HD12	1:B:473:LYS:HB2	1.49	0.91
2:D:403:MET:HA	2:D:421:SER:HA	1.51	0.89
2:C:520:THR:HG22	2:C:622:PHE:CD2	2.08	0.88
1:A:234:GLY:HA2	1:A:331:MET:HE2	1.56	0.88
1:B:84:TYR:CD1	1:B:118:GLN:HG2	2.10	0.87
1:B:44:ARG:NH1	1:B:155:LEU:O	2.08	0.86
1:A:391:ILE:HD13	1:B:391:ILE:HD13	1.58	0.85
1:B:480:ARG:HH21	1:B:484:LEU:HD11	1.42	0.84
1:A:99:MET:HE2	1:A:99:MET:H	1.40	0.84
1:B:234:GLY:HA2	1:B:331:MET:HE2	1.59	0.84
1:A:385:ASP:OD1	1:A:434:ARG:NH1	2.10	0.84
2:C:520:THR:HG22	2:C:622:PHE:HD2	1.42	0.82
1:A:119:ARG:HH11	1:A:119:ARG:HB2	1.43	0.82
2:D:520:THR:CG2	2:D:626:MET:HG3	2.09	0.81
2:D:520:THR:HG22	2:D:622:PHE:HD2	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ARG:NH1	1:A:119:ARG:HB2	1.96	0.81
2:D:520:THR:HG22	2:D:622:PHE:CD2	2.16	0.81
1:B:144:VAL:CG1	1:B:155:LEU:HD21	2.11	0.80
1:B:284:GLU:O	1:B:286:ILE:N	2.14	0.80
1:B:27:ILE:HG23	1:B:32:LEU:HD12	1.64	0.79
1:A:90:MET:HA	1:A:96:TYR:CD1	2.18	0.79
2:C:503:LEU:HD22	2:C:518:LEU:HD13	1.63	0.79
1:B:141:VAL:HG11	1:B:156:VAL:O	1.84	0.77
1:B:480:ARG:NH2	1:B:484:LEU:HD11	1.98	0.77
1:B:291:ASP:O	2:D:447:ARG:NH1	2.18	0.77
1:A:427:ARG:NH2	1:B:419:GLN:OE1	2.18	0.77
1:A:391:ILE:HD13	1:B:391:ILE:CD1	2.14	0.77
2:C:627:GLY:O	2:C:633:ARG:NH2	2.17	0.76
1:A:391:ILE:CD1	1:B:391:ILE:HD13	2.15	0.76
2:D:499:GLN:HA	2:D:534:TYR:CD2	2.21	0.75
2:C:520:THR:HG21	2:C:626:MET:HG3	1.67	0.74
1:B:385:ASP:OD1	1:B:434:ARG:NH1	2.21	0.74
1:A:171:GLY:HA2	1:A:178:THR:HG22	1.68	0.73
1:A:460:ARG:O	1:A:464:ILE:HG13	1.89	0.73
2:C:596:TRP:HA	2:C:600:MET:HB2	1.71	0.73
1:A:428:ARG:O	1:A:433:GLU:HG2	1.89	0.73
1:A:453:ASP:OD1	1:A:457:LYS:HE2	1.89	0.73
1:B:90:MET:HG2	1:B:96:TYR:HE2	1.53	0.73
1:B:164:LEU:HD21	1:B:180:ILE:HD12	1.70	0.72
1:A:141:VAL:HG11	1:A:156:VAL:O	1.89	0.72
1:B:484:LEU:H	1:B:484:LEU:HD12	1.53	0.72
2:D:604:HIS:O	2:D:605:ARG:HG2	1.90	0.71
4:F:3:DT:H2''	4:F:4:DC:O5'	1.90	0.71
1:A:181:PRO:HG3	1:A:329:PHE:CZ	2.25	0.71
1:B:474:ARG:O	1:B:474:ARG:HD2	1.91	0.71
1:A:72:MET:HE3	1:B:65:ALA:HB1	1.71	0.71
4:H:8:DC:H2''	4:H:9:DA:H5''	1.72	0.71
4:H:9:DA:H5'	4:H:9:DA:H8	1.56	0.70
2:C:442:LYS:O	2:C:445:ARG:NH1	2.18	0.70
1:B:50:MET:HB3	1:B:55:VAL:CG2	2.22	0.70
1:A:471:GLU:OE1	1:A:474:ARG:NH2	2.24	0.70
2:D:418:ASP:OD1	2:D:498:TYR:OH	2.09	0.70
1:A:177:ALA:O	1:A:330:ASN:ND2	2.25	0.69
1:B:310:ALA:O	1:B:314:LEU:N	2.18	0.69
1:B:84:TYR:O	1:B:88:VAL:HG23	1.92	0.69
2:D:633:ARG:NH1	4:F:9:DA:OP1	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:GLY:O	1:B:287:THR:N	2.25	0.68
2:C:502:VAL:HG22	2:C:607:MET:HE1	1.74	0.68
1:A:255:ARG:HG3	1:A:303:GLU:HG2	1.74	0.68
1:B:180:ILE:HG12	1:B:331:MET:HG2	1.75	0.68
2:C:406:GLY:O	2:C:408:GLU:N	2.25	0.68
1:A:255:ARG:NH1	1:A:303:GLU:OE2	2.26	0.68
1:B:22:TYR:O	1:B:26:VAL:HG23	1.93	0.68
1:B:125:MET:CE	1:B:133:LEU:HD12	2.23	0.68
1:A:474:ARG:HD2	1:A:474:ARG:O	1.94	0.68
1:A:261:PHE:CE1	1:A:267:LYS:HG2	2.29	0.67
1:A:249:THR:HG23	1:A:253:ARG:O	1.95	0.67
1:B:30:ARG:HH12	3:G:14:DA:H4'	1.55	0.67
