WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 07:00 PM EDT

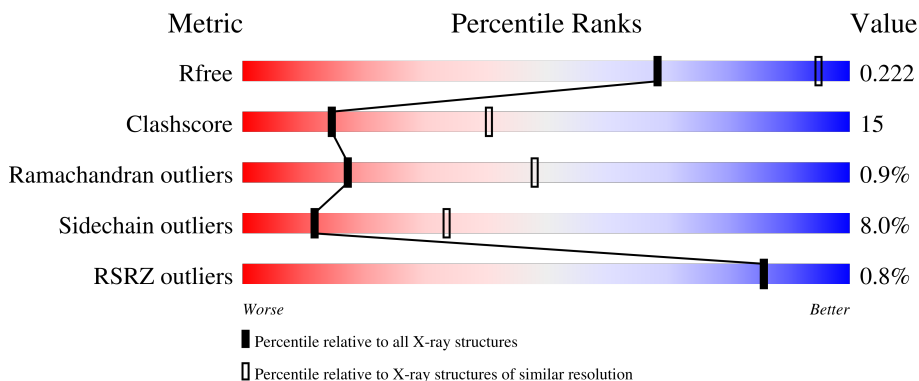|		
PDB ID	:	3RAE
Title	:	Quinolone(Levofloxacin)-DNA cleavage complex of type IV topoisomerase from S. pneumoniae
Authors	:	Laponogov, I.; Pan, X.-S.; Veselkov, D.A.; McAuley, K.E.; Fisher, L.M.; Sanderson, M.R.
Deposited on	:	2011-03-28
Resolution	:	2.90 Å(reported)

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.90 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.
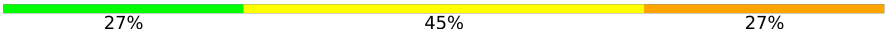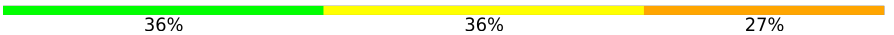
Metric	Percentile Ranks	Value
Rfree		0.222
Clashscore		15
Ramachandran outliers		0.9%
Sidechain outliers		8.0%
RSRZ outliers		0.8%

Worse *Better*

▎ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	496	71% 23% · ·
1	B	496	69% 26% · ·
2	C	268	3% 53% 21% · 22%
2	D	268	% 61% 14% · 22%

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Mol	Chain	Length	Quality of chain
3	E	7	29% 57% 14%
4	F	11	27% 45% 27%
5	G	7	57% 43%
6	H	11	36% 36% 27%

2 Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 11234 atoms, of which 38 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total 3736	C 2366	N 648	O 709	S 13	0	1	0
1	B	482	Total 3717	C 2359	N 640	O 705	S 13	0	1	0

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	208	Total 1445	C 917	N 254	O 268	S 6	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	209	1456	924	253	273	6	0	0	0

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
			Total	C	N	O	P			
3	E	7	140	69	27	38	6	0	0	0

- 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
			Total	C	N	O	P			
4	F	11	225	108	39	67	11	0	0	0

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

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

- 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
			Total	C	N	O	P			
6	H	11	226	107	43	65	11	0	0	0

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

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

- Molecule 8 is (3S)-9-fluoro-3-methyl-10-(4-methylpiperazin-1-yl)-7-oxo-2,3-dihydro-7H-[1,4]oxazino[2,3,4-ij]quinoline-6-carboxylic acid (three-letter code: LFX) (formula: $C_{18}H_{20}FN_3O_4$).
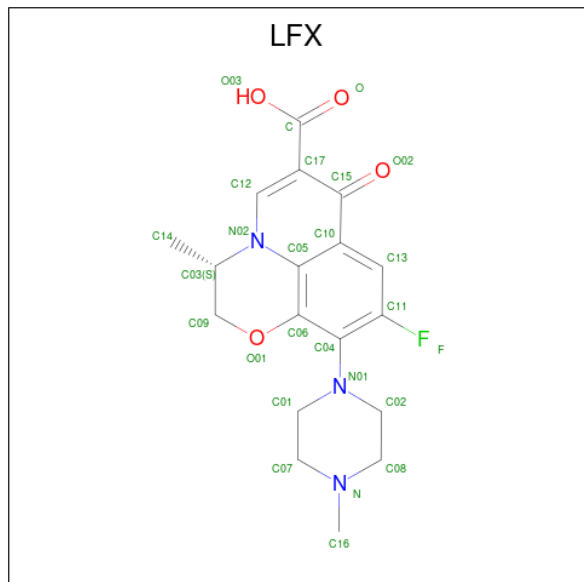
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	F	1	Total 45	C 18	F 1	H 19	N 3	O 4	0	0
8	H	1	Total 45	C 18	F 1	H 19	N 3	O 4	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	23	Total 23	O 23	0	0
9	B	21	Total 21	O 21	0	0

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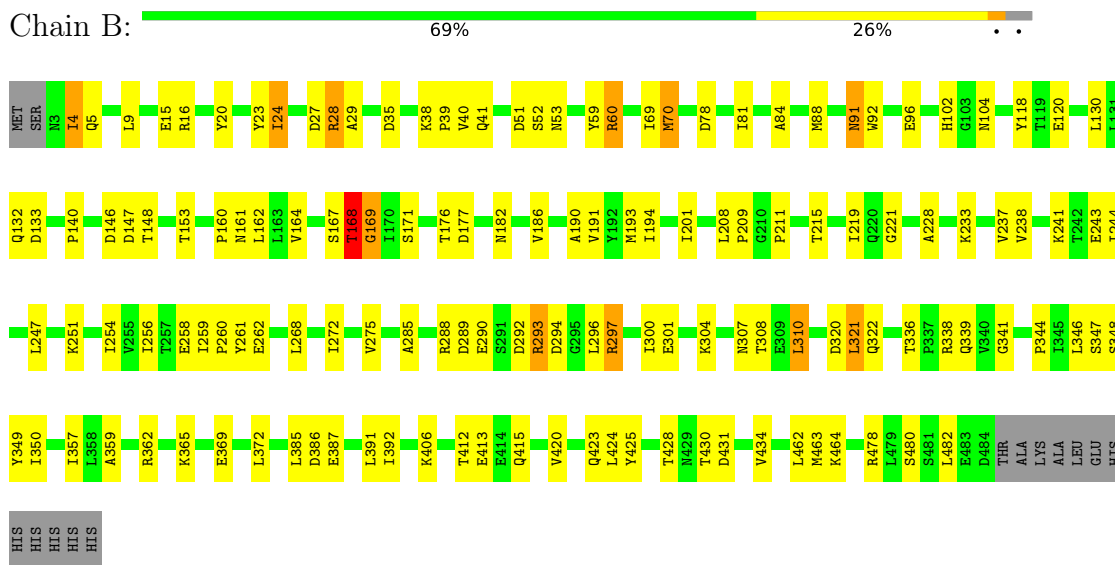| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total 1	O 1	0	0
9	D	3	Total 3	O 3	0	0
9	E	4	Total 4	O 4	0	0
9	G	2	Total 2	O 2	0	0

3 Residue-property plots ⓘ

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.

