



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:08 PM UTC

PDB ID : 3RAD / pdb_00003rad
Title : Quinolone(Clinafloxacin)-DNA cleavage complex of type IV topoisomerase from *S. pneumoniae*
Authors : Laponogov, I.; Pan, X.-S.; Veselkov, D.A.; McAuley, K.E.; Fisher, L.M.; Sanderson, M.R.
Deposited on : 2011-03-28
Resolution : 3.35 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

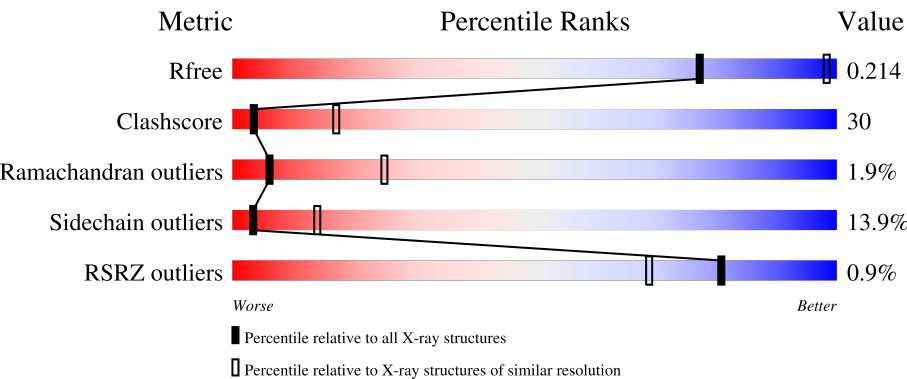
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.35 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.



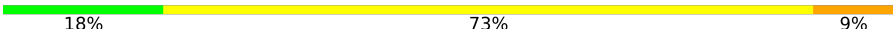
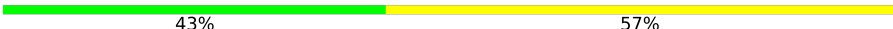
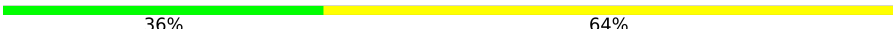
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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 $\leq 5\%$. 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	496	54%35%8%.
1	B	496	% 48%40%9%.
2	C	268	2% 46%27%.22%
2	D	268	2% 53%20%5%22%

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Mol	Chain	Length	Quality of chain
3	E	7	 43% 57%
4	F	11	 18% 73% 9%
5	G	7	 43% 57%
6	H	11	 36% 64%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11096 atoms, of which 32 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA topoisomerase 4 subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3702	2343	640	706	13			
1	B	482	Total	C	N	O	S	0	0	0
			3696	2345	635	703	13			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	257	THR	ILE	SEE REMARK 999	UNP P72525
A	489	LEU	-	expression tag	UNP P72525
A	490	GLU	-	expression tag	UNP P72525
A	491	HIS	-	expression tag	UNP P72525
A	492	HIS	-	expression tag	UNP P72525
A	493	HIS	-	expression tag	UNP P72525
A	494	HIS	-	expression tag	UNP P72525
A	495	HIS	-	expression tag	UNP P72525
A	496	HIS	-	expression tag	UNP P72525
B	257	THR	ILE	SEE REMARK 999	UNP P72525
B	489	LEU	-	expression tag	UNP P72525
B	490	GLU	-	expression tag	UNP P72525
B	491	HIS	-	expression tag	UNP P72525
B	492	HIS	-	expression tag	UNP P72525
B	493	HIS	-	expression tag	UNP P72525
B	494	HIS	-	expression tag	UNP P72525
B	495	HIS	-	expression tag	UNP P72525
B	496	HIS	-	expression tag	UNP P72525

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	209	Total	C	N	O	S	0	0	0
			1429	905	252	266	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	208	Total	C	N	O	S	0	0	0
			1417	898	247	267	5			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	380	MET	-	expression tag	UNP Q59961
C	381	GLY	-	expression tag	UNP Q59961
C	382	HIS	-	expression tag	UNP Q59961
C	383	HIS	-	expression tag	UNP Q59961
C	384	HIS	-	expression tag	UNP Q59961
C	385	HIS	-	expression tag	UNP Q59961
C	386	HIS	-	expression tag	UNP Q59961
C	387	HIS	-	expression tag	UNP Q59961
C	388	HIS	-	expression tag	UNP Q59961
C	389	HIS	-	expression tag	UNP Q59961
C	390	HIS	-	expression tag	UNP Q59961
C	391	HIS	-	expression tag	UNP Q59961
C	392	SER	-	expression tag	UNP Q59961
C	393	SER	-	expression tag	UNP Q59961
C	394	GLY	-	expression tag	UNP Q59961
C	395	HIS	-	expression tag	UNP Q59961
C	396	ILE	-	expression tag	UNP Q59961
C	397	ASP	-	expression tag	UNP Q59961
C	398	ASP	-	expression tag	UNP Q59961
C	399	ASP	-	expression tag	UNP Q59961
C	400	ASP	-	expression tag	UNP Q59961
C	401	LYS	-	expression tag	UNP Q59961
C	402	HIS	-	expression tag	UNP Q59961
C	403	MET	-	expression tag	UNP Q59961
C	460	ILE	VAL	SEE REMARK 999	UNP Q59961
C	644	ALA	THR	SEE REMARK 999	UNP Q59961
D	380	MET	-	expression tag	UNP Q59961
D	381	GLY	-	expression tag	UNP Q59961
D	382	HIS	-	expression tag	UNP Q59961
D	383	HIS	-	expression tag	UNP Q59961
D	384	HIS	-	expression tag	UNP Q59961
D	385	HIS	-	expression tag	UNP Q59961
D	386	HIS	-	expression tag	UNP Q59961
D	387	HIS	-	expression tag	UNP Q59961
D	388	HIS	-	expression tag	UNP Q59961
D	389	HIS	-	expression tag	UNP Q59961

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Chain	Residue	Modelled	Actual	Comment	Reference
D	390	HIS	-	expression tag	UNP Q59961
D	391	HIS	-	expression tag	UNP Q59961
D	392	SER	-	expression tag	UNP Q59961
D	393	SER	-	expression tag	UNP Q59961
D	394	GLY	-	expression tag	UNP Q59961
D	395	HIS	-	expression tag	UNP Q59961
D	396	ILE	-	expression tag	UNP Q59961
D	397	ASP	-	expression tag	UNP Q59961
D	398	ASP	-	expression tag	UNP Q59961
D	399	ASP	-	expression tag	UNP Q59961
D	400	ASP	-	expression tag	UNP Q59961
D	401	LYS	-	expression tag	UNP Q59961
D	402	HIS	-	expression tag	UNP Q59961
D	403	MET	-	expression tag	UNP Q59961
D	460	ILE	VAL	SEE REMARK 999	UNP Q59961
D	644	ALA	THR	SEE REMARK 999	UNP Q59961

- Molecule 3 is a DNA chain called 5'-D(*CP*AP*TP*GP*AP*AP*T)-3'.

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

- Molecule 4 is a DNA chain called 5'-D(P*AP*GP*TP*CP*AP*TP*TP*CP*AP*TP*G)-3'.

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

- Molecule 5 is a DNA chain called 5'-D(*CP*GP*TP*GP*CP*AP*T)-3'.

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

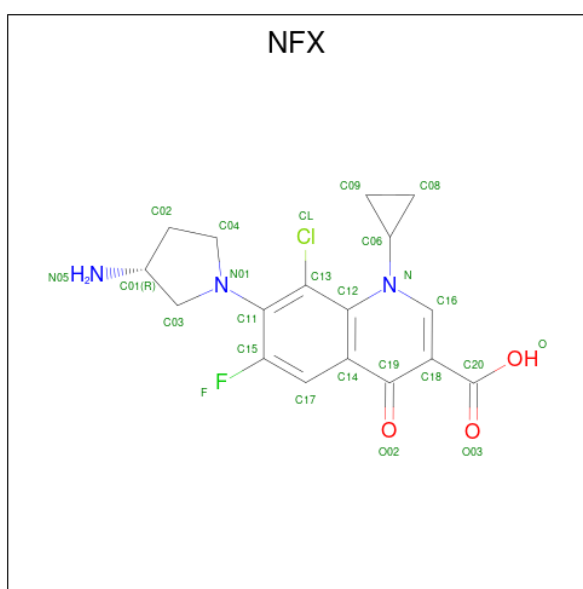
- Molecule 6 is a DNA chain called 5'-D(P*GP*AP*CP*TP*AP*TP*GP*CP*AP*CP*G)-3'.

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

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total Mg 2 2	0	0
7	B	2	Total Mg 2 2	0	0
7	C	1	Total Mg 1 1	0	0
7	D	1	Total Mg 1 1	0	0

- Molecule 8 is 7-[(3R)-3-aminopyrrolidin-1-yl]-8-chloro-1-cyclopropyl-6-fluoro-4-oxo-1,4-dihydroquinoline-3-carboxylic acid (CCD ID: NFX) (formula: C₁₇H₁₇ClFN₃O₃).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
8	F	1	Total	C	Cl	F	H	N	O	0	0
			41	17	1	1	16	3	3		
8	H	1	Total	C	Cl	F	H	N	O	0	0
			41	17	1	1	16	3	3		

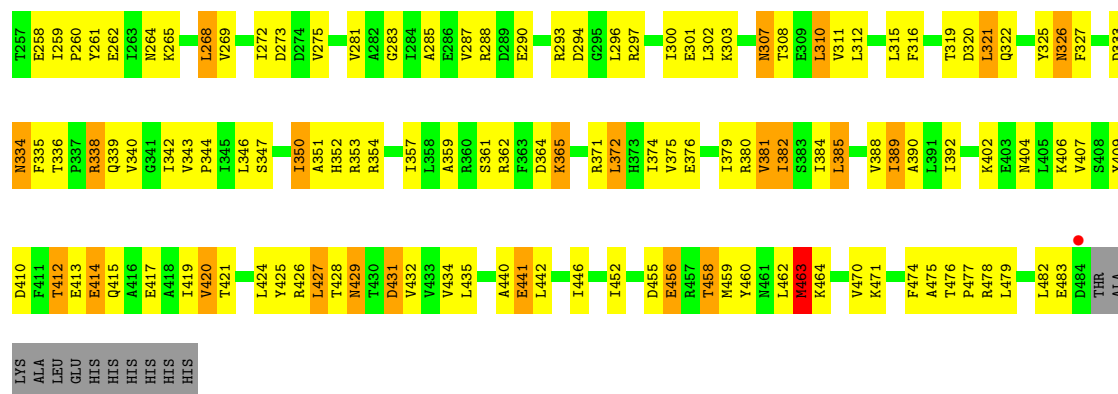
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	18	Total O 18 18	0	0
9	B	11	Total O 11 11	0	0
9	C	2	Total O 2 2	0	0