1:A:74:LYS:HD3	1:B:66:ARG:NH2	2.10	0.66
4:H:9:DA:H5'	4:H:9:DA:C8	2.30	0.66
3:G:13:DT:H2''	3:G:14:DA:O5'	1.94	0.66
2:C:422:ASN:O	2:C:424:PRO:HD3	1.96	0.66
2:C:429:LEU:HD12	2:C:501:LEU:CD1	2.25	0.66
1:B:354:HIS:O	1:B:358:VAL:HG23	1.96	0.66
2:D:499:GLN:HA	2:D:534:TYR:HD2	1.60	0.66
2:C:406:GLY:C	2:C:408:GLU:H	1.99	0.66
1:A:171:GLY:HA2	1:A:178:THR:CG2	2.26	0.65
1:A:125:MET:HE1	1:A:133:LEU:HD12	1.78	0.65
1:B:234:GLY:HA2	1:B:331:MET:CE	2.27	0.65
2:C:502:VAL:HG22	2:C:607:MET:CE	2.26	0.65
2:D:517:LEU:HD23	2:D:626:MET:HE1	1.79	0.65
1:B:187:GLU:OE1	1:B:211:PRO:HD2	1.96	0.65
1:B:90:MET:HG2	1:B:96:TYR:CE2	2.31	0.65
1:B:125:MET:HE1	1:B:133:LEU:HD12	1.76	0.64
1:B:140:THR:CB	1:B:358:VAL:HG13	2.16	0.64
2:C:602:PRO:HA	2:C:605:ARG:HG2	1.80	0.64
2:C:416:LEU:HA	2:C:452:ILE:O	1.98	0.64
1:A:72:MET:CE	1:B:65:ALA:HB1	2.27	0.63
1:A:389:GLU:O	1:A:393:ILE:HG13	1.98	0.63
1:B:142:ASP:OD1	1:B:361:ARG:NH2	2.31	0.63
1:A:383:ALA:HB2	1:A:421:ILE:HD13	1.79	0.63
2:C:633:ARG:HD3	1:B:19:PHE:HZ	1.63	0.63
1:B:97:ARG:HG3	1:B:98:TYR:CE1	2.34	0.63
2:C:441:ALA:O	2:C:445:ARG:HB3	1.98	0.62
2:D:627:GLY:O	2:D:633:ARG:NH2	2.32	0.62
1:B:90:MET:HA	1:B:96:TYR:CD2	2.35	0.62
1:B:484:LEU:N	1:B:484:LEU:HD12	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:SER:O	1:B:311:ASN:N	2.29	0.62
2:D:541:PRO:HG3	2:D:598:THR:HG21	1.80	0.61
2:C:446:ASN:O	2:C:448:GLU:N	2.29	0.61
1:A:172:ILE:HD12	3:E:12:DG:C2	2.35	0.61
4:H:8:DC:H2''	4:H:9:DA:C5'	2.30	0.61
2:D:623:ASP:O	2:D:627:GLY:HA3	2.01	0.61
1:A:196:MET:CG	1:A:352:ILE:HD13	2.31	0.61
1:B:471:GLU:O	1:B:475:LYS:HG3	2.00	0.60
1:A:66:ARG:HD3	1:B:70:ASP:HA	1.84	0.60
1:B:50:MET:HB3	1:B:55:VAL:HG23	1.83	0.60
2:C:459:ILE:O	2:C:517:LEU:HD13	2.02	0.60
1:B:236:GLY:O	1:B:329:PHE:N	2.35	0.60
1:A:56:THR:HB	1:A:57:PRO:HD2	1.85	0.59
2:C:432:VAL:HG12	2:C:433:GLU:N	2.17	0.59
2:C:440:SER:HB3	2:C:595:LEU:HD12	1.84	0.59
1:A:140:THR:HA	1:A:361:ARG:HD3	1.85	0.59
1:B:67:ILE:HG21	1:B:87:MET:HE1	1.83	0.59
2:D:466:SER:O	2:D:468:ASP:N	2.35	0.59
1:B:178:THR:HB	1:B:332:LEU:HB3	1.85	0.59
1:A:234:GLY:HA2	1:A:331:MET:CE	2.30	0.59
2:C:428:GLU:N	2:C:449:PHE:O	2.35	0.59
1:A:196:MET:HG2	1:A:352:ILE:HD13	1.85	0.59
1:A:243:ARG:HB3	1:A:260:GLU:HB2	1.85	0.59
1:B:271:HIS:O	1:B:275:VAL:HG23	2.03	0.59
2:C:539:GLN:HB2	2:C:606:LEU:O	2.03	0.59
1:A:380:LEU:HD22	1:A:424:MET:SD	2.43	0.59
1:A:72:MET:HB2	1:A:83:ILE:HD12	1.84	0.59
2:C:435:ASP:OD2	2:C:456:ARG:NH2	2.36	0.58
1:A:103:GLY:HA3	1:A:107:PHE:CZ	2.38	0.58
1:A:171:GLY:O	1:A:177:ALA:HA	2.03	0.58
1:B:244:THR:HG22	1:B:258:VAL:HG22	1.85	0.58
1:A:84:TYR:O	1:A:88:VAL:HG23	2.03	0.58
4:H:3:DT:H2''	4:H:4:DC:O5'	2.03	0.58
1:B:27:ILE:HG23	1:B:32:LEU:CD1	2.32	0.58
1:A:189:ILE:HD12	1:A:473:LYS:HB2	1.86	0.58
1:A:22:TYR:CD1	2:D:513:HIS:HB2	2.38	0.58
2:C:540:PRO:HA	2:C:599:THR:CG2	2.34	0.58
1:B:131:GLU:O	1:B:160:ARG:HG2	2.04	0.58
1:B:242:SER:OG	1:B:262:PRO:HD3	2.04	0.58
2:D:516:THR:O	2:D:520:THR:HG23	2.04	0.58