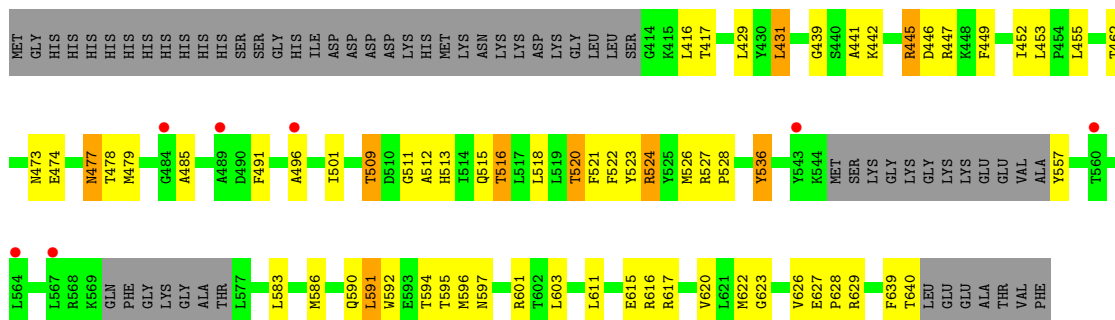• Molecule 1: DNA topoisomerase 4 subunit A
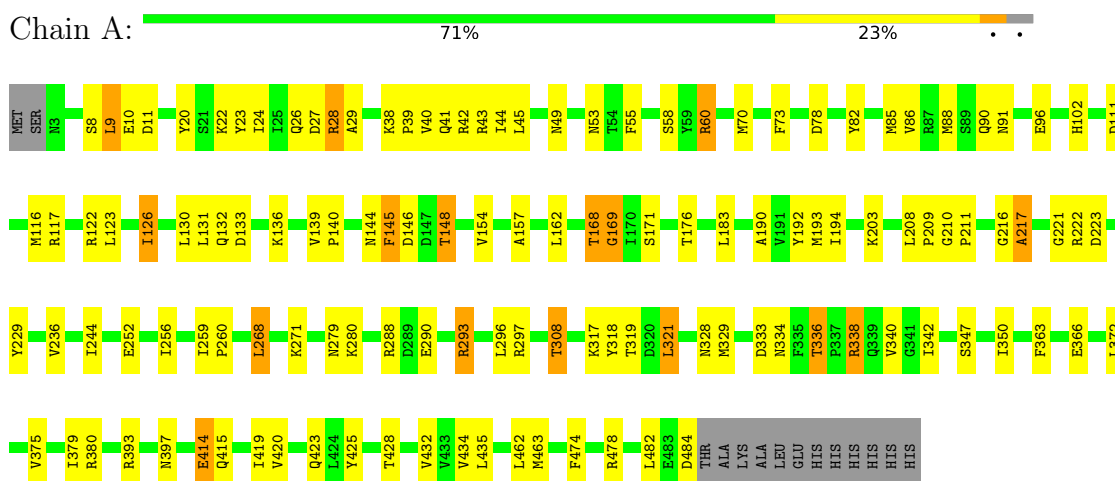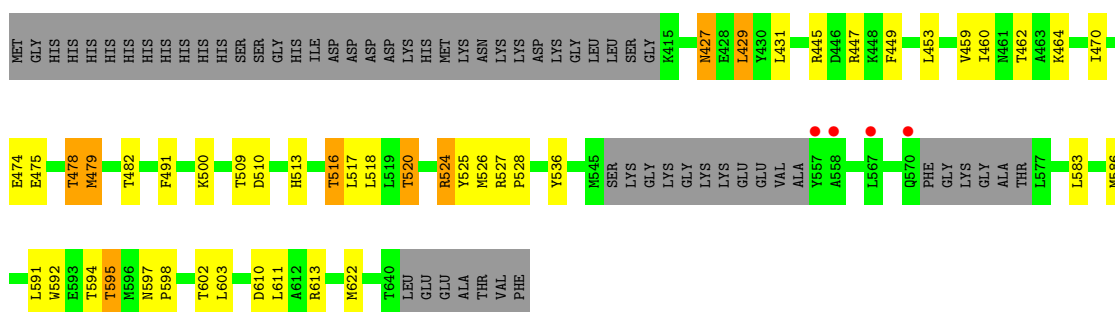

• Molecule 1: DNA topoisomerase 4 subunit A

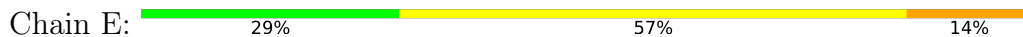• Molecule 2: DNA topoisomerase 4 subunit B

MET GLY HIS HIS HIS HIS HIS HIS HIS HIS SER SER GLY HIS ILE ASP ASP ASP ASP LYS HIS MET LYS ASN LYS LYS ASP LYS GLY LEU LEU SER G414 K415 L416 T417 L429 Y430 L431 G439 S440 A441 K442 R445 D446 R447 K448 F449 I452 L453 P454 L455 T462

N473 E474 N477 T478 M479 G484 A485 A489 D490 F491 A496 I501 T509 D510 G511 A512 H513 I514 Q515 T516 L517 L518 L519 T520 F521 F522 Y523 R524 Y525 M526 R527 P528 Y536 Y543 K544 MET SER LYS LYS GLY LYS LYS GLU VAL ALA Y557 T560

L564 L567 R568 K569 GLN PHE GLY LYS ALA THR L577 L583 M586 Q590 L591 W592 E593 T594 T595 M596 N597 R601 T602 L603 L611 E615 R616 R617 V620 L621 M622 G623 V626 E627 P628 R629 F639 T640 LEU GLU GLU ALA THR VAL PHE

• Molecule 2: DNA topoisomerase 4 subunit B

Chain D:

61%   14%   •   22%

MET GLY HIS HIS HIS HIS HIS HIS HIS HIS SER SER GLY HIS ILE ASP ASP ASP ASP LYS HIS MET LYS ASN LYS LYS ASP LYS GLY LEU LEU SER GLY K415 N427 E428 L429 Y430 L431 R445 D446 R447 K448 F449 L453 V459 I460 N461 T462 A463 K464 I470

E474 E475 T478 M479 T482 F491 K500 T509 D510 H513 T516 L517 L518 L519 T520 R524 Y525 M526 R527 P528 Y536 M545 SER LYS GLY LYS LYS GLY LYS GLU GLU VAL ALA Y557 A558 L567 Q570 PHE GLY LYS GLY ALA THR L577 L583 M586

L591 W592 E593 T594 T595 M596 N597 P598 T602 L603 D610 L611 A612 R613 M622 T640 LEU GLU GLU ALA THR VAL PHE

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

Chain E:

29%   57%   14%

C9 A10 T11 G12 A13 A14 T15

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

Chain F:

27%   45%   27%

A1 G2 T3 C4 A5 T6 T7 C8 A9 T10 G11
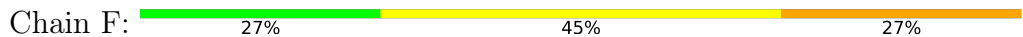
• Molecule 5: 5'-D(*CP*GP*TP*GP*CP*AP*T)-3'

Chain G:

57%   43%

C9 G12 C13 A14 T15
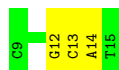
• Molecule 6: 5'-D(P*GP*AP*CP*TP*AP*TP*GP*CP*AP*CP*G)-3'

Chain H:

36%   36%   27%

G1 A2 C3 T4 A5 T6 C10 G11
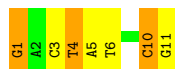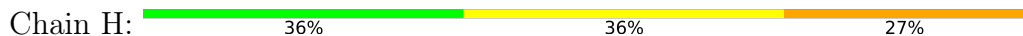
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	157.83Å　　157.83Å　　211.15Å 90.00°　　90.00°　　120.00°	Depositor
Resolution (Å)	41.83　–　2.90 41.83　–　2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (41.83-2.90) 99.0 (41.83-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.186　,　0.226 0.180　,　0.222	Depositor DCC
R_{free} test set	9357 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å^2)	61.9	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 50.5	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.048 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11234	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: LFX, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.45	0/3800	0.64	1/5146 (0.0%)
1	B	0.44	0/3781	0.60	0/5126
2	C	0.32	0/1471	0.52	0/2008
2	D	0.35	0/1482	0.54	0/2022
3	E	0.88	0/157	1.64	3/241 (1.2%)
4	F	0.83	0/251	1.80	12/385 (3.1%)
5	G	0.76	0/155	1.42	1/238 (0.4%)
6	H	0.76	0/253	1.67	4/388 (1.0%)
All	All	0.46	0/11350	0.74	21/15554 (0.1%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	10	DC	O4'-C4'-C3'	-12.00	98.80	106.00
4	F	1	DA	O4'-C1'-N9	10.84	115.59	108.00
3	E	10	DA	O4'-C1'-N9	8.06	113.64	108.00
6	H	1	DG	O4'-C1'-N9	7.97	113.58	108.00
4	F	3	DT	O4'-C4'-C3'	-7.87	101.28	106.00
4	F	6	DT	O4'-C4'-C3'	-6.72	101.81	104.50
4	F	5	DA	O4'-C1'-N9	6.56	112.59	108.00
3	E	11	DT	C4-C5-C7	6.00	122.60	119.00
4	F	3	DT	O4'-C1'-N1	5.98	112.19	108.00
1	A	183	LEU	CA-CB-CG	5.93	128.95	115.30
5	G	12	DG	O4'-C1'-N9	-5.92	103.86	108.00
4	F	6	DT	C4'-C3'-C2'	-5.81	97.87	103.10
4	F	6	DT	C1'-O4'-C4'	-5.78	104.32	110.10
4	F	8	DC	C1'-O4'-C4'	-5.60	104.50	110.10
4	F	3	DT	C5-C4-O4	-5.52	121.03	124.90
4	F	1	DA	C3'-C2'-C1'	-5.44	95.97	102.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	1	DA	C1'-O4'-C4'	-5.13	104.97	110.10
3	E	11	DT	C6-C5-C7	-5.10	119.84	122.90
4	F	1	DA	O4'-C1'-C2'	-5.09	101.83	105.90
6	H	10	DC	C1'-O4'-C4'	-5.08	105.02	110.10
6	H	4	DT	O4'-C4'-C3'	-5.06	102.47	104.50

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	3736	0	3650	111	0
1	B	3717	0	3630	118	0
2	C	1445	0	1242	57	0
2	D	1456	0	1243	44	0
3	E	140	0	78	2	0
4	F	225	0	126	5	0
5	G	139	0	78	2	0
6	H	226	0	124	9	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	G	1	0	0	0	0
8	F	26	19	19	0	0
8	H	26	19	19	1	0
9	A	23	0	0	1	0
9	B	21	0	0	0	0
9	C	1	0	0	0	0
9	D	3	0	0	0	0
9	E	4	0	0	0	0
9	G	2	0	0	0	0
All	All	11196	38	10209	327	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 15.

