Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2023 – 11:59 am GMT

PDB ID	:	2XKK
Title	:	CRYSTAL STRUCTURE OF MOXIFLOXACIN, DNA, and A. BAUMANNII TOPO IV (PARE-PARC FUSION TRUNCATE)
Authors	:	Wohlkonig, A.; Chan, P.F.; Fosberry, A.P.; Homes, P.; Huang, J.; Kranz, M.; Leydon, V.R.; Miles, T.J.; Pearson, N.D.; Perera, R.L.; Shillings, A.J.; Gwynn, M.N.; Bax, B.D.
Deposited on	:	2010-07-08
Resolution	:	3.25 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 (1)) were used in the production of this report:

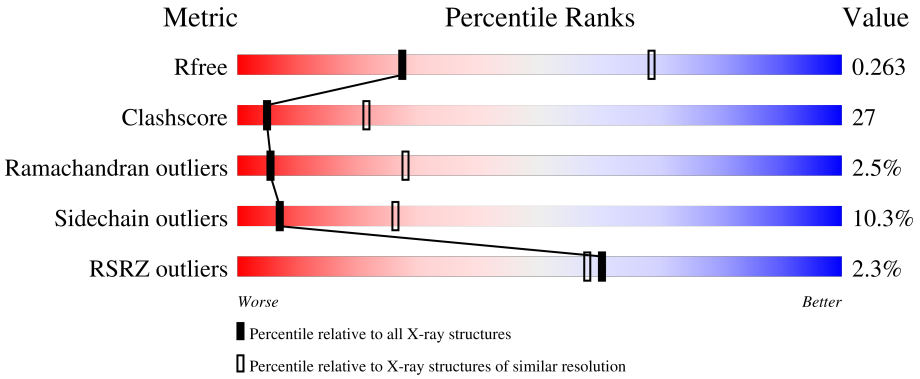
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	767	3% 46% 40% 5% 10%
1	C	767	% 47% 40% 6% 7%
2	E	34	. 38% 35% 24%
3	F	34	3% . 41% 32% 24%

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	MFX	E	1100	-	-	X	-
5	MFX	F	1100	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11873 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 TOPOISOMERASE IV.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	692	Total	C	N	O	P	S	0	1	0
			5249	3313	905	1011	1	19			
1	C	711	Total	C	N	O	P	S	0	1	0
			5464	3441	951	1051	1	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	346	MET	-	expression tag	UNP B0V9T6
C	346	MET	-	expression tag	UNP B0V9T6

- Molecule 2 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	26	Total	C	N	O	P	0	0	0
			534	256	104	149	25			

- Molecule 3 is a DNA chain called DNA.

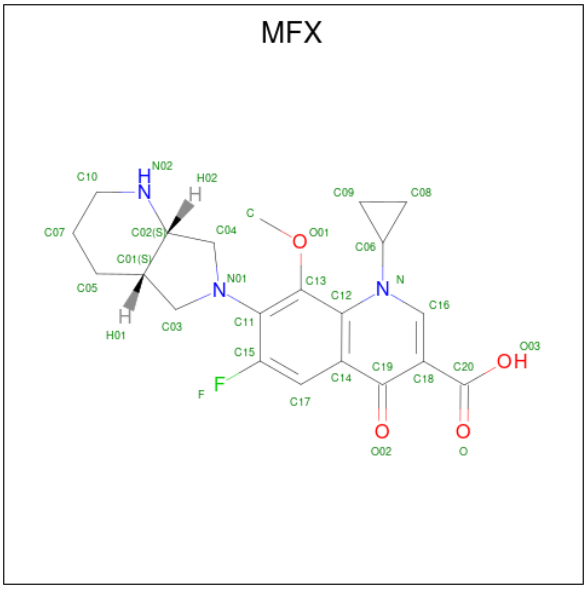
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	26	Total	C	N	O	P	0	0	0
			524	254	88	157	25			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		

- Molecule 5 is 1-cyclopropyl-6-fluoro-8-methoxy-7-[(4aS,7aS)-octahydro-6H-pyrrolo[3,4-b]pyr

idin-6-yl]-4-oxo-1,4-dihydroquinoline-3-carboxylic acid (three-letter code: MFX) (formula: $C_{21}H_{24}FN_3O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	E	1	Total	C	F	N	O	0	0
			29	21	1	3	4		
5	F	1	Total	C	F	N	O	0	0
			29	21	1	3	4		

- Molecule 6 is water.

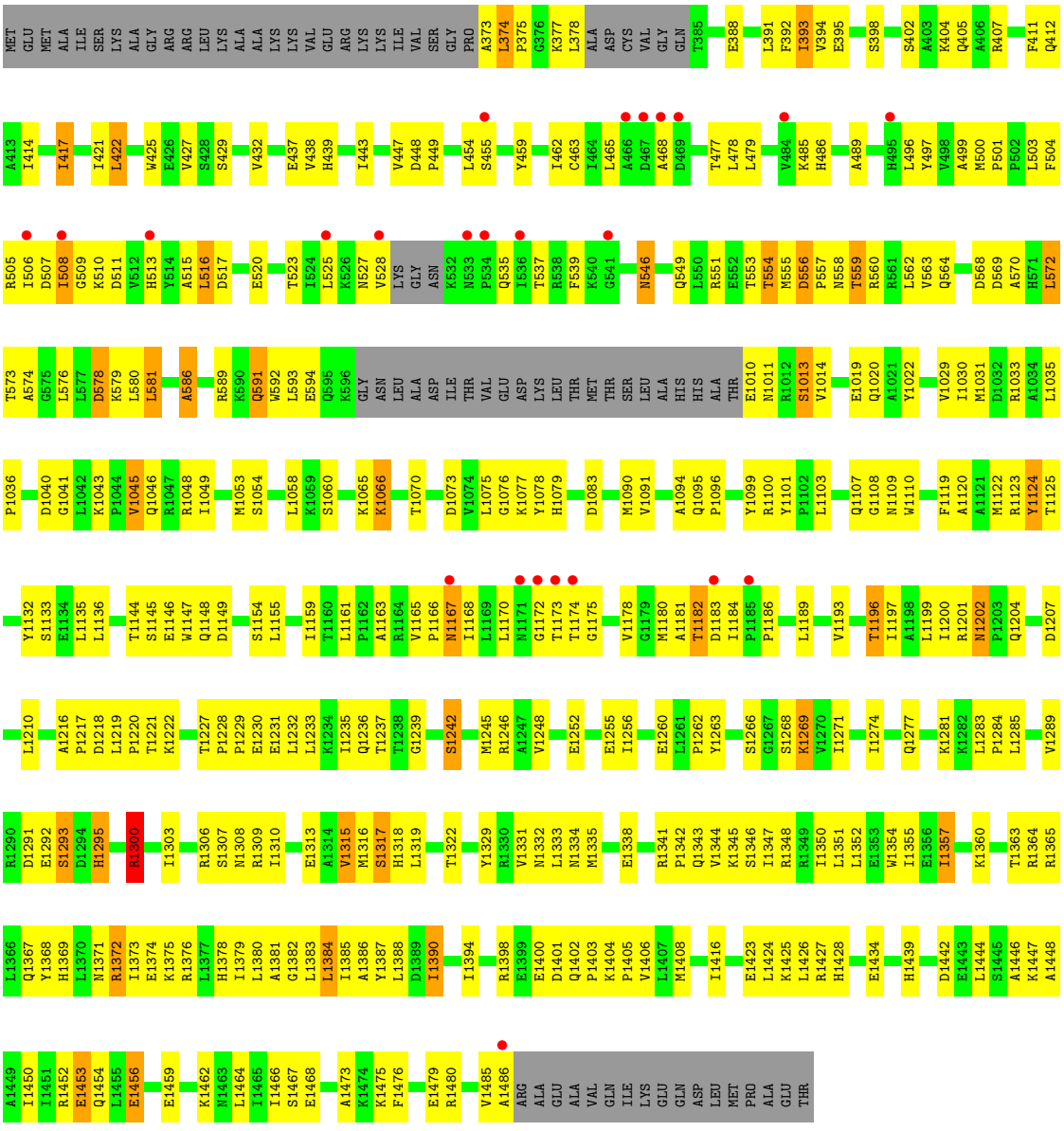
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	11	Total	O	0	0
			11	11		
6	C	20	Total	O	0	0
			20	20		
6	E	4	Total	O	0	0
			4	4		
6	F	5	Total	O	0	0
			5	5		

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.

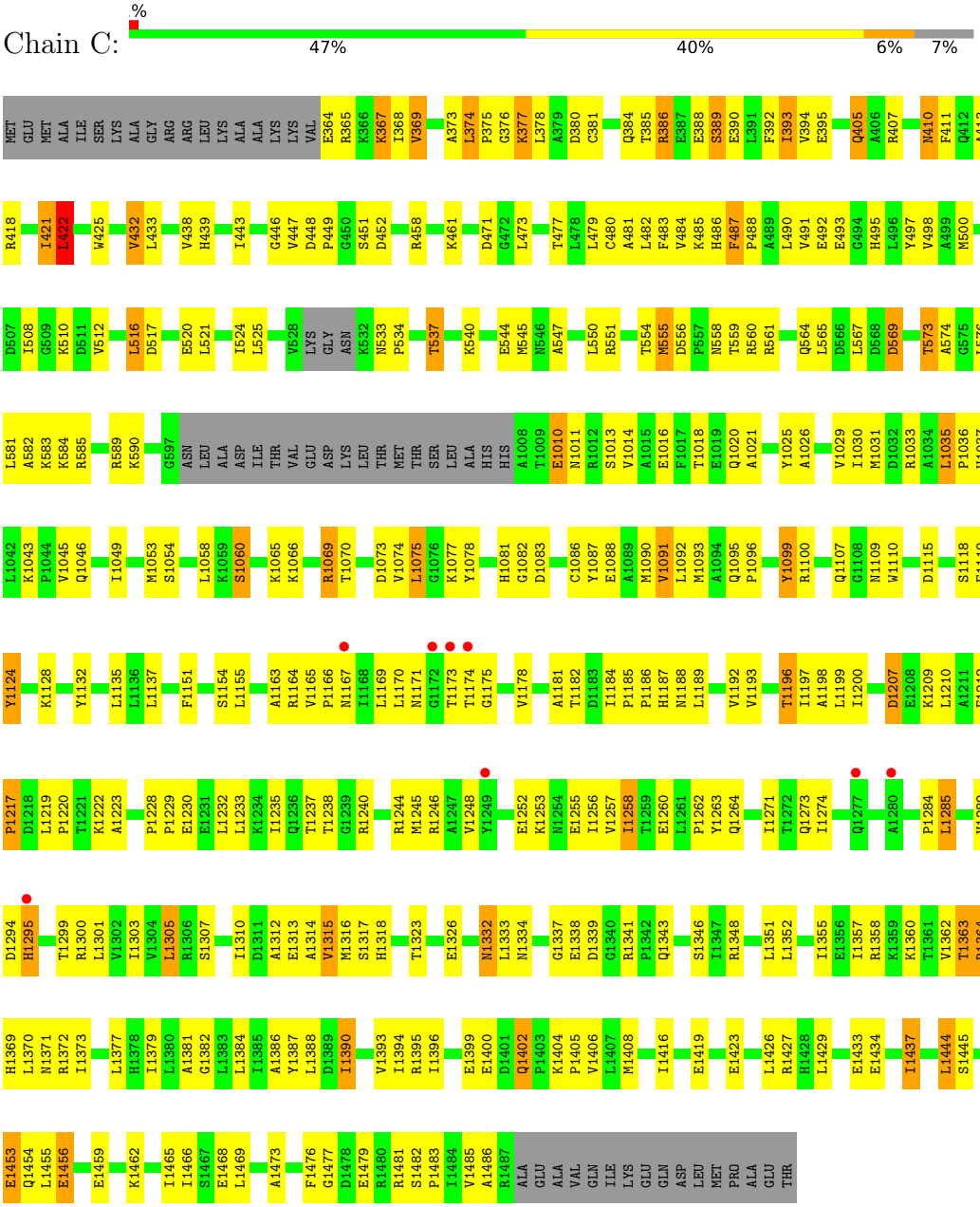
- Molecule 1: TOPOISOMERASE IV

Chain A:



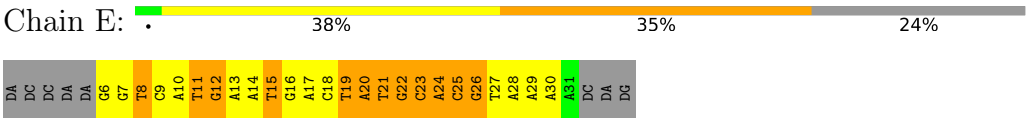
• Molecule 1: TOPOISOMERASE IV

Chain C:



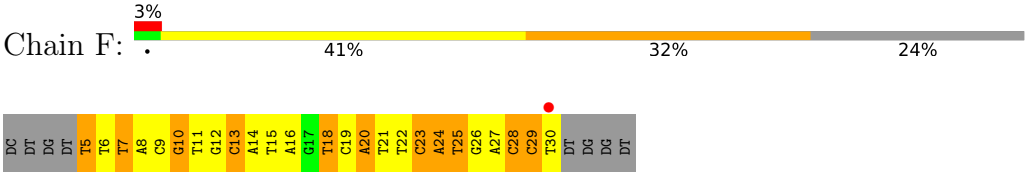
• Molecule 2: DNA

Chain E:



• Molecule 3: DNA

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	199.78Å 95.57Å 118.09Å 90.00° 108.27° 90.00°	Depositor
Resolution (Å)	36.17 – 3.25 36.17 – 3.26	Depositor EDS
% Data completeness (in resolution range)	96.8 (36.17-3.25) 96.9 (36.17-3.26)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.86 (at 3.25Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.194 , 0.270 0.188 , 0.263	Depositor DCC
R_{free} test set	1317 reflections (4.08%)	wwPDB-VP
Wilson B-factor (Å^2)	109.1	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 87.0	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	0.95	EDS
Total number of atoms	11873	wwPDB-VP
Average B, all atoms (Å^2)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.41	0/5320	0.61	0/7231
1	C	0.43	0/5537	0.64	1/7514 (0.0%)
2	E	0.93	0/600	1.92	21/923 (2.3%)
3	F	0.85	0/584	1.77	19/897 (2.1%)
All	All	0.49	0/12041	0.85	41/16565 (0.2%)

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	23	DC	O4'-C4'-C3'	-16.48	96.11	106.00
2	E	12	DG	O4'-C4'-C3'	-13.03	98.18	106.00
2	E	21	DT	C1'-O4'-C4'	-11.64	98.46	110.10
2	E	25	DC	O4'-C1'-N1	8.82	114.17	108.00
3	F	21	DT	O4'-C1'-N1	8.31	113.82	108.00
2	E	21	DT	O4'-C4'-C3'	-8.10	101.14	106.00
2	E	11	DT	P-O3'-C3'	7.96	129.25	119.70
2	E	22	DG	O4'-C1'-N9	-7.88	102.48	108.00
3	F	10	DG	O4'-C4'-C3'	-7.84	101.30	106.00
3	F	29	DC	O4'-C1'-N1	7.65	113.35	108.00
2	E	12	DG	C4'-C3'-C2'	-7.19	96.63	103.10
3	F	23	DC	C1'-O4'-C4'	-6.90	103.20	110.10
3	F	28	DC	O4'-C4'-C3'	-6.87	101.75	104.50
3	F	24	DA	O4'-C4'-C3'	-6.59	101.86	104.50
3	F	15	DT	N3-C4-O4	6.59	123.85	119.90
3	F	21	DT	C3'-C2'-C1'	-6.53	94.67	102.50
3	F	18	DT	P-O3'-C3'	6.48	127.47	119.70
2	E	26	DG	O4'-C1'-N9	6.44	112.51	108.00
3	F	10	DG	O4'-C1'-N9	-6.41	103.51	108.00
3	F	25	DT	O4'-C1'-N1	6.18	112.33	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	7	DT	O4'-C1'-N1	6.17	112.32	108.00
2	E	23	DC	C1'-O4'-C4'	-5.93	104.17	110.10
3	F	21	DT	C5-C4-O4	-5.89	120.77	124.90
3	F	21	DT	N3-C4-O4	5.85	123.41	119.90
2	E	24	DA	P-O3'-C3'	5.81	126.67	119.70
3	F	13	DC	C3'-C2'-C1'	-5.67	95.69	102.50
2	E	20	DA	C3'-C2'-C1'	-5.67	95.70	102.50
2	E	24	DA	O4'-C1'-N9	-5.65	104.04	108.00
2	E	11	DT	N3-C4-O4	5.63	123.28	119.90
2	E	11	DT	C5-C4-O4	-5.62	120.96	124.90
2	E	15	DT	C5-C4-O4	-5.59	120.99	124.90
3	F	20	DA	O4'-C1'-N9	5.47	111.83	108.00
2	E	21	DT	O4'-C1'-N1	5.36	111.75	108.00
2	E	8	DT	N3-C4-O4	5.27	123.06	119.90
2	E	8	DT	C5-C4-O4	-5.23	121.24	124.90
1	C	422	LEU	CA-CB-CG	5.22	127.32	115.30
2	E	21	DT	C4'-C3'-C2'	-5.16	98.46	103.10
3	F	25	DT	C5-C4-O4	-5.07	121.35	124.90
3	F	15	DT	C5-C4-O4	-5.06	121.36	124.90
2	E	19	DT	O4'-C1'-N1	5.04	111.53	108.00
3	F	5	DT	N3-C4-O4	5.01	122.91	119.90

