



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:55 PM UTC

PDB ID : 4JUO / pdb_00004juo
Title : A low-resolution three-gate structure of topoisomerase IV from *Streptococcus pneumoniae* in space group H32
Authors : Laponogov, I.; Veselkov, D.A.; Pan, X.-S.; Crevel, I.; Fisher, L.M.; Sanderson, M.R.
Deposited on : 2013-03-25
Resolution : 6.53 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

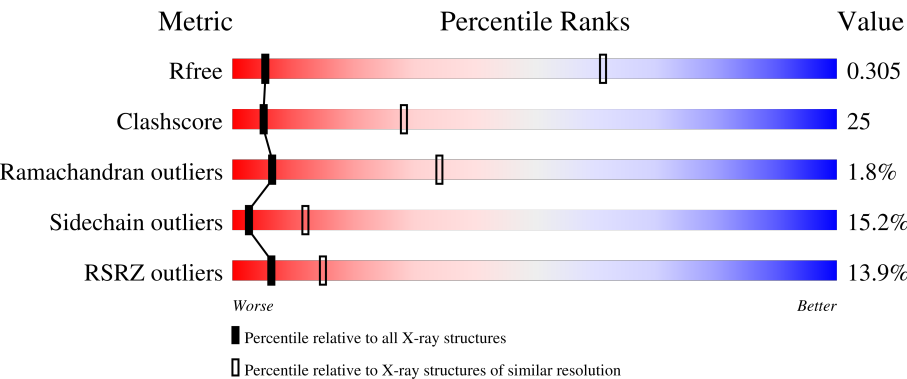
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 6.53 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



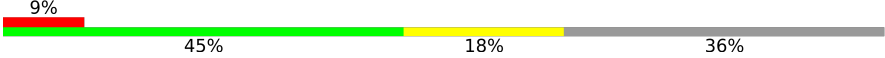
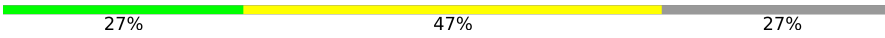
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1162 (9.00-4.00)
Clashscore	190562	1000 (9.00-4.04)
Ramachandran outliers	187476	1050 (9.00-4.00)
Sidechain outliers	187428	1014 (9.00-4.00)
RSRZ outliers	180081	1155 (9.00-4.00)

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	16% 63%29%5%
2	C	670	10% 50%23%8%19%
3	E	11	18% 27%36%36%
4	F	15	33%40%27%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	G	11	
6	H	15	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8283 atoms, of which 19 are hydrogens and 0 are deuteriums.

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

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

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

There are 9 discrepancies between the modelled and reference sequences:

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

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

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

There are 26 discrepancies between the modelled and reference sequences:

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

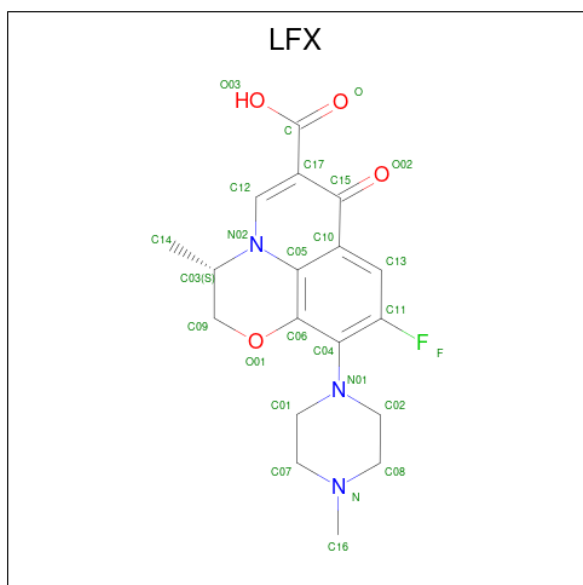
- Molecule 6 is a DNA chain called E-site DNA.

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

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

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

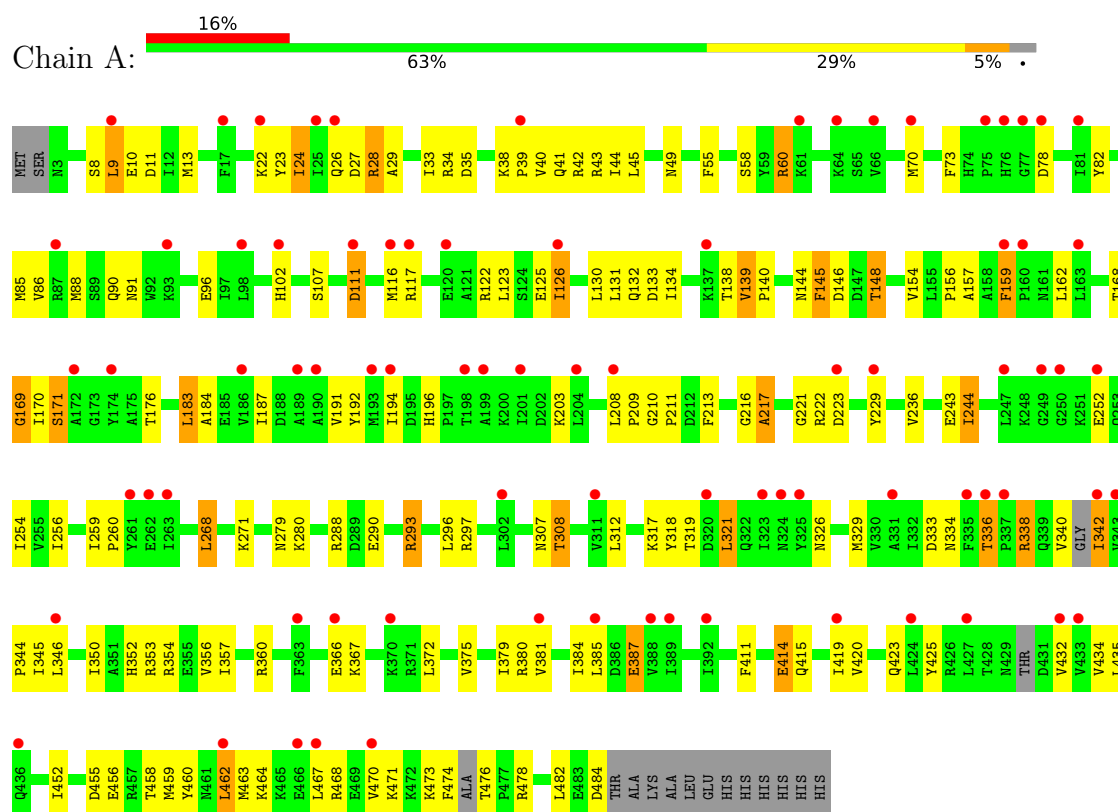
- Molecule 8 is (3S)-9-fluoro-3-methyl-10-(4-methylpiperazin-1-yl)-7-oxo-2,3-dihydro-7H-[1,4]oxazino[2,3,4-ij]quinoline-6-carboxylic acid (CCD ID: LFX) (formula: C₁₈H₂₀FN₃O₄).