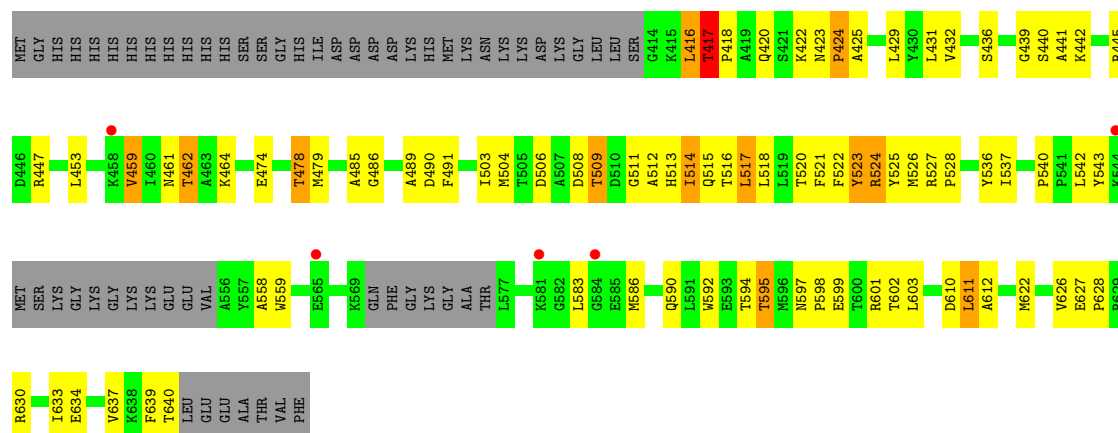
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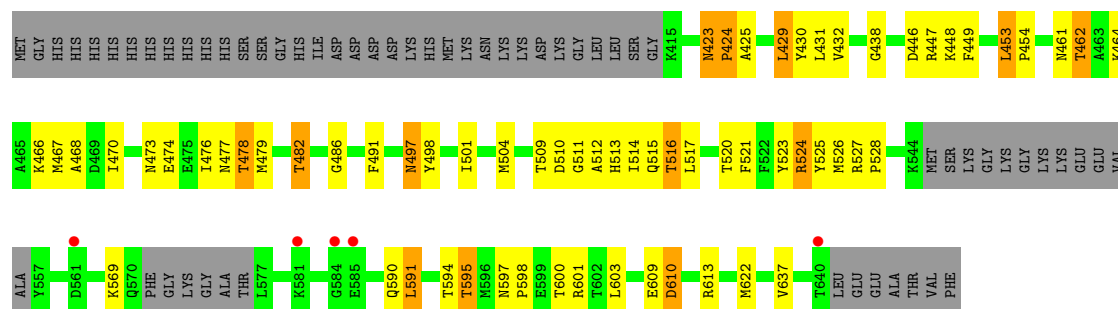
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	E	2	Total	O	0	0
			2	2		
9	G	1	Total	O	0	0
			1	1		



• Molecule 2: DNA topoisomerase 4 subunit B



• Molecule 2: DNA topoisomerase 4 subunit B



• Molecule 3: 5'-D(*CP*AP*TP*GP*AP*AP*T)-3'



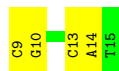
- Molecule 4: 5'-D(P*AP*GP*TP*CP*AP*TP*TP*CP*AP*TP*G)-3'

Chain F:  18% 73% 9%



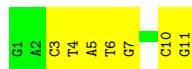
- Molecule 5: 5'-D(*CP*GP*TP*GP*CP*AP*T)-3'

Chain G:  43% 57%



- Molecule 6: 5'-D(P*GP*AP*CP*TP*AP*TP*GP*CP*AP*CP*G)-3'

Chain H:  36% 64%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.13Å 157.13Å 211.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.67 – 3.35 41.67 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.3 (41.67-3.35) 99.3 (41.67-3.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.177 , 0.228 0.167 , 0.214	Depositor DCC
R_{free} test set	5515 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å ²)	77.9	Xtriage
Anisotropy	0.599	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 63.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.063 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11096	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.58	0/3763	1.01	10/5104 (0.2%)
1	B	0.60	0/3757	0.96	4/5098 (0.1%)
2	C	0.51	0/1455	0.89	2/1991 (0.1%)
2	D	0.49	0/1443	0.89	3/1976 (0.2%)
3	E	0.34	0/157	1.03	0/241
4	F	0.36	0/251	1.24	1/385 (0.3%)
5	G	0.35	0/155	1.05	0/238
6	H	0.36	0/253	1.02	0/388
All	All	0.55	0/11234	0.97	20/15421 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	ILE	CA-C-N	-7.85	112.29	120.38
1	A	178	ILE	C-N-CA	-7.85	112.29	120.38
1	A	4	ILE	N-CA-C	7.25	117.95	110.05
1	B	208	LEU	CA-C-N	6.70	126.64	119.28
1	B	208	LEU	C-N-CA	6.70	126.64	119.28
1	A	196	HIS	CA-C-N	6.55	127.07	119.47
1	A	196	HIS	C-N-CA	6.55	127.07	119.47
1	A	194	ILE	N-CA-C	-5.97	104.69	110.72
1	A	139	VAL	CA-C-N	5.52	126.36	120.13
1	A	139	VAL	C-N-CA	5.52	126.36	120.13
2	C	417	THR	CA-C-N	5.46	125.66	120.31
2	C	417	THR	C-N-CA	5.46	125.66	120.31
1	B	196	HIS	CA-C-N	5.35	126.52	119.84
1	B	196	HIS	C-N-CA	5.35	126.52	119.84
1	A	128	GLY	N-CA-C	-5.27	106.41	112.73
1	A	479	LEU	N-CA-C	-5.25	106.81	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	423	ASN	CA-C-N	5.24	126.38	119.84
2	D	423	ASN	C-N-CA	5.24	126.38	119.84
4	F	1	DA	C3'-C2'-C1'	-5.06	94.00	101.60
2	D	511	GLY	N-CA-C	-5.04	106.39	112.49

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3702	0	3579	218	0
1	B	3696	0	3589	240	0
2	C	1429	0	1193	87	0
2	D	1417	0	1167	65	0
3	E	140	0	78	6	0
4	F	225	0	126	9	0
5	G	139	0	78	3	0
6	H	226	0	124	7	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	F	25	16	16	4	0
8	H	25	16	16	4	0
9	A	18	0	0	1	0
9	B	11	0	0	1	0
9	C	2	0	0	0	0
9	E	2	0	0	0	0
9	G	1	0	0	0	0
All	All	11064	32	9966	623	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 30.

