Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 10:35 PM EDT

PDB ID	:	4KPE
Title	:	Novel fluoroquinolones in complex with topoisomerase IV from S. pneumoniae and E-site G-gate
Authors	:	Laponogov, I.; Pan, X.-S.; Vesekov, D.A.; Cirz, R.T.; Wagman, A.S.; Moser, H.E.; Fisher, L.M.; Sanderson, M.R.
Deposited on	:	2013-05-13
Resolution	:	3.43 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 (i) 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 (i)) were used in the production of this report:

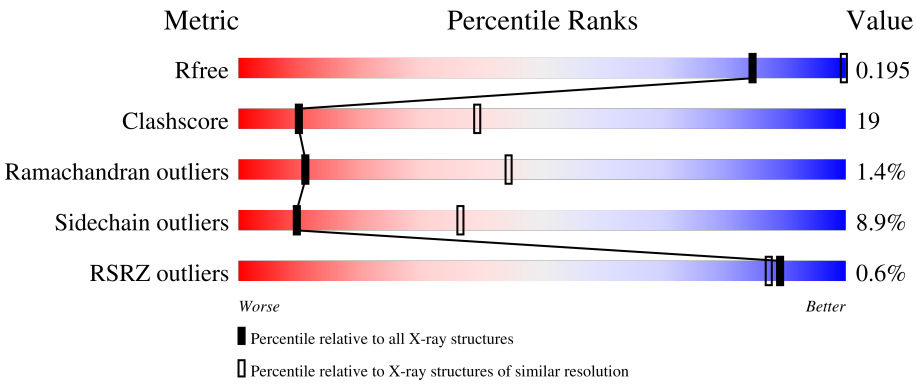
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.43 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1278 (3.50-3.38)
Clashscore	141614	1361 (3.50-3.38)
Ramachandran outliers	138981	1327 (3.50-3.38)
Sidechain outliers	138945	1328 (3.50-3.38)
RSRZ outliers	127900	1192 (3.50-3.38)

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	67% 27% • •
1	B	496	68% 25% • •
2	C	268	% 49% 25% • 22%
2	D	268	2% 54% 20% • 22%

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Mol	Chain	Length	Quality of chain
3	E	7	57% 43%
4	F	11	27% 64% 9%
5	G	7	14% 86%
6	H	11	18% 64% 18%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 11256 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
			Total	C	N	O	S			
1	A	482	3738	2371	645	709	13	0	1	0
1	B	482	3713	2358	638	704	13	0	1	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	257	THR	ILE	engineered mutation	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	engineered mutation	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
			Total	C	N	O	S			
2	C	208	1479	940	259	274	6	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	210	1474	939	256	274	5	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	engineered mutation	UNP Q59961
C	644	ALA	THR	engineered mutation	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	engineered mutation	UNP Q59961
D	644	ALA	THR	engineered mutation	UNP Q59961

- Molecule 3 is a DNA chain called E-site DNA1.

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 E-site DNA2.

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 E-site DNA3.

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

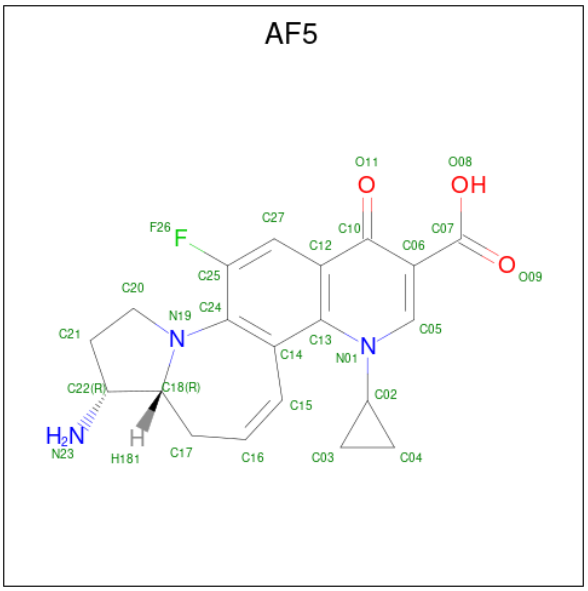
- Molecule 6 is a DNA chain called E-site DNA4.

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 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 (7aR,8R)-8-amino-4-cyclopropyl-12-fluoro-1-oxo-4,7,7a,8,9,10-hexahydro-1H-pyrrolo[1',2':1,7]azepino[2,3-h]quinoline-2-carboxylic acid (three-letter code: AF5) (formula: $C_{20}H_{20}FN_3O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	F	1	Total C F H N O 46 20 1 19 3 3	0	0
8	H	1	Total C F H N O 46 20 1 19 3 3	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	13	Total O 13 13	0	0
9	B	9	Total O 9 9	0	0
9	C	1	Total O 1 1	0	0