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	5249	0	5092	274	0
1	C	5464	0	5392	279	0
2	E	534	0	292	49	0
3	F	524	0	296	33	0
4	A	2	0	0	0	0
4	C	2	0	0	0	0
5	E	29	0	23	12	0
5	F	29	0	23	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	11	0	0	0	0
6	C	20	0	0	0	0
6	E	4	0	0	1	0
6	F	5	0	0	0	0
All	All	11873	0	11118	629	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (629) 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)
5:F:1100:MFX:HB	5:F:1100:MFX:C03	1.81	1.11
1:A:1300:ARG:HG3	1:A:1300:ARG:HH11	1.15	1.07
1:A:1256:ILE:HD13	1:A:1316:MET:HG2	1.31	1.06
1:C:386:ARG:HG2	1:C:386:ARG:HH21	1.12	1.05
5:F:1100:MFX:C03	5:F:1100:MFX:C	2.35	1.03
1:A:497:TYR:HB3	1:A:562:LEU:HD11	1.37	1.03
5:F:1100:MFX:C	5:F:1100:MFX:H03A	1.89	1.02
5:F:1100:MFX:HB	5:F:1100:MFX:H03A	1.38	1.00
5:E:1100:MFX:H06	5:E:1100:MFX:HA	1.40	1.00
1:A:508:ILE:HD13	1:A:528:VAL:HG11	1.44	0.99
1:C:1036:PRO:HG3	1:C:1173:THR:HG21	1.43	0.97
1:A:1036:PRO:HG2	1:A:1173:THR:HG21	1.50	0.93
5:E:1100:MFX:H06	5:E:1100:MFX:C	1.98	0.93
1:A:447:VAL:HG12	1:A:448:ASP:H	1.32	0.93
2:E:18:DC:H2'	2:E:19:DT:C6	2.05	0.91
1:C:1395:ARG:HG2	1:C:1399:GLU:HG3	1.53	0.90
1:C:1216:ALA:HB2	1:C:1232:LEU:HD13	1.52	0.90
3:F:20:DA:O4'	5:F:1100:MFX:H02	1.71	0.89
1:A:569:ASP:OD1	1:A:572:LEU:HB3	1.74	0.87
3:F:25:DT:H2"	3:F:26:DG:C8	2.10	0.87
1:C:1360:LYS:O	1:C:1364:ARG:HG2	1.74	0.86
1:A:392:PHE:HB2	1:A:414:ILE:HD13	1.57	0.86
1:C:373:ALA:O	1:C:374:LEU:HB2	1.74	0.86
5:F:1100:MFX:O01	5:F:1100:MFX:H03	1.77	0.85
5:F:1100:MFX:HB	5:F:1100:MFX:N01	1.89	0.84
1:C:1075:LEU:HD11	1:C:1083:ASP:HB3	1.55	0.84
5:E:1100:MFX:HB	5:E:1100:MFX:H01	1.56	0.84
1:C:1196:THR:HG23	1:C:1351:LEU:HD13	1.57	0.84
1:C:1274:ILE:HG21	1:C:1289:VAL:HG21	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ARG:HD2	1:A:412:GLN:O	1.78	0.83
1:A:1210:LEU:HD13	1:A:1348:ARG:HB2	1.60	0.83
1:A:1123[B]:ARG:HH12	3:F:16:DA:H2'	1.41	0.83
1:A:1295:HIS:CD2	1:A:1295:HIS:H	1.95	0.83
1:C:374:LEU:HD11	1:C:458:ARG:HH12	1.42	0.83
1:A:1300:ARG:HG3	1:A:1300:ARG:NH1	1.87	0.82
1:C:386:ARG:HH21	1:C:386:ARG:CG	1.93	0.81
1:C:386:ARG:HG2	1:C:386:ARG:NH2	1.92	0.81
5:E:1100:MFX:C	5:E:1100:MFX:H01	2.11	0.80
1:C:555:MET:O	1:C:560:ARG:HD3	1.82	0.79
1:C:393:ILE:O	1:C:393:ILE:HG22	1.82	0.79
1:C:1362:VAL:HG21	1:C:1465:ILE:HG12	1.64	0.78
1:C:1256:ILE:HD13	1:C:1316:MET:HG2	1.65	0.78
1:A:1207:ASP:OD1	1:A:1348:ARG:HD2	1.83	0.77
1:C:1037:HIS:O	1:C:1041:GLY:HA2	1.85	0.77
5:F:1100:MFX:O01	5:F:1100:MFX:C09	2.34	0.76
1:C:1213:TYR:O	1:C:1215:PRO:HD3	1.86	0.76
1:C:1164:ARG:HG2	1:C:1358:ARG:NH2	2.00	0.76
1:A:447:VAL:HG12	1:A:448:ASP:N	2.00	0.76
1:C:1025:TYR:O	1:C:1029:VAL:HG13	1.85	0.75
1:A:1382:GLY:HA2	1:A:1385:ILE:HD12	1.68	0.75
1:A:1132:TYR:OH	1:A:1167:ASN:ND2	2.19	0.75
1:A:1196:THR:HG23	1:A:1351:LEU:HD13	1.67	0.75
1:C:413:ALA:O	1:C:414:ILE:HD13	1.87	0.75
5:F:1100:MFX:C03	5:F:1100:MFX:O01	2.34	0.74
1:A:1459:GLU:OE2	1:A:1462:LYS:HD2	1.89	0.73
1:A:1475:LYS:HG2	1:A:1476:PHE:CZ	2.23	0.73
2:E:28:DA:H2'	2:E:29:DA:C8	2.24	0.73
1:C:1193:VAL:HG21	1:C:1473:ALA:HB2	1.71	0.72
1:C:1040:ASP:O	1:C:1167:ASN:HB3	1.90	0.72
1:C:1416:ILE:HD12	1:C:1416:ILE:H	1.53	0.72
1:A:1363:THR:HG22	1:A:1367:GLN:HE21	1.53	0.71
1:C:1167:ASN:HD21	1:C:1171:ASN:HD22	1.37	0.71
1:A:1154:SER:O	1:A:1155:LEU:HD23	1.91	0.71
1:A:417:ILE:HD12	1:A:479:LEU:HD11	1.73	0.70
1:C:487:PHE:N	1:C:488:PRO:HD3	2.06	0.70
1:C:1070:THR:O	1:C:1074:VAL:HG23	1.91	0.70
1:A:1382:GLY:O	1:A:1385:ILE:HB	1.90	0.70
1:C:503:LEU:HD12	1:C:503:LEU:O	1.91	0.70
3:F:20:DA:C4	5:F:1100:MFX:H04A	2.27	0.70
1:A:1170:LEU:CD2	1:A:1189:LEU:HA	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1178:VAL:HA	2:E:24:DA:OP1	1.92	0.69
1:C:381:CYS:HB2	1:C:410:ASN:O	1.92	0.69
1:A:374:LEU:N	1:A:375:PRO:HD3	2.06	0.69
1:C:1200:ILE:HG13	1:C:1355:ILE:HD13	1.74	0.69
1:A:551:ARG:HA	1:A:555:MET:HB2	1.75	0.69
2:E:19:DT:O2	5:E:1100:MFX:H03	1.93	0.68
1:A:1075:LEU:HD11	1:A:1083:ASP:HB3	1.74	0.68
3:F:27:DA:H5'	3:F:27:DA:C8	2.28	0.68
1:A:1390:ILE:HD11	1:A:1394:ILE:HD11	1.76	0.68
1:C:1036:PRO:CG	1:C:1173:THR:HG21	2.22	0.68
1:A:1040:ASP:O	1:A:1167:ASN:HB3	1.94	0.67
3:F:30:DT:P	3:F:30:DT:H3'	2.35	0.67
1:A:407:ARG:HD3	1:A:414:ILE:HG12	1.75	0.67
1:A:422:LEU:HD11	1:A:427:VAL:HG21	1.77	0.67
1:A:1360:LYS:O	1:A:1364:ARG:HG2	1.94	0.67
1:C:1193:VAL:O	1:C:1197:ILE:HG13	1.94	0.67
1:C:1258:ILE:O	1:C:1300:ARG:HA	1.93	0.67
3:F:25:DT:H2"	3:F:26:DG:N7	2.10	0.67
3:F:30:DT:H3'	3:F:30:DT:OP2	1.95	0.66
1:A:422:LEU:HD23	1:A:438:VAL:HG21	1.77	0.66
1:A:373:ALA:C	1:A:375:PRO:HD3	2.16	0.66
2:E:11:DT:H2"	2:E:12:DG:H5"	1.78	0.66
1:C:517:ASP:OD1	1:C:520:GLU:HG3	1.96	0.66
1:C:417:ILE:HD12	1:C:479:LEU:HD11	1.78	0.66
1:A:1043:LYS:HG3	1:A:1046:GLN:OE1	1.96	0.66
1:A:1049:ILE:HD13	1:A:1090:MET:HB2	1.76	0.66
2:E:19:DT:O2	5:E:1100:MFX:C03	2.44	0.65
1:A:1448:ALA:O	1:A:1452:ARG:HG2	1.97	0.65
1:C:461:LYS:HB3	1:C:497:TYR:CD1	2.32	0.65
1:A:1400:GLU:HG3	1:A:1406:VAL:HG21	1.79	0.65
1:C:1193:VAL:HG13	1:C:1469:LEU:HB3	1.79	0.65
1:C:1014:VAL:O	1:C:1018:THR:HG23	1.96	0.65
1:A:447:VAL:CG1	1:A:448:ASP:H	2.09	0.65
1:C:1395:ARG:HG2	1:C:1399:GLU:CG	2.27	0.65
2:E:18:DC:H2'	2:E:19:DT:C5	2.32	0.65
1:C:439:HIS:NE2	1:C:443:ILE:HD11	2.11	0.64
1:C:580:LEU:HA	1:C:589:ARG:HD2	1.79	0.64
1:C:1135:LEU:HD21	1:C:1476:PHE:HE2	1.61	0.64
1:C:1273:GLN:HB3	1:C:1323:THR:HG22	1.77	0.64
1:C:1363:THR:HG22	1:C:1367:GLN:HE21	1.61	0.64
1:C:1433:GLU:O	1:C:1437:ILE:HG23	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1367:GLN:HG2	1:C:1455:LEU:HD21	1.79	0.64
1:C:1295:HIS:CD2	1:C:1295:HIS:H	2.14	0.64
1:A:1107:GLN:HA	1:A:1107:GLN:OE1	1.97	0.63
1:C:1199:LEU:HD23	1:C:1352:LEU:HD23	1.80	0.63
1:C:1216:ALA:HB1	1:C:1217:PRO:HD2	1.80	0.63
1:A:1284:PRO:HD2	1:A:1285:LEU:HG	1.81	0.63
1:C:374:LEU:HD11	1:C:458:ARG:NH1	2.14	0.63
1:C:385:THR:HG22	1:C:388:GLU:H	1.64	0.63
1:C:1077:LYS:HE2	1:C:1078:TYR:CE2	2.34	0.63
1:A:425:TRP:O	1:A:485:LYS:HE3	1.98	0.63
1:C:477:THR:HG23	1:C:1018:THR:HB	1.81	0.62
1:C:1189:LEU:HD23	1:C:1477:GLY:HA2	1.81	0.62
1:A:1313:GLU:O	1:A:1317:SER:HB2	1.99	0.62
1:A:425:TRP:HE1	1:A:578:ASP:HA	1.64	0.62
1:A:1292:GLU:HB3	1:A:1300:ARG:HD3	1.79	0.62
1:C:589:ARG:NH2	2:E:24:DA:OP2	2.32	0.62
1:C:1256:ILE:HD13	1:C:1316:MET:CG	2.29	0.62
5:F:1100:MFX:N01	5:F:1100:MFX:H10	2.12	0.62
1:C:1135:LEU:HD21	1:C:1476:PHE:CE2	2.34	0.62
1:C:558:ASN:O	1:C:559:THR:HG23	2.00	0.62
2:E:22:DG:H1	3:F:13:DC:H42	1.46	0.62
1:C:446:GLY:O	1:C:447:VAL:HG23	1.99	0.61
5:F:1100:MFX:C03	5:F:1100:MFX:H10	2.30	0.61
1:A:1315:VAL:O	1:A:1319:LEU:HG	2.01	0.61
1:A:504:PHE:HB2	1:A:515:ALA:HB3	1.83	0.61
1:C:1452:ARG:O	1:C:1456:GLU:HB2	2.01	0.61
1:C:484:VAL:CG2	1:C:1014:VAL:HG11	2.30	0.61
1:A:392:PHE:HB2	1:A:414:ILE:CD1	2.30	0.61
1:C:388:GLU:O	1:C:411:PHE:HB2	2.00	0.61
1:A:1295:HIS:HB3	1:C:551:ARG:NH1	2.16	0.61
1:A:1189:LEU:O	1:A:1193:VAL:HG23	2.00	0.61
1:C:1453:GLU:HG3	1:C:1454:GLN:N	2.15	0.60
1:C:389:SER:O	1:C:390:GLU:HG3	2.01	0.60
1:A:477:THR:HG21	1:A:1022:TYR:HD1	1.67	0.60
1:A:1231:GLU:O	1:A:1235:ILE:HG13	2.01	0.60
1:A:1233:LEU:O	1:A:1237:THR:HG23	2.02	0.60
1:A:1307:SER:C	1:A:1309:ARG:H	2.04	0.60
1:C:556:ASP:OD2	1:C:556:ASP:C	2.39	0.60
1:C:491:VAL:HG12	1:C:567:LEU:HB2	1.83	0.60
1:A:421:ILE:HD12	1:A:422:LEU:O	2.02	0.60
2:E:28:DA:H2"	2:E:29:DA:H5'	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:LEU:C	1:A:572:LEU:HD23	2.21	0.59
1:A:1110:TRP:CZ2	1:A:1125:THR:HB	2.37	0.59
1:A:1306:ARG:H	1:A:1310:ILE:HD12	1.67	0.59
1:C:1107:GLN:HA	1:C:1107:GLN:OE1	2.02	0.59
1:C:1390:ILE:O	1:C:1393:VAL:HB	2.01	0.59
1:A:1173:THR:H	1:A:1184:ILE:HB	1.67	0.59
1:C:392:PHE:HB2	1:C:414:ILE:HD12	1.83	0.59
1:C:1213:TYR:C	1:C:1215:PRO:HD3	2.22	0.59
1:C:1132:TYR:OH	1:C:1167:ASN:ND2	2.36	0.59
1:A:500:MET:HB3	1:A:516:LEU:HD11	1.85	0.59
1:A:1300:ARG:NH1	1:A:1300:ARG:CG	2.63	0.59
2:E:12:DG:H5'	2:E:12:DG:C8	2.37	0.59
1:C:1448:ALA:O	1:C:1452:ARG:HG2	2.02	0.59
1:C:490:LEU:HG	1:C:495:HIS:HB2	1.84	0.59
5:F:1100:MFX:C03	5:F:1100:MFX:C10	2.77	0.59
1:C:1036:PRO:HG3	1:C:1173:THR:CG2	2.27	0.59
1:C:373:ALA:O	1:C:374:LEU:CB	2.50	0.58
1:C:422:LEU:HD23	1:C:438:VAL:HG21	1.82	0.58
1:C:1049:ILE:HD13	1:C:1090:MET:HB2	1.84	0.58
1:A:1108:GLY:HA2	1:C:545:MET:O	2.03	0.58
1:C:1386:ALA:HB1	1:C:1393:VAL:HG21	1.84	0.58
1:A:1193:VAL:HG21	1:A:1473:ALA:HB2	1.85	0.57
1:A:1335:MET:HE1	1:A:1350:ILE:HD11	1.85	0.57
1:A:1446:ALA:O	1:A:1450:ILE:HG13	2.04	0.57
1:A:506:ILE:HD12	1:A:506:ILE:N	2.19	0.57
1:A:1292:GLU:O	1:A:1300:ARG:HB3	2.04	0.57
1:A:508:ILE:HG13	1:A:511:ASP:O	2.03	0.57
1:C:448:ASP:O	1:C:451:SER:HB3	2.05	0.57
3:F:8:DA:H2"	3:F:9:DC:OP2	2.04	0.57
1:A:1281:LYS:HE3	1:A:1284:PRO:HB3	1.87	0.57
1:A:374:LEU:N	1:A:375:PRO:CD	2.67	0.57
1:A:1485:VAL:HG23	1:A:1486:ALA:N	2.20	0.57
1:A:425:TRP:CZ3	1:A:485:LYS:HB2	2.40	0.56
1:A:1073:ASP:OD2	1:C:1069:ARG:NH2	2.33	0.56
1:A:1163:ALA:HB1	1:A:1165:VAL:O	2.04	0.56
1:A:586:ALA:HA	1:A:589:ARG:HD3	1.85	0.56
1:A:1202:ASN:OD1	1:A:1202:ASN:C	2.44	0.56
1:A:1398:ARG:HG3	1:C:1429:LEU:O	2.05	0.56
1:A:1453:GLU:HG3	1:A:1454:GLN:N	2.19	0.56
1:A:1333:LEU:O	1:A:1344:VAL:HA	2.05	0.56
3:F:20:DA:O4'	5:F:1100:MFX:C02	2.48	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:LYS:HD2	1:C:415:MET:HG3	1.87	0.56
1:C:505:ARG:O	1:C:537:THR:HG23	2.05	0.56
1:A:546:ASN:HD21	1:A:549:GLN:CD	2.09	0.56
1:A:1197:ILE:HG23	1:A:1466:ILE:HD12	1.88	0.56
1:A:1135:LEU:HD11	1:A:1476:PHE:CD2	2.41	0.56
1:A:1010:GLU:C	1:A:1011:ASN:HD22	2.08	0.55
1:C:1197:ILE:HA	1:C:1200:ILE:HD12	1.88	0.55
1:A:546:ASN:N	1:A:546:ASN:HD22	2.03	0.55
1:A:432:VAL:HG13	1:A:438:VAL:HG11	1.88	0.55