All (623) 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:146:ASP:HB3	1:B:148:THR:HG23	1.27	1.15
1:B:70:MET:HE1	1:B:78:ASP:HB3	1.11	1.10
1:A:70:MET:HE1	1:A:78:ASP:HB3	1.11	1.08
1:B:307:ASN:ND2	1:B:310:LEU:HB2	1.69	1.07
1:A:60:ARG:HH11	1:A:60:ARG:HB2	1.18	1.07
1:A:354:ARG:HG3	1:A:459:MET:HE2	1.11	1.05
1:B:24:ILE:HD11	1:B:28:ARG:HE	1.16	1.05
1:B:307:ASN:HD21	1:B:310:LEU:HB2	0.89	1.05
1:B:70:MET:HE1	1:B:78:ASP:CB	1.86	1.05
1:A:443:ARG:HG3	1:A:443:ARG:HH11	0.97	1.04
1:B:354:ARG:HG3	1:B:459:MET:HE2	1.36	1.03
2:D:462:THR:HG21	2:D:521:PHE:HD2	1.17	1.02
1:A:139:VAL:HG11	1:A:154:VAL:O	1.61	1.00
1:B:24:ILE:HD11	1:B:28:ARG:NE	1.77	0.99
1:A:391:LEU:HD21	1:A:404:ASN:HB3	1.44	0.99
1:A:354:ARG:HG3	1:A:459:MET:CE	1.93	0.99
1:A:139:VAL:HG13	1:A:140:PRO:HD2	1.44	0.98
1:B:307:ASN:HD21	1:B:310:LEU:CB	1.75	0.98
2:C:486:GLY:O	2:C:491:PHE:HD2	1.48	0.96
1:A:21:SER:O	1:A:25:ILE:HG13	1.68	0.93
1:A:222:ARG:HD3	1:A:484:ASP:HA	1.47	0.93
1:B:41:GLN:HA	1:B:88:MET:HE1	1.50	0.93
1:A:60:ARG:HH11	1:A:60:ARG:CB	1.82	0.93
1:B:412:THR:HG23	1:B:415:GLN:NE2	1.82	0.92
1:A:443:ARG:HG3	1:A:443:ARG:NH1	1.77	0.92
1:B:9:LEU:HD23	1:B:9:LEU:O	1.69	0.92
1:A:70:MET:CE	1:A:78:ASP:HB3	2.00	0.91
1:A:443:ARG:HH11	1:A:443:ARG:CG	1.83	0.91
2:D:462:THR:HG21	2:D:521:PHE:CD2	2.05	0.89
8:H:101:NFX:H03	8:H:101:NFX:CL	2.10	0.89
2:D:431:LEU:HD22	2:D:479:MET:HE3	1.54	0.88
2:D:474:GLU:O	2:D:478:THR:HG23	1.75	0.87
1:B:9:LEU:HD23	1:B:9:LEU:C	2.00	0.87
2:D:524:ARG:HH11	2:D:524:ARG:HB3	1.40	0.87
1:A:91:ASN:HD22	1:A:91:ASN:H	1.23	0.86
1:B:219:ILE:HG23	1:B:236:VAL:HG21	1.57	0.86
1:B:256:ILE:HD13	1:B:321:LEU:HD21	1.57	0.86
2:D:590:GLN:O	2:D:594:THR:HG23	1.76	0.85
1:A:70:MET:HE1	1:A:78:ASP:CB	2.04	0.84
1:A:293:ARG:HH11	1:A:293:ARG:HB3	1.42	0.84
1:A:316:PHE:CE2	1:A:321:LEU:HD13	2.12	0.84
1:A:334:ASN:O	1:A:336:THR:HG22	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:520:THR:HG21	2:D:622:MET:HG3	1.60	0.84
1:B:194:ILE:HD11	1:B:463:MET:HE1	1.61	0.83
8:H:101:NFX:CL	8:H:101:NFX:C03	2.64	0.82
1:B:389:ILE:HD11	1:B:427:LEU:HD13	1.60	0.82
1:B:146:ASP:HB3	1:B:148:THR:CG2	2.09	0.82
2:C:491:PHE:CZ	2:C:526:MET:HE3	2.16	0.81
1:B:146:ASP:CB	1:B:148:THR:HG23	2.11	0.81
1:B:243:GLU:O	1:B:244:ILE:HD13	1.80	0.81
1:A:44:ILE:HD12	1:A:88:MET:CE	2.10	0.81
1:A:338:ARG:HD2	1:A:340:VAL:CG1	2.12	0.79
1:A:146:ASP:OD2	1:A:148:THR:HG22	1.82	0.79
1:B:41:GLN:HG2	1:B:88:MET:HE2	1.63	0.79
2:C:520:THR:HG21	2:C:622:MET:HG3	1.67	0.77
1:A:194:ILE:CD1	1:A:463:MET:HE2	2.14	0.77
1:B:254:ILE:HD13	1:B:312:LEU:HD13	1.67	0.77
2:C:611:LEU:HD13	2:C:611:LEU:O	1.84	0.77
1:A:139:VAL:HG13	1:A:140:PRO:CD	2.15	0.77
1:B:343:VAL:HB	1:B:344:PRO:HD3	1.66	0.77
1:A:354:ARG:CG	1:A:459:MET:HE2	2.05	0.76
1:B:95:ARG:HA	1:B:214:PRO:HG3	1.66	0.76
1:A:265:LYS:O	1:A:269:VAL:HG23	1.85	0.76
1:B:41:GLN:HA	1:B:88:MET:CE	2.15	0.76
4:F:9:DA:O5'	4:F:9:DA:H2'	1.85	0.75
1:B:385:LEU:HD21	1:B:427:LEU:HD22	1.69	0.75
1:A:442:LEU:O	1:A:446:ILE:HG13	1.85	0.75
1:B:24:ILE:CD1	1:B:28:ARG:NE	2.50	0.74
1:A:60:ARG:HB2	1:A:60:ARG:NH1	1.99	0.74
1:B:139:VAL:HG12	1:B:140:PRO:HD2	1.69	0.74
8:F:101:NFX:CL	8:F:101:NFX:H04A	2.25	0.73
1:B:354:ARG:HG3	1:B:459:MET:CE	2.14	0.73
1:B:431:ASP:O	1:B:434:VAL:HG12	1.87	0.73
1:B:412:THR:HG23	1:B:415:GLN:HE21	1.50	0.73
1:A:316:PHE:HE2	1:A:321:LEU:HD13	1.52	0.72
1:B:110:GLY:HA3	1:B:264:ASN:HD21	1.54	0.72
2:D:525:TYR:O	2:D:526:MET:HG3	1.89	0.72
1:B:160:PRO:O	1:B:164:VAL:HG23	1.89	0.72
2:C:491:PHE:CD1	2:C:528:PRO:HG2	2.25	0.72
2:C:524:ARG:HB3	2:C:525:TYR:CD1	2.25	0.72
1:B:95:ARG:HB2	1:B:180:PRO:HB3	1.72	0.72
1:B:381:VAL:HG12	1:B:382:ILE:N	2.03	0.72
8:F:101:NFX:CL	8:F:101:NFX:C04	2.75	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ASN:HD21	1:A:148:THR:HG23	1.56	0.71
1:B:48:MET:HE3	1:B:53:ASN:ND2	2.05	0.71
1:B:219:ILE:HG23	1:B:236:VAL:CG2	2.20	0.71
1:B:38:LYS:H	1:B:41:GLN:NE2	1.88	0.71
2:C:423:ASN:HD21	2:C:425:ALA:HB3	1.56	0.71
1:A:259:ILE:HB	1:A:260:PRO:CD	2.21	0.70
1:B:9:LEU:C	1:B:9:LEU:CD2	2.64	0.70
1:B:307:ASN:ND2	1:B:310:LEU:CB	2.44	0.70
1:A:24:ILE:HG22	1:A:171:SER:HB2	1.73	0.70
1:A:252:GLU:OE1	1:A:308:THR:HG21	1.91	0.70
1:B:41:GLN:CA	1:B:88:MET:HE1	2.21	0.70
1:B:167:SER:C	1:B:168:THR:HG22	2.15	0.69
1:B:236:VAL:CG2	1:B:237:VAL:N	2.55	0.69
1:A:194:ILE:HD11	1:A:463:MET:HE2	1.72	0.69
1:B:194:ILE:HD13	1:B:463:MET:HE2	1.75	0.69
2:C:462:THR:HG21	2:C:521:PHE:HD2	1.56	0.69
3:E:9:DC:H2''	3:E:10:DA:H5''	1.75	0.69
2:D:431:LEU:CD2	2:D:479:MET:HE3	2.21	0.69
1:A:144:ASN:C	1:A:146:ASP:H	2.01	0.69
1:B:70:MET:CE	1:B:78:ASP:HB3	2.06	0.69
2:C:474:GLU:O	2:C:478:THR:HG23	1.92	0.69
1:B:211:PRO:O	1:B:478:ARG:NH2	2.26	0.68
1:B:412:THR:CG2	1:B:415:GLN:NE2	2.56	0.68
1:A:60:ARG:HH11	1:A:60:ARG:CG	2.06	0.68
1:A:412:THR:HG23	1:A:415:GLN:OE1	1.94	0.68
1:B:43:ARG:HD3	1:B:73:PHE:HB3	1.73	0.68
2:D:486:GLY:O	2:D:491:PHE:HD2	1.76	0.68
8:F:101:NFX:CL	8:F:101:NFX:C06	2.78	0.68
8:H:101:NFX:CL	8:H:101:NFX:C06	2.78	0.68
1:A:244:ILE:HD12	1:A:244:ILE:N	2.09	0.68
1:B:357:ILE:HD12	1:B:463:MET:HG2	1.76	0.68
1:B:28:ARG:HG3	1:B:28:ARG:HH11	1.59	0.68
1:A:28:ARG:CZ	3:E:14:DA:H4'	2.24	0.67
1:A:40:VAL:O	1:A:44:ILE:HG13	1.94	0.67
1:B:389:ILE:HD11	1:B:427:LEU:CD1	2.23	0.67
1:A:169:GLY:HA2	1:A:176:THR:HG22	1.76	0.67
1:A:338:ARG:HD2	1:A:340:VAL:HG12	1.76	0.67
2:D:609:GLU:O	2:D:610:ASP:HB2	1.94	0.67
1:B:194:ILE:HD11	1:B:463:MET:CE	2.25	0.67
2:D:610:ASP:OD1	2:D:613:ARG:HB2	1.95	0.66
1:B:194:ILE:CD1	1:B:463:MET:CE	2.74	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:101:NFX:CL	8:H:101:NFX:C09	2.81	0.66
8:F:101:NFX:CL	8:F:101:NFX:C09	2.81	0.66
1:A:59:TYR:HB3	1:A:120:GLU:HG3	1.77	0.65
1:B:283:GLY:HA2	1:B:303:LYS:HD2	1.78	0.65
2:C:513:HIS:O	2:C:516:THR:HB	1.97	0.65
2:D:461:ASN:ND2	2:D:464:LYS:HG3	2.12	0.65
1:A:398:LYS:HD2	1:B:425:TYR:CD1	2.32	0.65
1:A:211:PRO:O	1:A:478:ARG:NH2	2.29	0.65
1:B:296:LEU:C	1:B:296:LEU:HD23	2.21	0.64
2:D:524:ARG:HB3	2:D:524:ARG:NH1	2.11	0.64
1:B:20:TYR:CD1	2:D:513:HIS:HB2	2.32	0.64
1:A:139:VAL:CG1	1:A:140:PRO:HD2	2.24	0.64
2:D:601:ARG:HH21	2:D:603:LEU:HD11	1.63	0.64
1:A:23:TYR:HB3	2:C:509:THR:HG21	1.78	0.64
1:B:95:ARG:HD2	1:B:95:ARG:O	1.97	0.64
1:B:28:ARG:CZ	5:G:14:DA:H4'	2.28	0.64
1:B:136:LYS:HE2	1:B:364:ASP:OD1	1.98	0.63
1:B:431:ASP:OD1	1:B:431:ASP:C	2.41	0.63
2:D:478:THR:O	2:D:482:THR:HG23	1.97	0.63
2:C:630:ARG:O	2:C:634:GLU:HG3	1.98	0.63
2:D:431:LEU:HD13	2:D:479:MET:CE	2.29	0.63
5:G:13:DC:H2''	5:G:14:DA:O5'	1.98	0.63
2:C:527:ARG:N	2:C:528:PRO:HD2	2.14	0.63
6:H:10:DC:H2''	6:H:11:DG:H5''	1.81	0.63
1:A:169:GLY:O	1:A:170:ILE:HG12	1.99	0.63
1:A:391:LEU:HD21	1:A:404:ASN:CB	2.26	0.63
1:B:44:ILE:HD12	1:B:88:MET:HE3	1.81	0.62
2:C:637:VAL:HG12	2:C:639:PHE:CE2	2.34	0.62
1:A:22:LYS:O	1:A:26:GLN:HG3	1.99	0.62
2:C:511:GLY:O	2:C:515:GLN:HG3	1.98	0.62
1:B:302:LEU:HD12	1:B:308:THR:HG22	1.80	0.62