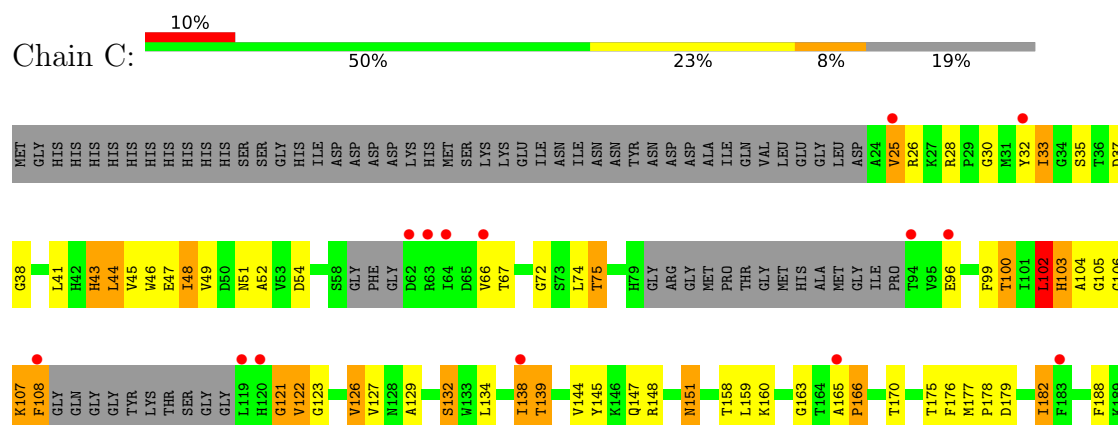
3 Residue-property plots

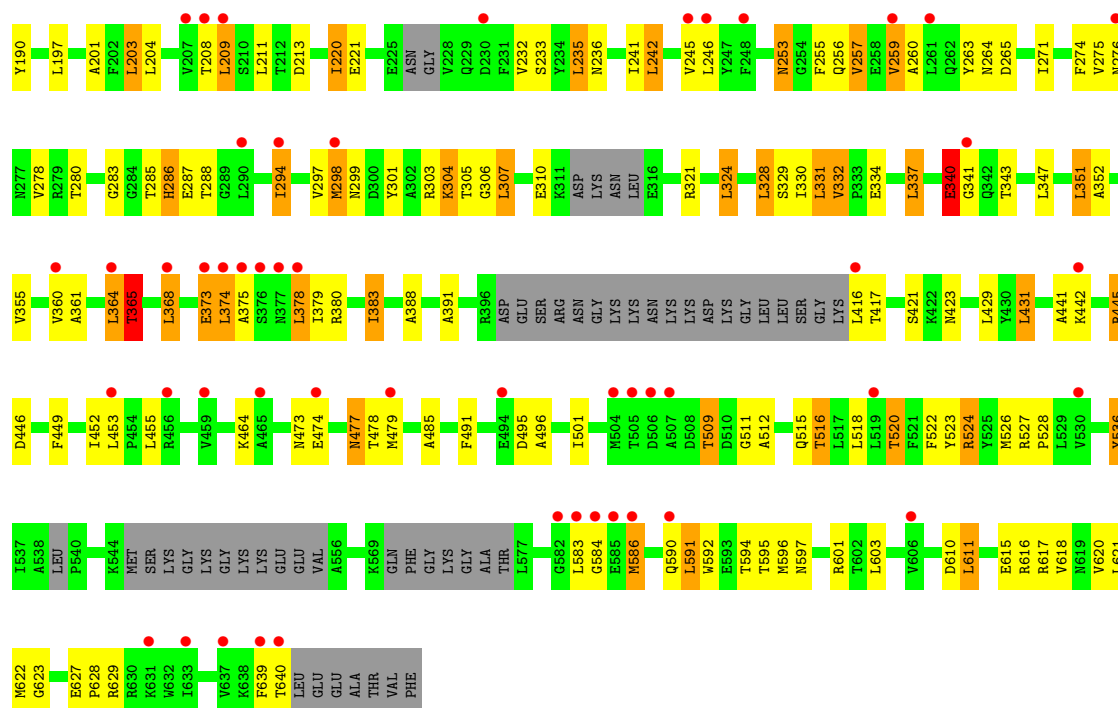
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

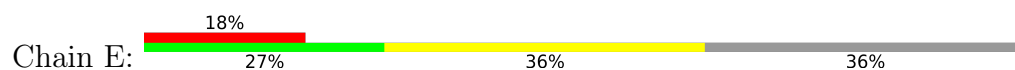


• Molecule 2: DNA topoisomerase 4 subunit B





- Molecule 3: E-site DNA



- Molecule 4: E-site DNA



- Molecule 5: E-site DNA



- Molecule 6: E-site DNA



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	213.58Å 213.58Å 211.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.44 – 6.53 46.44 – 6.53	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.44-6.53) 98.9 (46.44-6.53)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.83 (at 6.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.247 , 0.298 0.244 , 0.305	Depositor DCC
R_{free} test set	170 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	378.8	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 729.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	8283	wwPDB-VP
Average B, all atoms (Å ²)	183.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% of the height of the origin peak. No significant pseudotranslation is detected.*