All (327) 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:A:60:ARG:HH11	1:A:60:ARG:HB2	1.07	1.19
1:A:28:ARG:HG3	1:A:28:ARG:HH11	1.05	1.18
1:B:307:ASN:HD22	1:B:310:LEU:HB2	0.97	1.11
2:D:520:THR:HG21	2:D:622:MET:HG3	1.34	1.07
2:C:524:ARG:HH11	2:C:524:ARG:HG3	1.13	1.07
1:B:307:ASN:ND2	1:B:310:LEU:HB2	1.69	1.06
1:B:41:GLN:HG2	1:B:88:MET:HE2	1.36	1.06
1:B:146:ASP:HB3	1:B:148:THR:HG23	1.37	1.06
1:A:70:MET:HE1	1:A:78:ASP:HB3	1.37	1.05
2:D:524:ARG:HH11	2:D:524:ARG:HB3	1.23	1.02
1:B:256:ILE:HD13	1:B:321:LEU:HD21	1.46	0.98
2:D:583:LEU:HD23	2:D:586:MET:HE1	1.46	0.96
1:A:144:ASN:HD21	1:A:148:THR:HG23	1.31	0.94
1:A:60:ARG:HH11	1:A:60:ARG:CB	1.80	0.93
2:C:524:ARG:HH11	2:C:524:ARG:CG	1.81	0.92
1:B:28:ARG:HG3	1:B:28:ARG:HH11	1.33	0.91
1:B:70:MET:HE1	1:B:78:ASP:HB3	1.53	0.91
2:D:583:LEU:HA	2:D:586:MET:CE	2.01	0.91
1:A:60:ARG:HB2	1:A:60:ARG:NH1	1.86	0.90
1:B:20:TYR:CE1	1:B:24:ILE:HD13	2.06	0.90
1:A:293:ARG:HH11	1:A:293:ARG:HB3	1.36	0.90
2:D:431:LEU:HD13	2:D:479:MET:CE	2.02	0.88
1:A:28:ARG:HG3	1:A:28:ARG:NH1	1.86	0.88
2:D:611:LEU:HD13	2:D:611:LEU:O	1.73	0.87
2:D:583:LEU:HA	2:D:586:MET:HE2	1.56	0.86
1:A:256:ILE:HD13	1:A:321:LEU:HD21	1.56	0.86
2:D:524:ARG:HH11	2:D:524:ARG:CB	1.89	0.84
2:C:524:ARG:HG3	2:C:524:ARG:NH1	1.87	0.83
2:C:516:THR:O	2:C:520:THR:HG23	1.78	0.83
2:D:583:LEU:HD23	2:D:586:MET:CE	2.08	0.82
1:A:44:ILE:HD12	1:A:88:MET:CE	2.10	0.82
6:H:10:DC:H2"	6:H:11:DG:H5"	1.62	0.82
2:C:520:THR:HG21	2:C:622:MET:HG3	1.62	0.81
1:A:139:VAL:HG11	1:A:154:VAL:O	1.82	0.80
1:B:307:ASN:HD22	1:B:310:LEU:CB	1.89	0.80
1:B:431:ASP:O	1:B:434:VAL:HG12	1.84	0.78
2:D:516:THR:O	2:D:520:THR:HG23	1.85	0.76
1:A:38:LYS:H	1:A:41:GLN:NE2	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:474:GLU:O	2:D:478:THR:HG23	1.86	0.76
2:D:478:THR:O	2:D:482:THR:HG23	1.87	0.75
1:A:28:ARG:HH11	1:A:28:ARG:CG	1.94	0.75
1:A:169:GLY:HA2	1:A:176:THR:HG22	1.69	0.74
1:B:9:LEU:HD23	1:B:9:LEU:C	2.07	0.74
1:A:24:ILE:HG22	1:A:171:SER:HB2	1.70	0.73
1:B:28:ARG:HG3	1:B:28:ARG:NH1	1.94	0.73
1:A:8:SER:HB3	1:A:11:ASP:OD1	1.90	0.72
3:E:9:DC:H2"	3:E:10:DA:H5"	1.71	0.72
1:A:117[A]:ARG:HH22	4:F:1:DA:H8	1.34	0.72
1:B:146:ASP:CB	1:B:148:THR:HG23	2.18	0.72
1:A:146:ASP:HB3	1:A:148:THR:HG22	1.70	0.72
1:A:317:LYS:HE3	1:A:318:TYR:CE2	2.25	0.71
1:A:139:VAL:HG13	1:A:140:PRO:HD2	1.71	0.71
2:C:611:LEU:HD13	2:C:611:LEU:C	2.10	0.71
1:A:425:TYR:HB3	1:B:420:VAL:HG13	1.72	0.70
1:B:167:SER:C	1:B:168:THR:HG22	2.09	0.70
1:B:190:ALA:O	1:B:194:ILE:HG13	1.90	0.70
1:B:70:MET:CE	1:B:78:ASP:HB3	2.22	0.70
1:B:146:ASP:HB3	1:B:148:THR:CG2	2.17	0.70
2:D:431:LEU:HD13	2:D:479:MET:HE3	1.74	0.69
1:B:20:TYR:CZ	1:B:24:ILE:HD13	2.26	0.69
1:A:70:MET:CE	1:A:78:ASP:HB3	2.19	0.69
1:B:233:LYS:HG3	1:B:339:GLN:OE1	1.92	0.69
1:A:244:ILE:HD12	1:A:244:ILE:N	2.08	0.69
1:B:41:GLN:HA	1:B:88:MET:HE1	1.75	0.69
1:B:193:MET:CE	1:B:347:SER:HB3	2.22	0.69
2:D:516:THR:HG22	2:D:517:LEU:N	2.07	0.69
1:B:365:LYS:O	1:B:369:GLU:HG3	1.94	0.68
1:A:40:VAL:O	1:A:44:ILE:HG13	1.93	0.68
2:C:511:GLY:O	2:C:515:GLN:HG3	1.94	0.68
2:C:474:GLU:O	2:C:478:THR:HG23	1.93	0.67
1:A:350:ILE:HA	1:A:463:MET:HE1	1.75	0.67
1:A:146:ASP:CB	1:A:148:THR:HG22	2.25	0.67
1:B:423:GLN:NE2	1:B:425:TYR:HE1	1.92	0.67
1:A:252:GLU:OE1	1:A:308:THR:HG21	1.95	0.67
1:A:38:LYS:H	1:A:41:GLN:HE21	1.42	0.67
2:C:431:LEU:HD22	2:C:479:MET:HE3	1.74	0.67
1:A:70:MET:HE1	1:A:78:ASP:CB	2.21	0.66
1:A:271:LYS:HE3	1:A:319:THR:HB	1.75	0.66
6:H:5:DA:H2"	6:H:6:DT:O5'	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ASP:CG	1:A:148:THR:HG22	2.16	0.66
1:B:38:LYS:H	1:B:41:GLN:NE2	1.94	0.65
1:B:41:GLN:CG	1:B:88:MET:HE2	2.20	0.65
1:A:222:ARG:HD3	1:A:484:ASP:HA	1.77	0.65
1:A:209:PRO:HB2	1:A:482:LEU:CD1	2.26	0.65
1:A:146:ASP:OD2	1:A:148:THR:HG22	1.96	0.65
1:B:201:ILE:HD12	1:B:201:ILE:H	1.61	0.65
1:B:391:LEU:C	1:B:391:LEU:HD23	2.17	0.64
2:D:594:THR:OG1	2:D:595:THR:HG22	1.97	0.64
2:C:491:PHE:CE1	2:C:528:PRO:HG2	2.32	0.64
1:B:194:ILE:HD13	1:B:463:MET:HE2	1.80	0.64
1:A:169:GLY:CA	1:A:176:THR:HG22	2.27	0.64
1:A:60:ARG:HH11	1:A:60:ARG:CG	2.11	0.64
2:C:527:ARG:N	2:C:528:PRO:HD2	2.13	0.64
1:A:229:TYR:CD1	1:A:342:ILE:HD13	2.33	0.63
2:C:473:ASN:O	2:C:477:ASN:HB2	1.98	0.63
2:C:441:ALA:HB1	2:C:452:ILE:HD12	1.80	0.62
1:A:211:PRO:O	1:A:478:ARG:NH2	2.30	0.62
4:F:3:DT:H4'	4:F:4:DC:OP1	1.99	0.62
1:A:259:ILE:HB	1:A:260:PRO:CD	2.30	0.62
1:A:288:ARG:HD2	1:A:290:GLU:OE2	1.99	0.62
1:B:20:TYR:CE1	1:B:24:ILE:CD1	2.81	0.62
1:B:341:GLY:O	1:B:344:PRO:HD2	2.00	0.61
2:C:583:LEU:HA	2:C:586:MET:CE	2.30	0.61
2:D:611:LEU:HD13	2:D:611:LEU:C	2.20	0.61
1:B:357:ILE:HD12	1:B:463:MET:HG2	1.82	0.61
1:B:168:THR:HA	1:B:176:THR:O	2.01	0.60
1:B:211:PRO:O	1:B:478:ARG:NH2	2.31	0.60
2:D:431:LEU:CD1	2:D:479:MET:CE	2.79	0.60
1:A:22:LYS:O	1:A:26:GLN:HG3	2.01	0.60
1:A:23:TYR:HD1	1:A:24:ILE:HD13	1.66	0.60