1:B:139:VAL:HG11	1:B:154:VAL:O	1.99	0.62
2:C:461:ASN:ND2	2:C:464:LYS:HG3	2.14	0.62
1:A:22:LYS:HE2	1:A:26:GLN:OE1	2.00	0.62
2:C:489:ALA:C	2:C:491:PHE:H	2.08	0.62
1:B:139:VAL:HG12	1:B:154:VAL:HG13	1.82	0.61
1:B:259:ILE:HB	1:B:260:PRO:HD2	1.82	0.61
1:B:261:TYR:O	1:B:262:GLU:HB2	1.99	0.61
1:A:222:ARG:HD3	1:A:484:ASP:CA	2.24	0.61
2:C:540:PRO:HA	2:C:595:THR:HG21	1.81	0.61
1:A:194:ILE:HG23	1:A:460:TYR:CD1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:ILE:HB	1:B:260:PRO:CD	2.31	0.61
2:D:513:HIS:O	2:D:516:THR:HB	2.00	0.61
1:B:194:ILE:CD1	1:B:463:MET:HE1	2.30	0.61
1:B:296:LEU:HD23	1:B:297:ARG:N	2.14	0.61
1:A:389:ILE:HD11	1:A:427:LEU:HD13	1.83	0.61
1:B:139:VAL:CG1	1:B:154:VAL:HG13	2.31	0.61
2:C:442:LYS:O	2:C:445:ARG:HD3	2.00	0.61
1:B:389:ILE:HG22	1:B:390:ALA:N	2.15	0.60
2:C:491:PHE:HZ	2:C:526:MET:HE3	1.65	0.60
2:C:524:ARG:HB3	2:C:525:TYR:HD1	1.63	0.60
1:B:273:ASP:HA	1:B:287:VAL:HG21	1.83	0.60
1:A:219:ILE:HG23	1:A:236:VAL:HG11	1.84	0.60
1:B:354:ARG:CG	1:B:459:MET:HE2	2.23	0.60
2:C:542:LEU:HB2	2:C:543:TYR:CD2	2.37	0.60
1:A:139:VAL:CG1	1:A:140:PRO:CD	2.80	0.60
2:C:601:ARG:HD2	2:C:603:LEU:HD21	1.83	0.60
1:B:236:VAL:HG23	1:B:237:VAL:H	1.66	0.60
1:A:216:GLY:O	1:A:217:ALA:HB3	2.02	0.59
1:A:443:ARG:NH1	1:A:443:ARG:CG	2.49	0.59
1:A:48:MET:HE3	1:A:53:ASN:ND2	2.17	0.59
1:A:38:LYS:H	1:A:41:GLN:NE2	1.98	0.59
1:A:144:ASN:O	1:A:146:ASP:N	2.34	0.59
1:B:228:ALA:HA	1:B:233:LYS:O	2.02	0.59
2:C:459:VAL:HG11	2:C:518:LEU:HD23	1.84	0.59
6:H:3:DC:H2'	6:H:4:DT:C6	2.36	0.59
6:H:6:DT:C2'	6:H:7:DG:H5'	2.33	0.59
1:B:412:THR:H	1:B:415:GLN:HE21	1.51	0.58
1:A:385:LEU:HD22	1:A:389:ILE:HD12	1.85	0.58
1:A:167:SER:C	1:A:168:THR:HG22	2.27	0.58
1:A:23:TYR:CB	2:C:509:THR:HG21	2.34	0.58
1:B:87:ARG:HA	1:B:90:GLN:HG3	1.85	0.58
1:A:34:ARG:HD2	1:A:352:HIS:ND1	2.19	0.58
1:A:285:ALA:HB3	1:A:301:GLU:O	2.04	0.58
1:B:126:ILE:HG13	1:B:474:PHE:CD1	2.39	0.58
1:B:357:ILE:CD1	1:B:463:MET:HG2	2.33	0.58
1:A:355:GLU:OE2	1:A:355:GLU:HA	2.04	0.58
1:B:247:LEU:HB2	1:B:251:LYS:O	2.04	0.58
2:D:446:ASP:HB3	2:D:449:PHE:CE1	2.39	0.58
2:C:416:LEU:HG	2:C:417:THR:N	2.15	0.58
2:C:509:THR:O	2:C:512:ALA:HB3	2.04	0.58
1:A:63:ALA:HB1	1:A:116:MET:HE3	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:VAL:HG13	1:A:41:GLN:N	2.18	0.57
1:A:9:LEU:O	1:A:9:LEU:HD23	2.05	0.57
1:A:334:ASN:O	1:A:336:THR:CG2	2.52	0.57
1:B:84:ALA:O	1:B:88:MET:HG3	2.04	0.57
1:A:12:ILE:O	1:A:16:ARG:HG2	2.05	0.57
2:D:637:VAL:HG12	2:D:637:VAL:O	2.04	0.57
1:A:377:GLY:O	1:A:381:VAL:HG23	2.05	0.57
1:A:146:ASP:CG	1:A:148:THR:HG22	2.30	0.57
1:B:236:VAL:CG2	1:B:237:VAL:H	2.18	0.57
6:H:10:DC:C2'	6:H:11:DG:H5''	2.35	0.56
1:B:210:GLY:HA2	1:B:229:TYR:OH	2.05	0.56
6:H:5:DA:H2''	6:H:6:DT:O5'	2.05	0.56
2:C:486:GLY:O	2:C:491:PHE:CD2	2.41	0.56
1:A:190:ALA:O	1:A:194:ILE:HG13	2.06	0.56
2:C:516:THR:HG22	2:C:517:LEU:N	2.20	0.56
1:A:44:ILE:HD12	1:A:88:MET:HE3	1.86	0.56
1:B:236:VAL:HG22	1:B:237:VAL:N	2.19	0.56
2:D:516:THR:O	2:D:520:THR:HG23	2.06	0.56
1:A:391:LEU:HD23	1:A:391:LEU:O	2.06	0.56
1:A:455:ASP:HB3	1:A:458:THR:HB	1.87	0.55
2:D:597:ASN:HD22	2:D:600:THR:CB	2.18	0.55
1:A:59:TYR:CB	1:A:120:GLU:HG3	2.36	0.55
1:A:390:ALA:O	1:A:393:ARG:HB3	2.06	0.55
1:B:406:LYS:HE2	1:B:413:GLU:HA	1.88	0.55
1:A:44:ILE:O	1:A:48:MET:HG3	2.07	0.55
2:C:485:ALA:HB3	2:C:491:PHE:CE2	2.41	0.55
1:B:49:ASN:CB	1:B:131:LEU:HD13	2.36	0.55
1:A:194:ILE:HG23	1:A:460:TYR:HD1	1.70	0.55
1:B:89:SER:HA	1:B:99:VAL:O	2.06	0.55
2:C:627:GLU:N	2:C:628:PRO:CD	2.69	0.55
2:C:516:THR:CG2	2:C:622:MET:SD	2.95	0.55
1:A:139:VAL:CG1	1:A:154:VAL:O	2.47	0.55
1:A:160:PRO:HG2	1:A:186:VAL:HG12	1.87	0.55
1:B:343:VAL:HB	1:B:344:PRO:CD	2.37	0.55
2:C:479:MET:HE1	2:C:522:PHE:CZ	2.42	0.55
2:C:491:PHE:CE1	2:C:528:PRO:HG2	2.42	0.55
1:B:43:ARG:CD	1:B:73:PHE:HB3	2.37	0.55
1:A:181:HIS:CD2	1:A:211:PRO:HA	2.42	0.55
1:A:245:GLU:OE2	1:A:297:ARG:NH2	2.39	0.54
1:B:49:ASN:HB2	1:B:131:LEU:HD13	1.89	0.54
1:B:111:ASP:HB2	1:B:112:PRO:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ARG:HB3	1:A:293:ARG:NH1	2.18	0.54
1:B:91:ASN:H	1:B:91:ASN:HD22	1.55	0.54
1:B:28:ARG:HG3	1:B:28:ARG:NH1	2.20	0.54
1:B:243:GLU:C	1:B:244:ILE:HD13	2.32	0.54
3:E:13:DA:H2''	3:E:14:DA:O5'	2.07	0.54
1:A:391:LEU:HD23	1:A:391:LEU:C	2.33	0.54
1:B:471:LYS:O	1:B:475:ALA:HB2	2.07	0.54
1:B:35:ASP:O	1:B:161:ASN:HB3	2.07	0.54
1:B:429:ASN:CG	1:B:429:ASN:O	2.50	0.54
1:A:194:ILE:HD13	1:A:463:MET:HG2	1.89	0.54
1:A:448:MET:O	1:A:452:ILE:HG13	2.06	0.54
2:D:432:VAL:HG11	2:D:438:GLY:HA2	1.89	0.54
2:D:486:GLY:O	2:D:491:PHE:CD2	2.60	0.54
2:C:516:THR:HG21	2:C:622:MET:SD	2.48	0.53
1:A:87:ARG:C	1:A:89:SER:H	2.17	0.53
1:B:60:ARG:O	1:B:61:LYS:C	2.52	0.53
1:B:77:GLY:O	1:B:81:ILE:HG13	2.08	0.53
2:C:423:ASN:C	2:C:425:ALA:H	2.16	0.53
1:B:425:TYR:C	1:B:425:TYR:CD2	2.86	0.53
2:C:611:LEU:HD13	2:C:611:LEU:C	2.33	0.53
1:B:216:GLY:O	1:B:217:ALA:HB3	2.08	0.53
1:A:55:PHE:HA	1:A:122:ARG:HD2	1.90	0.53
1:B:194:ILE:CD1	1:B:463:MET:HE2	2.39	0.53
1:A:259:ILE:HB	1:A:260:PRO:HD2	1.89	0.53
2:C:626:VAL:HG11	4:F:9:DA:H3'	1.89	0.53
1:A:296:LEU:HD23	1:A:297:ARG:N	2.24	0.53
1:B:456:GLU:HG3	1:B:460:TYR:CE2	2.44	0.53
2:C:423:ASN:ND2	2:C:425:ALA:HB3	2.24	0.53
2:C:514:ILE:HG22	2:C:515:GLN:N	2.23	0.53
2:C:637:VAL:CG1	2:C:639:PHE:CE2	2.92	0.53
2:D:478:THR:O	2:D:482:THR:CG2	2.57	0.53
2:D:509:THR:O	2:D:512:ALA:HB3	2.09	0.53
1:A:97:ILE:O	1:A:97:ILE:HG12	2.09	0.53
1:B:75:PRO:HD3	1:B:145:PHE:CD2	2.43	0.53
1:B:381:VAL:O	1:B:384:ILE:N	2.31	0.53
3:E:9:DC:C2'	3:E:10:DA:H5''	2.38	0.53
2:D:516:THR:CG2	2:D:622:MET:SD	2.96	0.52
2:D:594:THR:OG1	2:D:595:THR:HG22	2.08	0.52
1:B:216:GLY:O	1:B:217:ALA:CB	2.58	0.52
1:B:285:ALA:HB3	1:B:301:GLU:O	2.09	0.52
1:A:20:TYR:CD1	2:C:513:HIS:HB2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:TYR:CD1	1:A:342:ILE:HD13	2.45	0.52
1:A:139:VAL:HG13	1:A:154:VAL:HG13	1.92	0.52
1:B:219:ILE:CG2	1:B:236:VAL:HG21	2.34	0.52
1:B:351:ALA:O	1:B:354:ARG:HB3	2.09	0.52
1:B:476:THR:HB	1:B:477:PRO:CD	2.38	0.52
1:B:107:SER:OG	1:B:109:ASP:HB2	2.08	0.52
1:B:209:PRO:HB2	1:B:482:LEU:CD1	2.40	0.52
1:A:44:ILE:HD12	1:A:88:MET:HE2	1.90	0.52
1:B:141:PHE:CE2	1:B:152:PRO:HD3	2.45	0.52
1:B:240:SER:OG	1:B:321:LEU:HD22	2.10	0.52
1:A:201:ILE:O	1:A:205:MET:HG3	2.09	0.51
1:B:40:VAL:HG13	1:B:41:GLN:N	2.26	0.51
1:A:40:VAL:CG1	1:A:41:GLN:N	2.73	0.51
2:D:431:LEU:CD1	2:D:479:MET:CE	2.89	0.51
1:B:272:ILE:O	1:B:275:VAL:N	2.44	0.51
1:B:273:ASP:CA	1:B:287:VAL:HG21	2.40	0.51
2:D:466:LYS:C	2:D:468:ALA:N	2.68	0.51
1:B:190:ALA:O	1:B:194:ILE:HG13	2.10	0.51
1:B:28:ARG:NH1	9:B:606:HOH:O	2.42	0.51
1:B:95:ARG:O	1:B:95:ARG:CD	2.58	0.51
1:A:91:ASN:H	1:A:91:ASN:ND2	2.01	0.51
1:B:96:GLU:OE2	1:B:96:GLU:HA	2.10	0.51
1:B:132:GLN:O	1:B:133:ASP:HB2	2.11	0.51
2:D:431:LEU:CD1	2:D:479:MET:HE2	2.40	0.51
1:A:213:PHE:CE2	1:A:219:ILE:HD11	2.46	0.51