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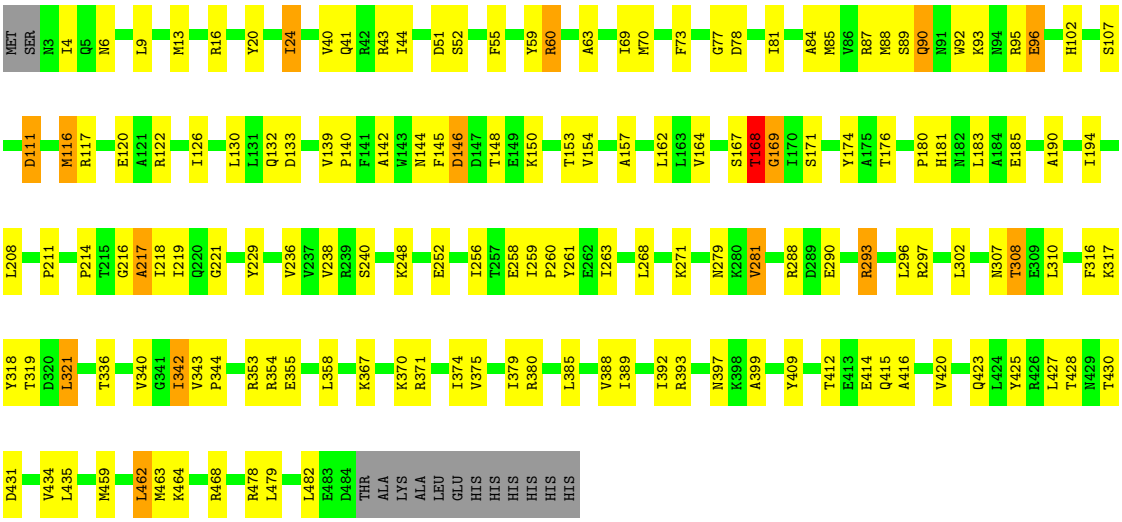
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	D	1	1	1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

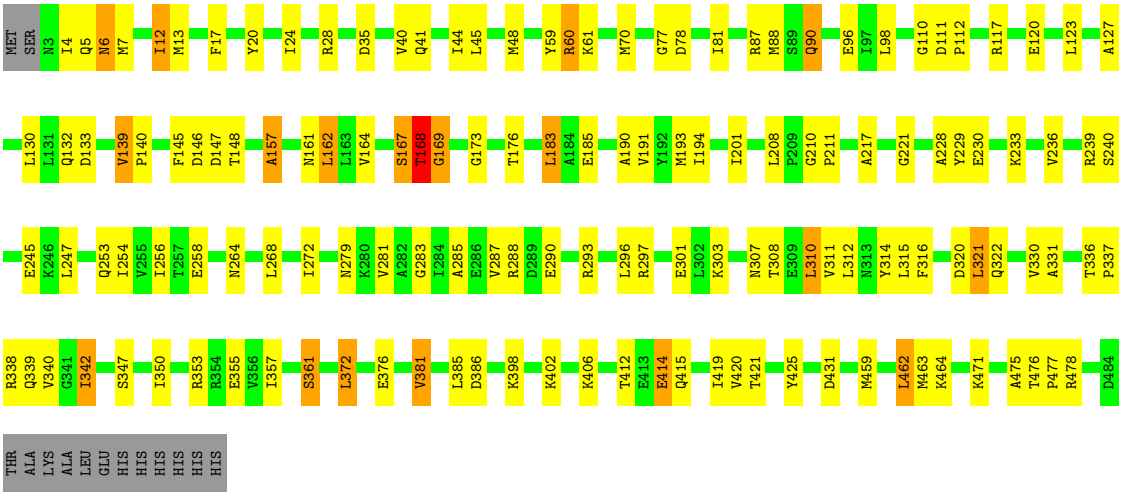
• Molecule 1: DNA topoisomerase 4 subunit A

Chain A: 67% 27%



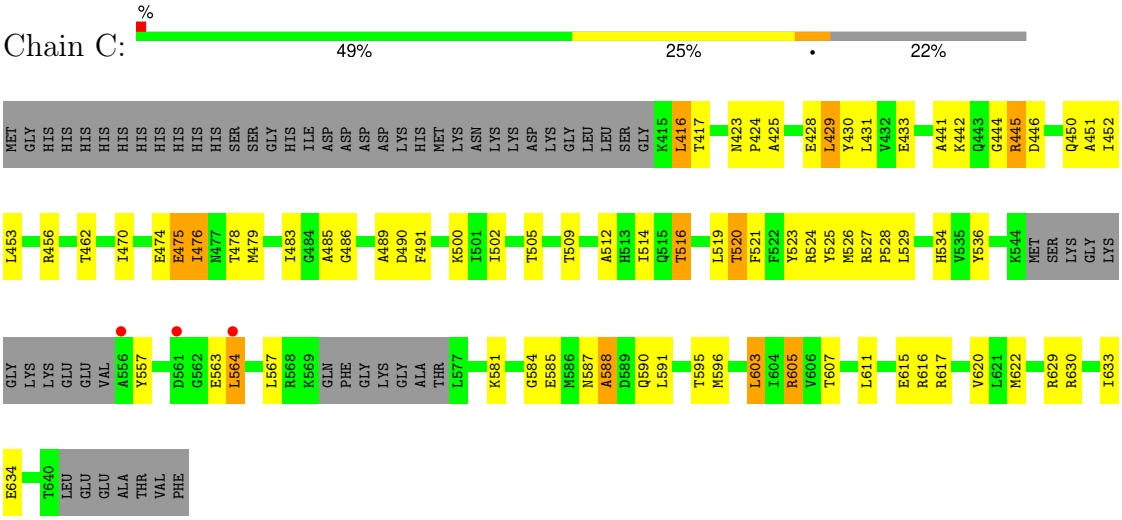
• Molecule 1: DNA topoisomerase 4 subunit A