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: 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	0.59	0/3779	0.95	9/5109 (0.2%)
2	C	0.54	0/3845	0.97	7/5251 (0.1%)
3	E	0.37	0/157	1.07	0/241
4	F	0.32	0/251	1.10	0/385
5	G	0.36	0/155	0.93	0/238
6	H	0.32	0/253	0.98	0/388
All	All	0.55	0/8440	0.97	16/11612 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	365	THR	N-CA-C	-6.70	104.12	112.90
1	A	171	SER	N-CA-C	6.39	114.89	108.75
1	A	170	ILE	CB-CA-C	-6.20	103.34	110.41
2	C	72	GLY	N-CA-C	-6.20	107.11	114.48
1	A	159	PHE	CA-C-N	5.94	127.26	119.84
1	A	159	PHE	C-N-CA	5.94	127.26	119.84
1	A	213	PHE	CA-C-N	5.59	125.25	119.05
1	A	213	PHE	C-N-CA	5.59	125.25	119.05
1	A	170	ILE	N-CA-C	5.53	116.74	107.18
1	A	196	HIS	CA-C-N	5.51	125.34	119.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	HIS	C-N-CA	5.51	125.34	119.28
2	C	241	ILE	N-CA-C	5.42	115.91	107.28
2	C	28	ARG	CA-C-N	5.41	124.93	119.19
2	C	28	ARG	C-N-CA	5.41	124.93	119.19
2	C	163	GLY	N-CA-C	5.18	118.54	110.88
2	C	103	HIS	N-CA-C	-5.10	99.93	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	102	LEU	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3720	0	3629	190	0
2	C	3786	0	3303	187	0
3	E	140	0	71	3	0
4	F	225	0	116	5	0
5	G	139	0	71	1	0
6	H	226	0	115	8	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	F	26	19	19	1	0
All	All	8264	19	7324	383	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (383) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:583:LEU:HB3	2:C:586:MET:CE	1.24	1.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:583:LEU:CB	2:C:586:MET:CE	1.75	1.57
2:C:583:LEU:CB	2:C:586:MET:HE3	1.36	1.46
2:C:583:LEU:HD22	2:C:586:MET:CE	1.56	1.35
2:C:583:LEU:CD2	2:C:586:MET:CE	2.06	1.32
2:C:583:LEU:CG	2:C:586:MET:CE	2.06	1.31
2:C:583:LEU:CD2	2:C:586:MET:HE1	1.62	1.30
1:A:338:ARG:HH12	1:A:344:PRO:CG	1.30	1.20
1:A:354:ARG:NE	1:A:456:GLU:OE1	1.76	1.18
2:C:583:LEU:CA	2:C:586:MET:HE2	1.75	1.17
1:A:60:ARG:HH11	1:A:60:ARG:HB2	1.07	1.15
1:A:28:ARG:HG3	1:A:28:ARG:HH11	1.05	1.14
1:A:354:ARG:CD	1:A:456:GLU:OE1	1.96	1.13
1:A:455:ASP:O	1:A:456:GLU:N	1.82	1.12
1:A:184:ALA:HB1	1:A:471:LYS:HE3	1.28	1.12
1:A:338:ARG:NH1	1:A:344:PRO:HG2	1.56	1.11
1:A:357:ILE:CG2	1:A:459:MET:HG2	1.79	1.11
1:A:455:ASP:C	1:A:456:GLU:N	2.09	1.10
2:C:583:LEU:CB	2:C:586:MET:HE2	1.55	1.09
1:A:354:ARG:HE	1:A:456:GLU:CD	1.62	1.08
1:A:33:ILE:HD11	1:A:345:ILE:CG1	1.84	1.06
1:A:33:ILE:HD11	1:A:345:ILE:HA	1.37	1.06
1:A:354:ARG:HD2	1:A:456:GLU:OE1	1.54	1.06
1:A:33:ILE:HD11	1:A:345:ILE:HG12	1.38	1.05
1:A:70:MET:HE1	1:A:78:ASP:HB3	1.36	1.04
2:C:524:ARG:HH11	2:C:524:ARG:HG3	1.13	1.04
2:C:583:LEU:HD22	2:C:586:MET:HE1	1.04	1.03
1:A:357:ILE:HG21	1:A:459:MET:CG	1.89	1.02
2:C:108:PHE:CD1	2:C:276:ASN:HB3	1.94	1.02
1:A:474:PHE:O	1:A:476:THR:HG23	1.61	1.00
2:C:583:LEU:HA	2:C:586:MET:HE2	1.43	0.97
2:C:583:LEU:CD2	2:C:586:MET:HE2	1.77	0.97
1:A:33:ILE:CD1	1:A:345:ILE:HG12	1.95	0.96
1:A:357:ILE:HG21	1:A:459:MET:HG2	0.98	0.96
1:A:338:ARG:HH12	1:A:344:PRO:HG3	1.28	0.96
2:C:431:LEU:HD22	2:C:479:MET:HE3	1.46	0.96
1:A:144:ASN:HD21	1:A:148:THR:HG23	1.31	0.95
1:A:60:ARG:HH11	1:A:60:ARG:CB	1.80	0.95
2:C:108:PHE:CE1	2:C:276:ASN:HA	1.99	0.95
1:A:33:ILE:CD1	1:A:345:ILE:HA	1.97	0.93
2:C:108:PHE:CE1	2:C:276:ASN:CA	2.46	0.93
1:A:10:GLU:O	2:C:617:ARG:HD2	1.68	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:583:LEU:CG	2:C:586:MET:HE1	1.85	0.91
2:C:524:ARG:HH11	2:C:524:ARG:CG	1.81	0.91
1:A:33:ILE:HD11	1:A:345:ILE:CA	2.01	0.91
1:A:338:ARG:NH1	1:A:344:PRO:CG	1.96	0.91
2:C:431:LEU:CD2	2:C:479:MET:HE3	2.00	0.90
1:A:60:ARG:HB2	1:A:60:ARG:NH1	1.86	0.89
1:A:293:ARG:HH11	1:A:293:ARG:HB3	1.36	0.89
1:A:357:ILE:CG2	1:A:459:MET:CG	2.50	0.88
1:A:384:ILE:O	1:A:387:GLU:HG2	1.74	0.86
2:C:524:ARG:HG3	2:C:524:ARG:NH1	1.87	0.86
1:A:28:ARG:HG3	1:A:28:ARG:NH1	1.86	0.86
1:A:256:ILE:HD13	1:A:321:LEU:HD21	1.56	0.85
2:C:516:THR:O	2:C:520:THR:HG23	1.78	0.83
6:H:10[B]:DC:H2"	6:H:11[B]:DG:H5"	1.62	0.81
1:A:44:ILE:HD12	1:A:88:MET:CE	2.10	0.81
2:C:108:PHE:HE1	2:C:276:ASN:HA	1.43	0.81
1:A:384:ILE:C	1:A:385:LEU:N	2.39	0.81
2:C:583:LEU:CD1	2:C:586:MET:HE1	2.11	0.81
1:A:125:GLU:OE2	1:A:473:LYS:NZ	2.13	0.80
2:C:583:LEU:CG	2:C:586:MET:HE2	1.94	0.80
1:A:34:ARG:HD2	1:A:352:HIS:CG	2.17	0.80
2:C:520:THR:HG21	2:C:622:MET:HG3	1.62	0.80
1:A:139:VAL:HG11	1:A:154:VAL:O	1.82	0.79
2:C:203:LEU:HD21	2:C:274:PHE:CD2	2.18	0.79
2:C:611:LEU:HD13	2:C:611:LEU:C	2.10	0.77
1:A:38:LYS:H	1:A:41:GLN:NE2	1.83	0.76
2:C:583:LEU:CA	2:C:586:MET:CE	2.47	0.76
1:A:33:ILE:HD11	1:A:345:ILE:CB	2.15	0.75
2:C:583:LEU:CD1	2:C:586:MET:CE	2.64	0.75
1:A:24:ILE:HG22	1:A:171:SER:HB2	1.70	0.74
1:A:28:ARG:HH11	1:A:28:ARG:CG	1.94	0.74
1:A:187:ILE:HD13	1:A:467:LEU:O	1.86	0.74
1:A:357:ILE:HD12	1:A:459:MET:SD	2.27	0.74
2:C:51:ASN:ND2	2:C:99:PHE:O	2.21	0.74
1:A:169:GLY:HA2	1:A:176:THR:HG22	1.69	0.73
2:C:304:LYS:O	2:C:306:GLY:N	2.21	0.73
1:A:146:ASP:HB3	1:A:148:THR:HG22	1.70	0.73
2:C:301:TYR:HD2	2:C:379:ILE:HD11	1.54	0.73
3:E:9[A]:DC:H2"	3:E:10[A]:DA:H5"	1.71	0.72
1:A:183:LEU:CD1	1:A:471:LYS:HA	2.19	0.72
2:C:256:GLN:HB3	2:C:331:LEU:HB2	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:VAL:HG13	1:A:140:PRO:HD2	1.71	0.72
2:C:203:LEU:CD2	2:C:274:PHE:CD2	2.73	0.72
1:A:317:LYS:HE3	1:A:318:TYR:CE2	2.25	0.71
2:C:259:VAL:HG22	2:C:328:LEU:HD23	1.70	0.71
2:C:584:GLY:CA	2:C:586:MET:N	2.50	0.71
1:A:8:SER:HB3	1:A:11:ASP:OD1	1.90	0.71
2:C:242:LEU:HD22	2:C:423:ASN:ND2	2.05	0.71
1:A:146:ASP:CG	1:A:148:THR:HG22	2.16	0.70
1:A:184:ALA:HB1	1:A:471:LYS:CE	2.15	0.70
1:A:138:THR:HG22	1:A:360:ARG:HB2	1.73	0.69
1:A:354:ARG:NE	1:A:456:GLU:CD	2.37	0.69
2:C:75:THR:HB	2:C:175:THR:HB	1.74	0.69
2:C:108:PHE:CG	2:C:276:ASN:HB3	2.27	0.69
2:C:332:VAL:HG12	2:C:334:GLU:H	1.56	0.69
1:A:40:VAL:O	1:A:44:ILE:HG13	1.93	0.69
2:C:583:LEU:HD13	2:C:586:MET:HE1	1.73	0.69
1:A:244:ILE:HD12	1:A:244:ILE:N	2.08	0.69
2:C:201:ALA:HB2	2:C:209:LEU:HD11	1.75	0.68
2:C:511:GLY:O	2:C:515:GLN:HG3	1.94	0.68
1:A:138:THR:O	1:A:356:VAL:HG22	1.94	0.67
1:A:156:PRO:O	1:A:353:ARG:NH1	2.27	0.67
2:C:67:THR:HB	2:C:75:THR:HG23	1.74	0.67
1:A:138:THR:HB	1:A:356:VAL:HG13	1.75	0.67
2:C:203:LEU:HD21	2:C:274:PHE:CE2	2.29	0.67