1:C:377:LYS:HD2	1:C:415:MET:CG	2.37	0.55
1:C:392:PHE:HB2	1:C:414:ILE:CD1	2.37	0.55
1:C:1369:HIS:O	1:C:1373:ILE:HG13	2.06	0.55
2:E:20:DA:H2'	2:E:20:DA:O5'	2.06	0.55
1:A:439:HIS:NE2	1:A:443:ILE:HD11	2.21	0.55
1:A:1292:GLU:CB	1:A:1300:ARG:HD3	2.37	0.55
5:F:1100:MFX:O01	5:F:1100:MFX:C06	2.54	0.55
1:A:1475:LYS:HG2	1:A:1476:PHE:CE2	2.41	0.55
1:A:560:ARG:O	1:A:560:ARG:HG3	2.06	0.55
1:A:1100:ARG:HB2	1:A:1186:PRO:HB3	1.89	0.55
2:E:20:DA:C4	5:E:1100:MFX:H04	2.41	0.54
1:A:1094:ALA:O	1:A:1096:PRO:HD3	2.06	0.54
1:C:1109:ASN:HB3	1:C:1120:ALA:HB2	1.88	0.54
1:C:1400:GLU:OE2	1:C:1400:GLU:HA	2.07	0.54
1:A:1216:ALA:HB2	1:A:1232:LEU:HD13	1.89	0.54
1:C:413:ALA:C	1:C:414:ILE:HD13	2.28	0.54
1:A:1200:ILE:HG13	1:A:1355:ILE:HD13	1.89	0.54
2:E:20:DA:C2	2:E:21:DT:C2	2.95	0.54
1:C:1284:PRO:HD2	1:C:1285:LEU:HG	1.90	0.54
2:E:29:DA:H2"	2:E:30:DA:O5'	2.08	0.54
5:E:1100:MFX:HB	5:E:1100:MFX:C01	2.32	0.54
1:C:488:PRO:O	1:C:492:GLU:HG3	2.08	0.54
1:A:1053:MET:HE3	1:A:1058:LEU:HD13	1.88	0.54
1:C:395:GLU:HG2	1:C:395:GLU:O	2.08	0.54
1:A:1045:VAL:HG23	1:A:1079:HIS:CE1	2.43	0.53
1:A:1384:LEU:HA	1:A:1387:TYR:HB2	1.88	0.53
1:A:1077:LYS:HE2	1:A:1078:TYR:CE2	2.43	0.53
1:C:1210:LEU:HD21	1:C:1214:ILE:HD12	1.90	0.53
2:E:8:DT:H3	3:F:27:DA:H2	1.55	0.53
1:A:425:TRP:NE1	1:A:578:ASP:HA	2.23	0.53
3:F:29:DC:H4'	3:F:30:DT:H5'	1.89	0.53
1:A:477:THR:HG21	1:A:1022:TYR:CD1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1199:LEU:HD23	1:A:1352:LEU:HD23	1.91	0.53
1:A:1343:GLN:HG2	1:A:1345:LYS:HG2	1.91	0.53
1:A:1374:GLU:O	1:A:1376:ARG:N	2.42	0.53
1:C:487:PHE:N	1:C:488:PRO:CD	2.71	0.53
1:C:1222:LYS:HA	1:C:1481:ARG:O	2.09	0.53
1:C:432:VAL:HG21	1:C:486:HIS:CE1	2.43	0.53
1:A:1148:GLN:C	1:A:1149:ASP:CA	2.77	0.53
1:C:1065:LYS:HZ3	1:C:1069:ARG:HH11	1.57	0.53
1:C:1167:ASN:HD21	1:C:1171:ASN:ND2	2.04	0.52
1:C:1334:ASN:HA	1:C:1343:GLN:O	2.10	0.52
1:A:398:SER:OG	1:C:1124:PTR:CE2	2.57	0.52
1:C:393:ILE:O	1:C:393:ILE:CG2	2.51	0.52
1:A:1479:GLU:CD	1:A:1479:GLU:H	2.12	0.52
2:E:24:DA:H1'	2:E:25:DC:H5'	1.90	0.52
1:A:454:LEU:HD11	1:A:489:ALA:HB1	1.91	0.52
1:A:1170:LEU:HD22	1:A:1189:LEU:HA	1.91	0.52
2:E:6:DG:H2"	2:E:7:DG:H8	1.75	0.52
1:A:1077:LYS:HG3	1:A:1078:TYR:CE2	2.45	0.52
1:C:380:ASP:HA	1:C:413:ALA:HB1	1.91	0.52
1:C:1077:LYS:HB2	1:C:1155:LEU:HD12	1.92	0.52
1:C:1402:GLN:O	1:C:1405:PRO:HD2	2.10	0.52
1:C:378:LEU:HD12	1:C:415:MET:HB2	1.92	0.51
1:C:1271:ILE:HD11	1:C:1291:ASP:HB2	1.92	0.51
1:A:1252:GLU:O	1:A:1255:GLU:HG3	2.11	0.51
1:A:1222:LYS:HB2	1:A:1260:GLU:OE1	2.11	0.51
1:C:1400:GLU:HG3	1:C:1406:VAL:HG21	1.93	0.51
1:C:1459:GLU:O	1:C:1459:GLU:HG3	2.11	0.51
1:A:1378:HIS:O	1:A:1381:ALA:HB3	2.10	0.51
1:C:1075:LEU:HD11	1:C:1083:ASP:CB	2.35	0.51
1:A:1076:GLY:HA3	1:C:1069:ARG:HD3	1.92	0.51
1:A:1416:ILE:HD12	1:A:1416:ILE:H	1.76	0.51
1:C:1123[A]:ARG:HH22	2:E:15:DT:P	2.33	0.51
1:C:1219:LEU:HD12	1:C:1263:TYR:CD1	2.46	0.51
1:C:1358:ARG:O	1:C:1362:VAL:HG23	2.09	0.51
2:E:6:DG:H2"	2:E:7:DG:C8	2.46	0.51
1:A:1022:TYR:OH	3:F:23:DC:H5"	2.10	0.51
1:C:1011:ASN:N	1:C:1011:ASN:HD22	2.09	0.51
1:C:1087:TYR:O	1:C:1090:MET:HB3	2.10	0.51
1:C:471:ASP:OD2	1:C:1033:ARG:NH2	2.40	0.51
1:C:1363:THR:O	1:C:1365:ARG:N	2.44	0.51
1:A:1381:ALA:O	1:A:1384:LEU:HD23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1363:THR:CG2	1:C:1367:GLN:HE21	2.24	0.50
1:A:393:ILE:O	1:A:393:ILE:HG22	2.10	0.50
1:C:1246:ARG:HG3	1:C:1326:GLU:HG3	1.93	0.50
1:C:473:LEU:HD23	1:C:1021:ALA:HA	1.94	0.50
1:C:1379:ILE:HD11	1:C:1416:ILE:HG22	1.92	0.50
1:C:390:GLU:OE2	1:C:461:LYS:HE2	2.11	0.50
1:A:421:ILE:HD11	1:A:478:LEU:O	2.12	0.50
1:C:374:LEU:CD1	1:C:458:ARG:HH12	2.19	0.50
1:C:1370:LEU:O	1:C:1372:ARG:N	2.45	0.50
3:F:26:DG:OP2	3:F:26:DG:H8	1.93	0.50
1:A:1145:SER:O	1:A:1147:TRP:HD1	1.95	0.49
1:C:1010:GLU:C	1:C:1011:ASN:HD22	2.14	0.49
1:C:1216:ALA:CB	1:C:1232:LEU:HD13	2.35	0.49
1:C:500:MET:HB3	1:C:516:LEU:HD11	1.94	0.49
1:C:582:ALA:HB3	1:C:585:ARG:HG3	1.94	0.49
1:A:576:LEU:HD21	1:A:1019:GLU:HB2	1.94	0.49
1:A:1306:ARG:CB	1:A:1310:ILE:HD11	2.42	0.49
1:C:1135:LEU:HD11	1:C:1476:PHE:CD2	2.47	0.49
1:A:1145:SER:O	1:A:1147:TRP:CD1	2.65	0.49
1:C:1164:ARG:HG2	1:C:1358:ARG:HH22	1.75	0.49
1:A:459:TYR:HB2	1:A:462:ILE:HD11	1.95	0.49
1:A:579:LYS:O	1:A:589:ARG:HD2	2.12	0.49
1:C:374:LEU:HD22	1:C:375:PRO:HD3	1.93	0.49
1:A:1178:VAL:HG22	3:F:23:DC:H4'	1.94	0.49
1:C:540:LYS:HD3	1:C:1151:PHE:CD2	2.46	0.49
1:C:1233:LEU:O	1:C:1237:THR:HG23	2.12	0.49
2:E:13:DA:C4	2:E:14:DA:C8	3.01	0.49
2:E:15:DT:H3	3:F:20:DA:H61	1.61	0.49
3:F:23:DC:H2"	3:F:24:DA:O5'	2.12	0.49
1:A:1274:ILE:CD1	1:A:1303:ILE:HD11	2.42	0.49
1:C:386:ARG:HH21	1:C:386:ARG:H	1.59	0.49
1:C:540:LYS:N	1:C:544:GLU:OE1	2.43	0.49
1:C:576:LEU:O	1:C:579:LYS:HB3	2.12	0.49
1:C:1207:ASP:OD1	1:C:1348:ARG:HD2	2.13	0.49
1:C:1073:ASP:O	1:C:1077:LYS:HG2	2.12	0.49
1:C:1174:THR:HG23	1:C:1174:THR:O	2.13	0.49
2:E:28:DA:H2"	2:E:29:DA:C5'	2.42	0.49
5:E:1100:MFX:C	5:E:1100:MFX:C01	2.88	0.49
1:C:1248:VAL:HB	1:C:1260:GLU:HB2	1.93	0.49
1:A:551:ARG:HA	1:A:555:MET:HG3	1.95	0.48
1:C:1404:LYS:O	1:C:1408:MET:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:LEU:HB3	1:A:581:LEU:HD23	1.95	0.48
1:A:1197:ILE:O	1:A:1201:ARG:HG3	2.14	0.48
1:C:380:ASP:HA	1:C:413:ALA:CB	2.44	0.48
1:C:1332:ASN:O	1:C:1334:ASN:N	2.37	0.48
1:C:1451:ILE:O	1:C:1455:LEU:HD12	2.14	0.48
1:A:546:ASN:ND2	1:A:549:GLN:HB2	2.28	0.48
1:A:1235:ILE:HD11	1:A:1242:SER:O	2.13	0.48
1:C:1100:ARG:HB2	1:C:1186:PRO:HB3	1.94	0.48
1:C:1209:LYS:O	1:C:1212:GLU:HB2	2.14	0.48
2:E:8:DT:O4	3:F:27:DA:N1	2.47	0.48
1:A:1452:ARG:O	1:A:1456:GLU:HB2	2.13	0.48
1:C:480:CYS:O	1:C:484:VAL:HG23	2.13	0.48
1:C:581:LEU:N	1:C:581:LEU:HD23	2.28	0.48
1:C:368:ILE:HG23	1:C:369:VAL:H	1.78	0.48
1:C:1255:GLU:HA	1:C:1303:ILE:O	2.14	0.48
1:C:1462:LYS:O	1:C:1466:ILE:HG12	2.13	0.48
1:A:553:THR:OG1	1:A:554:THR:HG23	2.14	0.48
1:C:1307:SER:O	1:C:1310:ILE:HG13	2.14	0.48
1:C:417:ILE:CD1	1:C:479:LEU:HD11	2.44	0.48
1:A:425:TRP:HE1	1:A:578:ASP:CA	2.25	0.48
1:C:422:LEU:HA	2:E:21:DT:O3'	2.14	0.48
1:A:549:GLN:O	1:A:553:THR:HG23	2.14	0.47
1:A:1174:THR:HG23	1:A:1183:ASP:OD1	2.14	0.47
1:A:1380:LEU:O	1:A:1384:LEU:HD22	2.13	0.47
1:C:1053:MET:HG2	1:C:1070:THR:HG23	1.95	0.47
1:C:1184:ILE:HA	1:C:1185:PRO:HD3	1.74	0.47
1:A:478:LEU:HD11	3:F:22:DT:H4'	1.96	0.47
1:C:1429:LEU:N	1:C:1429:LEU:HD23	2.29	0.47
1:A:1204:GLN:HE21	1:A:1204:GLN:HA	1.79	0.47
3:F:5:DT:H2"	3:F:6:DT:C6	2.50	0.47
1:C:1040:ASP:HA	1:C:1163:ALA:HB2	1.95	0.47
1:A:417:ILE:CD1	1:A:479:LEU:HD11	2.43	0.47
1:A:557:PRO:HA	1:A:560:ARG:HG2	1.96	0.47
1:A:1030:ILE:O	1:A:1035:LEU:HB2	2.14	0.47
1:A:505:ARG:HB2	1:A:539:PHE:CE2	2.49	0.47
1:A:1077:LYS:HB2	1:A:1155:LEU:HD12	1.96	0.47
1:A:1200:ILE:HB	1:A:1466:ILE:HD11	1.97	0.47
1:C:582:ALA:O	1:C:584:LYS:N	2.48	0.47
1:C:1256:ILE:CD1	1:C:1316:MET:HG2	2.42	0.47
1:C:1363:THR:O	1:C:1364:ARG:C	2.53	0.47
2:E:13:DA:H2"	2:E:14:DA:O5'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:27:DT:H2'	2:E:28:DA:C8	2.50	0.47
3:F:9:DC:H5"	3:F:9:DC:H6	1.78	0.47
1:A:557:PRO:HA	1:A:560:ARG:CD	2.45	0.47
1:C:1210:LEU:C	1:C:1210:LEU:HD23	2.34	0.47
1:C:1351:LEU:O	1:C:1355:ILE:HG13	2.14	0.47
2:E:23:DC:H2"	2:E:24:DA:H5'	1.95	0.47
1:A:562:LEU:HD12	1:A:563:VAL:N	2.30	0.47
1:C:1228:PRO:HA	1:C:1229:PRO:HD2	1.76	0.47
1:A:391:LEU:HD23	1:A:462:ILE:HG23	1.97	0.47
1:A:1236:GLN:HG2	1:A:1347:ILE:HG13	1.96	0.47
1:C:1124:PTR:HE2	1:C:1124:PTR:O1P	2.14	0.47
2:E:7:DG:H8	2:E:7:DG:OP2	1.98	0.47
1:A:402:SER:O	1:A:405:GLN:HB3	2.15	0.46
1:A:429:SER:HB3	1:A:449:PRO:HB2	1.96	0.46
1:A:581:LEU:HD23	1:A:581:LEU:N	2.30	0.46
1:A:1053:MET:HG2	1:A:1070:THR:HG23	1.97	0.46
1:A:1363:THR:O	1:A:1364:ARG:C	2.52	0.46
1:C:1026:ALA:O	1:C:1030:ILE:HG13	2.14	0.46
1:C:1054:SER:HB2	1:C:1137:LEU:HD11	1.98	0.46
1:C:1054:SER:HB2	1:C:1137:LEU:CD1	2.46	0.46
1:C:1175:GLY:O	1:C:1181:ALA:HB1	2.15	0.46
1:A:525:LEU:HD12	1:A:525:LEU:O	2.16	0.46
1:A:1013:SER:O	1:A:1014:VAL:C	2.54	0.46
1:A:1170:LEU:CD2	1:A:1189:LEU:HD12	2.46	0.46
1:A:391:LEU:HB2	1:A:459:TYR:CD1	2.51	0.46
1:A:523:THR:O	1:A:527:ASN:OD1	2.34	0.46
1:A:1424:LEU:HD12	1:A:1428:HIS:HD2	1.79	0.46
1:A:1073:ASP:O	1:A:1077:LYS:HG2	2.16	0.46
1:C:493:GLU:HB2	1:C:495:HIS:HD2	1.79	0.46
1:A:394:VAL:HG12	1:A:465:LEU:HD23	1.97	0.46
1:A:1189:LEU:HD23	1:A:1473:ALA:HA	1.97	0.46
1:A:1354:TRP:O	1:A:1357:ILE:N	2.46	0.46
1:C:1314:ALA:O	1:C:1315:VAL:C	2.53	0.46
1:A:1227:THR:HG23	1:A:1228:PRO:HD2	1.98	0.46
1:A:1245:MET:HE2	1:A:1262:PRO:HA	1.97	0.46
2:E:13:DA:C5	2:E:14:DA:N7	2.83	0.46
1:C:1220:PRO:HD2	1:C:1263:TYR:CD2	2.50	0.46
1:A:558:ASN:O	1:A:559:THR:HG23	2.16	0.46
1:A:1283:LEU:HD21	1:A:1318:HIS:CD2	2.50	0.46
1:A:1346:SER:OG	1:A:1347:ILE:N	2.48	0.46
1:A:1439:HIS:O	1:A:1442:ASP:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:471:ASP:CG	1:C:1033:ARG:HH22	2.17	0.46
2:E:15:DT:H3	3:F:20:DA:N6	2.14	0.46
1:A:404:LYS:HA	1:A:414:ILE:HG13	1.98	0.46
1:A:1108:GLY:O	1:A:1110:TRP:HD1	1.98	0.46
1:A:1136:LEU:O	1:A:1161:LEU:HB3	2.15	0.46
3:F:27:DA:H2"	3:F:28:DC:OP2	2.16	0.46
1:C:432:VAL:CG2	1:C:486:HIS:CE1	2.99	0.46
1:C:1030:ILE:HG23	1:C:1035:LEU:HD22	1.97	0.46
2:E:15:DT:H5"	6:E:2001:HOH:O	2.15	0.46
1:A:392:PHE:CE1	1:A:555:MET:HE2	2.51	0.45
1:A:1175:GLY:O	1:A:1181:ALA:HB1	2.16	0.45
1:C:425:TRP:CZ3	1:C:485:LYS:HB2	2.51	0.45
1:A:1221:THR:OG1	1:A:1222:LYS:N	2.50	0.45
1:A:1363:THR:CG2	1:A:1367:GLN:HE21	2.25	0.45
1:C:1223:ALA:HB1	1:C:1246:ARG:O	2.16	0.45
1:A:1091:VAL:O	1:A:1095:GLN:HG3	2.16	0.45
2:E:20:DA:C4	2:E:21:DT:C6	3.04	0.45
5:F:1100:MFX:F	5:F:1100:MFX:C04	2.54	0.45
1:A:463:CYS:HA	1:A:497:TYR:O	2.16	0.45
1:A:497:TYR:CE2	1:A:564:GLN:HG3	2.52	0.45