Chain B: 68% 25%



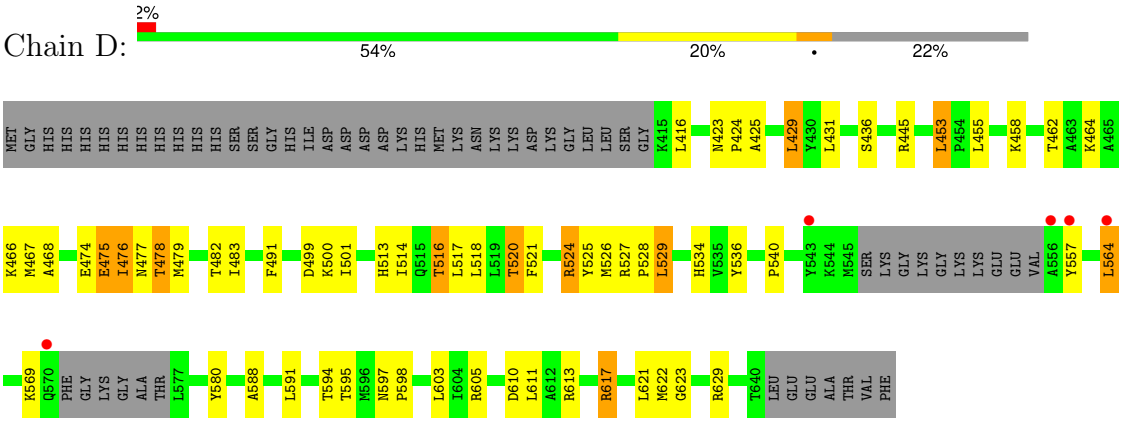
• Molecule 2: DNA topoisomerase 4 subunit B

Chain C:



• Molecule 2: DNA topoisomerase 4 subunit B

Chain D:



• Molecule 3: E-site DNA1

Chain E:

• Molecule 4: E-site DNA2

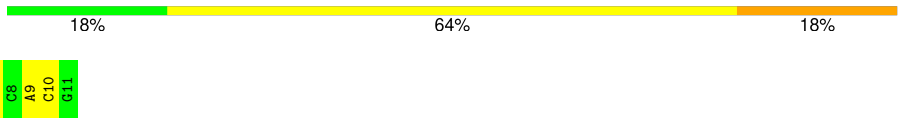
Chain F:

• Molecule 5: E-site DNA3

Chain G:

• Molecule 6: E-site DNA4

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	157.83Å 157.83Å 210.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.82 – 3.43 43.81 – 3.43	Depositor EDS
% Data completeness (in resolution range)	97.1 (41.82-3.43) 97.2 (43.81-3.43)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.13 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.154 , 0.195 0.157 , 0.195	Depositor DCC
R_{free} test set	2002 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	54.2	Xtriage
Anisotropy	0.621	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 44.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11256	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: AF5, 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	0.43	0/3802	0.62	0/5150
1	B	0.45	0/3777	0.62	0/5122
2	C	0.35	0/1505	0.56	0/2053
2	D	0.35	0/1500	0.55	0/2049
3	E	0.87	0/157	1.54	2/241 (0.8%)
4	F	0.86	0/251	1.80	10/385 (2.6%)
5	G	0.78	0/155	1.56	3/238 (1.3%)
6	H	0.79	0/253	1.69	7/388 (1.8%)
All	All	0.46	0/11400	0.75	22/15626 (0.1%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	1	DG	O4'-C1'-N9	8.93	114.25	108.00
6	H	10	DC	O4'-C4'-C3'	-7.95	101.23	106.00
4	F	3	DT	O4'-C4'-C3'	-7.53	101.48	106.00
4	F	10	DT	O4'-C4'-C3'	-7.50	101.50	106.00
6	H	1	DG	C4'-C3'-C2'	-7.35	96.48	103.10
6	H	2	DA	O4'-C4'-C3'	-7.23	101.61	104.50
6	H	4	DT	C5-C4-O4	-7.11	119.93	124.90
6	H	4	DT	N3-C4-O4	6.54	123.82	119.90
4	F	9	DA	O4'-C1'-N9	-6.53	103.43	108.00
4	F	6	DT	O4'-C1'-N1	6.39	112.47	108.00
3	E	14	DA	O4'-C4'-C3'	-6.33	101.97	104.50
6	H	1	DG	C3'-C2'-C1'	-6.13	95.14	102.50
4	F	8	DC	O4'-C1'-N1	6.13	112.29	108.00
5	G	11	DT	N3-C4-O4	6.12	123.57	119.90
4	F	6	DT	O4'-C4'-C3'	-6.07	102.07	104.50
5	G	15	DT	N3-C4-O4	5.84	123.41	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	6	DT	C1'-O4'-C4'	-5.64	104.46	110.10
4	F	6	DT	C4'-C3'-C2'	-5.63	98.03	103.10
3	E	15	DT	N3-C4-O4	5.24	123.04	119.90
5	G	15	DT	O4'-C1'-N1	5.19	111.64	108.00
4	F	7	DT	N3-C2-O2	-5.12	119.23	122.30
4	F	8	DC	C1'-O4'-C4'	-5.03	105.08	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3738	0	3664	138	1
1	B	3713	0	3628	131	1
2	C	1479	0	1308	70	0
2	D	1474	0	1287	57	0
3	E	140	0	78	1	0
4	F	225	0	126	6	0
5	G	139	0	78	5	0
6	H	226	0	124	14	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	27	19	18	6	0
8	H	27	19	18	5	0
9	A	13	0	0	3	0
9	B	9	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
All	All	11218	38	10329	409	1