1:B:28:ARG:HH11	1:B:28:ARG:CG	2.09	0.60
6:H:3:DC:H2'	6:H:4:DT:C6	2.37	0.59
2:D:525:TYR:O	2:D:526:MET:HG3	2.03	0.59
1:A:146:ASP:OD2	1:A:148:THR:CG2	2.50	0.59
1:A:145:PHE:CE1	1:A:146:ASP:HB2	2.38	0.59
2:C:431:LEU:HD22	2:C:479:MET:CE	2.32	0.59
1:B:256:ILE:CD1	1:B:321:LEU:HD21	2.28	0.58
2:D:500:LYS:HG2	2:D:536:TYR:CE2	2.38	0.58
1:A:192:TYR:CZ	1:A:203:LYS:HE2	2.39	0.58
1:B:243:GLU:C	1:B:244:ILE:HD13	2.24	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:583:LEU:HA	2:C:586:MET:HE2	1.86	0.57
1:B:243:GLU:O	1:B:244:ILE:HD13	2.04	0.57
2:D:602:THR:O	2:D:603:LEU:HD23	2.05	0.57
1:A:317:LYS:HE3	1:A:318:TYR:CZ	2.38	0.57
2:C:616:ARG:O	2:C:620:VAL:HG23	2.04	0.57
1:B:241:LYS:HD3	1:B:258:GLU:OE2	2.04	0.57
2:C:626:VAL:HG11	4:F:10:DT:OP2	2.05	0.57
2:D:431:LEU:CD1	2:D:479:MET:HE2	2.35	0.57
1:B:406:LYS:HE2	1:B:413:GLU:HA	1.86	0.56
1:A:259:ILE:HB	1:A:260:PRO:HD2	1.86	0.56
2:C:446:ASP:OD1	2:C:449:PHE:CE1	2.58	0.56
1:B:412:THR:H	1:B:415:GLN:HE21	1.54	0.56
1:A:139:VAL:HG13	1:A:140:PRO:CD	2.36	0.56
1:B:359:ALA:HA	1:B:362:ARG:NH1	2.20	0.56
1:B:29:ALA:HB3	1:B:171:SER:HB3	1.86	0.55
2:C:416:LEU:HG	2:C:417:THR:N	2.20	0.55
1:B:288:ARG:NH1	1:B:290:GLU:OE2	2.39	0.55
2:C:524:ARG:CG	2:C:524:ARG:NH1	2.54	0.55
1:B:285:ALA:HB3	1:B:301:GLU:HG2	1.89	0.55
2:D:464:LYS:HG3	2:D:622:MET:O	2.07	0.55
1:A:210:GLY:HA2	1:A:229:TYR:OH	2.07	0.55
1:A:193:MET:HE1	1:A:347:SER:HB3	1.88	0.54
2:C:491:PHE:HE1	2:C:528:PRO:HG2	1.71	0.54
1:B:146:ASP:O	1:B:147:ASP:HB2	2.07	0.54
6:H:11:DG:C8	6:H:11:DG:H5'	2.42	0.54
1:A:193:MET:CE	1:A:347:SER:HB3	2.37	0.54
1:B:118:TYR:HE2	6:H:1:DG:H5'	1.73	0.54
1:B:307:ASN:ND2	1:B:310:LEU:CB	2.59	0.54
2:C:442:LYS:O	2:C:445:ARG:HD3	2.08	0.54
2:D:610:ASP:OD1	2:D:613:ARG:HB2	2.07	0.53
1:B:38:LYS:NZ	5:G:13:DC:OP1	2.36	0.53
1:B:194:ILE:CD1	1:B:463:MET:HE2	2.38	0.53
1:A:216:GLY:O	1:A:217:ALA:HB3	2.08	0.53
1:B:53:ASN:ND2	1:B:60:ARG:HD2	2.24	0.53
2:C:431:LEU:HD11	2:C:501:ILE:CG2	2.39	0.53
1:B:24:ILE:HD11	1:B:28:ARG:HE	1.73	0.53
1:A:256:ILE:CD1	1:A:321:LEU:HD21	2.33	0.53
2:C:479:MET:HE1	2:C:522:PHE:CZ	2.44	0.53
1:B:209:PRO:HB2	1:B:482:LEU:CD1	2.38	0.52
2:C:591:LEU:HD22	2:C:596:MET:HG3	1.91	0.52
1:A:38:LYS:N	1:A:41:GLN:HE21	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:TYR:OH	1:A:203:LYS:HE2	2.10	0.52
1:B:91:ASN:C	1:B:91:ASN:HD22	2.13	0.52
1:A:290:GLU:HB2	1:A:297:ARG:HG2	1.90	0.52
1:A:146:ASP:CG	1:A:148:THR:CG2	2.78	0.52
1:B:69:ILE:HG22	1:B:81:ILE:HD13	1.92	0.52
1:B:35:ASP:O	1:B:161:ASN:HB3	2.10	0.52
2:D:479:MET:HE1	2:D:518:LEU:HD22	1.92	0.52
2:D:491:PHE:HD1	2:D:528:PRO:HG2	1.75	0.51
1:A:288:ARG:NH1	1:A:290:GLU:OE2	2.29	0.51
1:A:293:ARG:HB3	1:A:293:ARG:NH1	2.15	0.51
1:B:23:TYR:HB2	2:D:509:THR:HG21	1.93	0.51
2:C:590:GLN:O	2:C:594:THR:HG23	2.11	0.51
2:C:611:LEU:HD13	2:C:611:LEU:O	2.10	0.51
2:D:524:ARG:HB3	2:D:524:ARG:NH1	2.08	0.51
1:A:23:TYR:CB	2:C:509:THR:HG21	2.40	0.51
1:A:434:VAL:HG13	1:A:435:LEU:N	2.25	0.51
1:B:104:ASN:ND2	2:C:439:GLY:HA3	2.26	0.50
1:B:430:THR:HG23	1:B:430:THR:O	2.11	0.50
2:C:479:MET:CE	2:C:522:PHE:CZ	2.94	0.50
1:A:117[A]:ARG:NH2	4:F:1:DA:H8	2.07	0.50
1:B:201:ILE:HD12	1:B:201:ILE:N	2.25	0.50
1:B:20:TYR:CD1	2:D:513:HIS:HB2	2.47	0.50
1:B:24:ILE:HD11	1:B:28:ARG:NE	2.26	0.50
1:A:144:ASN:HD21	1:A:148:THR:CG2	2.14	0.49
1:A:10:GLU:O	2:C:617:ARG:HD2	2.12	0.49
2:C:611:LEU:C	2:C:611:LEU:CD1	2.81	0.49
1:A:393:ARG:HH12	1:B:386:ASP:CG	2.16	0.49
1:B:9:LEU:HD23	1:B:9:LEU:O	2.12	0.49
1:B:169:GLY:HA3	1:B:176:THR:O	2.13	0.49
6:H:3:DC:H4'	6:H:4:DT:OP1	2.12	0.49
1:B:254:ILE:HB	1:B:300:ILE:HB	1.95	0.49
2:D:592:TRP:CE2	2:D:597:ASN:HB2	2.48	0.49
1:B:132:GLN:O	1:B:133:ASP:HB2	2.13	0.49
1:B:290:GLU:OE1	1:B:297:ARG:NH1	2.41	0.49
2:D:611:LEU:C	2:D:611:LEU:CD1	2.81	0.49
2:C:592:TRP:CE2	2:C:597:ASN:HB2	2.47	0.49
1:B:91:ASN:HD22	1:B:92:TRP:N	2.11	0.48
1:B:118:TYR:CE2	6:H:1:DG:H5'	2.49	0.48
1:B:423:GLN:NE2	1:B:425:TYR:CE1	2.79	0.48
1:A:44:ILE:HD13	1:A:85:MET:HB2	1.96	0.47
1:A:96:GLU:HG2	1:A:126:ILE:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ASN:O	1:A:336:THR:HG23	2.15	0.47
1:B:41:GLN:HA	1:B:88:MET:CE	2.41	0.47
1:A:130:LEU:HD23	1:A:157:ALA:HA	1.96	0.47
1:B:84:ALA:O	1:B:88:MET:HG3	2.15	0.47
1:A:49:ASN:HB2	1:A:131:LEU:HD13	1.97	0.47
1:B:91:ASN:C	1:B:91:ASN:ND2	2.67	0.47
1:B:191:VAL:HG13	1:B:464:LYS:HG2	1.96	0.47
1:B:201:ILE:H	1:B:201:ILE:CD1	2.27	0.47
6:H:4:DT:O2	8:H:101:LFX:H01	2.15	0.46
1:A:146:ASP:OD2	1:A:146:ASP:O	2.33	0.46
1:A:244:ILE:N	1:A:244:ILE:CD1	2.79	0.46
1:A:268:LEU:HD11	1:A:321:LEU:HD23	1.97	0.46
1:A:338:ARG:HB3	1:A:340:VAL:HG13	1.98	0.46
1:B:15:GLU:OE1	1:B:16:ARG:NH1	2.49	0.46
1:B:167:SER:C	1:B:168:THR:CG2	2.80	0.46
1:B:23:TYR:CB	2:D:509:THR:HG21	2.46	0.46
2:D:427:ASN:HA	2:D:449:PHE:O	2.15	0.46
1:B:296:LEU:HD23	1:B:297:ARG:N	2.31	0.46
2:C:509:THR:O	2:C:512:ALA:HB3	2.16	0.46
2:D:474:GLU:O	2:D:478:THR:CG2	2.60	0.46