1:A:132:GLN:O	1:A:133:ASP:HB2	2.10	0.51
1:A:164:VAL:HG21	1:A:183:LEU:HD23	1.93	0.51
2:D:453:LEU:C	2:D:453:LEU:HD22	2.36	0.51
1:B:440:ALA:C	1:B:442:LEU:N	2.68	0.51
1:B:293:ARG:NH2	2:C:592:TRP:CE2	2.80	0.50
1:B:236:VAL:CG1	1:B:327:PHE:HE2	2.24	0.50
1:B:440:ALA:O	1:B:441:GLU:C	2.53	0.50
1:A:146:ASP:OD2	1:A:148:THR:CG2	2.56	0.50
1:B:455:ASP:OD2	1:B:458:THR:HB	2.12	0.50
2:D:446:ASP:O	2:D:448:LYS:N	2.44	0.50
2:D:453:LEU:HD22	2:D:454:PRO:N	2.26	0.50
1:A:371:ARG:O	1:A:371:ARG:HG3	2.12	0.50
1:A:236:VAL:CG1	1:A:237:VAL:N	2.75	0.50
1:B:265:LYS:O	1:B:269:VAL:HG23	2.11	0.50
2:C:597:ASN:O	2:C:601:ARG:HG2	2.11	0.50
4:F:5:DA:H2'	4:F:6:DT:H71	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:TYR:CG	2:C:509:THR:HG21	2.46	0.50
1:A:329:MET:HE3	1:A:345:ILE:HD11	1.93	0.50
1:B:226:LYS:O	1:B:230:GLU:HB2	2.12	0.50
2:C:523:TYR:C	2:C:523:TYR:CD2	2.90	0.50
1:A:20:TYR:HA	2:C:509:THR:HG22	1.93	0.50
1:A:194:ILE:HD11	1:A:463:MET:CE	2.42	0.50
1:A:229:TYR:CD1	1:A:342:ILE:CD1	2.95	0.50
1:A:429:ASN:OD1	1:A:430:THR:N	2.44	0.50
1:A:423:GLN:NE2	1:A:425:TYR:HE1	2.10	0.50
1:B:187:ILE:O	1:B:191:VAL:HG23	2.12	0.49
1:B:412:THR:HG23	1:B:415:GLN:CD	2.33	0.49
2:D:527:ARG:N	2:D:528:PRO:HD2	2.26	0.49
2:C:542:LEU:HB3	2:C:543:TYR:CE2	2.47	0.49
2:D:504:MET:HE1	2:D:591:LEU:HD21	1.92	0.49
1:A:134:ILE:HG23	1:A:135:GLU:N	2.26	0.49
1:A:371:ARG:HG2	1:A:442:LEU:HD11	1.95	0.49
2:C:597:ASN:C	2:C:599:GLU:H	2.20	0.49
1:A:23:TYR:CD1	2:C:509:THR:HG21	2.47	0.49
1:A:378:LEU:O	1:A:382:ILE:HG13	2.13	0.49
1:A:425:TYR:C	1:A:425:TYR:CD2	2.90	0.49
1:B:169:GLY:O	1:B:170:ILE:HG12	2.13	0.49
1:A:8:SER:HB3	1:A:11:ASP:OD1	2.13	0.49
1:A:41:GLN:HA	1:A:88:MET:HE1	1.93	0.49
1:A:144:ASN:HD21	1:A:148:THR:CG2	2.24	0.49
1:B:44:ILE:HD12	1:B:88:MET:CE	2.43	0.49
4:F:9:DA:O5'	4:F:9:DA:C2'	2.60	0.49
1:B:143:TRP:CE2	1:B:150:LYS:HE2	2.47	0.49
1:B:307:ASN:O	1:B:307:ASN:CG	2.56	0.49
2:C:520:THR:CG2	2:C:622:MET:HG3	2.40	0.49
1:A:63:ALA:CB	1:A:116:MET:HE3	2.41	0.48
1:B:456:GLU:HG3	1:B:460:TYR:HE2	1.77	0.48
2:C:583:LEU:HA	2:C:586:MET:HE3	1.94	0.48
2:D:597:ASN:ND2	2:D:600:THR:CB	2.76	0.48
1:A:352:HIS:O	1:A:353:ARG:C	2.56	0.48
1:B:25:ILE:HG22	1:B:26:GLN:N	2.28	0.48
2:D:423:ASN:O	2:D:425:ALA:N	2.46	0.48
1:B:131:LEU:O	1:B:134:ILE:HG22	2.13	0.48
2:D:516:THR:HG22	2:D:517:LEU:N	2.27	0.48
2:D:429:LEU:HD22	2:D:430:TYR:N	2.28	0.48
1:A:169:GLY:O	1:A:170:ILE:CG1	2.61	0.48
1:A:192:TYR:OH	1:A:203:LYS:HE2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ASN:HB3	1:B:114:ALA:HB2	1.96	0.48
2:D:477:ASN:C	2:D:479:MET:H	2.21	0.48
1:A:169:GLY:HA3	1:A:176:THR:O	2.12	0.48
1:A:316:PHE:CD2	1:A:321:LEU:HD13	2.48	0.48
1:B:462:LEU:O	1:B:463:MET:C	2.56	0.48
2:C:514:ILE:HA	2:C:517:LEU:HD12	1.94	0.48
2:D:523:TYR:C	2:D:523:TYR:CD2	2.91	0.48
2:C:479:MET:CE	2:C:522:PHE:CZ	2.97	0.48
1:A:45:LEU:CD2	1:A:123:LEU:HD22	2.43	0.48
1:A:412:THR:O	1:A:413:GLU:C	2.55	0.48
1:B:38:LYS:H	1:B:41:GLN:HE21	1.58	0.48
1:B:95:ARG:CA	1:B:214:PRO:HG3	2.40	0.48
1:B:283:GLY:CA	1:B:303:LYS:HD2	2.44	0.48
1:B:359:ALA:HA	1:B:362:ARG:NH1	2.29	0.48
2:C:626:VAL:HG11	4:F:10:DT:OP2	2.14	0.48
3:E:9:DC:H2''	3:E:10:DA:C5'	2.43	0.48
4:F:2:DG:C8	4:F:3:DT:H72	2.49	0.48
1:B:452:ILE:HA	1:B:458:THR:HG22	1.96	0.48
1:B:194:ILE:HG13	1:B:350:ILE:CD1	2.43	0.48
1:B:319:THR:OG1	1:B:321:LEU:HB2	2.14	0.48
2:C:540:PRO:HA	2:C:595:THR:CG2	2.44	0.48
1:B:380:ARG:NH2	1:B:409:TYR:O	2.32	0.47
1:A:254:ILE:HD13	1:A:312:LEU:HD12	1.96	0.47
1:B:385:LEU:HD22	1:B:389:ILE:HD12	1.96	0.47
2:C:439:GLY:C	2:C:441:ALA:N	2.72	0.47
2:C:479:MET:CE	2:C:522:PHE:HZ	2.28	0.47
2:C:558:ALA:C	2:C:559:TRP:CE3	2.92	0.47
1:A:187:ILE:O	1:A:188:ASP:C	2.57	0.47
1:A:452:ILE:HA	1:A:458:THR:HG22	1.95	0.47
1:B:326:ASN:N	1:B:326:ASN:HD22	2.10	0.47
1:A:259:ILE:HB	1:A:260:PRO:HD3	1.94	0.47
2:C:536:TYR:C	2:C:537:ILE:HG13	2.39	0.47
2:C:542:LEU:CB	2:C:543:TYR:CD2	2.96	0.47
1:B:412:THR:O	1:B:413:GLU:C	2.57	0.47
2:D:473:ASN:OD1	2:D:476:ILE:HG12	2.14	0.47
2:C:602:THR:C	2:C:603:LEU:HD23	2.40	0.47
1:B:43:ARG:NH1	1:B:74:HIS:ND1	2.62	0.47
1:B:34:ARG:HD2	1:B:352:HIS:ND1	2.30	0.47
1:B:333:ASP:O	1:B:334:ASN:C	2.58	0.47
2:C:610:ASP:O	2:C:612:ALA:N	2.48	0.47
1:A:219:ILE:CG2	1:A:236:VAL:HG11	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:PRO:HD3	2:C:639:PHE:CE1	2.51	0.46
1:A:350:ILE:HG12	1:A:463:MET:CE	2.45	0.46
2:D:466:LYS:C	2:D:468:ALA:H	2.23	0.46
1:A:60:ARG:NH1	1:A:60:ARG:CG	2.72	0.46
1:B:159:PHE:HB3	1:B:470:VAL:HG11	1.96	0.46
1:B:288:ARG:NH1	1:B:290:GLU:OE2	2.48	0.46
1:A:82:TYR:O	1:A:86:VAL:HG23	2.15	0.46
2:D:432:VAL:HG11	2:D:438:GLY:CA	2.44	0.46
1:A:36:GLY:CA	1:A:162:LEU:HB2	2.46	0.46
1:A:41:GLN:HA	1:A:88:MET:CE	2.45	0.46
1:A:334:ASN:O	1:A:335:PHE:HB2	2.14	0.46
1:B:44:ILE:CD1	1:B:88:MET:HE3	2.44	0.46
1:B:157:ALA:O	1:B:353:ARG:HD3	2.15	0.46
1:B:228:ALA:C	1:B:230:GLU:H	2.23	0.46
1:A:260:PRO:O	1:A:263:ILE:HB	2.16	0.46
2:C:639:PHE:O	2:C:640:THR:CB	2.63	0.46
1:B:91:ASN:HD22	1:B:91:ASN:N	2.13	0.46
2:D:423:ASN:O	2:D:423:ASN:CG	2.56	0.46
1:A:343:VAL:HB	1:A:344:PRO:HD3	1.98	0.46
1:A:382:ILE:HD12	1:A:432:VAL:HG22	1.98	0.46
1:B:49:ASN:HB2	1:B:131:LEU:CD1	2.46	0.46
1:B:53:ASN:ND2	1:B:60:ARG:HD2	2.31	0.46
1:B:70:MET:HE1	1:B:78:ASP:CA	2.45	0.46
1:B:285:ALA:HB3	1:B:301:GLU:HG2	1.97	0.46
1:B:338:ARG:HB3	1:B:340:VAL:HG13	1.98	0.46
1:B:372:LEU:HD22	1:B:376:GLU:HG3	1.98	0.46
2:C:542:LEU:CB	2:C:543:TYR:CE2	2.98	0.46
1:A:391:LEU:C	1:A:391:LEU:CD2	2.89	0.46
1:B:141:PHE:HE2	1:B:152:PRO:HD3	1.81	0.46
1:B:307:ASN:ND2	1:B:307:ASN:O	2.49	0.46
2:D:497:ASN:HB3	2:D:498:TYR:CD2	2.51	0.46
2:D:598:PRO:HA	2:D:601:ARG:HD3	1.98	0.46
1:A:190:ALA:HB2	1:A:346:LEU:HD22	1.98	0.45
1:A:280:LYS:HB3	1:A:280:LYS:HE3	1.60	0.45
1:A:381:VAL:O	1:A:385:LEU:N	2.49	0.45
1:B:325:TYR:CD1	1:B:325:TYR:C	2.94	0.45
1:A:73:PHE:O	1:A:75:PRO:HD3	2.16	0.45
1:A:100:GLU:O	1:A:121:ALA:HA	2.16	0.45
1:A:9:LEU:O	1:A:9:LEU:CD2	2.63	0.45
1:A:187:ILE:O	1:A:191:VAL:HG23	2.16	0.45
1:A:195:ASP:O	1:A:197:PRO:HD3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:ILE:HA	1:A:463:MET:HE1	1.97	0.45
1:A:28:ARG:NH1	3:E:14:DA:H4'	2.31	0.45
1:B:201:ILE:O	1:B:205:MET:HG3	2.17	0.45
1:B:321:LEU:HD23	1:B:321:LEU:HA	1.75	0.45
1:B:388:VAL:O	1:B:392:ILE:HG13	2.17	0.45
1:A:45:LEU:HD23	1:A:123:LEU:CD2	2.46	0.45
1:B:110:GLY:HA3	1:B:264:ASN:ND2	2.26	0.45
1:B:126:ILE:HG13	1:B:474:PHE:CE1	2.52	0.45
1:B:320:ASP:C	1:B:322:GLN:N	2.74	0.45
2:C:637:VAL:HG12	2:C:639:PHE:CD2	2.52	0.45
1:A:452:ILE:HA	1:A:458:THR:CG2	2.47	0.45
1:B:415:GLN:O	1:B:419:ILE:HG13	2.16	0.45
2:C:491:PHE:CD1	2:C:528:PRO:CG	2.99	0.45
2:D:467:MET:HA	2:D:470:ILE:HD12	1.99	0.45
1:A:24:ILE:HD12	1:A:28:ARG:NE	2.32	0.45
1:A:272:ILE:O	1:A:275:VAL:HB	2.17	0.45
1:B:239:ARG:NH1	1:B:316:PHE:CE1	2.84	0.45
1:B:242:THR:HG21	1:B:312:LEU:HD11	1.99	0.45
2:C:491:PHE:HD1	2:C:528:PRO:CG	2.30	0.45