1:B:164:LEU:HD21	1:B:180:ILE:CD1	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:520:THR:HG22	2:C:622:PHE:CE2	2.39	0.57
2:D:517:LEU:HD23	2:D:626:MET:CE	2.33	0.57
1:A:106:ASN:HB3	1:A:116:ALA:HB2	1.86	0.57
2:C:608:ALA:HA	1:B:7:VAL:O	2.05	0.57
2:C:445:ARG:HD2	2:C:452:ILE:HG12	1.87	0.57
2:D:459:ILE:O	2:D:517:LEU:HD13	2.04	0.57
1:A:23:ALA:O	1:A:27:ILE:HG13	2.05	0.57
1:B:471:GLU:OE1	1:B:474:ARG:NH2	2.37	0.57
1:B:216:PRO:HA	1:B:481:ARG:HH11	1.69	0.57
1:A:294:ASN:O	1:A:296:GLU:N	2.29	0.57
1:B:480:ARG:NE	1:B:484:LEU:HD11	2.20	0.57
1:A:374:ALA:O	1:A:378:GLU:HG3	2.05	0.56
1:B:194:LEU:HD23	1:B:194:LEU:O	2.04	0.56
1:B:480:ARG:CZ	1:B:484:LEU:HD11	2.35	0.56
2:D:422:ASN:O	2:D:424:PRO:HD3	2.06	0.56
1:A:125:MET:CE	1:A:133:LEU:HD12	2.34	0.56
1:B:41:PRO:O	1:B:45:ARG:HG3	2.05	0.56
1:A:67:ILE:O	1:A:71:VAL:HG23	2.06	0.56
1:A:99:MET:H	1:A:99:MET:HE3	1.65	0.56
1:B:480:ARG:HE	1:B:484:LEU:HD11	1.69	0.56
1:A:146:ASN:ND2	1:A:151:GLU:HB2	2.20	0.56
2:D:423:ASN:C	2:D:425:ALA:H	2.08	0.56
4:F:3:DT:H4'	4:F:4:DC:OP1	2.05	0.56
1:A:404:GLN:HG3	1:A:418:SER:HB2	1.88	0.56
2:D:445:ARG:HA	2:D:600:MET:HE2	1.86	0.56
1:A:294:ASN:C	1:A:296:GLU:H	2.09	0.56
1:B:84:TYR:CE1	1:B:118:GLN:HG2	2.40	0.56
2:D:423:ASN:O	2:D:425:ALA:N	2.37	0.56
1:B:192:VAL:O	1:B:196:MET:HG3	2.06	0.56
2:C:440:SER:CB	2:C:595:LEU:HD12	2.35	0.56
2:C:429:LEU:HD12	2:C:501:LEU:HD11	1.88	0.56
1:A:98:TYR:CZ	1:A:185:LEU:HB2	2.41	0.56
1:B:284:GLU:C	1:B:286:ILE:H	2.07	0.56
1:B:72:MET:HE1	1:B:80:ASP:N	2.20	0.56
1:B:67:ILE:CG2	1:B:87:MET:HE1	2.36	0.56
1:A:119:ARG:HD3	1:A:120:TYR:CE2	2.41	0.55
1:B:131:GLU:OE2	1:B:134:ARG:NH1	2.39	0.55
2:D:541:PRO:HG3	2:D:598:THR:CG2	2.36	0.55
1:A:42:VAL:O	1:A:46:ILE:HG13	2.06	0.55
1:A:304:VAL:HG22	1:A:313:ILE:HD12	1.89	0.55
1:A:399:THR:HG22	1:A:401:ALA:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:442:LYS:HA	2:C:445:ARG:HD3	1.88	0.55
2:D:499:GLN:CA	2:D:534:TYR:HD2	2.19	0.55
1:A:422:LEU:HB3	1:B:427:ARG:HB3	1.87	0.55
1:A:230:ALA:HB1	1:A:329:PHE:CD1	2.42	0.55
1:A:235:LYS:HE2	1:A:341:ILE:HD13	1.88	0.55
1:B:389:GLU:O	1:B:393:ILE:HG12	2.07	0.54
1:B:460:ARG:O	1:B:464:ILE:HG13	2.07	0.54
1:B:50:MET:O	1:B:55:VAL:HG22	2.07	0.54
2:D:427:THR:HG22	2:D:498:TYR:HD2	1.72	0.54
2:C:435:ASP:N	4:F:2:DA:OP1	2.37	0.54
1:B:27:ILE:CG2	1:B:32:LEU:HD12	2.36	0.54
1:B:343:SER:O	1:B:347:ILE:HG13	2.06	0.54
1:A:355:GLN:NE2	1:A:355:GLN:HA	2.22	0.54
1:A:74:LYS:HD3	1:B:66:ARG:HH21	1.72	0.54
1:A:84:TYR:CD1	1:A:118:GLN:HG2	2.43	0.54
1:B:244:THR:HG22	1:B:258:VAL:HA	1.90	0.54
1:A:132:MET:O	1:A:158:PRO:HD2	2.08	0.54
3:E:13:DT:H2''	3:E:14:DA:O5'	2.07	0.54
1:B:203:THR:HG21	1:B:228:HIS:CE1	2.43	0.53
2:D:446:ASN:O	2:D:448:GLU:N	2.37	0.53
1:B:189:ILE:CD1	1:B:473:LYS:HB2	2.30	0.53
1:A:36:ARG:NH2	1:A:156:VAL:HB	2.24	0.53
1:A:131:GLU:O	1:A:160:ARG:HG2	2.09	0.53
1:B:42:VAL:HG13	1:B:43:HIS:N	2.23	0.53
1:B:77:PRO:O	1:B:78:HIS:ND1	2.41	0.53
1:A:332:LEU:HD12	1:A:340:LYS:O	2.09	0.53
2:C:540:PRO:HA	2:C:599:THR:HG21	1.90	0.52