1:A:10:GLU:O	2:C:617:ARG:CD	2.43	0.67
1:A:271:LYS:HE3	1:A:319:THR:HB	1.75	0.67
1:A:252:GLU:OE1	1:A:308:THR:HG21	1.95	0.67
1:A:70:MET:CE	1:A:78:ASP:HB3	2.19	0.67
2:C:33:ILE:HD11	2:C:44:LEU:HB3	1.76	0.67
2:C:474:GLU:O	2:C:478:THR:HG23	1.93	0.66
2:C:265:ASP:O	2:C:421:SER:CB	2.44	0.66
1:A:146:ASP:CB	1:A:148:THR:HG22	2.25	0.66
1:A:38:LYS:H	1:A:41:GLN:HE21	1.42	0.66
8:F:101:LFX:H01	6:H:4[B]:DT:O2	1.95	0.66
6:H:5[B]:DA:H2"	6:H:6[B]:DT:O5'	1.96	0.66
1:A:146:ASP:OD2	1:A:148:THR:HG22	1.96	0.65
2:C:102:LEU:HD21	2:C:127:VAL:HG22	1.79	0.65
2:C:294:ILE:HA	2:C:297:VAL:HG12	1.78	0.65
2:C:203:LEU:CD2	2:C:274:PHE:CE2	2.80	0.65
2:C:104:ALA:O	2:C:106:GLY:N	2.30	0.64
1:A:13:MET:HE2	2:C:618:VAL:HA	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:491:PHE:CE1	2:C:528:PRO:HG2	2.32	0.64
1:A:126:ILE:HG13	1:A:474:PHE:CD2	2.32	0.64
1:A:222:ARG:HD3	1:A:484:ASP:HA	1.78	0.64
1:A:209:PRO:HB2	1:A:482:LEU:CD1	2.26	0.64
1:A:169:GLY:CA	1:A:176:THR:HG22	2.27	0.64
1:A:60:ARG:HH11	1:A:60:ARG:CG	2.11	0.64
2:C:527:ARG:N	2:C:528:PRO:HD2	2.13	0.63
2:C:583:LEU:HB3	2:C:586:MET:HB2	1.80	0.63
2:C:441:ALA:HB1	2:C:452:ILE:HD12	1.80	0.63
2:C:473:ASN:O	2:C:477:ASN:HB2	1.98	0.63
1:A:288:ARG:HD2	1:A:290:GLU:OE2	1.99	0.63
4:F:3[A]:DT:H4'	4:F:4[A]:DC:OP1	1.99	0.62
2:C:102:LEU:HD23	2:C:126:VAL:HG22	1.81	0.62
2:C:583:LEU:HA	2:C:586:MET:CE	2.21	0.62
1:A:211:PRO:O	1:A:478:ARG:NH2	2.30	0.62
1:A:259:ILE:HB	1:A:260:PRO:CD	2.30	0.62
2:C:583:LEU:HD13	2:C:586:MET:CE	2.30	0.62
1:A:13:MET:HE1	2:C:622:MET:CG	2.30	0.61
2:C:132:SER:O	2:C:151:ASN:N	2.25	0.61
1:A:194:ILE:CD1	1:A:464:LYS:HG3	2.31	0.61
1:A:381:VAL:HG23	1:A:411:PHE:CZ	2.36	0.61
2:C:301:TYR:CD2	2:C:379:ILE:HD11	2.37	0.60
1:A:338:ARG:HH12	1:A:344:PRO:HG2	1.19	0.60
1:A:22:LYS:O	1:A:26:GLN:HG3	2.01	0.60
1:A:23:TYR:HD1	1:A:24:ILE:HD13	1.66	0.60
2:C:584:GLY:C	2:C:586:MET:N	2.59	0.60
6:H:3[B]:DC:H2'	6:H:4[B]:DT:C6	2.37	0.60
1:A:381:VAL:CG2	1:A:411:PHE:CZ	2.85	0.59
2:C:139:THR:HG23	2:C:144:VAL:HB	1.84	0.59
1:A:145:PHE:CE1	1:A:146:ASP:HB2	2.38	0.59
1:A:146:ASP:OD2	1:A:148:THR:CG2	2.50	0.59
1:A:381:VAL:HG23	1:A:411:PHE:CE1	2.37	0.59
2:C:583:LEU:CB	2:C:586:MET:HB2	2.32	0.59
1:A:33:ILE:CD1	1:A:345:ILE:CG1	2.64	0.58
2:C:271:ILE:HD11	2:C:324:LEU:HD13	1.85	0.58
2:C:583:LEU:HD23	2:C:586:MET:HE2	1.80	0.58
1:A:184:ALA:CB	1:A:471:LYS:HE3	2.19	0.58
1:A:183:LEU:HD11	1:A:470:VAL:HG12	1.86	0.58
2:C:134:LEU:HD12	2:C:176:PHE:HB3	1.86	0.58
1:A:317:LYS:HE3	1:A:318:TYR:CZ	2.38	0.57
2:C:446:ASP:OD1	2:C:449:PHE:CE1	2.58	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:51:ASN:HD21	2:C:99:PHE:HA	1.68	0.57
1:A:192:TYR:CZ	1:A:203:LYS:HE2	2.39	0.57
1:A:146:ASP:CG	1:A:148:THR:CG2	2.78	0.57
2:C:373:GLU:C	2:C:375:ALA:H	2.11	0.57
2:C:616:ARG:O	2:C:620:VAL:HG23	2.04	0.57
2:C:416:LEU:HG	2:C:417:THR:N	2.20	0.57
2:C:583:LEU:CA	2:C:586:MET:HB2	2.32	0.57
2:C:48:ILE:HD11	2:C:127:VAL:HG11	1.85	0.57
1:A:259:ILE:HB	1:A:260:PRO:HD2	1.86	0.56
1:A:13:MET:HE1	2:C:622:MET:HG2	1.88	0.56
1:A:288:ARG:NH1	1:A:290:GLU:OE2	2.30	0.56
2:C:584:GLY:HA2	2:C:586:MET:N	2.21	0.55
2:C:190:TYR:CD2	2:C:213:ASP:HB2	2.42	0.55
2:C:48:ILE:HD11	2:C:127:VAL:HG21	1.87	0.55
1:A:210:GLY:HA2	1:A:229:TYR:OH	2.07	0.55
6:H:11[B]:DG:H5'	6:H:11[B]:DG:C8	2.42	0.55
1:A:139:VAL:HG13	1:A:140:PRO:CD	2.36	0.55
2:C:257:VAL:HB	2:C:330:ILE:HG22	1.88	0.54
2:C:197:LEU:HD22	2:C:209:LEU:HD22	1.90	0.54
1:A:184:ALA:HA	1:A:471:LYS:HD2	1.90	0.54
2:C:253:ASN:O	2:C:253:ASN:ND2	2.36	0.54
1:A:13:MET:O	2:C:621:LEU:CD1	2.56	0.54
2:C:380:ARG:HD3	2:C:495:ASP:HA	1.89	0.54
2:C:491:PHE:HE1	2:C:528:PRO:HG2	1.71	0.54
2:C:431:LEU:HD11	2:C:501:ILE:CG2	2.39	0.53
1:A:117[A]:ARG:HH22	4:F:1[A]:DA:H8	1.56	0.53
2:C:442:LYS:O	2:C:445:ARG:HD3	2.08	0.53
1:A:290:GLU:HB2	1:A:297:ARG:HG2	1.90	0.53
2:C:285:THR:HG23	2:C:347:LEU:O	2.09	0.53
1:A:293:ARG:HB3	1:A:293:ARG:NH1	2.15	0.53
1:A:326:ASN:ND2	4:F:11[A]:DG:H4'	2.24	0.53
2:C:52:ALA:HB2	2:C:99:PHE:CE1	2.44	0.53
1:A:192:TYR:OH	1:A:203:LYS:HE2	2.09	0.52
1:A:194:ILE:HD13	1:A:464:LYS:HG3	1.91	0.52
2:C:591:LEU:HD22	2:C:596:MET:HG3	1.91	0.52
1:A:216:GLY:O	1:A:217:ALA:HB3	2.08	0.52
1:A:452:ILE:HG12	1:A:458:THR:CG2	2.40	0.52
1:A:357:ILE:CD1	1:A:459:MET:SD	2.97	0.52
1:A:33:ILE:HD13	1:A:345:ILE:HA	1.89	0.51
2:C:611:LEU:C	2:C:611:LEU:CD1	2.81	0.51
1:A:126:ILE:HG13	1:A:474:PHE:CE2	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:139:THR:O	2:C:170:THR:HA	2.10	0.51
2:C:96:GLU:HG2	2:C:138:ILE:HD11	1.91	0.51
2:C:373:GLU:O	2:C:375:ALA:N	2.43	0.51
1:A:434:VAL:HG13	1:A:435:LEU:N	2.25	0.51
2:C:304:LYS:C	2:C:306:GLY:H	2.18	0.51
1:A:256:ILE:CD1	1:A:321:LEU:HD21	2.33	0.51
2:C:590:GLN:O	2:C:594:THR:HG23	2.11	0.51
2:C:54:ASP:OD1	2:C:107:LYS:HA	2.11	0.50
2:C:479:MET:CE	2:C:522:PHE:CZ	2.94	0.50
2:C:611:LEU:HD13	2:C:611:LEU:O	2.10	0.50
2:C:132:SER:N	2:C:177:MET:O	2.42	0.50
2:C:526:MET:C	2:C:528:PRO:HD2	2.36	0.50
2:C:321:ARG:HG2	2:C:324:LEU:HD12	1.92	0.50
2:C:43:HIS:O	2:C:47:GLU:HG2	2.12	0.49
2:C:464:LYS:HD2	6:H:8[B]:DC:OP2	2.12	0.49
1:A:350:ILE:HG23	1:A:460:TYR:CE1	2.48	0.49
1:A:159:PHE:HB3	1:A:470:VAL:HG11	1.94	0.49
2:C:431:LEU:HD22	2:C:479:MET:CE	2.32	0.49
1:A:194:ILE:HG21	1:A:464:LYS:CD	2.42	0.49
1:A:296:LEU:C	1:A:296:LEU:HD23	2.38	0.49
6:H:3[B]:DC:H4'	6:H:4[B]:DT:OP1	2.12	0.49
1:A:357:ILE:CG2	1:A:459:MET:HG3	2.40	0.49
2:C:360:VAL:O	2:C:364:LEU:HD12	2.13	0.49
1:A:38:LYS:N	1:A:41:GLN:HE21	2.07	0.48
1:A:354:ARG:NE	1:A:456:GLU:OE2	2.40	0.48
2:C:263:TYR:CE2	2:C:378:LEU:HD21	2.47	0.48
2:C:592:TRP:CE2	2:C:597:ASN:HB2	2.47	0.48
1:A:452:ILE:HG12	1:A:458:THR:HG22	1.96	0.48
2:C:351:LEU:HD22	2:C:355:VAL:HG13	1.95	0.48
1:A:326:ASN:CG	4:F:11[A]:DG:H4'	2.39	0.48
2:C:516:THR:O	2:C:520:THR:CG2	2.57	0.48
1:A:194:ILE:HD12	1:A:464:LYS:CG	2.43	0.48
2:C:203:LEU:HD23	2:C:274:PHE:CD2	2.46	0.48
1:A:360:ARG:HH12	1:A:462:LEU:HD13	1.79	0.47
1:A:381:VAL:HG22	1:A:411:PHE:CZ	2.49	0.47
2:C:246:LEU:O	2:C:260:ALA:HA	2.15	0.47
2:C:242:LEU:CD2	2:C:423:ASN:ND2	2.76	0.47
2:C:361:ALA:O	2:C:365:THR:OG1	2.32	0.47
2:C:179:ASP:OD1	2:C:182:ILE:HG23	2.15	0.47
2:C:190:TYR:HD2	2:C:213:ASP:HB2	1.79	0.47
1:A:96:GLU:HG2	1:A:126:ILE:HD12	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:LEU:HD23	1:A:157:ALA:HA	1.96	0.47