1:A:517:ASP:OD1	1:A:520:GLU:HG3	2.16	0.45
1:C:481:ALA:O	1:C:482:LEU:C	2.54	0.45
1:C:580:LEU:C	1:C:581:LEU:HD23	2.37	0.45
2:E:22:DG:H1	3:F:13:DC:N4	2.11	0.45
1:A:1048:ARG:HD3	1:A:1079:HIS:HB2	1.99	0.45
1:A:1398:ARG:CZ	1:C:1390:ILE:HG21	2.46	0.45
1:A:1100:ARG:HG3	1:A:1101:TYR:CE2	2.52	0.45
1:A:1103:LEU:N	1:A:1103:LEU:HD23	2.27	0.45
1:A:1219:LEU:N	1:A:1219:LEU:HD22	2.32	0.45
1:A:1274:ILE:HD11	1:A:1303:ILE:HD11	1.98	0.45
1:C:1038:ILE:CG2	1:C:1337:GLY:HA2	2.47	0.45
1:C:1045:VAL:O	1:C:1049:ILE:HG13	2.17	0.45
1:A:1220:PRO:HD2	1:A:1263:TYR:CD2	2.52	0.45
1:A:1277:GLN:HE22	1:A:1322:THR:HB	1.81	0.45
1:C:1031:MET:HE3	1:C:1031:MET:HA	1.98	0.45
1:A:1447:LYS:HA	1:A:1450:ILE:HD12	1.99	0.45
1:C:506:ILE:H	1:C:506:ILE:HD12	1.82	0.45
1:C:1043:LYS:HG3	1:C:1046:GLN:OE1	2.16	0.45
1:C:1077:LYS:HE2	1:C:1078:TYR:HE2	1.78	0.45
1:C:1093:MET:HA	1:C:1099:TYR:CD1	2.52	0.45
1:C:1305:LEU:HD11	1:C:1312:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1293:SER:OG	1:C:1299:THR:HA	2.18	0.44
1:C:1170:LEU:CD2	1:C:1189:LEU:HA	2.47	0.44
1:C:1232:LEU:HD23	1:C:1235:ILE:HD12	1.98	0.44
1:C:1238:THR:C	1:C:1240:ARG:H	2.20	0.44
1:A:508:ILE:O	1:A:510:LYS:N	2.50	0.44
1:C:1170:LEU:HD22	1:C:1189:LEU:HA	2.00	0.44
1:C:1189:LEU:CD2	1:C:1477:GLY:HA2	2.47	0.44
1:C:1240:ARG:NH2	2:E:26:DG:OP1	2.51	0.44
1:C:1377:LEU:HD23	1:C:1377:LEU:HA	1.84	0.44
1:A:1239:GLY:O	1:A:1331:VAL:HG12	2.18	0.44
1:A:1307:SER:C	1:A:1309:ARG:N	2.71	0.44
1:A:1408:MET:HE3	1:A:1408:MET:HB2	1.84	0.44
1:A:1123[A]:ARG:HG3	1:A:1124:PTR:CD2	2.47	0.44
1:C:1167:ASN:HA	1:C:1170:LEU:HD12	1.99	0.44
1:C:1365:ARG:NH2	1:C:1468:GLU:OE2	2.50	0.44
1:C:1390:ILE:HD11	1:C:1429:LEU:HD13	1.98	0.44
1:A:508:ILE:HD11	1:A:513:HIS:CD2	2.53	0.44
1:A:1424:LEU:HD12	1:A:1428:HIS:CD2	2.52	0.44
3:F:9:DC:H2'	3:F:10:DG:C8	2.53	0.44
1:A:564:GLN:HB3	1:A:1011:ASN:ND2	2.32	0.44
1:C:405:GLN:HG2	1:C:547:ALA:HB2	1.98	0.44
1:C:1060:SER:O	1:C:1128:LYS:HE3	2.18	0.44
1:C:1165:VAL:HB	1:C:1166:PRO:CD	2.47	0.44
1:A:1394:ILE:HD13	1:C:1394:ILE:HD13	2.00	0.44
1:C:1091:VAL:HG12	1:C:1092:LEU:N	2.33	0.44
1:A:551:ARG:HA	1:A:555:MET:CB	2.45	0.44
1:A:1073:ASP:CG	1:C:1069:ARG:HH21	2.20	0.44
1:C:392:PHE:CG	1:C:555:MET:HE1	2.53	0.44
1:C:1210:LEU:HD23	1:C:1210:LEU:O	2.18	0.44
3:F:18:DT:H2"	3:F:19:DC:C6	2.52	0.44
1:A:374:LEU:CD1	1:A:378:LEU:HD22	2.48	0.43
1:A:1146:GLU:HB3	1:A:1159:ILE:HD12	1.99	0.43
1:A:1216:ALA:HB1	1:A:1217:PRO:HD2	1.98	0.43
1:C:1245:MET:HE2	1:C:1262:PRO:HA	1.98	0.43
2:E:22:DG:N2	3:F:14:DA:C4	2.86	0.43
3:F:26:DG:H2"	3:F:27:DA:C8	2.53	0.43
1:A:1274:ILE:HG21	1:A:1289:VAL:HG21	2.00	0.43
1:A:546:ASN:HD21	1:A:549:GLN:CG	2.31	0.43
1:A:1383:LEU:O	1:A:1386:ALA:N	2.50	0.43
1:C:1095:GLN:HA	1:C:1096:PRO:HD3	1.82	0.43
1:A:454:LEU:CD1	1:A:489:ALA:HB1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1334:ASN:O	1:A:1335:MET:HB3	2.19	0.43
1:C:1263:TYR:O	1:C:1264:GLN:HB2	2.18	0.43
1:A:546:ASN:HD21	1:A:549:GLN:HB2	1.84	0.43
1:A:546:ASN:N	1:A:546:ASN:ND2	2.67	0.43
1:A:1030:ILE:HG23	1:A:1035:LEU:HD22	2.01	0.43
1:C:377:LYS:HD2	1:C:415:MET:SD	2.58	0.43
1:C:1115:ASP:CG	1:C:1118:SER:HB3	2.39	0.43
1:C:1373:ILE:HG23	1:C:1444:LEU:HD13	1.99	0.43
2:E:23:DC:H4'	2:E:24:DA:OP1	2.19	0.43
1:A:1048:ARG:CD	1:A:1079:HIS:HB2	2.49	0.43
1:A:1248:VAL:HB	1:A:1260:GLU:HB2	2.00	0.43
1:A:1398:ARG:NH2	1:C:1390:ILE:HG21	2.34	0.43
1:C:1154:SER:O	1:C:1155:LEU:HD23	2.19	0.43
1:C:1427:ARG:HB2	1:C:1427:ARG:NH1	2.34	0.43
1:A:496:LEU:HD12	1:A:496:LEU:HA	1.86	0.43
1:A:1065:LYS:O	1:A:1066:LYS:C	2.56	0.43
1:C:1167:ASN:ND2	1:C:1171:ASN:HD22	2.11	0.43
1:A:1292:GLU:O	1:A:1300:ARG:O	2.37	0.43
1:A:1464:LEU:O	1:A:1468:GLU:HG3	2.18	0.43
1:C:484:VAL:HG22	1:C:1014:VAL:HG11	1.99	0.43
1:A:1268:SER:O	1:A:1269:LYS:C	2.57	0.43
1:A:1426:LEU:HD23	1:A:1426:LEU:HA	1.78	0.43
1:C:1293:SER:O	1:C:1294:ASP:HB3	2.19	0.43
1:C:1482:SER:HA	1:C:1483:PRO:HD3	1.83	0.43
1:A:1277:GLN:O	1:A:1281:LYS:N	2.52	0.43
1:C:1396:ILE:HD13	1:C:1406:VAL:HG12	2.01	0.43
2:E:18:DC:C2'	2:E:19:DT:C6	2.90	0.43
2:E:24:DA:C1'	2:E:25:DC:H5'	2.49	0.43
1:A:377:LYS:HE3	1:A:437:GLU:OE1	2.19	0.42
1:A:468:ALA:HB1	1:A:503:LEU:HD13	2.00	0.42
1:A:1363:THR:O	1:A:1365:ARG:N	2.52	0.42
1:C:479:LEU:HD23	1:C:479:LEU:HA	1.84	0.42
1:C:520:GLU:O	1:C:524:ILE:HG13	2.19	0.42
2:E:24:DA:H2"	2:E:25:DC:H2'	2.01	0.42
1:A:1189:LEU:CD2	1:A:1473:ALA:HA	2.49	0.42
1:C:452:ASP:O	1:C:452:ASP:CG	2.58	0.42
1:C:564:GLN:HB3	1:C:1011:ASN:ND2	2.34	0.42
2:E:9:DC:H2"	2:E:10:DA:H5'	2.00	0.42
1:A:1165:VAL:HB	1:A:1166:PRO:CD	2.49	0.42
1:C:483:PHE:O	1:C:484:VAL:C	2.56	0.42
1:A:1204:GLN:HA	1:A:1204:GLN:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1245:MET:HB2	1:A:1329:TYR:HE1	1.85	0.42
1:A:1341:ARG:HA	1:A:1342:PRO:HD3	1.84	0.42
1:A:1372:ARG:HE	1:A:1372:ARG:HB2	1.36	0.42
1:A:1170:LEU:HD21	1:A:1189:LEU:HA	2.01	0.42
1:C:498:VAL:CG2	1:C:565:LEU:HD11	2.48	0.42
1:C:1035:LEU:CD1	1:C:1035:LEU:N	2.83	0.42
1:C:1252:GLU:HB3	1:C:1253:LYS:NZ	2.35	0.42
1:C:1387:TYR:CE1	1:C:1434:GLU:HB2	2.54	0.42
3:F:6:DT:H2'	3:F:7:DT:H71	2.01	0.42
1:A:1045:VAL:HG23	1:A:1079:HIS:NE2	2.35	0.42
1:A:1109:ASN:HB3	1:A:1120:ALA:HB2	2.01	0.42
3:F:6:DT:C5	3:F:7:DT:H73	2.55	0.42
1:A:388:GLU:O	1:A:411:PHE:HD2	2.03	0.42
1:A:425:TRP:CE3	1:A:485:LYS:HB2	2.54	0.42
1:A:1365:ARG:O	1:A:1368:TYR:HB3	2.20	0.42
1:C:510:LYS:HA	1:C:510:LYS:HD3	1.68	0.42
1:C:1485:VAL:CG1	1:C:1486:ALA:N	2.82	0.42
2:E:16:DG:N2	2:E:17:DA:C2	2.88	0.42
1:A:1031:MET:HE2	1:A:1031:MET:HB3	1.91	0.42
1:C:422:LEU:CD2	1:C:438:VAL:HG21	2.48	0.42
1:C:1091:VAL:HA	1:C:1110:TRP:HZ3	1.85	0.42
1:A:1053:MET:HG2	1:A:1070:THR:CG2	2.49	0.42
1:A:1065:LYS:O	1:A:1066:LYS:O	2.38	0.42
1:A:1427:ARG:NH2	1:C:1419:GLU:OE1	2.52	0.42
1:C:506:ILE:HD12	1:C:506:ILE:N	2.34	0.42
1:C:1088:GLU:HG2	1:C:1119:PHE:CZ	2.55	0.42
2:E:16:DG:C2	5:F:1100:MFX:HA	2.54	0.42
1:A:395:GLU:O	1:A:395:GLU:HG2	2.20	0.42
1:A:591:GLN:O	1:A:594:GLU:N	2.52	0.42
1:A:1439:HIS:O	1:A:1442:ASP:N	2.52	0.42
1:C:1065:LYS:HZ2	1:C:1069:ARG:HE	1.67	0.42
1:C:1169:LEU:O	1:C:1187:HIS:ND1	2.50	0.42
1:C:1313:GLU:OE2	1:C:1313:GLU:HA	2.20	0.42
1:C:1373:ILE:HG23	1:C:1444:LEU:HB3	2.02	0.42
1:C:1405:PRO:HA	1:C:1408:MET:CE	2.49	0.42
5:E:1100:MFX:H06	5:E:1100:MFX:O01	2.14	0.42
1:A:1219:LEU:HA	1:A:1219:LEU:HD13	1.79	0.41
1:A:1231:GLU:O	1:A:1231:GLU:HG3	2.20	0.41
1:A:1401:ASP:O	1:A:1403:PRO:HD3	2.20	0.41
1:C:407:ARG:HD3	1:C:414:ILE:HG12	2.02	0.41
1:C:1109:ASN:OD1	1:C:1109:ASN:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:13:DA:H2'	2:E:14:DA:H8	1.84	0.41
1:A:589:ARG:O	1:A:593:LEU:HG	2.19	0.41
1:C:415:MET:HA	1:C:416:PRO:HD3	1.90	0.41
1:C:569:ASP:O	1:C:569:ASP:CG	2.58	0.41
1:C:1291:ASP:OD1	1:C:1291:ASP:C	2.59	0.41
1:C:448:ASP:HA	1:C:449:PRO:HD3	1.93	0.41
1:C:461:LYS:HB3	1:C:497:TYR:CE1	2.54	0.41
1:C:589:ARG:O	1:C:590:LYS:C	2.56	0.41
1:C:1199:LEU:HD23	1:C:1352:LEU:CD2	2.48	0.41
1:C:1315:VAL:O	1:C:1318:HIS:HB3	2.19	0.41
1:A:499:ALA:O	1:A:501:PRO:HD3	2.20	0.41
1:C:1196:THR:O	1:C:1197:ILE:C	2.56	0.41
1:A:556:ASP:HA	1:A:557:PRO:HD3	1.80	0.41
1:A:1229:PRO:O	1:A:1230:GLU:C	2.59	0.41
1:A:1291:ASP:O	1:A:1291:ASP:OD1	2.38	0.41
1:C:376:GLY:C	1:C:378:LEU:N	2.73	0.41
1:C:1188:ASN:O	1:C:1192:VAL:HG23	2.20	0.41
2:E:24:DA:C2'	2:E:25:DC:H5'	2.51	0.41
1:A:551:ARG:HA	1:A:555:MET:CG	2.50	0.41
1:A:1199:LEU:HD11	1:A:1210:LEU:HD12	2.02	0.41
1:A:1387:TYR:CD1	1:A:1434:GLU:HG3	2.55	0.41
1:C:573:THR:HG22	1:C:574:ALA:N	2.35	0.41
2:E:18:DC:H2"	2:E:19:DT:H5'	2.03	0.41
1:A:1182:THR:HB	1:A:1334:ASN:HB3	2.02	0.41
1:A:1218:ASP:OD2	1:A:1480:ARG:HA	2.21	0.41
1:A:1300:ARG:O	1:A:1300:ARG:HG2	2.21	0.41
1:C:367:LYS:H	1:C:367:LYS:HG3	1.72	0.41
1:C:1040:ASP:OD1	1:C:1041:GLY:N	2.54	0.41
1:C:1077:LYS:HG3	1:C:1078:TYR:CE2	2.55	0.41
2:E:13:DA:C4	2:E:14:DA:N7	2.89	0.41
1:A:1119:PHE:CD2	1:A:1119:PHE:C	2.94	0.41
1:A:1374:GLU:C	1:A:1376:ARG:N	2.75	0.41
1:A:1402:GLN:HA	1:A:1403:PRO:HD3	1.80	0.41
1:C:386:ARG:HG2	1:C:386:ARG:H	1.55	0.41
1:C:417:ILE:CD1	1:C:479:LEU:HD21	2.51	0.41
1:C:421:ILE:CD1	1:C:479:LEU:HD23	2.51	0.41
1:C:1169:LEU:HD23	1:C:1169:LEU:HA	1.70	0.41
1:C:1285:LEU:HG	1:C:1285:LEU:H	1.59	0.41
2:E:20:DA:C4	5:E:1100:MFX:C04	3.03	0.41
3:F:11:DT:H2"	3:F:12:DG:H5'	2.01	0.41
1:A:1041:GLY:HA2	1:A:1168:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1404:LYS:N	1:A:1405:PRO:CD	2.84	0.41
5:E:1100:MFX:H16	5:E:1100:MFX:H08	1.66	0.41
1:A:429:SER:HA	1:A:486:HIS:CE1	2.56	0.40
1:A:586:ALA:O	1:A:589:ARG:HB2	2.21	0.40
1:A:1390:ILE:CD1	1:A:1394:ILE:HD11	2.48	0.40
1:A:1450:ILE:O	1:A:1454:GLN:HG3	2.21	0.40
1:C:533:ASN:HA	1:C:534:PRO:HD3	1.85	0.40
1:C:1182:THR:HG23	1:C:1182:THR:O	2.21	0.40
1:C:1271:ILE:O	1:C:1274:ILE:HB	2.21	0.40
1:A:1030:ILE:HD13	1:A:1180:MET:CE	2.51	0.40
1:A:1369:HIS:O	1:A:1373:ILE:HG13	2.22	0.40
1:C:1093:MET:HB2	1:C:1093:MET:HE3	1.85	0.40
2:E:20:DA:C6	2:E:21:DT:C4	3.08	0.40
1:A:1172:GLY:HA3	1:A:1184:ILE:O	2.21	0.40
1:A:1379:ILE:HD11	1:A:1416:ILE:HG22	2.03	0.40
1:C:1479:GLU:OE2	1:C:1479:GLU:N	2.41	0.40
1:A:507:ASP:HB2	1:A:535:GLN:HG3	2.02	0.40
1:A:570:ALA:O	1:A:574:ALA:N	2.54	0.40
1:C:505:ARG:HG3	1:C:512:VAL:CG1	2.52	0.40
1:C:1058:LEU:HD21	1:C:1065:LYS:HB3	2.02	0.40
1:C:1081:HIS:HB3	1:C:1082:GLY:H	1.76	0.40
1:C:1245:MET:CE	1:C:1263:TYR:H	2.35	0.40
1:C:1462:LYS:O	1:C:1466:ILE:CG1	2.70	0.40
1:A:1268:SER:O	1:A:1271:ILE:N	2.55	0.40
1:C:485:LYS:CG	1:C:486:HIS:CD2	3.05	0.40
3:F:19:DC:H2"	3:F:20:DA:H5'	2.02	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	682/767 (89%)	564 (83%)	103 (15%)	15 (2%)	6 31
1	C	705/767 (92%)	615 (87%)	70 (10%)	20 (3%)	5 25
All	All	1387/1534 (90%)	1179 (85%)	173 (12%)	35 (2%)	5 28