1:B:160:PRO:O	1:B:164:VAL:HG23	2.15	0.45
2:C:455:LEU:CD1	2:C:518:LEU:HD11	2.46	0.45
2:C:526:MET:C	2:C:528:PRO:HD2	2.36	0.45
1:A:45:LEU:HD22	1:A:123:LEU:HD22	1.98	0.45
2:D:524:ARG:HH11	2:D:524:ARG:CG	2.26	0.45
1:A:23:TYR:CG	2:C:509:THR:HG21	2.51	0.45
2:D:462:THR:HA	2:D:470:ILE:HD11	1.98	0.45
1:B:59:TYR:HB3	1:B:120:GLU:HB2	1.99	0.45
1:A:86:VAL:O	1:A:90:GLN:HG3	2.16	0.45
2:D:527:ARG:N	2:D:528:PRO:HD2	2.32	0.45
1:A:82:TYR:CD1	1:A:116:MET:HB3	2.51	0.45
1:B:9:LEU:C	1:B:9:LEU:CD2	2.80	0.45
1:B:28:ARG:NH2	2:D:510:ASP:OD1	2.50	0.45
2:C:516:THR:O	2:C:520:THR:CG2	2.57	0.45
1:B:321:LEU:HD23	1:B:321:LEU:HA	1.78	0.45
3:E:13:DA:H2"	3:E:14:DA:O5'	2.17	0.45
1:A:42:ARG:NE	1:A:154:VAL:HA	2.32	0.44
2:C:523:TYR:OH	2:C:615:GLU:HB2	2.16	0.44
2:D:597:ASN:HA	2:D:598:PRO:HD3	1.86	0.44
1:A:415:GLN:O	1:A:419:ILE:HG13	2.18	0.44
1:A:169:GLY:HA3	1:A:176:THR:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:LEU:C	1:A:296:LEU:HD23	2.38	0.44
2:C:441:ALA:CB	2:C:452:ILE:HD12	2.48	0.44
2:C:623:GLY:O	2:C:629:ARG:NH2	2.38	0.44
1:B:387:GLU:OE1	1:B:387:GLU:N	2.48	0.44
2:D:583:LEU:CD2	2:D:586:MET:CE	2.90	0.44
1:B:247:LEU:HB2	1:B:251:LYS:O	2.18	0.44
1:A:132:GLN:O	1:A:133:ASP:HB2	2.18	0.44
6:H:10:DC:H2"	6:H:11:DG:C5'	2.40	0.44
1:A:24:ILE:HD13	1:A:24:ILE:N	2.29	0.43
1:A:414:GLU:CD	1:A:414:GLU:H	2.22	0.43
1:B:4:ILE:HG13	1:B:5:GLN:N	2.32	0.43
1:A:280:LYS:HB3	1:A:280:LYS:HE3	1.79	0.43
1:A:393:ARG:NH1	1:B:386:ASP:OD2	2.51	0.43
2:C:431:LEU:CD2	2:C:479:MET:CE	2.96	0.43
1:A:44:ILE:HD12	1:A:88:MET:HE1	1.96	0.43
1:A:126:ILE:HG13	1:A:474:PHE:CD1	2.53	0.43
1:B:310:LEU:HD23	1:B:310:LEU:HA	1.64	0.43
2:C:536:TYR:N	2:C:536:TYR:CD2	2.87	0.43
1:A:20:TYR:CD1	2:C:513:HIS:HB2	2.54	0.43
1:B:168:THR:HA	1:B:169:GLY:HA3	1.84	0.43
1:B:228:ALA:HA	1:B:233:LYS:O	2.18	0.43
1:B:320:ASP:C	1:B:322:GLN:N	2.72	0.43
1:B:406:LYS:NZ	1:B:413:GLU:HB2	2.33	0.43
2:C:446:ASP:OD1	2:C:449:PHE:HE1	2.00	0.43
1:A:29:ALA:O	1:A:38:LYS:HE2	2.19	0.43
2:D:429:LEU:HD23	2:D:429:LEU:HA	1.71	0.43
2:D:475:GLU:O	2:D:479:MET:HB2	2.19	0.43
1:A:43:ARG:HG2	1:A:73:PHE:HB3	2.00	0.43
1:B:261:TYR:CD2	1:B:262:GLU:HG3	2.53	0.43
1:A:397:ASN:HA	1:B:428:THR:OG1	2.19	0.43
1:B:146:ASP:HB3	1:B:148:THR:H	1.83	0.43
1:B:346:LEU:O	1:B:350:ILE:HG13	2.18	0.43
5:G:13:DC:H2"	5:G:14:DA:O5'	2.19	0.43
1:A:28:ARG:NH1	1:A:28:ARG:CG	2.64	0.43
2:C:639:PHE:O	2:C:640:THR:CB	2.67	0.43
1:A:375:VAL:O	1:A:379:ILE:HG13	2.19	0.43
1:B:40:VAL:HG13	1:B:41:GLN:N	2.33	0.43
1:B:292:ASP:O	1:B:294:ASP:N	2.51	0.43
2:D:516:THR:HG23	2:D:622:MET:SD	2.59	0.43
1:A:55:PHE:HA	1:A:122:ARG:HD2	2.00	0.42
1:A:423:GLN:NE2	1:A:425:TYR:HE1	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:VAL:CG1	1:B:238:VAL:N	2.82	0.42
2:C:431:LEU:HD11	2:C:501:ILE:HG22	2.01	0.42
2:C:557:TYR:OH	2:C:590:GLN:HG2	2.18	0.42
1:A:44:ILE:HB	1:A:88:MET:HE1	2.01	0.42
1:B:259:ILE:HB	1:B:260:PRO:CD	2.48	0.42
1:B:424:LEU:HD23	1:B:424:LEU:HA	1.79	0.42
2:C:601:ARG:CZ	2:C:603:LEU:HD11	2.49	0.42
2:C:441:ALA:O	2:C:445:ARG:HB3	2.20	0.42
4:F:6:DT:H2"	4:F:7:DT:H5'	2.02	0.42
1:B:130:LEU:HD21	1:B:161:ASN:HB2	2.01	0.42
1:A:29:ALA:HB3	1:A:171:SER:HB3	2.02	0.42
1:B:140:PRO:HG2	1:B:153:THR:OG1	2.19	0.42
2:D:459:VAL:HG12	2:D:460:ILE:N	2.35	0.41
1:A:334:ASN:O	1:A:336:THR:CG2	2.69	0.41
1:B:24:ILE:HG23	1:B:171:SER:HB2	2.01	0.41
1:B:182:ASN:O	1:B:186:VAL:HG23	2.19	0.41
1:A:169:GLY:CA	1:A:176:THR:CG2	2.95	0.41
1:B:38:LYS:H	1:B:41:GLN:HE21	1.65	0.41
1:B:219:ILE:HB	1:B:482:LEU:HD23	2.03	0.41
2:C:479:MET:CE	2:C:522:PHE:HZ	2.32	0.41
1:B:272:ILE:O	1:B:275:VAL:HB	2.20	0.41
1:A:146:ASP:OD2	1:A:148:THR:HB	2.20	0.41
2:C:627:GLU:N	2:C:628:PRO:CD	2.84	0.41
1:A:428:THR:HG22	1:B:392:ILE:O	2.20	0.41
1:B:146:ASP:HB3	1:B:148:THR:N	2.36	0.41
1:A:168:THR:HA	1:A:169:GLY:HA3	1.94	0.41
1:B:423:GLN:HE21	1:B:425:TYR:HE1	1.60	0.41
2:C:462:THR:HG21	2:C:521:PHE:HD2	1.86	0.41
1:A:9:LEU:CD2	1:A:9:LEU:O	2.69	0.41
1:A:27:ASP:HA	1:A:39:PRO:HG2	2.03	0.41
1:A:136:LYS:HG2	1:A:363:PHE:CD2	2.56	0.41
1:A:333:ASP:O	1:A:334:ASN:C	2.60	0.41
1:B:259:ILE:HB	1:B:260:PRO:HD2	2.02	0.40
1:A:53:ASN:HA	9:A:805:HOH:O	2.21	0.40
1:B:51:ASP:O	1:B:52:SER:HB2	2.22	0.40
1:B:160:PRO:HG3	1:B:349:TYR:CE2	2.56	0.40
2:C:485:ALA:HB3	2:C:491:PHE:CE2	2.55	0.40
1:A:190:ALA:O	1:A:194:ILE:HG13	2.21	0.40
2:C:524:ARG:HH11	2:C:524:ARG:CB	2.32	0.40
1:B:27:ASP:HA	1:B:39:PRO:HG2	2.04	0.40
1:B:289:ASP:HB3	2:C:447:ARG:NH2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ARG:NH1	1:A:60:ARG:CG	2.78	0.40
2:D:524:ARG:NH1	2:D:524:ARG:CG	2.84	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	481/496 (97%)	454 (94%)	22 (5%)	5 (1%)	15	45
1	B	481/496 (97%)	447 (93%)	29 (6%)	5 (1%)	15	45
2	C	202/268 (75%)	186 (92%)	15 (7%)	1 (0%)	29	61
2	D	203/268 (76%)	191 (94%)	11 (5%)	1 (0%)	29	61
All	All	1367/1528 (90%)	1278 (94%)	77 (6%)	12 (1%)	17	48