1:A:268:LEU:HD11	1:A:321:LEU:HD23	1.97	0.47
1:A:334:ASN:O	1:A:336:THR:HG23	2.15	0.47
1:A:44:ILE:HD13	1:A:85:MET:HB2	1.96	0.47
1:A:360:ARG:HH12	1:A:462:LEU:CD1	2.28	0.47
1:A:414:GLU:CD	1:A:414:GLU:H	2.22	0.47
2:C:524:ARG:CG	2:C:524:ARG:NH1	2.54	0.47
1:A:44:ILE:HD12	1:A:88:MET:HE1	1.95	0.47
2:C:303:ARG:NH1	2:C:310:GLU:HA	2.30	0.46
1:A:146:ASP:OD2	1:A:146:ASP:O	2.33	0.46
2:C:255:PHE:CE2	2:C:332:VAL:HG22	2.50	0.46
1:A:49:ASN:HB2	1:A:131:LEU:HD13	1.97	0.46
1:A:194:ILE:HD12	1:A:464:LYS:HG3	1.97	0.46
2:C:41:LEU:HD11	2:C:178:PRO:HG3	1.98	0.46
2:C:99:PHE:CD1	2:C:99:PHE:C	2.93	0.46
2:C:374:LEU:O	2:C:378:LEU:HB2	2.16	0.46
1:A:44:ILE:HB	1:A:88:MET:HE1	1.97	0.46
1:A:338:ARG:HB3	1:A:340:VAL:HG13	1.98	0.46
1:A:229:TYR:O	1:A:342:ILE:HB	2.15	0.46
2:C:263:TYR:CZ	2:C:378:LEU:HD21	2.50	0.46
2:C:455:LEU:CD1	2:C:518:LEU:HD11	2.46	0.46
1:A:24:ILE:HD13	1:A:24:ILE:N	2.29	0.45
2:C:583:LEU:HB3	2:C:586:MET:HE3	0.49	0.45
1:A:33:ILE:CG1	1:A:345:ILE:HG12	2.44	0.45
1:A:86:VAL:O	1:A:90:GLN:HG3	2.16	0.45
2:C:623:GLY:O	2:C:629:ARG:NH2	2.38	0.45
2:C:75:THR:HB	2:C:175:THR:CB	2.43	0.45
2:C:25:VAL:HB	2:C:32:TYR:CZ	2.51	0.45
2:C:242:LEU:CD2	2:C:423:ASN:HD22	2.30	0.45
2:C:523:TYR:OH	2:C:615:GLU:HB2	2.16	0.45
2:C:100:THR:O	2:C:102:LEU:HD13	2.17	0.45
2:C:265:ASP:HB2	2:C:421:SER:CB	2.47	0.45
1:A:187:ILE:HG12	1:A:467:LEU:HD22	1.99	0.45
2:C:334:GLU:HA	2:C:337:LEU:HB2	1.98	0.45
1:A:70:MET:HE1	1:A:78:ASP:CB	2.25	0.45
1:A:82:TYR:CD1	1:A:116:MET:HB3	2.51	0.45
2:C:307:LEU:HD13	2:C:307:LEU:N	2.32	0.45
1:A:144:ASN:C	1:A:146:ASP:H	2.25	0.44
2:C:121:GLY:C	2:C:123:GLY:H	2.23	0.44
2:C:509:THR:O	2:C:512:ALA:HB3	2.16	0.44
1:A:333:ASP:O	1:A:334:ASN:C	2.60	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ASP:OD1	1:A:35:ASP:C	2.61	0.44
1:A:42:ARG:NE	1:A:154:VAL:HA	2.32	0.44
1:A:45:LEU:HD22	1:A:123:LEU:HD22	1.98	0.44
1:A:194:ILE:HG21	1:A:464:LYS:HD2	2.00	0.44
1:A:415:GLN:O	1:A:419:ILE:HG13	2.18	0.44
1:A:169:GLY:HA3	1:A:176:THR:O	2.18	0.44
2:C:304:LYS:C	2:C:306:GLY:N	2.75	0.44
1:A:243:GLU:C	1:A:244:ILE:HD12	2.42	0.44
2:C:373:GLU:C	2:C:375:ALA:N	2.75	0.44
3:E:13[A]:DA:H2''	3:E:14[A]:DA:O5'	2.17	0.44
1:A:132:GLN:O	1:A:133:ASP:HB2	2.18	0.44
2:C:30:GLY:HA2	2:C:35:SER:H	1.83	0.44
2:C:108:PHE:CD1	2:C:276:ASN:CB	2.69	0.44
1:A:144:ASN:HD21	1:A:148:THR:CG2	2.14	0.43
2:C:26:ARG:HD2	2:C:129:ALA:O	2.18	0.43
1:A:43:ARG:HG2	1:A:73:PHE:HB3	2.01	0.43
2:C:352:ALA:HA	2:C:355:VAL:HG22	2.00	0.43
1:A:29:ALA:O	1:A:38:LYS:HE2	2.19	0.43
2:C:203:LEU:HD21	2:C:274:PHE:CG	2.53	0.43
2:C:388:ALA:HA	2:C:391:ALA:HB3	2.00	0.43
1:A:9:LEU:C	1:A:9:LEU:CD2	2.91	0.43
2:C:285:THR:OG1	2:C:352:ALA:HB3	2.18	0.43
2:C:298:MET:SD	2:C:368:LEU:HD21	2.58	0.43
2:C:583:LEU:CD1	2:C:586:MET:HE3	2.44	0.43
1:A:55:PHE:HA	1:A:122:ARG:HD2	2.00	0.43
2:C:341:GLY:O	2:C:343:THR:N	2.44	0.43
2:C:524:ARG:HH11	2:C:524:ARG:CB	2.32	0.43
6:H:10[B]:DC:H2''	6:H:11[B]:DG:C5'	2.40	0.43
1:A:169:GLY:CA	1:A:176:THR:CG2	2.95	0.43
2:C:283:GLY:HA2	2:C:287:GLU:OE1	2.19	0.42
1:A:423:GLN:NE2	1:A:425:TYR:HE1	2.17	0.42
2:C:328:LEU:HD22	2:C:329:SER:N	2.34	0.42
5:G:13[B]:DC:H2''	5:G:14[B]:DA:O5'	2.19	0.42
1:A:191:VAL:HG22	1:A:464:LYS:HG2	2.00	0.42
1:A:194:ILE:CG2	1:A:464:LYS:HD2	2.49	0.42
1:A:312:LEU:HA	1:A:312:LEU:HD12	1.80	0.42
1:A:375:VAL:O	1:A:379:ILE:HG13	2.19	0.42
2:C:639:PHE:O	2:C:640:THR:CB	2.67	0.42
1:A:184:ALA:HB2	1:A:471:LYS:HG3	2.00	0.42
1:A:353:ARG:HG3	1:A:463:MET:HE3	2.01	0.42
2:C:37:ASP:HA	2:C:38:GLY:HA2	1.71	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:197:LEU:HD23	2:C:197:LEU:HA	1.87	0.42
2:C:536:TYR:N	2:C:536:TYR:CD2	2.87	0.42
1:A:191:VAL:HG11	1:A:468:ARG:NH2	2.35	0.42
1:A:346:LEU:HD23	1:A:346:LEU:HA	1.84	0.42
1:A:125:GLU:CD	1:A:473:LYS:NZ	2.76	0.42
2:C:297:VAL:HG11	2:C:364:LEU:HD11	2.01	0.42
2:C:431:LEU:HD11	2:C:501:ILE:HG22	2.02	0.42
4:F:6[A]:DT:H2''	4:F:7[A]:DT:H5'	2.02	0.42
1:A:146:ASP:OD2	1:A:148:THR:HB	2.20	0.42
2:C:380:ARG:CD	2:C:495:ASP:HA	2.49	0.42
1:A:184:ALA:CB	1:A:471:LYS:HG3	2.50	0.42
1:A:280:LYS:HB3	1:A:280:LYS:HE3	1.79	0.42
2:C:297:VAL:HG11	2:C:364:LEU:CD1	2.50	0.42
2:C:441:ALA:O	2:C:445:ARG:HB3	2.20	0.42
1:A:385:LEU:HA	1:A:385:LEU:HD23	1.86	0.41
2:C:102:LEU:HB2	2:C:103:HIS:H	1.71	0.41
2:C:601:ARG:CZ	2:C:603:LEU:HD11	2.50	0.41
1:A:23:TYR:CD1	1:A:24:ILE:HD13	2.52	0.41
1:A:144:ASN:C	1:A:146:ASP:N	2.77	0.41
1:A:334:ASN:O	1:A:336:THR:CG2	2.69	0.41
2:C:96:GLU:O	2:C:99:PHE:HB3	2.19	0.41
2:C:145:TYR:HA	2:C:160:LYS:O	2.19	0.41
2:C:485:ALA:HB3	2:C:491:PHE:CE2	2.56	0.41
2:C:610:ASP:O	2:C:611:LEU:C	2.62	0.41
1:A:169:GLY:HA2	1:A:176:THR:CG2	2.46	0.41
1:A:357:ILE:CB	1:A:459:MET:CG	2.99	0.41
2:C:165:ALA:HA	2:C:166:PRO:HD3	1.90	0.41
1:A:244:ILE:N	1:A:244:ILE:CD1	2.79	0.41
2:C:74:LEU:HB2	2:C:188:PHE:CE2	2.55	0.41
2:C:446:ASP:OD1	2:C:449:PHE:HE1	2.00	0.41
1:A:184:ALA:HA	1:A:471:LYS:CD	2.50	0.41
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.89	0.41
2:C:220:ILE:HG22	2:C:221:GLU:H	1.86	0.41
1:A:27:ASP:HA	1:A:39:PRO:HG2	2.03	0.41
1:A:307:ASN:OD1	1:A:307:ASN:C	2.64	0.41
2:C:337:LEU:HD23	2:C:337:LEU:HA	1.81	0.41
2:C:627:GLU:N	2:C:628:PRO:CD	2.84	0.41
1:A:340:VAL:HB	1:A:345:ILE:HG13	1.85	0.41
2:C:147:GLN:HB2	2:C:159:LEU:HA	2.03	0.41
1:A:29:ALA:HB3	1:A:171:SER:HB3	2.02	0.40
1:A:107:SER:OG	1:A:111:ASP:OD2	2.37	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:9[A]:DC:C2'	3:E:10[A]:DA:H5''	2.48	0.40
1:A:28:ARG:NH1	1:A:28:ARG:CG	2.64	0.40
2:C:383:ILE:H	2:C:383:ILE:HG13	1.62	0.40
1:A:254:ILE:HD13	1:A:312:LEU:HD13	2.04	0.40
2:C:41:LEU:O	2:C:44:LEU:HD12	2.21	0.40
2:C:235:LEU:HD12	2:C:235:LEU:HA	1.88	0.40
2:C:340:GLU:HB3	2:C:341:GLY:H	1.50	0.40
2:C:520:THR:CG2	2:C:622:MET:HG3	2.44	0.40
1:A:13:MET:O	2:C:621:LEU:HD13	2.21	0.40
2:C:236:ASN:ND2	2:C:264:ASN:HD22	2.20	0.40
1:A:9:LEU:CD2	1:A:9:LEU:O	2.69	0.40
2:C:236:ASN:HD21	2:C:264:ASN:HD22	1.69	0.40
2:C:283:GLY:O	2:C:286:HIS:HE1	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [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	468/496 (94%)	443 (95%)	20 (4%)	5 (1%)	11	46
2	C	524/670 (78%)	455 (87%)	56 (11%)	13 (2%)	4	26
All	All	992/1166 (85%)	898 (90%)	76 (8%)	18 (2%)	6	34