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	LEU
1	C	508	ILE
1	A	509	GLY
1	A	1066	LYS
1	C	374	LEU
1	C	410	ASN
1	C	583	LYS
1	C	1333	LEU
1	C	1363	THR
1	C	1364	ARG
1	C	1371	ASN
1	C	1381	ALA
1	A	573	THR
1	A	1371	ASN
1	A	1375	LYS
1	C	573	THR
1	C	1039	SER
1	C	1198	ALA
1	C	1217	PRO
1	C	1388	LEU
1	A	586	ALA
1	A	592	TRP
1	A	1293	SER
1	C	1066	LYS
1	C	1305	LEU
1	A	568	ASP
1	A	591	GLN
1	A	1033	ARG
1	A	1308	ASN
1	A	1388	LEU
1	C	367	LYS
1	A	1300	ARG
1	C	1382	GLY
1	C	487	PHE
1	C	1315	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	537/656 (82%)	488 (91%)	49 (9%)	9 31
1	C	572/656 (87%)	507 (89%)	65 (11%)	5 22
All	All	1109/1312 (84%)	995 (90%)	114 (10%)	7 26

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	393	ILE
1	A	417	ILE
1	A	422	LEU
1	A	455	SER
1	A	508	ILE
1	A	516	LEU
1	A	537	THR
1	A	546	ASN
1	A	554	THR
1	A	556	ASP
1	A	559	THR
1	A	572	LEU
1	A	578	ASP
1	A	581	LEU
1	A	1013	SER
1	A	1020	GLN
1	A	1029	VAL
1	A	1045	VAL
1	A	1054	SER
1	A	1060	SER
1	A	1099	TYR
1	A	1122	MET
1	A	1133	SER
1	A	1144	THR
1	A	1167	ASN
1	A	1182	THR
1	A	1196	THR