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	PHE
1	A	329	MET
1	B	168	THR
1	B	293	ARG
2	C	496	ALA
2	D	427	ASN
1	A	169	GLY
1	A	217	ALA
1	A	221	GLY
1	B	304	LYS
1	B	169	GLY
1	B	221	GLY

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	378/431 (88%)	349 (92%)	29 (8%)	13	35
1	B	376/431 (87%)	350 (93%)	26 (7%)	15	41
2	C	111/224 (50%)	99 (89%)	12 (11%)	6	20
2	D	111/224 (50%)	100 (90%)	11 (10%)	8	24
All	All	976/1310 (74%)	898 (92%)	78 (8%)	12	33

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	28	ARG
1	A	58	SER
1	A	60	ARG
1	A	91	ASN
1	A	102	HIS
1	A	111	ASP
1	A	126	ILE
1	A	148	THR
1	A	162	LEU
1	A	168	THR
1	A	208	LEU
1	A	223	ASP
1	A	236	VAL
1	A	268	LEU
1	A	279	ASN
1	A	293	ARG
1	A	308	THR
1	A	321	LEU
1	A	328	ASN
1	A	336	THR
1	A	338	ARG
1	A	366	GLU
1	A	372	LEU

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Mol	Chain	Res	Type
1	A	380	ARG
1	A	414	GLU
1	A	420	VAL
1	A	432	VAL
1	A	462	LEU
1	B	4	ILE
1	B	24	ILE
1	B	28	ARG
1	B	60	ARG
1	B	70	MET
1	B	91	ASN
1	B	96	GLU
1	B	102	HIS
1	B	162	LEU
1	B	168	THR
1	B	177	ASP
1	B	208	LEU
1	B	215	THR
1	B	268	LEU
1	B	293	ARG
1	B	297	ARG
1	B	308	THR
1	B	310	LEU
1	B	321	LEU
1	B	336	THR
1	B	338	ARG
1	B	348	SER
1	B	372	LEU
1	B	385	LEU
1	B	462	LEU
1	B	480	SER
2	C	429	LEU
2	C	431	LEU
2	C	445	ARG
2	C	453	LEU
2	C	477	ASN
2	C	509	THR
2	C	516	THR
2	C	520	THR
2	C	524	ARG
2	C	536	TYR
2	C	591	LEU

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Mol	Chain	Res	Type
2	C	595	THR
2	D	429	LEU
2	D	445	ARG
2	D	447	ARG
2	D	453	LEU
2	D	478	THR
2	D	479	MET
2	D	516	THR
2	D	520	THR
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 (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	68	ASN
1	A	91	ASN
1	A	102	HIS
1	A	267	ASN
1	A	328	ASN
1	A	423	GLN
1	B	41	GLN
1	B	91	ASN
1	B	102	HIS
1	B	267	ASN
1	B	307	ASN
1	B	313	ASN
1	B	328	ASN
1	B	404	ASN
1	B	415	GLN
1	B	423	GLN
2	C	420	GLN
2	C	477	ASN
2	D	619	ASN

5.3.3 RNA (i)

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 monosaccharides 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	LFX	H	101	7	29,29,29	0.82	1 (3%)	44,44,44	1.40	10 (22%)
8	LFX	F	101	7	29,29,29	0.83	1 (3%)	44,44,44	1.58	11 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	LFX	H	101	7	-	0/8/27/27	0/4/4/4
8	LFX	F	101	7	-	0/8/27/27	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	101	LFX	O02-C15	3.08	1.29	1.23
8	H	101	LFX	O02-C15	2.70	1.28	1.23

All (21) bond angle outliers are listed below:

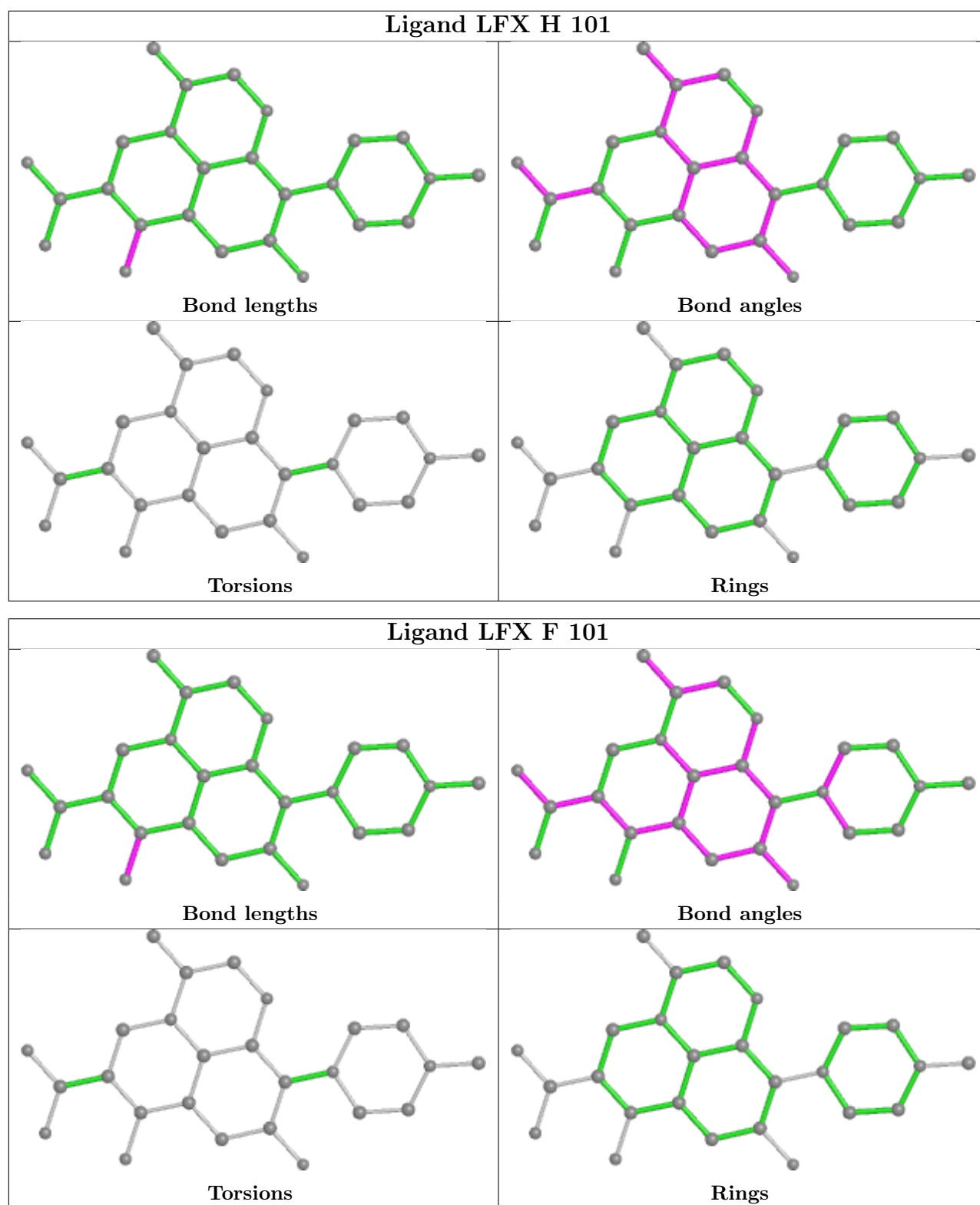| Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	F	101	LFX	O-C-C17	-3.51	114.76	122.46
8	F	101	LFX	C06-C05-N02	-3.39	117.77	119.89
8	H	101	LFX	C14-C03-C09	-2.85	103.75	112.58
8	H	101	LFX	C06-C04-C11	-2.81	113.65	116.02
8	H	101	LFX	O01-C06-C04	-2.79	115.06	117.90
8	H	101	LFX	O-C-C17	-2.58	116.80	122.46
8	H	101	LFX	F-C11-C04	-2.56	114.64	118.36
8	F	101	LFX	C06-C04-C11	-2.51	113.90	116.02
8	F	101	LFX	O01-C06-C04	-2.42	115.44	117.90
8	F	101	LFX	C10-C05-C06	2.42	122.77	120.07
8	F	101	LFX	C14-C03-C09	-2.40	105.16	112.58
8	F	101	LFX	C13-C11-C04	2.38	126.67	123.22
8	F	101	LFX	C10-C15-C17	-2.34	112.62	115.59
8	H	101	LFX	C06-C05-N02	-2.33	118.43	119.89
8	F	101	LFX	C02-N01-C01	2.31	116.61	111.52
8	F	101	LFX	F-C11-C04	-2.29	115.04	118.36
8	F	101	LFX	C13-C10-C05	-2.19	115.97	118.84
8	H	101	LFX	C13-C11-C04	2.15	126.33	123.22
8	H	101	LFX	C13-C10-C05	-2.06	116.14	118.84
8	H	101	LFX	C10-C05-C06	2.03	122.34	120.07
8	H	101	LFX	C09-C03-N02	2.01	111.33	107.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	H	101	LFX	1	0