1:A:343:SER:O	1:A:347:ILE:HG13	2.09	0.52
1:B:34:ASP:HB3	1:B:37:ASP:OD1	2.09	0.52
2:D:427:THR:HG22	2:D:498:TYR:CD2	2.43	0.52
1:B:380:LEU:O	1:B:384:LEU:HG	2.10	0.52
1:B:441:TYR:CZ	1:B:445:LEU:HD21	2.44	0.52
2:C:432:VAL:CG1	2:C:437:ALA:HB3	2.38	0.52
2:D:416:LEU:HA	2:D:452:ILE:O	2.09	0.52
1:B:28:VAL:O	1:B:29:ALA:HB2	2.09	0.52
2:D:509:VAL:O	2:D:512:ALA:HB3	2.09	0.52
1:A:257:VAL:HG22	1:A:301:VAL:HG22	1.92	0.52
1:B:55:VAL:O	1:B:124:ARG:HB2	2.09	0.52
1:A:99:MET:HE2	1:A:99:MET:N	2.17	0.52
2:D:510:ASP:HB3	3:E:15:DT:H4'	1.91	0.52
1:A:156:VAL:HG22	1:A:157:LEU:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:633:ARG:NH1	4:H:9:DA:OP1	2.42	0.52
1:A:447:LEU:O	1:A:451:LEU:HG	2.10	0.51
1:B:98:TYR:CZ	1:B:185:LEU:HB2	2.46	0.51
2:D:466:SER:O	2:D:469:LYS:N	2.43	0.51
2:D:509:VAL:HG23	2:D:510:ASP:N	2.25	0.51
1:B:30:ARG:NH1	3:G:14:DA:C4'	2.66	0.51
2:C:541:PRO:HG3	2:C:598:THR:HB	1.92	0.51
4:F:8:DC:H2''	4:F:9:DA:H5''	1.92	0.51
1:B:377:LEU:HG	1:B:437:ILE:CG2	2.40	0.51
1:B:97:ARG:HA	1:B:216:PRO:HB3	1.93	0.51
2:D:435:ASP:N	4:H:2:DA:OP1	2.36	0.51
2:D:520:THR:HA	2:D:622:PHE:CE2	2.45	0.51
1:B:376:ILE:N	1:B:376:ILE:HD12	2.26	0.51
2:C:423:ASN:O	2:C:425:ALA:N	2.38	0.51
1:A:444:LEU:O	1:A:448:ILE:HG13	2.10	0.51
2:D:427:THR:HG22	2:D:428:GLU:N	2.26	0.51
1:A:174:VAL:HG22	4:F:8:DC:H4'	1.92	0.51
1:A:75:TYR:O	1:A:77:PRO:HD3	2.11	0.51
1:A:383:ALA:HB2	1:A:421:ILE:CD1	2.40	0.51
2:D:428:GLU:N	2:D:449:PHE:O	2.44	0.51
1:A:59:LYS:O	1:A:124:ARG:NH1	2.41	0.50
1:B:268:THR:O	1:B:271:HIS:HB3	2.11	0.50
1:A:441:TYR:CZ	1:A:445:LEU:HD21	2.46	0.50
1:B:22:TYR:CZ	1:B:26:VAL:HG21	2.46	0.50
2:D:618:ALA:O	2:D:622:PHE:HD1	1.94	0.50
2:C:423:ASN:C	2:C:425:ALA:H	2.12	0.50
4:F:9:DA:C8	4:F:9:DA:H5'	2.46	0.50
1:B:40:LYS:HG3	1:B:43:HIS:ND1	2.26	0.50
1:A:404:GLN:HG3	1:A:418:SER:CB	2.41	0.50
1:B:90:MET:HA	1:B:96:TYR:CE2	2.47	0.50
1:B:227:ILE:HG22	1:B:231:TYR:CE2	2.46	0.50
2:D:529:ILE:HG22	2:D:535:VAL:HG23	1.93	0.50
1:A:132:MET:HA	1:A:159:ALA:HA	1.93	0.50
2:C:631:GLU:CB	2:C:632:PRO:HD3	2.42	0.50
1:B:433:GLU:O	1:B:436:LYS:N	2.44	0.49
1:A:203:THR:O	1:A:207:MET:HG3	2.12	0.49
2:C:432:VAL:CG1	2:C:433:GLU:N	2.75	0.49
2:D:491:PHE:CG	2:D:491:PHE:O	2.66	0.49
1:A:46:ILE:HG21	1:A:90:MET:CE	2.42	0.49
1:B:131:GLU:OE1	1:B:134:ARG:HD2	2.12	0.49
1:B:441:TYR:CE2	1:B:445:LEU:HD21	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:520:THR:CG2	2:C:626:MET:HG3	2.39	0.49
1:B:244:THR:CG2	1:B:258:VAL:HG22	2.43	0.49
1:B:98:TYR:CD1	1:B:166:VAL:CG1	2.95	0.49
2:D:525:TYR:O	2:D:526:MET:HG3	2.12	0.49
2:C:504:MET:HE1	2:C:595:LEU:CD2	2.42	0.49
1:A:196:MET:HG3	1:A:352:ILE:HD13	1.95	0.49
1:B:97:ARG:HG3	1:B:98:TYR:CD1	2.48	0.49
2:D:449:PHE:CD1	2:D:450:GLN:HG3	2.48	0.49
2:D:599:THR:O	2:D:605:ARG:HD2	2.13	0.49
2:C:509:VAL:HG11	1:B:25:SER:CB	2.43	0.49
2:C:536:TYR:CB	2:C:607:MET:HE1	2.42	0.49
2:D:527:LYS:N	2:D:528:PRO:CD	2.76	0.49
2:C:590:MET:HG2	2:C:594:GLN:CB	2.43	0.48
2:C:633:ARG:O	2:C:637:ILE:HG13	2.14	0.48