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 19.

All (409) 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:70:MET:HE1	1:A:78:ASP:CB	1.75	1.16
2:C:526:MET:CE	2:C:529:LEU:HD12	1.80	1.11
1:A:146:ASP:HB3	1:A:148:THR:HG23	1.33	1.10
1:B:146:ASP:HB3	1:B:148:THR:HG23	1.14	1.08
1:A:60:ARG:HG3	1:A:60:ARG:HH11	1.16	1.06
1:B:117[B]:ARG:HG3	1:B:117[B]:ARG:HH11	1.21	1.05
1:A:70:MET:HE1	1:A:78:ASP:HB3	1.11	1.05
1:A:194:ILE:CD1	1:A:463:MET:HE2	1.88	1.04
1:B:70:MET:HE1	1:B:78:ASP:HB3	1.37	1.04
1:A:117[B]:ARG:HH11	1:A:117[B]:ARG:HG3	0.88	1.03
1:A:117[B]:ARG:HG3	1:A:117[B]:ARG:NH1	1.69	1.02
1:B:146:ASP:HB3	1:B:148:THR:CG2	1.94	0.97
1:A:194:ILE:HD11	1:A:463:MET:HE2	1.49	0.95
1:A:96:GLU:HG2	1:A:126:ILE:HD13	1.48	0.94
1:A:60:ARG:HH11	1:A:60:ARG:CG	1.80	0.93
2:C:526:MET:HE3	2:C:529:LEU:HD12	1.49	0.92
1:A:194:ILE:HD11	1:A:463:MET:CE	2.00	0.91
1:B:350:ILE:HG23	1:B:463:MET:CE	2.01	0.91
2:D:520:THR:HG21	2:D:622:MET:HG3	1.53	0.90
1:A:117[B]:ARG:HH11	1:A:117[B]:ARG:CG	1.80	0.90
8:F:101:AF5:H042	6:H:1:DG:H5”	1.52	0.90
1:A:288:ARG:NH1	1:A:290:GLU:OE2	2.04	0.89
1:A:293:ARG:HH11	1:A:293:ARG:HB3	1.38	0.89
1:B:70:MET:HE1	1:B:78:ASP:CB	2.02	0.88
1:B:350:ILE:HG23	1:B:463:MET:HE1	1.56	0.87
2:C:616:ARG:O	2:C:620:VAL:HG23	1.73	0.87
1:A:70:MET:CE	1:A:78:ASP:HB3	2.04	0.86
1:B:256:ILE:HD13	1:B:321:LEU:HD21	1.56	0.86
1:A:139:VAL:HG11	1:A:154:VAL:O	1.75	0.86
1:B:167:SER:C	1:B:168:THR:HG22	1.96	0.86
2:D:474:GLU:O	2:D:478:THR:HG22	1.77	0.85
2:C:536:TYR:HD1	2:C:603:LEU:HD12	1.41	0.84
5:G:13:DC:H42	6:H:7:DG:H1	1.25	0.83
2:D:516:THR:O	2:D:520:THR:HG23	1.78	0.83
1:A:60:ARG:HG3	1:A:60:ARG:NH1	1.90	0.83
1:B:288:ARG:NH1	1:B:290:GLU:OE2	2.12	0.83
1:A:252:GLU:OE1	1:A:308:THR:HG21	1.79	0.82
1:B:164:VAL:HG21	1:B:183:LEU:HD23	1.62	0.81
1:A:167:SER:C	1:A:168:THR:HG22	2.03	0.79
1:B:117[B]:ARG:HG3	1:B:117[B]:ARG:NH1	1.94	0.79
1:A:229:TYR:CD1	1:A:342:ILE:HD13	2.18	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:ILE:HD12	1:B:201:ILE:H	1.47	0.79
1:B:350:ILE:HA	1:B:463:MET:HE1	1.64	0.79
1:A:194:ILE:HD13	1:A:463:MET:HE2	1.64	0.78
2:C:536:TYR:CD1	2:C:603:LEU:HD12	2.18	0.78
8:F:101:AF5:H151	8:F:101:AF5:H031	1.64	0.78
2:C:462:THR:HG21	2:C:521:PHE:HD2	1.49	0.78
1:B:44:ILE:HD12	1:B:88:MET:CE	2.14	0.77
2:C:470:ILE:O	2:C:476:ILE:HG21	1.85	0.77
2:C:536:TYR:HB3	2:C:603:LEU:CD1	2.14	0.76
1:A:146:ASP:CB	1:A:148:THR:HG23	2.12	0.76
8:F:101:AF5:H151	8:F:101:AF5:C03	2.16	0.76
2:C:486:GLY:O	2:C:491:PHE:HD2	1.70	0.75
2:C:591:LEU:HD22	2:C:596:MET:HG3	1.68	0.75