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	305	THR
2	C	373	GLU
1	A	145	PHE
1	A	329	MET
2	C	105	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	122	VAL
2	C	304	LYS
2	C	340	GLU
2	C	496	ALA
2	C	107	LYS
2	C	151	ASN
2	C	374	LEU
1	A	169	GLY
2	C	132	SER
1	A	217	ALA
1	A	221	GLY
2	C	121	GLY
2	C	166	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	377/431 (88%)	341 (90%)	36 (10%)	8	25
2	C	313/558 (56%)	244 (78%)	69 (22%)	1	6
All	All	690/989 (70%)	585 (85%)	105 (15%)	3	12

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	24	ILE
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	134	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	139	VAL
1	A	148	THR
1	A	162	LEU
1	A	168	THR
1	A	183	LEU
1	A	208	LEU
1	A	223	ASP
1	A	236	VAL
1	A	244	ILE
1	A	268	LEU
1	A	279	ASN
1	A	293	ARG
1	A	308	THR
1	A	321	LEU
1	A	336	THR
1	A	338	ARG
1	A	342	ILE
1	A	366	GLU
1	A	367	LYS
1	A	372	LEU
1	A	380	ARG
1	A	387	GLU
1	A	414	GLU
1	A	420	VAL
1	A	432	VAL
1	A	462	LEU
2	C	25	VAL
2	C	33	ILE
2	C	43	HIS
2	C	44	LEU
2	C	45	VAL
2	C	46	TRP
2	C	48	ILE
2	C	49	VAL
2	C	66	VAL
2	C	75	THR
2	C	100	THR
2	C	102	LEU
2	C	108	PHE
2	C	122	VAL
2	C	126	VAL
2	C	138	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	139	THR
2	C	148	ARG
2	C	158	THR
2	C	182	ILE
2	C	203	LEU
2	C	204	LEU
2	C	208	THR
2	C	209	LEU
2	C	211	LEU
2	C	220	ILE
2	C	232	VAL
2	C	233	SER
2	C	235	LEU
2	C	242	LEU
2	C	245	VAL
2	C	253	ASN
2	C	257	VAL
2	C	259	VAL
2	C	275	VAL
2	C	278	VAL
2	C	280	THR
2	C	286	HIS
2	C	288	THR
2	C	294	ILE
2	C	298	MET
2	C	299	ASN
2	C	307	LEU
2	C	324	LEU
2	C	328	LEU
2	C	331	LEU
2	C	332	VAL
2	C	337	LEU
2	C	340	GLU
2	C	351	LEU
2	C	364	LEU
2	C	365	THR
2	C	368	LEU
2	C	378	LEU
2	C	383	ILE
2	C	429	LEU
2	C	431	LEU
2	C	445	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	586	MET
2	C	591	LEU
2	C	595	THR
2	C	611	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	68	ASN
1	A	91	ASN
1	A	196	HIS
1	A	267	ASN
1	A	324	ASN
1	A	328	ASN
1	A	423	GLN
2	C	51	ASN
2	C	69	ASN
2	C	128	ASN
2	C	198	ASN
2	C	264	ASN
2	C	477	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	LFX	F	101	7	29,29,29	0.84	1 (3%)	44,44,44	1.45	9 (20%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	101	LFX	O02-C15	3.10	1.29	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	101	LFX	O-C-C17	-3.81	114.78	122.67
8	F	101	LFX	O01-C06-C04	-2.41	115.37	117.90
8	F	101	LFX	C10-C15-C17	-2.39	112.63	115.64
8	F	101	LFX	C06-C05-N02	-2.32	117.79	119.84
8	F	101	LFX	C02-N01-C01	2.25	116.62	111.57
8	F	101	LFX	C13-C11-C04	2.24	126.67	123.34
8	F	101	LFX	C10-C05-C06	2.14	122.73	120.32
8	F	101	LFX	C06-C04-C11	-2.08	113.89	115.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	101	LFX	F-C11-C04	-2.00	114.99	118.28