1:B:40:LYS:HD2	1:B:43:HIS:HE1	1.79	0.48
1:B:450:ASP:O	1:B:454:ILE:HG13	2.13	0.48
1:B:156:VAL:HG22	1:B:157:LEU:N	2.28	0.48
1:B:177:ALA:O	1:B:330:ASN:ND2	2.47	0.48
1:B:308:ALA:C	1:B:310:ALA:H	2.16	0.48
1:B:133:LEU:O	1:B:136:ILE:HG22	2.13	0.48
1:A:189:ILE:CD1	1:A:473:LYS:HB2	2.42	0.48
1:B:63:LYS:O	1:B:66:ARG:HB2	2.13	0.48
2:C:406:GLY:C	2:C:408:GLU:N	2.66	0.48
1:A:441:TYR:O	1:A:445:LEU:HD23	2.14	0.48
2:C:508:ASP:OD1	2:C:511:GLY:N	2.43	0.48
1:B:172:ILE:HD11	4:H:9:DA:C2	2.49	0.48
1:A:97:ARG:HB2	1:A:182:PRO:HB3	1.96	0.48
2:C:416:LEU:HB2	2:C:453:LEU:HD23	1.95	0.48
1:B:30:ARG:HH11	3:G:14:DA:H4'	1.69	0.48
1:A:90:MET:HB3	1:A:96:TYR:CZ	2.49	0.47
1:B:360:VAL:O	1:B:364:ARG:HG3	2.14	0.47
2:D:432:VAL:HG22	2:D:433:GLU:N	2.29	0.47
2:C:527:LYS:N	2:C:528:PRO:CD	2.77	0.47
1:A:143:PHE:HB3	1:A:152:ARG:HG2	1.95	0.47
1:A:363:THR:HG21	1:A:455:LEU:HG	1.96	0.47
1:B:117:ALA:C	1:B:119:ARG:H	2.16	0.47
1:B:291:ASP:CG	2:D:447:ARG:HH12	2.17	0.47
2:C:618:ALA:O	2:C:622:PHE:HD1	1.97	0.47
1:A:128:ILE:HG12	1:A:161:PHE:CE1	2.49	0.47
2:D:541:PRO:CG	2:D:598:THR:HG21	2.44	0.47
1:A:46:ILE:O	1:A:50:MET:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:ALA:O	1:B:27:ILE:HG13	2.14	0.47
2:C:435:ASP:CG	2:C:456:ARG:HH21	2.17	0.47
2:D:445:ARG:O	2:D:446:ASN:HB3	2.14	0.47
1:A:93:TRP:CD1	1:A:94:TRP:HE3	2.33	0.47
1:B:374:ALA:O	1:B:378:GLU:HG3	2.15	0.47
1:A:393:ILE:HD12	1:A:407:LEU:HD23	1.97	0.47
1:B:164:LEU:C	1:B:164:LEU:HD23	2.35	0.47
1:B:480:ARG:HE	1:B:484:LEU:CD1	2.28	0.47
1:A:19:PHE:HZ	2:D:633:ARG:HD3	1.80	0.47
2:D:449:PHE:CE1	2:D:450:GLN:HG3	2.49	0.47
1:A:146:ASN:CG	1:A:151:GLU:HB2	2.35	0.46
1:A:461:VAL:O	1:A:465:ILE:HG13	2.15	0.46
2:D:466:SER:C	2:D:468:ASP:N	2.67	0.46
1:A:164:LEU:HD21	1:A:180:ILE:HD12	1.97	0.46
1:A:213:PRO:O	1:A:480:ARG:NH2	2.47	0.46
1:B:59:LYS:O	1:B:124:ARG:NH1	2.42	0.46
2:C:471:LEU:O	2:C:477:ARG:NH2	2.43	0.46
1:A:447:LEU:HD11	1:A:451:LEU:HD11	1.97	0.46
1:B:196:MET:HG2	1:B:352:ILE:HD13	1.98	0.46
1:B:203:THR:HG21	1:B:228:HIS:ND1	2.31	0.46
1:B:42:VAL:HG13	1:B:43:HIS:H	1.81	0.46
1:B:474:ARG:C	1:B:474:ARG:HD2	2.36	0.46
1:A:363:THR:CG2	1:A:455:LEU:HG	2.45	0.46
1:A:76:HIS:HB3	1:A:83:ILE:HD11	1.97	0.46
1:A:140:THR:HB	1:A:358:VAL:HG13	1.97	0.46
1:B:161:PHE:O	1:B:163:ASN:N	2.49	0.46
1:B:185:LEU:O	1:B:189:ILE:HG13	2.16	0.46
1:B:93:TRP:O	1:B:216:PRO:HB2	2.16	0.46
2:C:633:ARG:HD2	4:H:9:DA:OP1	2.16	0.46
1:A:31:ALA:CB	1:A:173:ALA:HB2	2.46	0.46
1:A:304:VAL:HG12	1:A:305:LYS:N	2.31	0.46
1:A:56:THR:HB	1:A:57:PRO:CD	2.46	0.46
1:B:134:ARG:O	1:B:135:ASP:HB2	2.16	0.46
1:B:387:ILE:O	1:B:391:ILE:HG13	2.16	0.46
2:C:427:THR:HA	2:C:449:PHE:O	2.16	0.45
1:B:415:GLU:O	1:B:418:SER:OG	2.30	0.45
2:D:466:SER:C	2:D:468:ASP:H	2.19	0.45
1:A:441:TYR:CE2	1:A:445:LEU:HD21	2.52	0.45
2:C:445:ARG:O	2:C:450:GLN:HB2	2.16	0.45
1:A:156:VAL:HG22	1:A:157:LEU:H	1.81	0.45
1:A:235:LYS:CE	1:A:341:ILE:HD13	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:ILE:O	1:B:468:GLU:HG3	2.17	0.45