6:H:6:DT:H2''	6:H:7:DG:H5'	1.98	0.45
1:A:139:VAL:HG21	1:A:154:VAL:O	2.17	0.45
1:A:403:GLU:O	1:A:407:VAL:HG23	2.18	0.44
2:C:514:ILE:O	2:C:515:GLN:C	2.59	0.44
1:A:350:ILE:HG12	1:A:463:MET:HE1	2.00	0.44
2:D:423:ASN:C	2:D:425:ALA:H	2.24	0.44
1:A:259:ILE:CB	1:A:260:PRO:CD	2.89	0.44
2:D:497:ASN:HB3	2:D:498:TYR:CE2	2.52	0.44
1:A:216:GLY:O	1:A:217:ALA:CB	2.65	0.44
1:B:90:GLN:NE2	1:B:92:TRP:CZ2	2.86	0.44
1:B:167:SER:O	1:B:168:THR:HG22	2.17	0.44
1:B:371:ARG:O	1:B:375:VAL:HG23	2.17	0.44
2:C:417:THR:HA	2:C:418:PRO:HD3	1.70	0.44
1:A:35:ASP:OD1	1:A:35:ASP:C	2.59	0.44
1:A:87:ARG:C	1:A:89:SER:N	2.75	0.44
1:A:320:ASP:C	1:A:322:GLN:N	2.74	0.44
1:B:217:ALA:N	1:B:258:GLU:OE1	2.44	0.44
1:B:459:MET:SD	1:B:459:MET:C	3.00	0.44
2:D:525:TYR:O	2:D:526:MET:CG	2.62	0.44
1:B:135:GLU:HG2	1:B:136:LYS:N	2.33	0.44
2:C:429:LEU:HD11	2:C:431:LEU:HD21	1.98	0.44
5:G:9:DC:H2''	5:G:10:DG:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:ILE:CD1	1:A:427:LEU:HD13	2.48	0.43
1:B:462:LEU:O	1:B:464:LYS:N	2.51	0.43
1:B:478:ARG:O	1:B:479:LEU:HD23	2.17	0.43
2:D:453:LEU:HD22	2:D:454:PRO:CD	2.48	0.43
1:A:87:ARG:O	1:A:89:SER:N	2.51	0.43
1:A:276:ARG:HD3	1:A:287:VAL:HG23	1.99	0.43
1:B:426:ARG:C	1:B:428:THR:H	2.26	0.43
1:B:288:ARG:HG2	2:C:420:GLN:NE2	2.33	0.43
1:B:414:GLU:H	1:B:414:GLU:CD	2.26	0.43
2:D:432:VAL:HG11	2:D:438:GLY:N	2.34	0.43
1:A:397:ASN:O	1:A:398:LYS:C	2.62	0.43
1:B:162:LEU:O	1:B:162:LEU:HD22	2.18	0.43
1:B:169:GLY:HA2	1:B:176:THR:HG22	2.00	0.43
1:B:346:LEU:O	1:B:350:ILE:CG1	2.66	0.43
2:D:466:LYS:O	2:D:468:ALA:N	2.51	0.43
1:A:213:PHE:CE2	1:A:219:ILE:CD1	3.01	0.43
1:B:311:VAL:O	1:B:315:LEU:HG	2.18	0.43
1:B:375:VAL:HG13	1:B:435:LEU:HD22	2.00	0.43
1:A:20:TYR:CZ	1:A:24:ILE:HG13	2.53	0.43
1:A:321:LEU:HD22	1:A:321:LEU:O	2.19	0.43
1:B:201:ILE:HD12	1:B:201:ILE:H	1.84	0.43
1:B:228:ALA:C	1:B:230:GLU:N	2.76	0.43
2:D:491:PHE:HD1	2:D:528:PRO:HG2	1.84	0.43
1:A:144:ASN:OD1	1:A:147:ASP:N	2.52	0.43
1:A:342:ILE:HA	1:A:342:ILE:HD12	1.72	0.43
1:B:41:GLN:CG	1:B:88:MET:HE2	2.41	0.43
1:B:342:ILE:HD12	1:B:342:ILE:HA	1.89	0.43
1:B:352:HIS:O	1:B:353:ARG:C	2.61	0.43
1:B:385:LEU:HD21	1:B:427:LEU:CD2	2.43	0.43
1:A:194:ILE:CG1	1:A:463:MET:HE2	2.48	0.43
1:A:451:ALA:O	1:A:452:ILE:C	2.61	0.43
1:B:28:ARG:HH11	1:B:28:ARG:CG	2.31	0.43
1:B:357:ILE:HD12	1:B:463:MET:CG	2.47	0.43
1:B:236:VAL:HG12	1:B:327:PHE:HE2	1.84	0.43
1:B:285:ALA:CB	1:B:301:GLU:HG2	2.48	0.43
1:B:375:VAL:O	1:B:379:ILE:HD12	2.19	0.43
2:D:466:LYS:O	2:D:470:ILE:HG13	2.19	0.43
1:A:244:ILE:N	1:A:244:ILE:CD1	2.79	0.43
1:B:146:ASP:O	1:B:147:ASP:HB2	2.18	0.43
1:B:440:ALA:O	1:B:442:LEU:N	2.52	0.43
1:A:276:ARG:HG2	1:A:276:ARG:HH11	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:VAL:O	1:A:420:VAL:HG13	2.18	0.42
1:B:254:ILE:HB	1:B:300:ILE:HB	2.01	0.42
1:B:442:LEU:O	1:B:446:ILE:HG13	2.18	0.42
1:A:464:LYS:HB2	1:A:464:LYS:HE2	1.87	0.42
1:B:49:ASN:CG	1:B:131:LEU:HD13	2.44	0.42
1:B:352:HIS:C	1:B:354:ARG:N	2.77	0.42
2:D:597:ASN:O	2:D:601:ARG:HB3	2.19	0.42
1:A:185:GLU:OE1	1:A:209:PRO:HD2	2.20	0.42
1:A:385:LEU:HD23	1:A:385:LEU:HA	1.78	0.42
1:B:167:SER:O	1:B:168:THR:CB	2.67	0.42
1:B:296:LEU:C	1:B:296:LEU:CD2	2.91	0.42
1:A:56:ASP:OD1	1:A:56:ASP:N	2.51	0.42
1:B:195:ASP:C	1:B:197:PRO:HD3	2.44	0.42
1:B:361:SER:O	1:B:365:LYS:HB2	2.19	0.42
1:B:476:THR:CB	1:B:477:PRO:CD	2.96	0.42
1:A:163:LEU:HG	1:A:345:ILE:HG21	2.00	0.42
1:B:420:VAL:HG12	1:B:421:THR:HG23	2.00	0.42
1:B:204:LEU:HD23	1:B:204:LEU:HA	1.88	0.42
6:H:3:DC:H4'	6:H:4:DT:OP1	2.19	0.42
1:A:87:ARG:HA	1:A:90:GLN:CG	2.50	0.42
1:A:471:LYS:O	1:A:475:ALA:HB2	2.20	0.42
2:C:489:ALA:C	2:C:491:PHE:N	2.74	0.42
2:C:524:ARG:CB	2:C:525:TYR:HD1	2.31	0.42
2:D:431:LEU:HD11	2:D:479:MET:HE2	2.02	0.42
2:D:514:ILE:O	2:D:515:GLN:C	2.62	0.42
1:A:146:ASP:OD2	1:A:146:ASP:C	2.63	0.42
1:A:207:PHE:O	1:A:209:PRO:HD3	2.19	0.42
1:A:240:SER:HB2	1:A:321:LEU:HD22	2.02	0.42
1:B:220:GLN:HA	1:B:483:GLU:O	2.20	0.42
1:B:112:PRO:HA	1:B:113:PRO:HD3	1.84	0.42
1:B:334:ASN:O	1:B:335:PHE:HB2	2.19	0.42
1:A:355:GLU:OE2	1:A:355:GLU:CA	2.67	0.42
2:C:491:PHE:CE2	2:C:526:MET:HE3	2.53	0.42
2:C:633:ILE:O	2:C:637:VAL:HB	2.20	0.42
1:A:44:ILE:HB	1:A:88:MET:HE1	2.01	0.41
1:A:459:MET:SD	1:A:459:MET:C	3.03	0.41
1:B:402:LYS:NZ	1:B:417:GLU:OE1	2.53	0.41
1:A:326:ASN:OD1	4:F:11:DG:H5''	2.20	0.41
1:A:403:GLU:HA	1:A:406:LYS:HD2	2.01	0.41
1:B:53:ASN:CG	1:B:60:ARG:HD2	2.44	0.41
1:A:90:GLN:HE21	1:A:90:GLN:HB3	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:LEU:HD23	1:A:435:LEU:HA	1.64	0.41
2:C:439:GLY:C	2:C:441:ALA:H	2.26	0.41
2:C:630:ARG:HG2	2:C:634:GLU:OE2	2.20	0.41
1:A:95:ARG:HA	1:A:214:PRO:HB3	2.03	0.41
1:B:353:ARG:HD2	1:B:353:ARG:HA	1.79	0.41
1:A:29:ALA:HB3	1:A:171:SER:HB3	2.02	0.41
1:B:141:PHE:CD2	1:B:151:GLU:C	2.99	0.41
1:B:463:MET:HE2	1:B:463:MET:HB3	1.14	0.41
2:C:506:ASP:C	2:C:508:ASP:H	2.28	0.41
2:C:590:GLN:O	2:C:594:THR:HG23	2.20	0.41
1:A:325:TYR:CD1	1:A:325:TYR:C	2.98	0.41
1:B:462:LEU:C	1:B:464:LYS:N	2.79	0.41
1:A:24:ILE:HA	1:A:28:ARG:HB2	2.02	0.41
1:A:194:ILE:HG12	1:A:463:MET:HE2	2.03	0.41
1:A:350:ILE:HG23	1:A:463:MET:HE1	2.03	0.41
1:B:9:LEU:CD1	2:D:523:TYR:HD1	2.34	0.41
1:B:28:ARG:NH2	2:D:510:ASP:OD2	2.54	0.41
2:C:503:ILE:CG2	2:C:518:LEU:HD12	2.51	0.41
2:D:424:PRO:HA	2:D:497:ASN:O	2.21	0.41
1:B:37:LEU:HD23	1:B:37:LEU:HA	1.89	0.41
1:B:139:VAL:CG1	1:B:140:PRO:HD2	2.45	0.41
1:B:190:ALA:HB2	1:B:346:LEU:CD2	2.51	0.41
2:C:422:LYS:O	2:C:424:PRO:HD3	2.20	0.41
1:A:48:MET:HE2	1:A:48:MET:HB3	1.83	0.41
1:A:96:GLU:OE2	1:A:96:GLU:HA	2.20	0.41
1:B:168:THR:HA	1:B:169:GLY:HA3	1.74	0.41
1:B:268:LEU:O	1:B:272:ILE:HG13	2.21	0.41
1:B:353:ARG:O	1:B:357:ILE:HG13	2.20	0.41
1:B:424:LEU:HD23	1:B:424:LEU:HA	1.93	0.41
2:C:429:LEU:CD1	2:C:431:LEU:HD21	2.51	0.41
2:C:622:MET:HE3	2:C:622:MET:HB3	1.86	0.41
1:A:108:MET:HE3	9:A:618:HOH:O	2.20	0.41
1:A:243:GLU:C	1:A:244:ILE:HD12	2.46	0.41
1:B:455:ASP:OD2	1:B:458:THR:CB	2.69	0.41
1:A:159:PHE:HB3	1:A:470:VAL:HG11	2.03	0.40
1:A:168:THR:HA	1:A:169:GLY:HA3	1.77	0.40
1:A:329:MET:HE1	1:A:345:ILE:HD12	2.03	0.40
1:A:329:MET:HE3	1:A:329:MET:HB3	1.87	0.40
1:B:201:ILE:HD12	1:B:201:ILE:N	2.35	0.40
4:F:1:DA:C2	4:F:2:DG:C6	3.09	0.40
1:A:260:PRO:HG2	1:A:320:ASP:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:ILE:CB	1:B:260:PRO:CD	2.92	0.40
2:C:432:VAL:HA	2:C:504:MET:O	2.21	0.40
1:A:387:GLU:HA	1:A:390:ALA:HB3	2.03	0.40
1:A:49:ASN:HB2	1:A:131:LEU:HD13	2.02	0.40
1:A:337:PRO:HD3	2:C:639:PHE:HE1	1.86	0.40
2:D:461:ASN:OD1	2:D:461:ASN:C	2.63	0.40
4:F:3:DT:H4'	4:F:4:DC:OP1	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	480/496 (97%)	432 (90%)	40 (8%)	8 (2%)	7	27
1	B	480/496 (97%)	414 (86%)	57 (12%)	9 (2%)	6	25
2	C	203/268 (76%)	175 (86%)	23 (11%)	5 (2%)	4	20
2	D	202/268 (75%)	176 (87%)	22 (11%)	4 (2%)	6	24
All	All	1365/1528 (89%)	1197 (88%)	142 (10%)	26 (2%)	6	25