There are no chirality outliers.

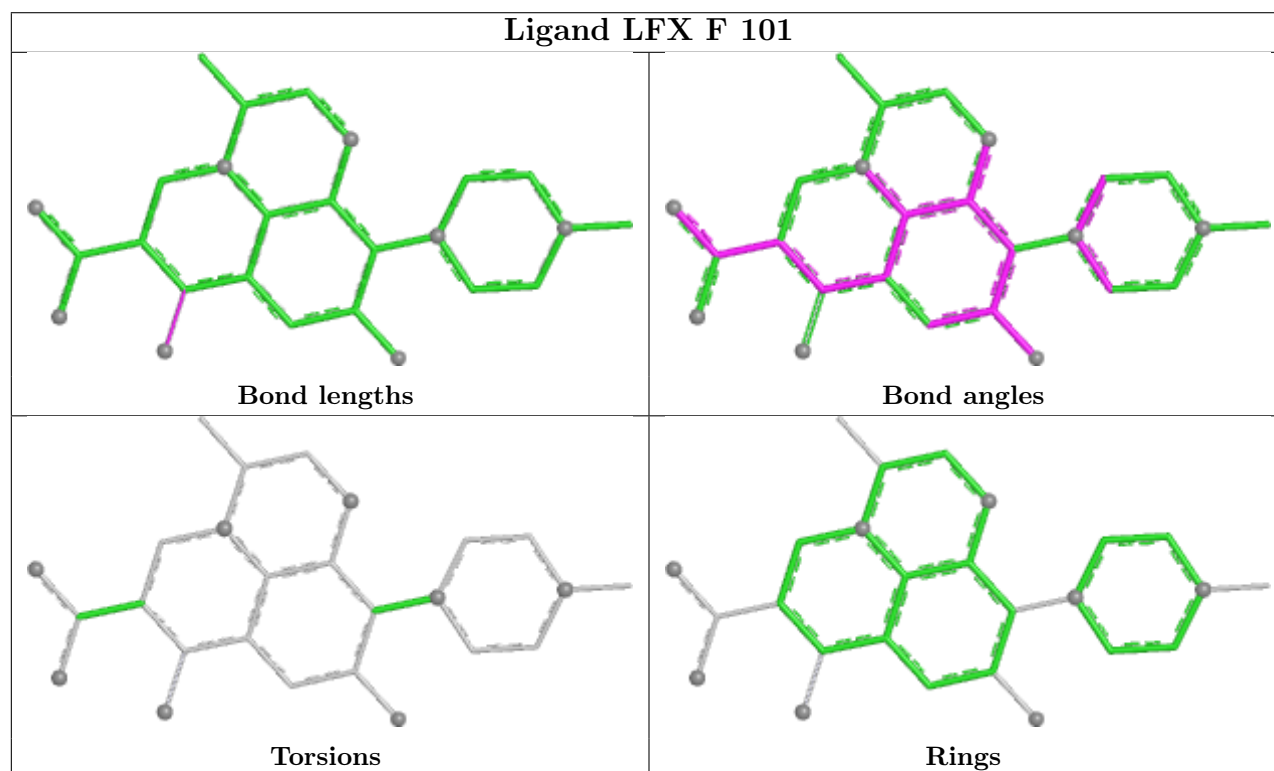
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
2	C	1

All chain breaks are listed below:

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

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	479/496 (96%)	1.01	80 (16%) 4 12	23, 120, 215, 273	1 (0%)
2	C	546/670 (81%)	0.68	64 (11%) 9 17	62, 212, 491, 533	0
3	E	7/11 (63%)	0.92	2 (28%) 1 7	27, 30, 65, 72	7 (100%)
4	F	11/15 (73%)	0.31	0 100 100	27, 46, 56, 68	11 (100%)
5	G	7/11 (63%)	0.90	1 (14%) 6 14	27, 30, 64, 72	7 (100%)
6	H	11/15 (73%)	0.45	0 100 100	28, 47, 56, 67	11 (100%)
All	All	1061/1218 (87%)	0.82	147 (13%) 6 15	23, 161, 464, 533	37 (3%)

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	262	GLU	20.3
2	C	583	LEU	17.3
2	C	639	PHE	11.5
2	C	585	GLU	11.1
1	A	320	ASP	10.8
1	A	335	PHE	10.2
1	A	78	ASP	10.0
1	A	160	PRO	9.0
1	A	389	ILE	8.8
1	A	388	VAL	8.7
2	C	586	MET	8.1
1	A	229	TYR	7.7
2	C	376	SER	7.5
1	A	261	TYR	7.5
2	C	582	GLY	7.0
1	A	323	ILE	7.0
2	C	377	ASN	6.7
1	A	337	PRO	6.5
2	C	507	ALA	6.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	427	LEU	6.2
2	C	96	GLU	5.8
1	A	9	LEU	5.8
2	C	290	LEU	5.8
2	C	374	LEU	5.8
1	A	199	ALA	5.8
2	C	375	ALA	5.5
1	A	174	TYR	5.4
2	C	506	ASP	5.4
2	C	259	VAL	5.4
1	A	342	ILE	5.4
1	A	325	TYR	5.4
2	C	294	ILE	5.3
1	A	198	THR	5.1
1	A	190	ALA	5.1
2	C	119	LEU	4.9
1	A	381	VAL	4.6
2	C	606	VAL	4.6
1	A	75	PRO	4.6
1	A	204	LEU	4.6
1	A	249	GLY	4.6
2	C	637	VAL	4.5
2	C	360	VAL	4.4
1	A	70	MET	4.4
2	C	640	THR	4.3
2	C	341	GLY	4.2
1	A	392	ILE	4.2
1	A	163	LEU	4.2
1	A	61	LYS	4.1
1	A	159	PHE	4.1
2	C	364	LEU	4.1
1	A	366	GLU	4.0
1	A	102	HIS	4.0
1	A	223	ASP	3.9
1	A	81	ILE	3.9
1	A	87	ARG	3.9
1	A	76	HIS	3.9
1	A	186	VAL	3.9
1	A	424	LEU	3.8
1	A	250	GLY	3.8
2	C	63	ARG	3.7
1	A	208	LEU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	116	MET	3.7
1	A	26	GLN	3.7
1	A	343	VAL	3.7
2	C	584	GLY	3.7
1	A	467	LEU	3.6
1	A	189	ALA	3.6
1	A	462	LEU	3.6
1	A	263	ILE	3.5
1	A	22	LYS	3.5
2	C	442	LYS	3.5
1	A	346	LEU	3.4
1	A	120	GLU	3.4
2	C	373	GLU	3.4
1	A	470	VAL	3.4
2	C	479	MET	3.4
2	C	108	PHE	3.3
2	C	64	ILE	3.3
1	A	93	LYS	3.3
1	A	432	VAL	3.3
2	C	246	LEU	3.3
2	C	261	LEU	3.3
1	A	172	ALA	3.2
2	C	276	ASN	3.2
2	C	32	TYR	3.2
2	C	62	ASP	3.2
2	C	504	MET	3.2
1	A	193	MET	3.2
1	A	252	GLU	3.1
2	C	209	LEU	3.1
2	C	505	THR	3.1
1	A	137	LYS	3.1
1	A	66	VAL	3.0
1	A	247	LEU	3.0
1	A	370	LYS	3.0
1	A	419	ILE	3.0
1	A	111	ASP	2.9
1	A	324	ASN	2.9
1	A	98	LEU	2.9
2	C	416	LEU	2.9
1	A	363	PHE	2.9
2	C	453	LEU	2.8
2	C	94	THR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	474	GLU	2.8
1	A	385	LEU	2.8
2	C	530	VAL	2.8
1	A	117[A]	ARG	2.7
2	C	590	GLN	2.7
1	A	336	THR	2.7
3	E	11[A]	DT	2.7
2	C	183	PHE	2.7
1	A	77	GLY	2.6
1	A	64	LYS	2.6
1	A	331	ALA	2.6
2	C	208	THR	2.5
2	C	519	LEU	2.5
1	A	433	VAL	2.5
1	A	194	ILE	2.5
2	C	120	HIS	2.5
2	C	25	VAL	2.5
2	C	207	VAL	2.5
2	C	248	PHE	2.5
2	C	459	VAL	2.5
3	E	12[A]	DG	2.5
2	C	631	LYS	2.4
2	C	368	LEU	2.4
2	C	230	ASP	2.4
2	C	66	VAL	2.3
2	C	298	MET	2.3
1	A	311	VAL	2.3
2	C	494	GLU	2.3
5	G	11[B]	DT	2.3
1	A	302	LEU	2.2
2	C	245	VAL	2.2
2	C	138	ILE	2.2
1	A	201	ILE	2.2
2	C	165	ALA	2.1
1	A	126	ILE	2.1
2	C	378	LEU	2.1
1	A	25	ILE	2.1
1	A	436	GLN	2.1
1	A	466	GLU	2.1
2	C	465	ALA	2.1
1	A	17	PHE	2.1
2	C	456	ARG	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	39	PRO	2.0
2	C	633	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

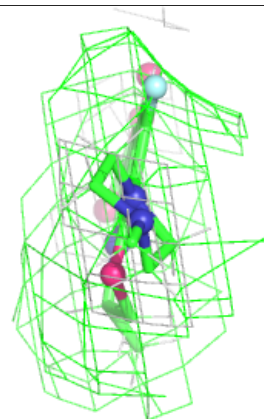
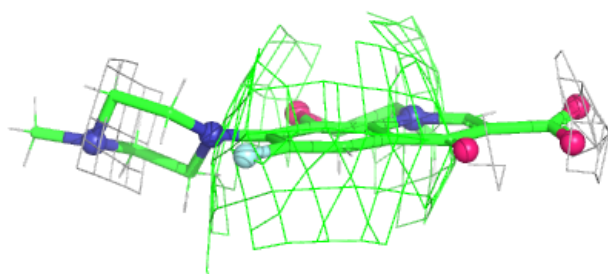
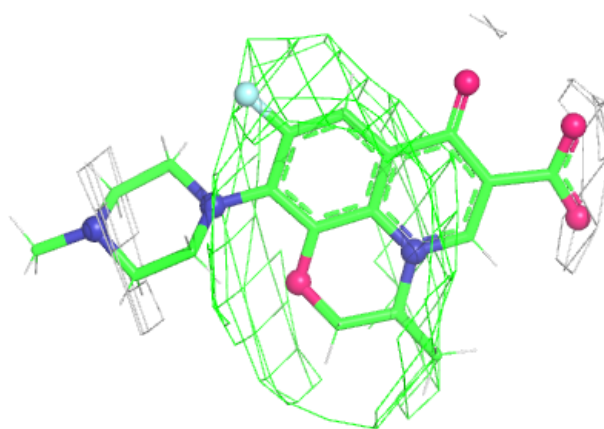
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	501	1/1	0.86	0.17	64,64,64,64	0
8	LFX	F	101	26/26	0.92	0.18	63,89,142,148	0
7	MG	C	701	1/1	0.94	0.13	71,71,71,71	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 F 101:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.