1:A:447:LEU:HD12	1:A:451:LEU:HG	1.99	0.45
2:D:625:LEU:O	2:D:633:ARG:NE	2.38	0.45
1:A:318:PHE:O	1:A:324:GLN:HB3	2.17	0.45
1:B:441:TYR:O	1:B:445:LEU:HD23	2.16	0.45
1:B:444:LEU:O	1:B:448:ILE:HG13	2.17	0.45
2:C:409:ILE:O	2:C:411:ASN:N	2.46	0.45
1:A:294:ASN:C	1:A:296:GLU:N	2.70	0.45
1:B:92:GLN:HB3	1:B:94:TRP:CE2	2.52	0.45
2:C:429:LEU:HD12	2:C:501:LEU:HD12	1.97	0.45
1:A:144:VAL:HG11	1:A:155:LEU:HD21	1.98	0.44
2:C:429:LEU:C	2:C:429:LEU:HD13	2.38	0.44
2:C:445:ARG:HA	2:C:600:MET:HE2	2.00	0.44
2:C:525:TYR:O	2:C:526:MET:HG3	2.17	0.44
4:F:8:DC:H2''	4:F:9:DA:C5'	2.46	0.44
1:A:181:PRO:HG3	1:A:329:PHE:CE1	2.53	0.44
1:A:100:LEU:HA	1:A:126:SER:OG	2.17	0.44
1:A:235:LYS:NZ	1:A:341:ILE:HD13	2.33	0.44
2:D:476:ILE:O	2:D:480:PHE:HD2	2.00	0.44
1:A:181:PRO:O	1:A:183:HIS:CE1	2.71	0.44
1:A:352:ILE:O	1:A:356:LYS:HG3	2.17	0.44
1:A:97:ARG:HG3	1:A:98:TYR:CD1	2.53	0.44
1:A:133:LEU:O	1:A:136:ILE:HB	2.18	0.44
1:A:426:LEU:HB3	1:B:394:ILE:CD1	2.48	0.44
2:D:432:VAL:HG21	2:D:437:ALA:CB	2.48	0.44
1:A:243:ARG:HG2	1:A:259:THR:OG1	2.17	0.44
2:D:433:GLU:O	2:D:433:GLU:HG3	2.17	0.43
1:A:25:SER:O	1:A:29:ALA:HB3	2.17	0.43
1:B:162:PRO:O	1:B:166:VAL:HG23	2.18	0.43
1:B:164:LEU:O	1:B:164:LEU:HD23	2.18	0.43
1:A:355:GLN:NE2	1:A:355:GLN:CA	2.80	0.43
1:A:98:TYR:CD1	1:A:166:VAL:CG1	3.01	0.43
2:C:503:LEU:HD22	2:C:518:LEU:CD1	2.41	0.43
4:F:5:DA:C2	4:F:6:DT:C2	3.06	0.43
2:D:499:GLN:CA	2:D:534:TYR:CD2	2.95	0.43
1:A:230:ALA:O	1:A:234:GLY:N	2.48	0.43
1:A:304:VAL:HG21	1:A:310:ALA:HA	2.00	0.43
1:A:50:MET:O	1:A:55:VAL:HG22	2.18	0.43
2:D:432:VAL:CG2	2:D:437:ALA:HB3	2.48	0.43
1:B:391:ILE:O	1:B:395:ARG:HG3	2.19	0.43
2:D:631:GLU:N	2:D:632:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:GLY:C	1:A:480:ARG:HH22	2.22	0.43
1:B:75:TYR:O	1:B:77:PRO:HD3	2.18	0.43
2:D:537:ILE:HB	2:D:608:ALA:HB3	2.01	0.43
2:C:430:PHE:HB2	2:C:452:ILE:HD13	2.00	0.43
1:A:186:GLY:HA2	1:A:473:LYS:HG3	2.01	0.42
1:B:50:MET:CB	1:B:55:VAL:CG2	2.95	0.42
1:A:97:ARG:HG3	1:A:98:TYR:CE1	2.54	0.42
1:B:194:LEU:HD23	1:B:194:LEU:C	2.39	0.42
4:H:5:DA:C2	4:H:6:DT:C2	3.07	0.42
1:B:148:ASP:O	1:B:149:ALA:HB3	2.19	0.42
1:B:29:ALA:O	1:B:30:ARG:HB2	2.20	0.42
1:B:40:LYS:CG	1:B:43:HIS:ND1	2.82	0.42
2:C:633:ARG:HD3	1:B:19:PHE:CZ	2.49	0.42
1:A:119:ARG:HG3	1:A:119:ARG:H	1.44	0.42
1:A:66:ARG:CG	1:B:73:GLY:HA3	2.50	0.42
1:B:376:ILE:HG23	1:B:420:ALA:CB	2.49	0.42
1:A:309:SER:CB	1:A:312:VAL:HG23	2.50	0.42
2:D:539:GLN:HB2	2:D:606:LEU:O	2.20	0.42
1:A:25:SER:CB	2:D:509:VAL:HG11	2.50	0.42
2:D:532:ALA:HB3	2:D:534:TYR:CD1	2.54	0.42
1:A:377:LEU:HD23	1:A:441:TYR:HB2	2.02	0.42
1:A:72:MET:CE	1:B:65:ALA:CB	2.96	0.42
1:B:132:MET:O	1:B:157:LEU:HB3	2.20	0.42
2:C:527:LYS:N	2:C:528:PRO:HD2	2.35	0.42
1:A:181:PRO:HA	1:A:182:PRO:HD3	1.87	0.42
1:A:276:ARG:O	1:A:280:GLU:HB2	2.20	0.42
2:C:504:MET:HE1	2:C:595:LEU:HD22	2.00	0.41
1:B:111:ASP:C	1:B:266:ASN:HD21	2.23	0.41
1:A:378:GLU:O	1:A:382:ILE:HG13	2.20	0.41