1:B:239:ARG:HB2	1:B:322:GLN:HG3	1.69	0.74
1:A:317:LYS:HE2	1:A:318:TYR:CZ	2.22	0.74
1:A:44:ILE:HD12	1:A:88:MET:CE	2.18	0.74
1:A:20:TYR:OH	9:A:612:HOH:O	2.06	0.74
1:A:146:ASP:HB3	1:A:148:THR:CG2	2.14	0.73
2:D:524:ARG:HH11	2:D:524:ARG:HB3	1.53	0.73
1:A:355:GLU:OE2	1:A:355:GLU:HA	1.85	0.73
1:B:211:PRO:O	1:B:478:ARG:NH2	2.23	0.72
6:H:4:DT:H2"	6:H:5:DA:H5'	1.70	0.71
1:B:146:ASP:CB	1:B:148:THR:HG23	2.07	0.71
1:B:281:VAL:HG21	1:B:314:TYR:CB	2.20	0.70
2:C:629:ARG:O	2:C:633:ILE:HG13	1.90	0.70
2:C:516:THR:O	2:C:520:THR:HG23	1.91	0.70
1:B:193:MET:HE1	1:B:347:SER:HB3	1.74	0.70
5:G:13:DC:N3	6:H:7:DG:N2	2.36	0.70
1:B:201:ILE:HD12	1:B:201:ILE:N	2.07	0.70
1:A:70:MET:CE	1:A:78:ASP:CB	2.66	0.69
1:A:307:ASN:ND2	1:A:310:LEU:HB2	2.08	0.69
2:C:520:THR:HG21	2:C:622:MET:HG3	1.72	0.69
2:D:423:ASN:O	2:D:425:ALA:N	2.25	0.68
1:B:194:ILE:HG12	1:B:350:ILE:HD13	1.75	0.68
2:C:527:ARG:N	2:C:528:PRO:HD2	2.09	0.67
2:C:591:LEU:CD2	2:C:596:MET:HG3	2.23	0.67
1:A:296:LEU:HD23	1:A:297:ARG:N	2.09	0.67
1:A:293:ARG:HB3	1:A:293:ARG:NH1	2.07	0.67
2:D:525:TYR:O	2:D:526:MET:HG3	1.94	0.67
1:A:211:PRO:O	1:A:478:ARG:NH2	2.28	0.67
1:B:281:VAL:HG21	1:B:314:TYR:CG	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:3:DC:H2'	6:H:4:DT:C5	2.29	0.66
2:C:536:TYR:CD1	2:C:603:LEU:CD1	2.78	0.66
2:C:564:LEU:O	2:C:567:LEU:N	2.27	0.66
1:B:4:ILE:HG12	1:B:5:GLN:N	2.09	0.66
2:C:491:PHE:HD1	2:C:528:PRO:HG2	1.61	0.66
1:B:350:ILE:CA	1:B:463:MET:HE1	2.26	0.65
5:G:13:DC:N4	6:H:7:DG:H1	1.93	0.65
1:B:117[B]:ARG:HH11	1:B:117[B]:ARG:CG	2.04	0.65
1:A:216:GLY:O	1:A:217:ALA:HB3	1.96	0.65
2:C:536:TYR:HB3	2:C:603:LEU:HD11	1.77	0.64
1:B:7:MET:HB3	1:B:12:ILE:CD1	2.27	0.64
1:A:397:ASN:OD1	1:A:399:ALA:HB3	1.98	0.64
6:H:3:DC:H4'	6:H:4:DT:OP1	1.98	0.64
1:B:350:ILE:CG2	1:B:463:MET:HE1	2.27	0.64
2:D:516:THR:HG23	2:D:622:MET:CE	2.28	0.63
1:B:350:ILE:HG23	1:B:463:MET:HE2	1.76	0.63
4:F:3:DT:H4'	4:F:4:DC:OP1	1.98	0.63
1:B:4:ILE:HG12	1:B:5:GLN:H	1.61	0.63
1:B:59:TYR:HB3	1:B:120:GLU:HB3	1.79	0.62
1:B:168:THR:HA	1:B:176:THR:O	1.99	0.62
8:F:101:AF5:C04	6:H:1:DG:H5"	2.27	0.62
1:B:307:ASN:ND2	1:B:310:LEU:HB2	2.14	0.62
2:C:489:ALA:C	2:C:491:PHE:H	2.02	0.62
1:A:194:ILE:CD1	1:A:463:MET:CE	2.66	0.62
8:H:101:AF5:H151	8:H:101:AF5:H031	1.80	0.62
1:A:139:VAL:HG13	1:A:140:PRO:HD2	1.82	0.61
1:B:201:ILE:H	1:B:201:ILE:CD1	2.11	0.61
6:H:3:DC:H2'	6:H:4:DT:C6	2.35	0.61
2:C:431:LEU:HD13	2:C:479:MET:CE	2.29	0.61
2:C:536:TYR:CB	2:C:603:LEU:HD11	2.31	0.61
1:B:281:VAL:CG2	1:B:314:TYR:CG	2.82	0.61
1:A:317:LYS:HD3	1:A:318:TYR:CE2	2.35	0.61