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	PHE
1	B	168	THR
1	B	217	ALA
2	D	569	LYS
2	D	610	ASP
1	A	169	GLY
1	A	217	ALA
1	A	305	ASP

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Mol	Chain	Res	Type
2	C	611	LEU
2	D	424	PRO
2	D	447	ARG
1	A	88	MET
1	B	382	ILE
1	B	463	MET
2	C	436	SER
1	A	168	THR
1	B	334	ASN
1	B	427	LEU
2	C	424	PRO
1	A	170	ILE
1	B	441	GLU
2	C	490	ASP
1	B	169	GLY
2	C	598	PRO
1	A	221	GLY
1	B	221	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	371/431 (86%)	322 (87%)	49 (13%)	4	15
1	B	372/431 (86%)	314 (84%)	58 (16%)	2	10
2	C	104/224 (46%)	90 (86%)	14 (14%)	4	15
2	D	102/224 (46%)	91 (89%)	11 (11%)	6	22
All	All	949/1310 (72%)	817 (86%)	132 (14%)	3	14

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	28	ARG
1	A	34	ARG

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Mol	Chain	Res	Type
1	A	48	MET
1	A	60	ARG
1	A	90	GLN
1	A	91	ASN
1	A	96	GLU
1	A	97	ILE
1	A	102	HIS
1	A	111	ASP
1	A	117	ARG
1	A	134	ILE
1	A	146	ASP
1	A	154	VAL
1	A	168	THR
1	A	183	LEU
1	A	208	LEU
1	A	236	VAL
1	A	237	VAL
1	A	242	THR
1	A	268	LEU
1	A	279	ASN
1	A	293	ARG
1	A	321	LEU
1	A	322	GLN
1	A	329	MET
1	A	336	THR
1	A	338	ARG
1	A	342	ILE
1	A	355	GLU
1	A	360	ARG
1	A	366	GLU
1	A	371	ARG
1	A	380	ARG
1	A	385	LEU
1	A	387	GLU
1	A	389	ILE
1	A	391	LEU
1	A	412	THR
1	A	414	GLU
1	A	420	VAL
1	A	433	VAL
1	A	434	VAL
1	A	443	ARG

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Mol	Chain	Res	Type
1	A	452	ILE
1	A	458	THR
1	A	462	LEU
1	A	469	GLU
1	B	4	ILE
1	B	9	LEU
1	B	24	ILE
1	B	26	GLN
1	B	28	ARG
1	B	34	ARG
1	B	58	SER
1	B	70	MET
1	B	79	SER
1	B	81	ILE
1	B	90	GLN
1	B	91	ASN
1	B	95	ARG
1	B	96	GLU
1	B	98	LEU
1	B	117	ARG
1	B	120	GLU
1	B	126	ILE
1	B	139	VAL
1	B	146	ASP
1	B	162	LEU
1	B	167	SER
1	B	168	THR
1	B	177	ASP
1	B	198	THR
1	B	208	LEU
1	B	236	VAL
1	B	238	VAL
1	B	268	LEU
1	B	281	VAL
1	B	294	ASP
1	B	307	ASN
1	B	310	LEU
1	B	321	LEU
1	B	326	ASN
1	B	336	THR
1	B	338	ARG
1	B	339	GLN

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Mol	Chain	Res	Type
1	B	347	SER
1	B	350	ILE
1	B	365	LYS
1	B	372	LEU
1	B	374	ILE
1	B	381	VAL
1	B	385	LEU
1	B	389	ILE
1	B	404	ASN
1	B	407	VAL
1	B	410	ASP
1	B	412	THR
1	B	414	GLU
1	B	420	VAL
1	B	429	ASN
1	B	431	ASP
1	B	432	VAL
1	B	456	GLU
1	B	458	THR
1	B	463	MET
2	C	416	LEU
2	C	417	THR
2	C	440	SER
2	C	447	ARG
2	C	453	LEU
2	C	459	VAL
2	C	462	THR
2	C	478	THR
2	C	509	THR
2	C	514	ILE
2	C	517	LEU
2	C	523	TYR
2	C	524	ARG
2	C	595	THR
2	D	429	LEU
2	D	453	LEU
2	D	462	THR
2	D	478	THR
2	D	482	THR
2	D	497	ASN
2	D	501	ILE
2	D	516	THR

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Mol	Chain	Res	Type
2	D	524	ARG
2	D	591	LEU
2	D	595	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	53	ASN
1	A	68	ASN
1	A	90	GLN
1	A	91	ASN
1	A	94	ASN
1	A	181	HIS
1	A	253	GLN
1	A	267	ASN
1	A	313	ASN
1	A	334	ASN
1	A	339	GLN
1	B	41	GLN
1	B	53	ASN
1	B	68	ASN
1	B	76	HIS
1	B	91	ASN
1	B	196	HIS
1	B	253	GLN
1	B	264	ASN
1	B	267	ASN
1	B	307	ASN
1	B	322	GLN
1	B	326	ASN
1	B	415	GLN
2	C	420	GLN
2	C	423	ASN
2	C	427	ASN
2	C	461	ASN
2	C	477	ASN
2	C	636	ASN
2	D	497	ASN
2	D	597	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 6 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
8	NFX	H	101	7	28,28,28	1.22	3 (10%)	35,43,43	1.41	5 (14%)
8	NFX	F	101	7	28,28,28	1.21	3 (10%)	35,43,43	1.42	6 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NFX	H	101	7	-	5/12/23/23	0/4/4/4
8	NFX	F	101	7	-	4/12/23/23	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	101	NFX	C11-C13	2.52	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	101	NFX	C11-C13	2.51	1.43	1.40
8	H	101	NFX	C12-N	2.42	1.43	1.40
8	F	101	NFX	C12-N	2.40	1.43	1.40
8	F	101	NFX	C12-C13	2.19	1.43	1.40
8	H	101	NFX	C12-C13	2.19	1.43	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	101	NFX	C06-N-C16	-3.46	114.67	119.74
8	H	101	NFX	C06-N-C16	-3.46	114.67	119.74
8	F	101	NFX	C16-C18-C19	-3.01	117.73	119.94
8	H	101	NFX	C16-C18-C19	-3.00	117.74	119.94
8	F	101	NFX	C09-C06-N	2.68	123.11	118.87
8	H	101	NFX	C09-C06-N	2.66	123.08	118.87
8	F	101	NFX	O02-C19-C18	-2.32	119.34	123.07
8	H	101	NFX	O02-C19-C18	-2.30	119.38	123.07
8	F	101	NFX	C12-N-C06	2.09	124.54	122.35
8	H	101	NFX	C12-N-C06	2.08	124.53	122.35
8	F	101	NFX	C08-C06-N	2.01	122.05	118.87

There are no chirality outliers.

All (9) torsion outliers are listed below:

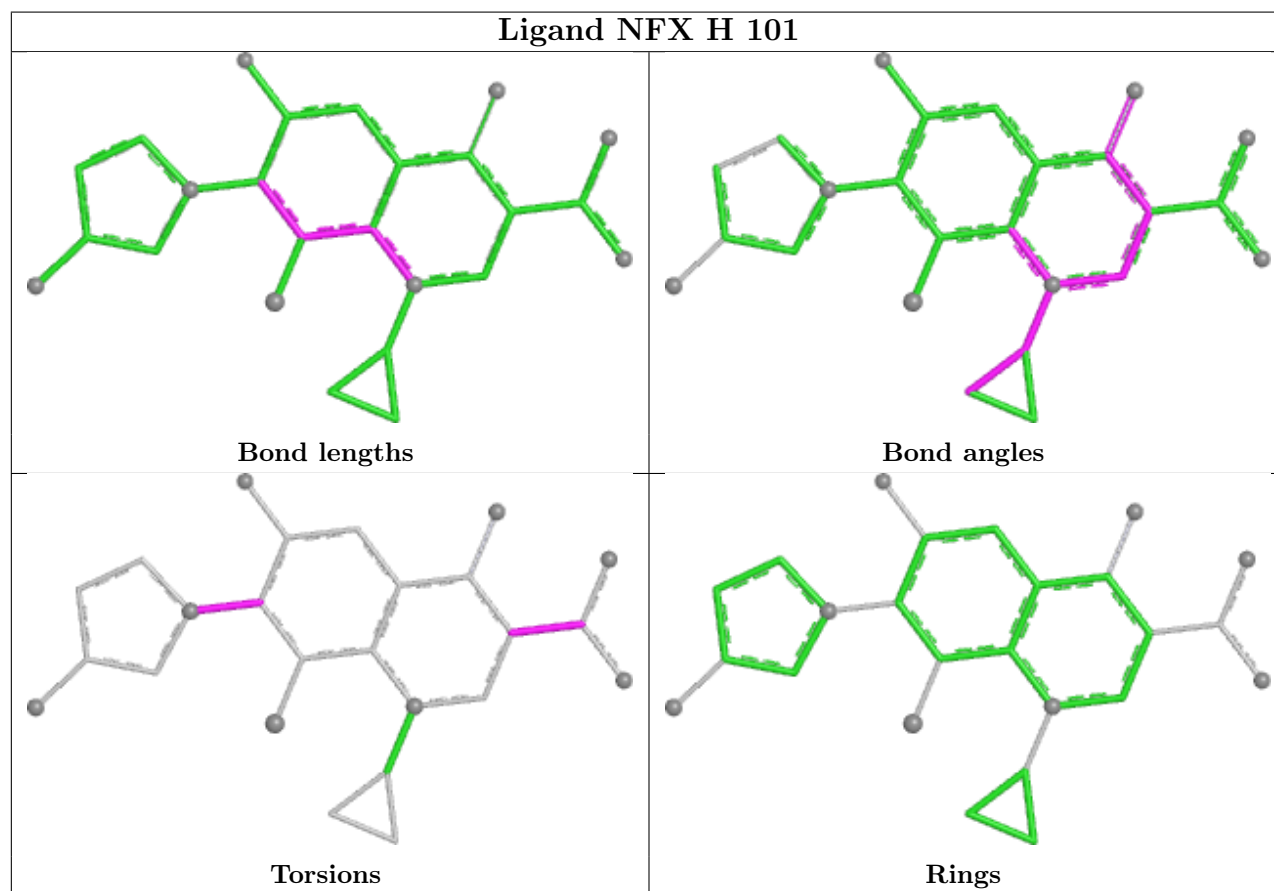
Mol	Chain	Res	Type	Atoms
8	F	101	NFX	C19-C18-C20-O03
8	H	101	NFX	C19-C18-C20-O03
8	F	101	NFX	C19-C18-C20-O
8	H	101	NFX	C19-C18-C20-O
8	F	101	NFX	C16-C18-C20-O03
8	F	101	NFX	C16-C18-C20-O
8	H	101	NFX	C16-C18-C20-O03
8	H	101	NFX	C16-C18-C20-O
8	H	101	NFX	C13-C11-N01-C03

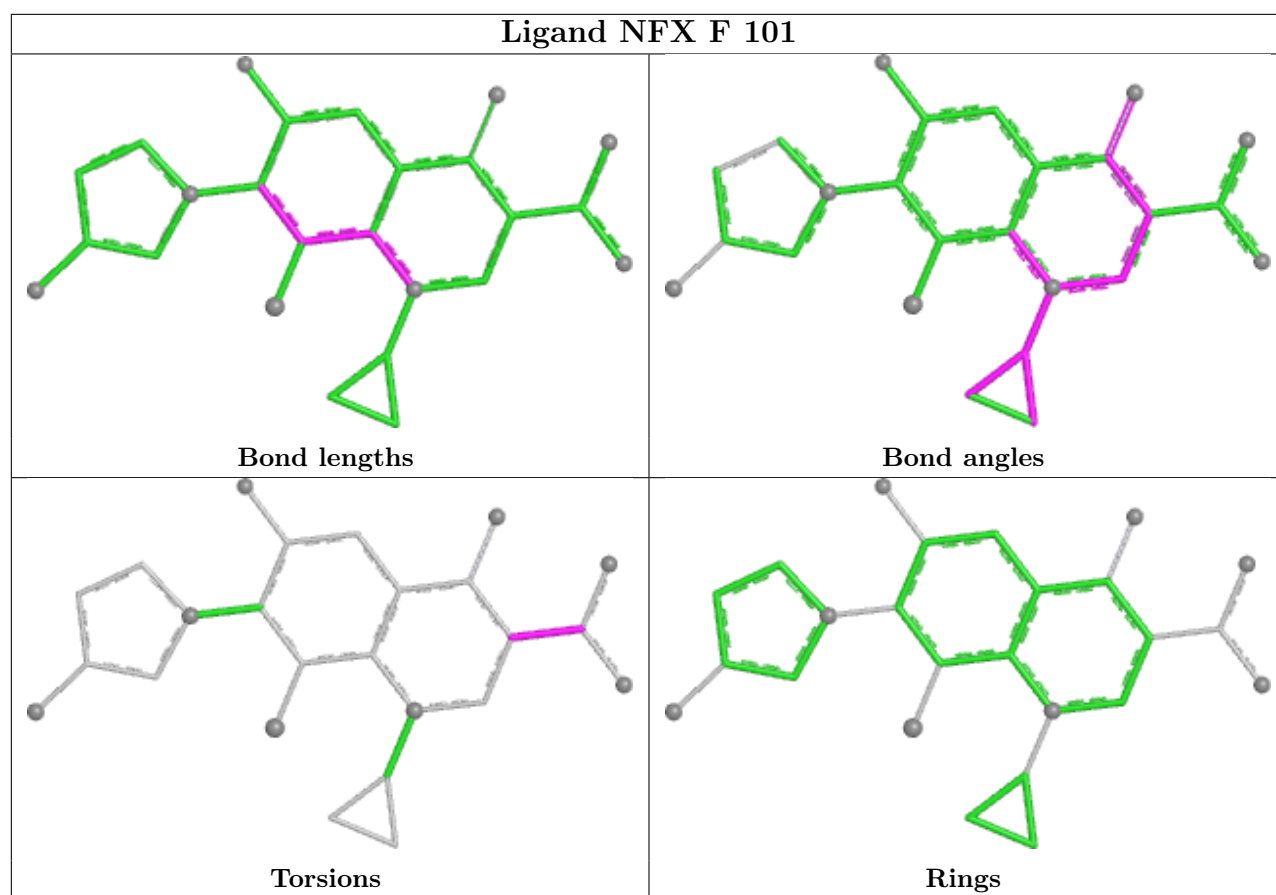
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	H	101	NFX	4	0
8	F	101	NFX	4	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 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 [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	482/496 (97%)	-0.59	0 100 100	55, 80, 119, 141	0
1	B	482/496 (97%)	-0.48	3 (0%) 85 75	50, 79, 114, 146	0
2	C	209/268 (77%)	0.01	5 (2%) 59 44	88, 119, 153, 173	0
2	D	208/268 (77%)	0.08	5 (2%) 59 44	82, 119, 155, 174	0
3	E	7/7 (100%)	-0.07	0 100 100	86, 91, 128, 158	0
4	F	11/11 (100%)	-0.34	0 100 100	98, 113, 140, 158	0
5	G	7/7 (100%)	0.24	0 100 100	77, 87, 126, 149	0
6	H	11/11 (100%)	-0.58	0 100 100	90, 104, 130, 145	0
All	All	1417/1564 (90%)	-0.36	13 (0%) 81 69	50, 90, 140, 174	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	581	LYS	3.2
2	D	584	GLY	3.2
2	D	640	THR	2.7
1	B	3	ASN	2.7
1	B	252	GLU	2.4
2	C	584	GLY	2.4
2	D	585	GLU	2.4
2	D	561	ASP	2.4
2	C	544	LYS	2.3
2	C	581	LYS	2.3
1	B	484	ASP	2.3
2	C	565	GLU	2.1
2	C	458	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

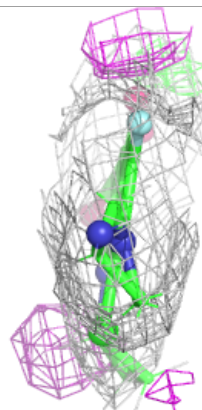
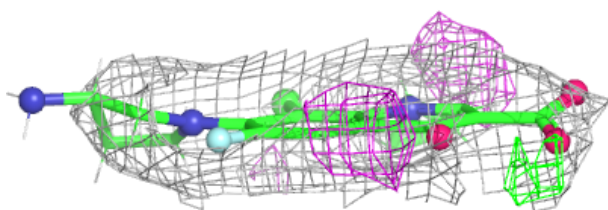
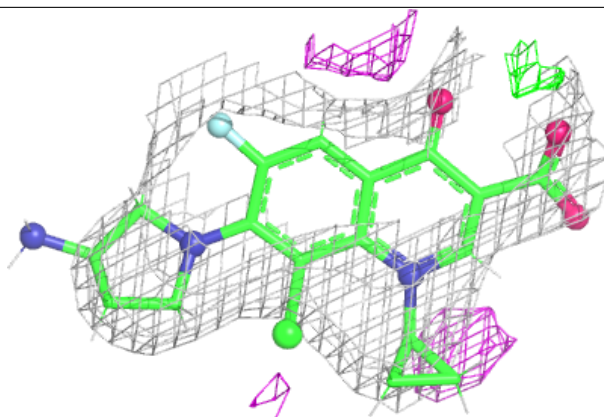
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MG	A	502	1/1	0.84	0.23	121,121,121,121	0
7	MG	C	701	1/1	0.86	0.22	87,87,87,87	0
7	MG	B	502	1/1	0.89	0.18	119,119,119,119	0
7	MG	D	701	1/1	0.89	0.23	78,78,78,78	0
7	MG	B	501	1/1	0.90	0.07	101,101,101,101	0
7	MG	A	501	1/1	0.93	0.06	87,87,87,87	0
8	NFX	F	101	25/25	0.93	0.12	120,135,161,235	0
8	NFX	H	101	25/25	0.94	0.10	118,143,190,200	0

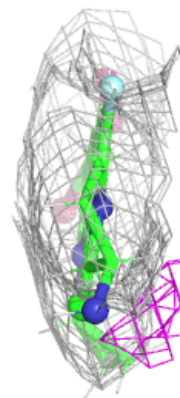
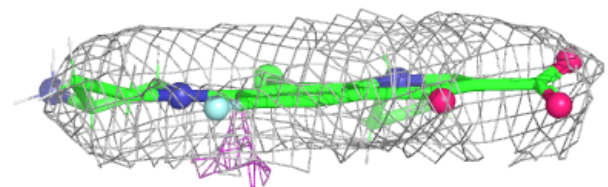
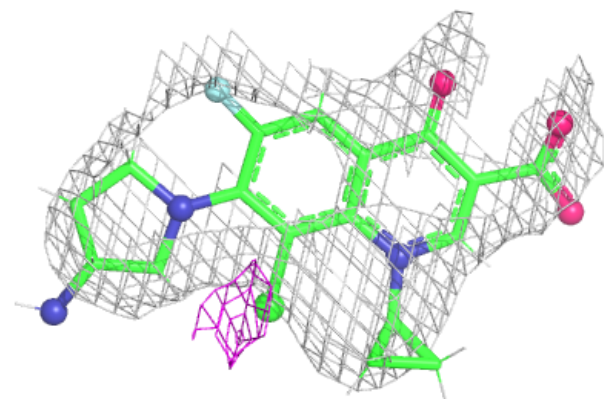
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NFX F 101:

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

**Electron density around NFX H 101:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.