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Mol	Chain	Res	Type
1	A	1202	ASN
1	A	1242	SER
1	A	1246	ARG
1	A	1266	SER
1	A	1269	LYS
1	A	1293	SER
1	A	1295	HIS
1	A	1300	ARG
1	A	1315	VAL
1	A	1317	SER
1	A	1332	ASN
1	A	1338	GLU
1	A	1357	ILE
1	A	1372	ARG
1	A	1384	LEU
1	A	1390	ILE
1	A	1423	GLU
1	A	1425	LYS
1	A	1444	LEU
1	A	1453	GLU
1	A	1456	GLU
1	A	1467	SER
1	C	364	GLU
1	C	365	ARG
1	C	369	VAL
1	C	377	LYS
1	C	384	GLN
1	C	386	ARG
1	C	389	SER
1	C	393	ILE
1	C	394	VAL
1	C	405	GLN
1	C	414	ILE
1	C	418	ARG
1	C	421	ILE
1	C	422	LEU
1	C	432	VAL
1	C	433	LEU
1	C	505	ARG
1	C	516	LEU
1	C	521	LEU
1	C	525	LEU

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Mol	Chain	Res	Type
1	C	537	THR
1	C	550	LEU
1	C	554	THR
1	C	555	MET
1	C	561	ARG
1	C	569	ASP
1	C	578	ASP
1	C	1010	GLU
1	C	1013	SER
1	C	1016	GLU
1	C	1020	GLN
1	C	1035	LEU
1	C	1060	SER
1	C	1069	ARG
1	C	1075	LEU
1	C	1086	CYS
1	C	1091	VAL
1	C	1099	TYR
1	C	1122	MET
1	C	1196	THR
1	C	1207	ASP
1	C	1230	GLU
1	C	1244	ARG
1	C	1257	VAL
1	C	1258	ILE
1	C	1285	LEU
1	C	1295	HIS
1	C	1301	LEU
1	C	1317	SER
1	C	1332	ASN
1	C	1338	GLU
1	C	1339	ASP
1	C	1341	ARG
1	C	1346	SER
1	C	1357	ILE
1	C	1384	LEU
1	C	1390	ILE
1	C	1402	GLN
1	C	1423	GLU
1	C	1426	LEU
1	C	1437	ILE
1	C	1444	LEU

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Mol	Chain	Res	Type
1	C	1445	SER
1	C	1453	GLU
1	C	1456	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	513	HIS
1	A	527	ASN
1	A	546	ASN
1	A	1011	ASN
1	A	1020	GLN
1	A	1167	ASN
1	A	1171	ASN
1	A	1204	GLN
1	A	1295	HIS
1	A	1332	ASN
1	A	1367	GLN
1	A	1428	HIS
1	C	486	HIS
1	C	495	HIS
1	C	1011	ASN
1	C	1020	GLN
1	C	1167	ASN
1	C	1204	GLN
1	C	1295	HIS
1	C	1332	ASN
1	C	1367	GLN
1	C	1428	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	PTR	C	1124	1,2	15,16,17	2.02	1 (6%)	19,22,24	0.76	1 (5%)
1	PTR	A	1124	1,3	15,16,17	1.89	1 (6%)	19,22,24	0.99	1 (5%)

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
1	PTR	C	1124	1,2	-	2/10/11/13	0/1/1/1
1	PTR	A	1124	1,3	-	1/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1124	PTR	OH-CZ	-7.61	1.23	1.40
1	A	1124	PTR	OH-CZ	-7.02	1.24	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1124	PTR	CB-CA-C	-3.27	105.33	111.47
1	C	1124	PTR	CB-CA-C	-2.11	107.51	111.47

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1124	PTR	CZ-OH-P-O1P
1	C	1124	PTR	CA-CB-CG-CD1
1	C	1124	PTR	CA-CB-CG-CD2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	1124	PTR	2	0
1	A	1124	PTR	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
5	MFX	E	1100	4	33,33,33	1.14	1 (3%)	46,50,50	2.75	19 (41%)
5	MFX	F	1100	4	33,33,33	0.97	3 (9%)	46,50,50	2.18	12 (26%)

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
5	MFX	E	1100	4	-	4/14/35/35	1/5/5/5
5	MFX	F	1100	4	-	2/14/35/35	1/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1100	MFX	C14-C12	-2.16	1.37	1.40
5	F	1100	MFX	C14-C12	-2.15	1.37	1.40
5	F	1100	MFX	C01-C02	-2.09	1.50	1.53
5	F	1100	MFX	C16-C18	-2.04	1.32	1.38

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	1100	MFX	C03-N01-C11	-7.49	108.80	123.04
5	E	1100	MFX	C04-N01-C11	-7.05	109.63	123.04
5	F	1100	MFX	C04-N01-C11	-6.27	111.12	123.04
5	F	1100	MFX	C03-N01-C11	-5.76	112.08	123.04
5	E	1100	MFX	C13-C11-C15	5.33	120.53	116.02
5	E	1100	MFX	C10-N02-C02	-5.18	108.39	111.62
5	F	1100	MFX	C-O01-C13	-4.77	101.70	114.78
5	E	1100	MFX	C16-C18-C19	-4.62	116.45	119.88
5	E	1100	MFX	C12-N-C16	4.20	122.80	119.81
5	F	1100	MFX	O-C20-C18	-4.06	113.55	122.46
5	F	1100	MFX	C20-C18-C19	4.02	127.69	121.56
5	E	1100	MFX	C17-C14-C12	3.69	123.67	118.84
5	E	1100	MFX	C06-N-C16	-3.57	114.34	119.73
5	E	1100	MFX	C-O01-C13	-3.55	105.04	114.78
5	E	1100	MFX	C13-C12-N	3.41	126.85	123.05
5	F	1100	MFX	O03-C20-O	3.33	131.22	123.61
5	E	1100	MFX	C14-C12-C13	-3.18	116.53	120.07
5	E	1100	MFX	C15-C11-N01	-3.17	113.41	121.57
5	E	1100	MFX	C09-C06-N	-3.06	114.24	118.84
5	F	1100	MFX	C01-C03-N01	3.00	107.23	102.99
5	E	1100	MFX	C14-C19-C18	2.84	119.20	115.59
5	F	1100	MFX	C13-C11-C15	2.78	118.38	116.02
5	F	1100	MFX	F-C15-C11	2.78	122.40	118.36
5	F	1100	MFX	C16-C18-C20	-2.69	113.88	118.35
5	E	1100	MFX	C07-C05-C01	-2.68	107.36	111.93
5	E	1100	MFX	C17-C14-C19	-2.49	115.69	119.95
5	E	1100	MFX	O03-C20-O	2.36	129.00	123.61
5	F	1100	MFX	C17-C15-C11	-2.29	119.92	123.22
5	E	1100	MFX	C17-C15-C11	-2.25	119.97	123.22
5	E	1100	MFX	C14-C12-N	-2.18	116.62	118.91
5	F	1100	MFX	C14-C12-C13	-2.00	117.84	120.07

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	1100	MFX	C09-C06-N-C16
5	E	1100	MFX	C08-C06-N-C16
5	E	1100	MFX	C09-C06-N-C12
5	E	1100	MFX	C08-C06-N-C12
5	F	1100	MFX	C13-C11-N01-C04

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Mol	Chain	Res	Type	Atoms
5	F	1100	MFX	C11-C13-O01-C

All (2) ring outliers are listed below:

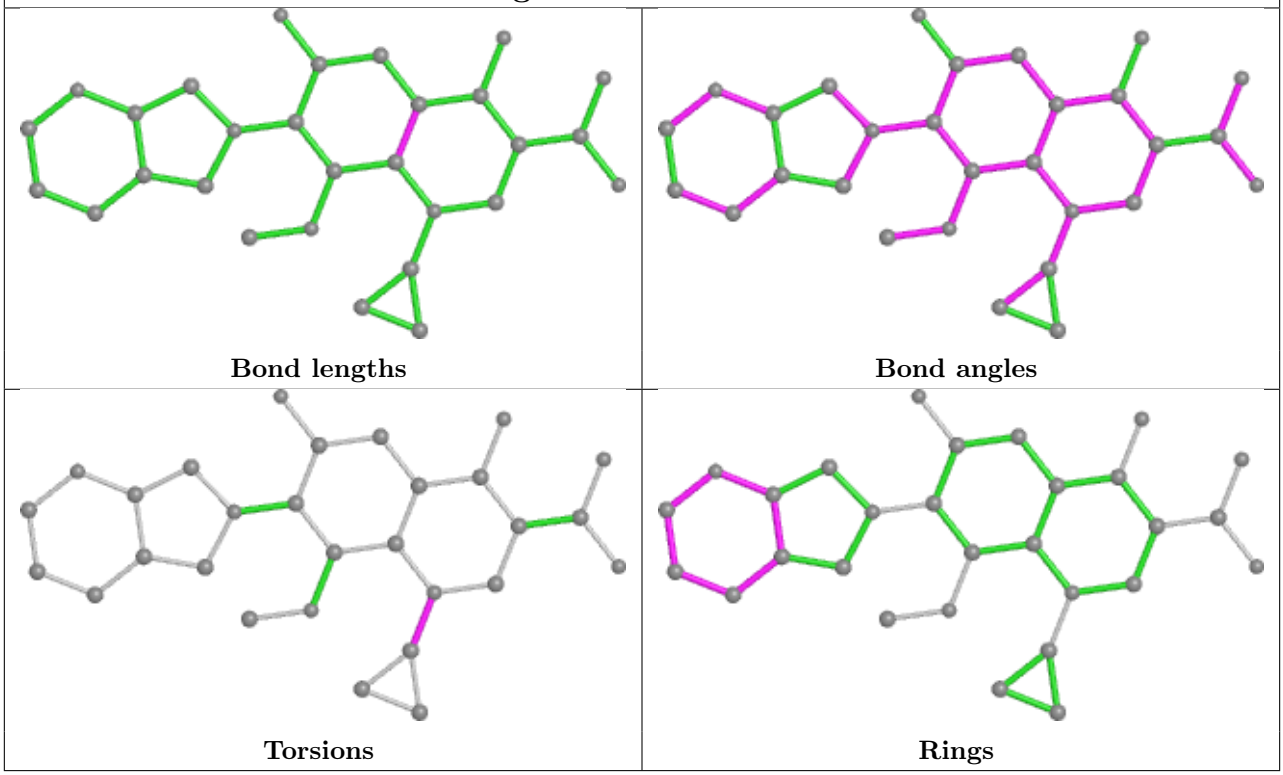
Mol	Chain	Res	Type	Atoms
5	F	1100	MFX	C01-C02-C05-C07-C10-N02
5	E	1100	MFX	C01-C02-C05-C07-C10-N02

2 monomers are involved in 29 short contacts:

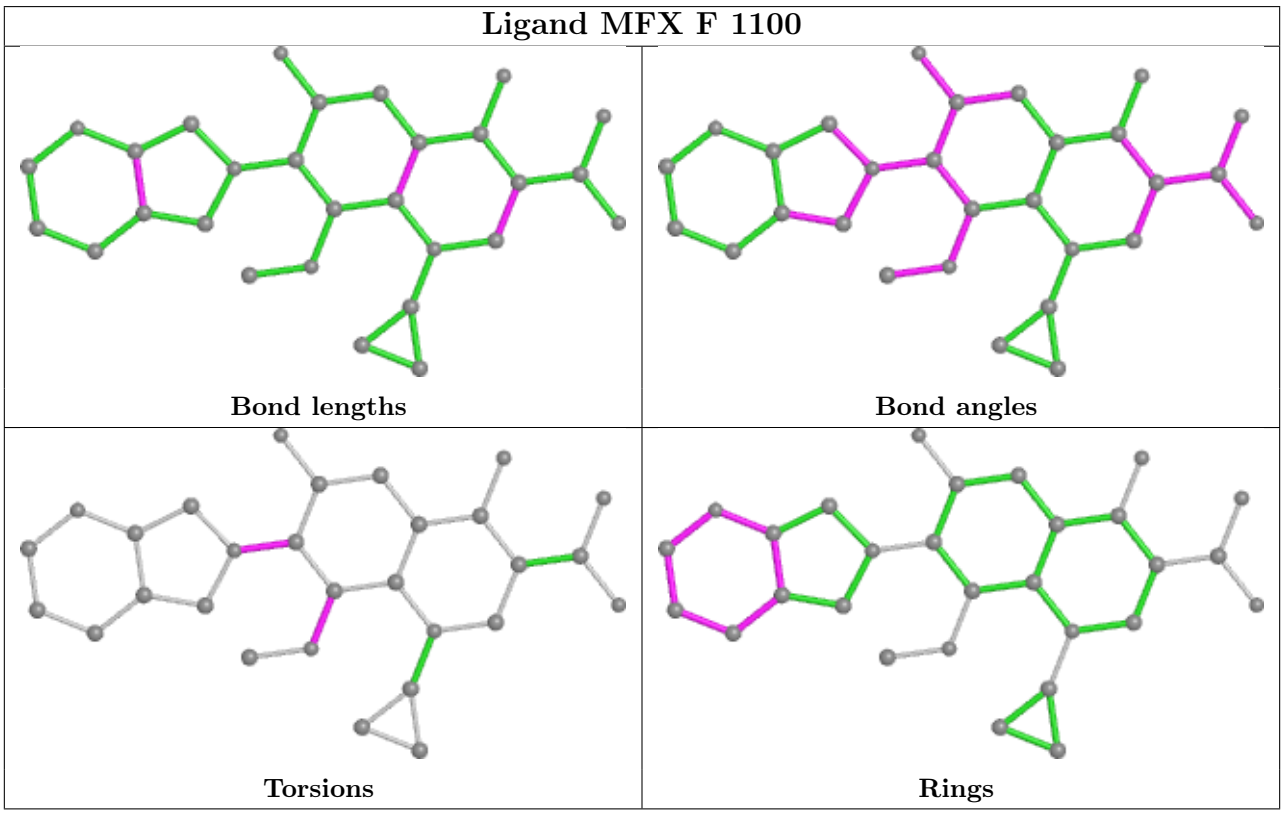
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1100	MFX	12	0
5	F	1100	MFX	17	0

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 MFX E 1100



Ligand MFX F 1100



5.7 Other polymers

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	691/767 (90%)	-0.06	24 (3%) 44 40	74, 138, 203, 247	0
1	C	710/767 (92%)	-0.18	8 (1%) 80 80	74, 125, 185, 222	0
2	E	26/34 (76%)	0.09	0 100 100	105, 127, 234, 250	0
3	F	26/34 (76%)	0.05	1 (3%) 40 37	98, 142, 225, 251	0
All	All	1453/1602 (90%)	-0.11	33 (2%) 60 58	74, 131, 197, 251	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	534	PRO	4.7
1	A	1172	GLY	4.1
1	A	1173	THR	3.5
1	A	533	ASN	3.4
1	C	1172	GLY	3.4
1	A	536	ILE	3.3
1	A	1174	THR	3.2
1	A	1183	ASP	3.1
1	A	506	ILE	3.0
1	C	1173	THR	3.0
1	C	1174	THR	2.9
1	A	513	HIS	2.9
1	A	525	LEU	2.8
1	A	1171	ASN	2.8
1	A	467	ASP	2.8
1	A	528	VAL	2.8
1	C	1295	HIS	2.7
1	A	1486	ALA	2.6
1	C	1277	GLN	2.5
1	A	484	VAL	2.5
1	C	1249	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	468	ALA	2.4
1	A	1167	ASN	2.4
1	A	455	SER	2.3
1	A	1185	PRO	2.3
1	C	1280	ALA	2.2
1	A	469	ASP	2.2
1	C	1167	ASN	2.2
1	A	508	ILE	2.2
1	A	466	ALA	2.1
1	A	495	HIS	2.1
3	F	30	DT	2.1
1	A	541	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	PTR	C	1124	16/17	0.97	0.18	112,119,127,129	0
1	PTR	A	1124	16/17	0.98	0.15	84,90,97,104	0

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
5	MFX	F	1100	29/29	0.93	0.24	123,139,149,153	0
4	MG	A	1504	1/1	0.95	0.13	103,103,103,103	0
5	MFX	E	1100	29/29	0.97	0.19	92,109,119,124	0
4	MG	C	2488	1/1	0.98	0.24	75,75,75,75	0

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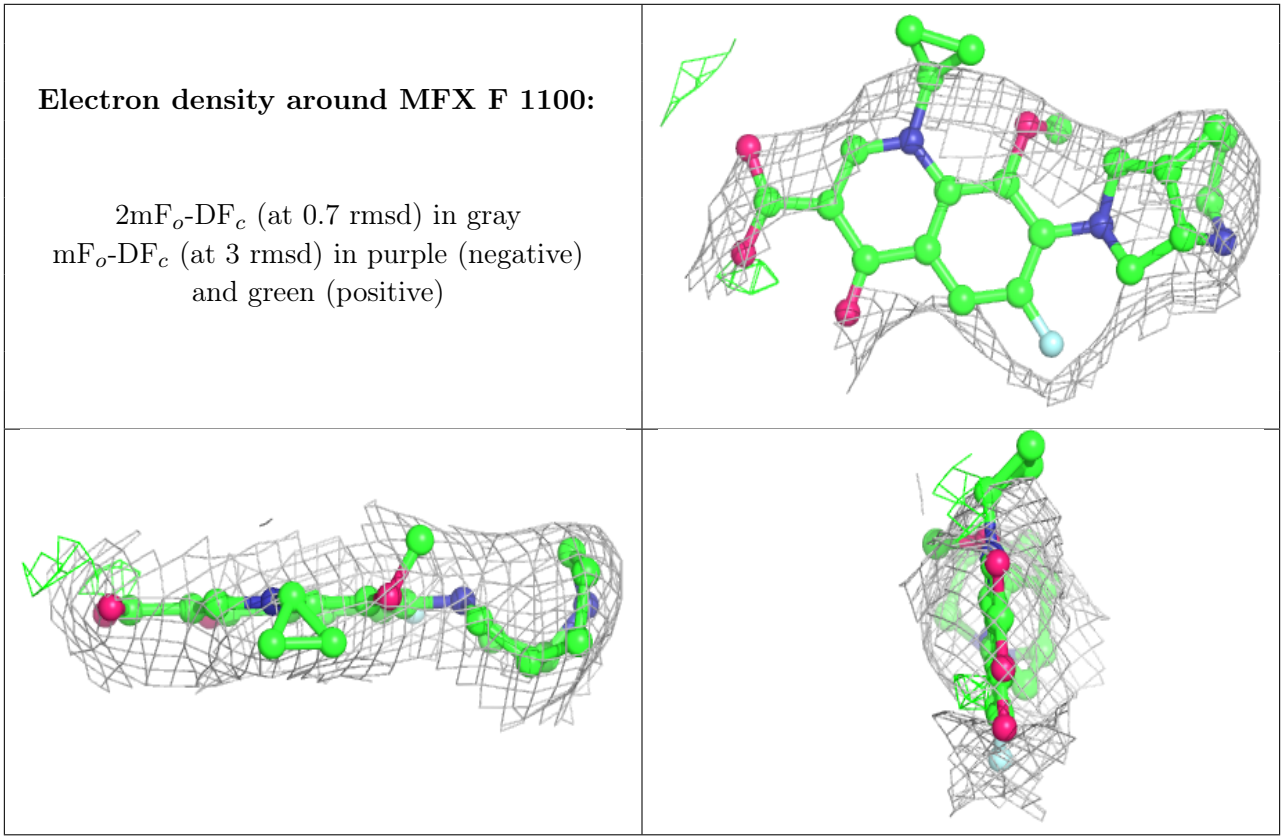
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	C	1504	1/1	0.99	0.08	89,89,89,89	0
4	MG	A	2487	1/1	0.99	0.39	114,114,114,114	0

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.

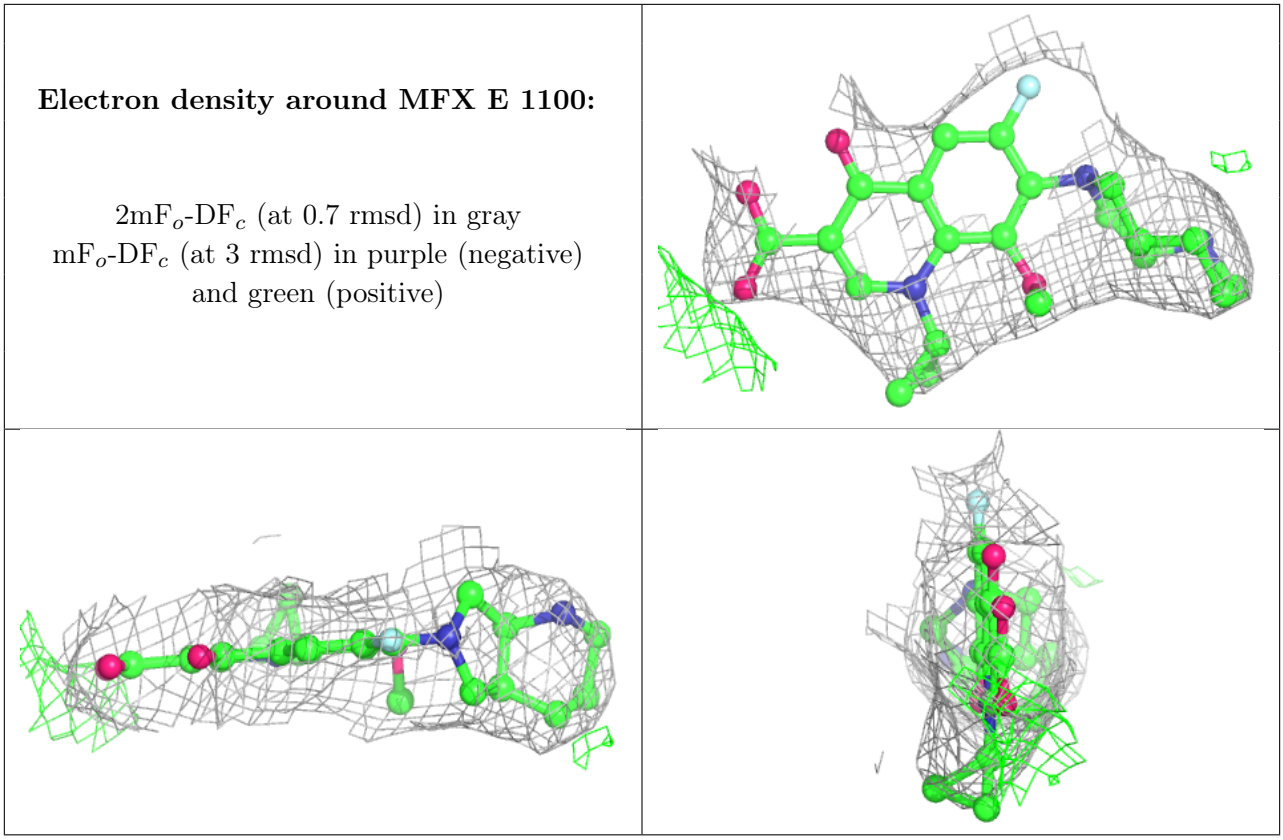
Electron density around MFX F 1100:

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



Electron density around MFX E 1100:

$2mF_o$-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.