2:C:483:MET:O	2:C:497:ARG:HG3	2.21	0.41
2:D:441:ALA:O	2:D:445:ARG:HB3	2.19	0.41
2:D:520:THR:HG22	2:D:622:PHE:CE2	2.54	0.41
1:A:105:GLY:O	1:A:107:PHE:HD1	2.04	0.41
1:B:169:ALA:O	1:B:170:THR:HB	2.21	0.41
2:D:499:GLN:C	2:D:534:TYR:HD2	2.24	0.41
1:A:35:VAL:HG12	1:A:334:ILE:O	2.21	0.41
1:A:474:ARG:HD2	1:A:474:ARG:C	2.40	0.41
1:A:187:GLU:OE1	1:A:480:ARG:NH1	2.53	0.41
1:B:117:ALA:C	1:B:119:ARG:N	2.73	0.41
2:D:527:LYS:HB3	2:D:528:PRO:HD3	2.03	0.41
1:B:129:ALA:O	1:B:132:MET:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:TYR:CE1	1:B:26:VAL:CG2	3.04	0.41
2:C:538:ALA:C	2:C:540:PRO:HD3	2.40	0.41
1:A:196:MET:CE	1:A:462:SER:HB2	2.51	0.41
1:B:187:GLU:O	1:B:190:ASP:HB2	2.21	0.41
1:B:363:THR:CG2	1:B:455:LEU:HD21	2.51	0.41
3:G:14:DA:H2''	3:G:15:DT:H5'	2.02	0.41
1:B:22:TYR:CE1	1:B:26:VAL:HG21	2.55	0.41
1:B:30:ARG:HH11	3:G:14:DA:C4'	2.31	0.41
1:A:242:SER:OG	1:A:262:PRO:HD3	2.21	0.41
1:A:258:VAL:HB	1:A:300:PHE:HB3	2.02	0.41
1:A:359:VAL:HG21	1:A:465:ILE:HG12	2.03	0.41
1:B:230:ALA:HB1	1:B:329:PHE:CG	2.56	0.41
1:A:404:GLN:O	1:A:408:MET:HG3	2.21	0.41
1:A:67:ILE:HB	1:A:87:MET:HE1	2.03	0.41
1:A:93:TRP:CD1	1:A:94:TRP:CE3	3.09	0.41
1:B:45:ARG:HD3	1:B:75:TYR:CB	2.51	0.41
1:A:148:ASP:HB3	1:A:150:ASN:OD1	2.21	0.41
1:A:161:PHE:C	1:A:161:PHE:CD2	2.95	0.41
1:B:419:GLN:NE2	1:B:419:GLN:HA	2.37	0.40
1:A:404:GLN:HG3	1:A:418:SER:OG	2.20	0.40
1:B:131:GLU:HA	1:B:134:ARG:HG3	2.04	0.40
1:B:181:PRO:HD3	1:B:327:PHE:CE2	2.56	0.40
1:B:376:ILE:O	1:B:380:LEU:HG	2.22	0.40
1:B:171:GLY:HA2	1:B:178:THR:O	2.21	0.40
1:B:40:LYS:HB2	1:B:41:PRO:HD2	2.02	0.40
1:B:454:ILE:HG12	1:B:460:ARG:CZ	2.52	0.40
1:A:66:ARG:HG3	1:B:73:GLY:HA3	2.03	0.40
1:A:172:ILE:HB	3:E:12:DG:N2	2.36	0.40
1:B:453:ASP:HB3	1:B:460:ARG:NH1	2.36	0.40
1:B:321:THR:OG1	1:B:322:GLN:N	2.54	0.40
2:C:475:GLU:OE2	2:C:475:GLU:HA	2.22	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	483/499 (97%)	442 (92%)	33 (7%)	8 (2%)	9	36
1	B	463/499 (93%)	416 (90%)	35 (8%)	12 (3%)	5	28
2	C	194/269 (72%)	168 (87%)	21 (11%)	5 (3%)	5	28
2	D	188/269 (70%)	158 (84%)	23 (12%)	7 (4%)	3	22
All	All	1328/1536 (86%)	1184 (89%)	112 (8%)	32 (2%)	6	30

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	29	ALA
1	B	286	ILE
2	D	408	GLU
1	A	30	ARG
1	A	295	ARG
2	C	407	LEU
2	C	415	LYS
2	C	447	ARG
1	B	30	ARG
1	B	283	ILE
1	B	285	GLY
1	B	331	MET
2	D	447	ARG
1	A	106	ASN
1	A	170	THR
1	B	280	GLU
2	D	416	LEU
2	D	467	MET
1	A	296	GLU
1	B	321	THR
2	D	424	PRO
2	D	605	ARG
1	A	159	ALA
2	C	416	LEU
2	C	424	PRO
1	B	162	PRO
1	B	170	THR
2	D	404	LYS
1	A	162	PRO
1	A	283	ILE

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Mol	Chain	Res	Type
1	B	171	GLY
1	B	28	VAL

### 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	302/433 (70%)	293 (97%)	9 (3%)	41	69
1	B	272/433 (63%)	264 (97%)	8 (3%)	42	70
2	C	88/226 (39%)	88 (100%)	0	100	100
2	D	83/226 (37%)	81 (98%)	2 (2%)	49	74
All	All	745/1318 (56%)	726 (97%)	19 (3%)	46	72

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LEU