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

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Ligand LFX H 101

Bond lengths

Bond angles

Torsions

Rings

Ligand LFX F 101

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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(Å²)	Q<0.9
1	A	482/496 (97%)	-0.70	0	100	100	44, 63, 101, 138	0
1	B	482/496 (97%)	-0.67	0	100	100	43, 63, 95, 135	0
2	C	208/268 (77%)	-0.32	7 (3%)	45	40	67, 105, 148, 170	0
2	D	209/268 (77%)	-0.41	4 (1%)	66	65	68, 99, 133, 167	0
3	E	7/7 (100%)	-0.38	0	100	100	62, 70, 102, 151	0
4	F	11/11 (100%)	-0.73	0	100	100	71, 91, 121, 146	0
5	G	7/7 (100%)	-0.14	0	100	100	57, 70, 105, 139	0
6	H	11/11 (100%)	-0.69	0	100	100	67, 86, 111, 122	0
All	All	1417/1564 (90%)	-0.58	11 (0%)	86	86	43, 71, 127, 170	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	560	THR	3.6
2	D	557	TYR	2.8
2	C	484	GLY	2.6
2	C	496	ALA	2.6
2	C	489	ALA	2.5
2	C	567	LEU	2.4
2	D	567	LEU	2.4
2	C	543	TYR	2.3
2	C	564	LEU	2.2
2	D	558	ALA	2.2
2	D	570	GLN	2.2

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 monosaccharides 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(Å^2)	Q<0.9
7	MG	A	501	1/1	0.83	0.11	72,72,72,72	0
7	MG	B	700	1/1	0.88	0.08	70,70,70,70	0
7	MG	C	701	1/1	0.88	0.60	98,98,98,98	0
7	MG	D	701	1/1	0.89	0.35	72,72,72,72	0
8	LFX	H	101	26/26	0.92	0.18	85,102,118,125	0
7	MG	A	502	1/1	0.93	0.35	89,89,89,89	0
8	LFX	F	101	26/26	0.94	0.18	78,96,121,127	0
7	MG	G	101	1/1	0.94	0.30	103,103,103,103	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 LFX H 101:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
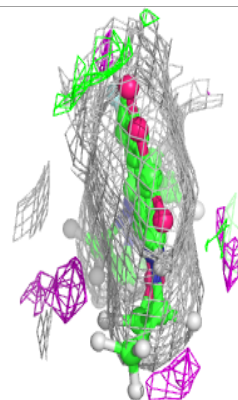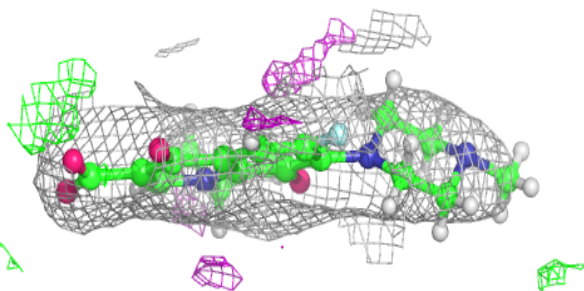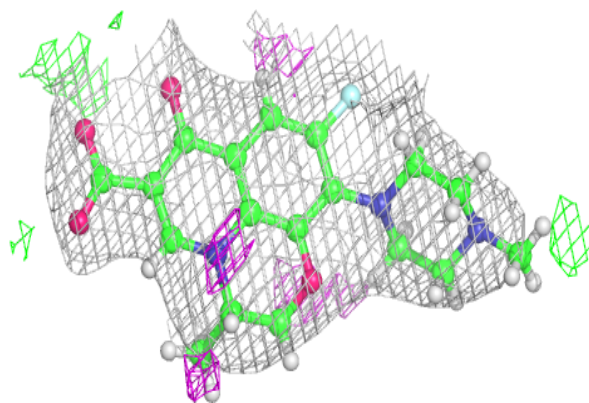
Electron density around LFX F 101:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
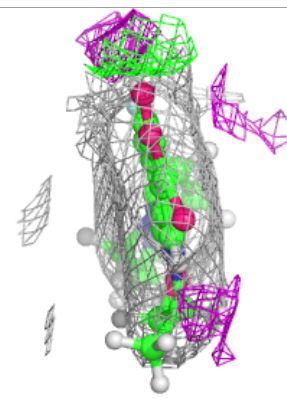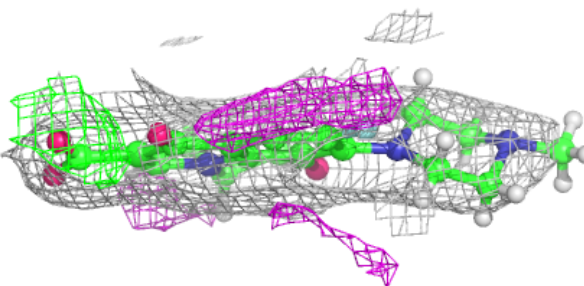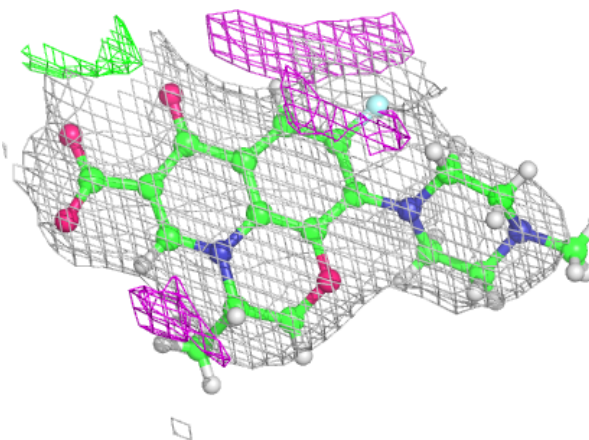
6.5 Other polymers (i)

There are no such residues in this entry.