2:D:610:ASP:OD2	2:D:613:ARG:HB2	2.01	0.60
1:B:169:GLY:HA3	1:B:176:THR:O	2.00	0.60
2:C:431:LEU:HD13	2:C:479:MET:HE3	1.81	0.60
1:A:169:GLY:HA2	1:A:176:THR:HG22	1.81	0.60
2:C:536:TYR:HD1	2:C:603:LEU:CD1	2.12	0.60
4:F:3:DT:H2'	4:F:4:DC:C6	2.37	0.60
2:D:527:ARG:N	2:D:528:PRO:HD2	2.17	0.60
1:A:4:ILE:HD11	2:C:605:ARG:HG3	1.83	0.59
1:A:164:VAL:HG21	1:A:183:LEU:HD23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:MET:CE	1:B:347:SER:HB3	2.32	0.59
1:B:240:SER:OG	1:B:321:LEU:O	2.17	0.59
2:D:474:GLU:O	2:D:478:THR:CG2	2.49	0.59
2:D:623:GLY:O	2:D:629:ARG:NH2	2.32	0.59
2:D:423:ASN:C	2:D:425:ALA:H	2.05	0.59
1:A:367:LYS:NZ	1:A:367:LYS:HB3	2.17	0.58
1:B:169:GLY:HA2	1:B:176:THR:HG22	1.85	0.58
1:A:169:GLY:HA2	1:A:176:THR:CG2	2.34	0.58
1:B:355:GLU:OE2	1:B:355:GLU:HA	2.03	0.58
2:D:527:ARG:N	2:D:528:PRO:CD	2.66	0.58
1:B:77:GLY:O	1:B:81:ILE:HG13	2.04	0.58
2:C:491:PHE:HE1	2:C:528:PRO:HB2	1.69	0.58
2:C:491:PHE:CD1	2:C:528:PRO:HG2	2.38	0.57
1:A:84:ALA:O	1:A:88:MET:HG3	2.04	0.57
6:H:4:DT:C2'	6:H:5:DA:H5'	2.35	0.57
1:A:434:VAL:HG13	1:A:435:LEU:N	2.19	0.57
2:C:423:ASN:O	2:C:425:ALA:N	2.37	0.57
1:A:423:GLN:NE2	1:B:421:THR:HB	2.20	0.56
8:F:101:AF5:C15	8:F:101:AF5:C02	2.83	0.56
1:A:296:LEU:HD23	1:A:296:LEU:C	2.25	0.56
2:C:527:ARG:N	2:C:528:PRO:CD	2.69	0.56
2:D:516:THR:HG22	2:D:517:LEU:HG	1.88	0.56
2:C:474:GLU:O	2:C:478:THR:HG23	2.05	0.55
8:H:101:AF5:H151	8:H:101:AF5:C03	2.37	0.55
1:A:63:ALA:HB2	1:A:116:MET:HG2	1.87	0.55
2:D:458:LYS:HB2	6:H:6:DT:O2	2.05	0.55
1:B:190:ALA:O	1:B:194:ILE:HG13	2.07	0.55
1:A:117[A]:ARG:NH2	4:F:1:DA:H2'	2.22	0.55
1:A:431:ASP:OD1	1:A:434:VAL:HG12	2.06	0.55
2:C:630:ARG:O	2:C:634:GLU:HG3	2.06	0.55
1:B:35:ASP:O	1:B:161:ASN:HB3	2.07	0.54
1:A:181:HIS:CD2	1:A:211:PRO:HA	2.42	0.54
1:A:44:ILE:HD12	1:A:88:MET:HE3	1.88	0.54
1:A:130:LEU:HD23	1:A:157:ALA:HA	1.90	0.54
1:A:240:SER:OG	1:A:321:LEU:HD22	2.07	0.54
2:C:431:LEU:CD1	2:C:479:MET:CE	2.85	0.54
1:A:425:TYR:O	1:A:428:THR:OG1	2.22	0.54
2:C:444:GLY:HA2	2:C:588:ALA:HB1	1.90	0.54
1:A:354:ARG:HG3	1:A:459:MET:CE	2.38	0.54
1:A:70:MET:HE2	1:A:78:ASP:HA	1.89	0.54
1:A:371:ARG:O	1:A:375:VAL:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:GLY:HA2	1:B:303:LYS:HD2	1.89	0.53
1:A:388:VAL:O	1:A:392:ILE:HD12	2.08	0.53
1:A:44:ILE:HG12	1:A:69:ILE:HD13	1.90	0.53
2:C:591:LEU:HD23	2:C:591:LEU:O	2.09	0.53
1:B:281:VAL:HG23	1:B:314:TYR:CD2	2.43	0.53
1:B:240:SER:OG	1:B:321:LEU:HD22	2.09	0.53
1:A:70:MET:HE1	1:A:78:ASP:CA	2.37	0.53
1:B:167:SER:O	1:B:168:THR:HG22	2.08	0.53
2:C:526:MET:CE	2:C:529:LEU:CD1	2.73	0.53