1	A	99	MET
1	A	119	ARG
1	A	148	ASP
1	A	164	LEU
1	A	185	LEU
1	A	244	THR
1	A	271	HIS
1	A	381	LEU
1	B	11	LEU
1	B	53	LEU
1	B	66	ARG
1	B	93	TRP
1	B	185	LEU
1	B	228	HIS
1	B	381	LEU
1	B	416	ARG
2	D	447	ARG
2	D	449	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	404	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
6	LFX	F	102	5	21,29,29	1.07	2 (9%)	25,44,44	1.32	4 (16%)
6	LFX	H	101	5	21,29,29	1.08	2 (9%)	25,44,44	1.36	4 (16%)

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
6	LFX	F	102	5	-	0/4/27/27	0/3/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	LFX	H	101	5	-	0/4/27/27	0/3/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	101	LFX	C17-C	3.86	1.51	1.47
6	F	102	LFX	C17-C	3.73	1.51	1.47
6	H	101	LFX	O02-C15	2.34	1.27	1.23
6	F	102	LFX	O02-C15	2.30	1.27	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
6	H	101	LFX	C02-N01-C01	3.36	118.94	111.52
6	F	102	LFX	C02-N01-C01	3.33	118.87	111.52
6	F	102	LFX	C12-C17-C15	-2.70	118.61	119.97
6	H	101	LFX	C12-C17-C15	-2.56	118.68	119.97
6	H	101	LFX	C15-C10-C05	2.22	121.66	119.98
6	F	102	LFX	C15-C10-C05	2.22	121.65	119.98
6	H	101	LFX	C14-C03-C09	-2.10	106.06	112.50
6	F	102	LFX	C14-C03-C09	-2.04	106.25	112.50

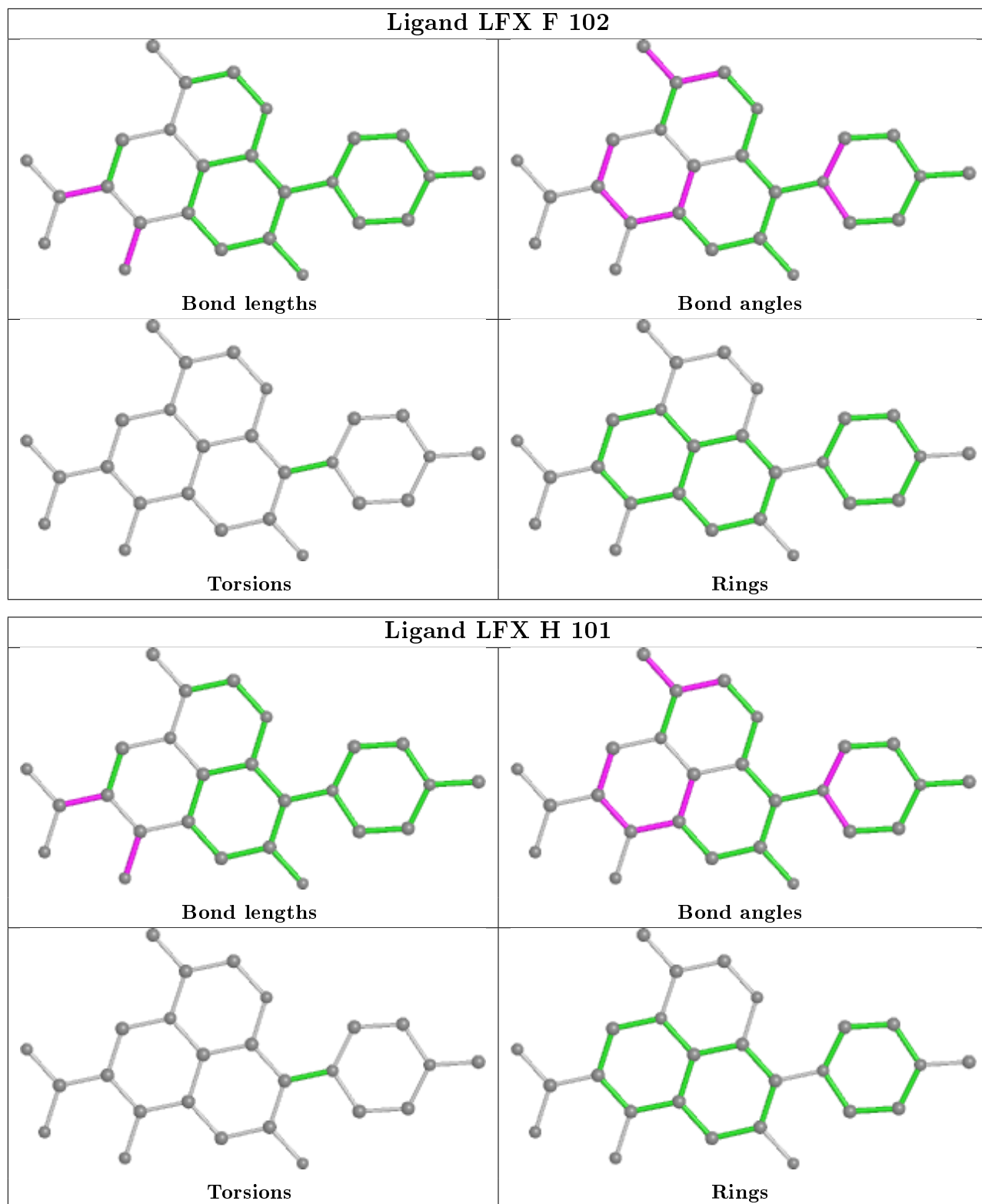
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	485/499 (97%)	-0.54	0 <a href="#">100</a> <a href="#">100</a>	64, 93, 126, 156	0
1	B	471/499 (94%)	-0.39	5 (1%) <a href="#">80</a> <a href="#">84</a>	69, 102, 149, 191	0
2	C	198/269 (73%)	-0.35	2 (1%) <a href="#">82</a> <a href="#">86</a>	85, 115, 151, 170	0
2	D	194/269 (72%)	-0.20	0 <a href="#">100</a> <a href="#">100</a>	83, 123, 160, 226	0
3	E	7/15 (46%)	0.11	0 <a href="#">100</a> <a href="#">100</a>	99, 104, 151, 167	0
3	G	7/15 (46%)	0.13	0 <a href="#">100</a> <a href="#">100</a>	100, 102, 158, 190	0
4	F	11/19 (57%)	0.57	2 (18%) <a href="#">1</a> <a href="#">1</a>	103, 121, 160, 174	0
4	H	11/19 (57%)	0.68	2 (18%) <a href="#">1</a> <a href="#">1</a>	101, 119, 146, 171	0
All	All	1384/1604 (86%)	-0.39	11 (0%) <a href="#">86</a> <a href="#">89</a>	64, 105, 150, 226	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	288	ALA	3.3
4	F	4	DC	2.8
4	H	4	DC	2.5
1	B	163	ASN	2.3
1	B	257	VAL	2.3
2	C	485	THR	2.2
1	B	285	GLY	2.2
4	H	1	DG	2.2
2	C	431	ILE	2.2
4	F	3	DT	2.0
1	B	256	ILE	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](#)

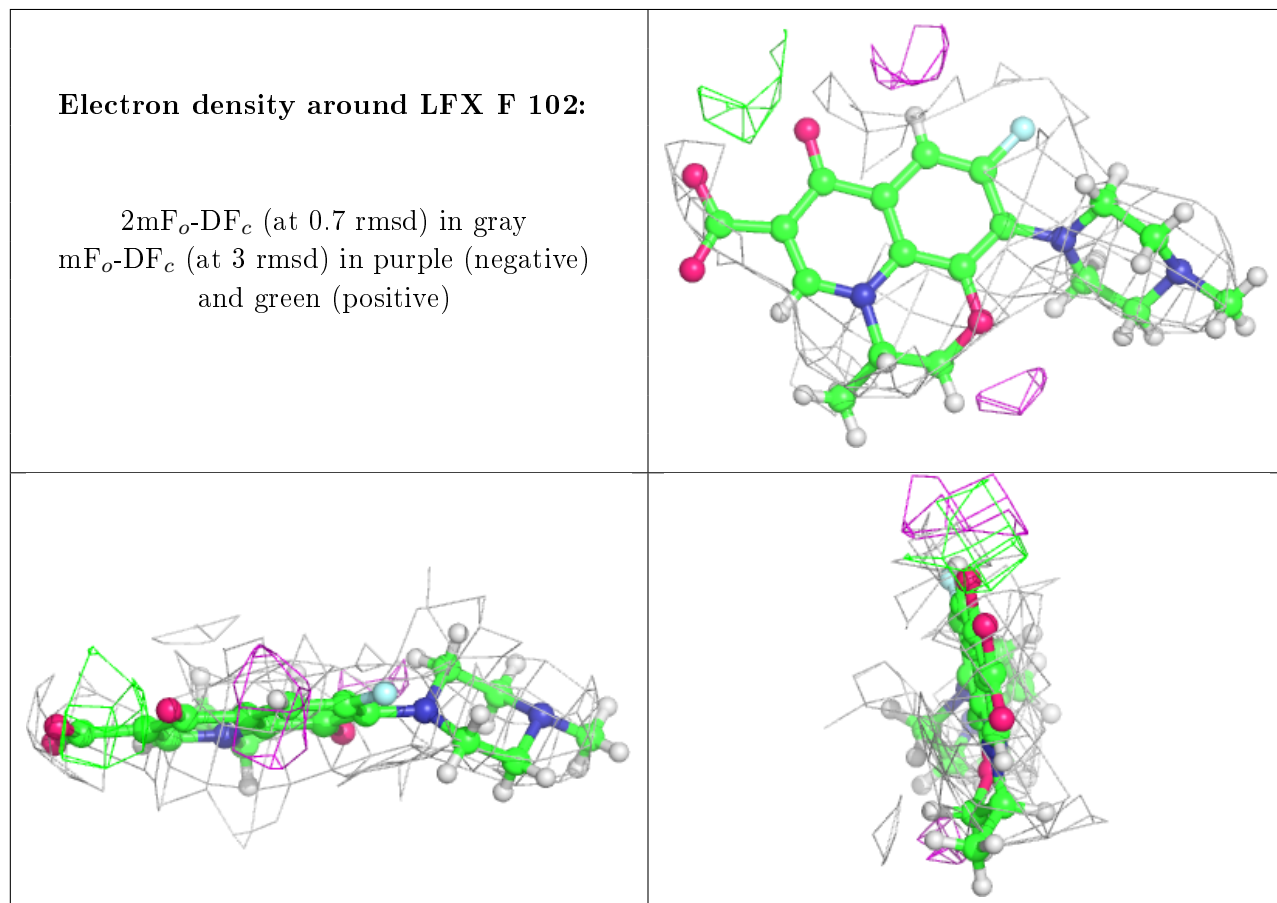
There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

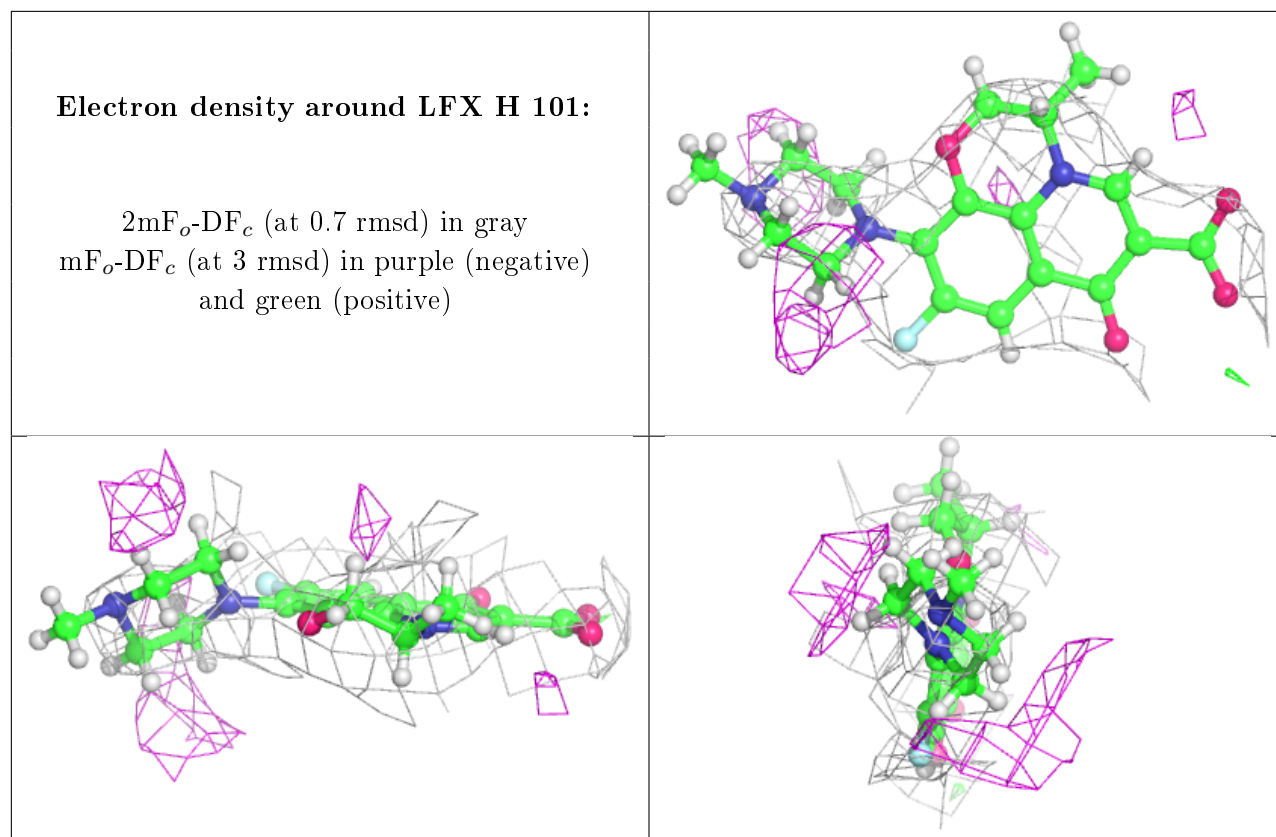
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	MG	F	101	1/1	0.72	0.55	228,228,228,228	0
5	MG	E	101	1/1	0.73	0.29	143,143,143,143	0
6	LFX	F	102	26/26	0.83	0.29	225,236,284,285	0
6	LFX	H	101	26/26	0.86	0.40	140,164,189,204	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.







## 6.5 Other polymers [i](#)

There are no such residues in this entry.