2:C:587:ASN:O	2:C:590:GLN:N	2.41	0.53
2:C:486:GLY:O	2:C:491:PHE:CD2	2.56	0.52
2:D:516:THR:HG22	2:D:517:LEU:N	2.22	0.52
1:A:256:ILE:HD13	1:A:321:LEU:HD21	1.90	0.52
1:B:229:TYR:CG	1:B:342:ILE:HG12	2.44	0.52
1:B:372:LEU:HD22	1:B:376:GLU:HG3	1.91	0.52
2:D:464:LYS:HG3	2:D:622:MET:O	2.09	0.52
1:A:229:TYR:CD1	1:A:342:ILE:CD1	2.90	0.52
1:B:45:LEU:HD22	1:B:123:LEU:HD22	1.92	0.52
2:C:485:ALA:HB3	2:C:491:PHE:CE2	2.44	0.52
1:B:40:VAL:HG13	1:B:41:GLN:N	2.24	0.52
1:B:44:ILE:CD1	1:B:88:MET:CE	2.88	0.52
1:A:171:SER:HB3	1:A:174:TYR:O	2.10	0.52
1:A:240:SER:HB3	1:A:258:GLU:O	2.11	0.52
1:A:43:ARG:HG2	1:A:73:PHE:HB3	1.91	0.51
1:A:51:ASP:O	1:A:52:SER:HB2	2.10	0.51
1:A:271:LYS:HE3	1:A:319:THR:HB	1.92	0.51
1:B:290:GLU:OE1	1:B:297:ARG:NH1	2.41	0.51
2:C:431:LEU:CD1	2:C:479:MET:HE3	2.39	0.51
2:D:524:ARG:HH11	2:D:524:ARG:CB	2.22	0.51
1:B:471:LYS:O	1:B:475:ALA:HB2	2.10	0.51
1:B:7:MET:HB3	1:B:12:ILE:HD12	1.92	0.51
1:B:146:ASP:O	1:B:147:ASP:HB2	2.11	0.51
4:F:3:DT:H2'	4:F:4:DC:C5	2.45	0.51
8:H:101:AF5:C02	8:H:101:AF5:C15	2.88	0.51
1:B:357:ILE:O	1:B:361:SER:OG	2.28	0.51
2:D:540:PRO:HA	2:D:595:THR:HG22	1.93	0.51
1:B:17:PHE:CD1	2:D:621:LEU:HD22	2.46	0.51
1:A:167:SER:C	1:A:168:THR:CG2	2.74	0.50
1:B:13:MET:CE	2:D:520:THR:HG22	2.42	0.50
1:B:44:ILE:O	1:B:48:MET:HG3	2.12	0.50
1:B:194:ILE:CD1	1:B:463:MET:HG2	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:LEU:HD11	1:B:253:GLN:HB2	1.92	0.50
2:C:536:TYR:HB3	2:C:603:LEU:HD13	1.90	0.50
1:A:107:SER:OG	1:A:111:ASP:OD2	2.22	0.50
1:A:157:ALA:O	1:A:353:ARG:HD3	2.12	0.50
1:A:6:ASN:HD22	2:C:607:THR:HG21	1.76	0.50
1:A:214:PRO:HA	1:A:479:LEU:HD12	1.93	0.50
1:B:201:ILE:HG12	1:B:230:GLU:HG3	1.94	0.50
2:D:516:THR:CG2	2:D:622:MET:HE1	2.42	0.50
1:A:41:GLN:HA	1:A:88:MET:HE1	1.94	0.49
1:A:77:GLY:O	1:A:81:ILE:HG13	2.12	0.49
2:C:591:LEU:HD22	2:C:596:MET:CG	2.40	0.49
1:A:464:LYS:O	1:A:468:ARG:HG3	2.12	0.49
2:C:525:TYR:O	2:C:526:MET:HG3	2.12	0.49
2:C:557:TYR:OH	2:C:590:GLN:HG2	2.12	0.49
1:A:169:GLY:HA3	1:A:176:THR:O	2.12	0.49
1:A:185:GLU:OE1	1:A:478:ARG:NH1	2.45	0.49
1:B:24:ILE:HG13	1:B:28:ARG:HD2	1.94	0.49
1:B:281:VAL:CG2	1:B:314:TYR:CD2	2.95	0.49
1:A:302:LEU:CD1	1:A:308:THR:HB	2.42	0.49
2:D:526:MET:CE	2:D:529:LEU:HD12	2.42	0.49
1:A:70:MET:CE	1:A:78:ASP:HA	2.42	0.49
2:C:462:THR:HG21	2:C:521:PHE:CD2	2.38	0.49
2:C:509:THR:O	2:C:512:ALA:HB3	2.13	0.49
2:D:455:LEU:CD1	2:D:518:LEU:HD21	2.43	0.49
1:A:60:ARG:CG	1:A:60:ARG:NH1	2.52	0.49
2:D:564:LEU:C	2:D:564:LEU:CD2	2.81	0.49
2:C:442:LYS:O	2:C:445:ARG:HD3	2.13	0.48
2:C:446:ASP:O	2:C:450:GLN:HB2	2.13	0.48
4:F:1:DA:H5"	8:H:101:AF5:C04	2.42	0.48
4:F:1:DA:H5"	8:H:101:AF5:H042	1.94	0.48
1:B:194:ILE:HG12	1:B:350:ILE:CD1	2.42	0.48
2:D:491:PHE:CE1	2:D:528:PRO:HB2	2.48	0.48
2:D:500:LYS:HG3	2:D:536:TYR:CE2	2.49	0.48
1:B:20:TYR:CD1	2:D:513:HIS:HB2	2.49	0.48
1:A:70:MET:CE	1:A:78:ASP:CA	2.91	0.48
1:B:157:ALA:O	1:B:353:ARG:HD3	2.13	0.48
2:D:478:THR:O	2:D:478:THR:OG1	2.27	0.48
1:A:140:PRO:HG2	1:A:153:THR:OG1	2.14	0.48
1:B:307:ASN:CG	1:B:310:LEU:HB2	2.34	0.48
2:D:478:THR:O	2:D:482:THR:OG1	2.28	0.48
1:A:425:TYR:HB3	1:B:420:VAL:HG13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:101:AF5:C03	8:F:101:AF5:C15	2.89	0.48
1:A:367:LYS:NZ	1:A:367:LYS:CB	2.76	0.47
2:D:594:THR:OG1	2:D:595:THR:HG23	2.13	0.47
2:D:525:TYR:C	2:D:526:MET:HG3	2.35	0.47
1:A:290:GLU:HB2	1:A:297:ARG:HG2	1.95	0.47
1:B:311:VAL:O	1:B:315:LEU:HG	2.14	0.47
1:B:350:ILE:CB	1:B:463:MET:HE1	2.44	0.47
1:B:381:VAL:HG21	1:B:419:ILE:HD13	1.96	0.47
1:A:371:ARG:HG3	1:A:375:VAL:HG23	1.96	0.47
1:A:144:ASN:HA	9:A:605:HOH:O	2.14	0.47
2:D:529:LEU:CD2	2:D:534:HIS:HB2	2.44	0.47
2:D:617:ARG:O	2:D:617:ARG:HG3	2.14	0.47
2:D:629:ARG:HD2	6:H:9:DA:OP1	2.14	0.47
1:A:20:TYR:O	1:A:24:ILE:HG22	2.15	0.47
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.76	0.47
1:B:185:GLU:OE1	1:B:478:ARG:NH1	2.47	0.47
1:B:139:VAL:HG22	1:B:140:PRO:HD2	1.96	0.47
1:B:167:SER:C	1:B:168:THR:CG2	2.68	0.47
1:B:169:GLY:CA	1:B:176:THR:HG22	2.45	0.47
1:A:420:VAL:HG13	1:B:425:TYR:HB3	1.97	0.47
1:B:217:ALA:N	1:B:258:GLU:OE1	2.28	0.47
2:D:557:TYR:HE2	2:D:580:TYR:HH	1.63	0.47
1:A:40:VAL:HG13	1:A:41:GLN:N	2.31	0.46
1:B:296:LEU:C	1:B:296:LEU:HD23	2.35	0.46
1:A:144:ASN:C	1:A:146:ASP:H	2.19	0.46
1:A:219:ILE:HB	1:A:482:LEU:HD23	1.97	0.46
1:A:367:LYS:HB3	1:A:367:LYS:HZ3	1.80	0.46
1:A:425:TYR:CD2	1:B:398:LYS:HB2	2.51	0.46
1:B:288:ARG:NH2	1:B:301:GLU:OE2	2.47	0.46
2:C:441:ALA:O	2:C:445:ARG:HB3	2.16	0.46
2:C:429:LEU:HA	2:C:429:LEU:HD23	1.67	0.46
1:B:459:MET:SD	1:B:459:MET:C	2.94	0.46
1:A:259:ILE:HB	1:A:260:PRO:CD	2.46	0.46
2:C:416:LEU:HG	2:C:417:THR:N	2.31	0.46
1:B:194:ILE:HD13	1:B:463:MET:HG2	1.97	0.46
1:B:350:ILE:HG12	1:B:463:MET:CE	2.46	0.46
1:A:169:GLY:CA	1:A:176:THR:CG2	2.94	0.45
1:B:110:GLY:HA3	1:B:264:ASN:HD21	1.81	0.45
1:B:281:VAL:HG23	1:B:314:TYR:CG	2.51	0.45
2:C:516:THR:HG23	2:C:622:MET:SD	2.56	0.45
1:A:260:PRO:O	1:A:263:ILE:HB	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:526:MET:HE2	2:C:529:LEU:HD12	1.86	0.45
1:B:281:VAL:HG21	1:B:314:TYR:HB2	1.96	0.45
2:C:523:TYR:OH	2:C:615:GLU:HB2	2.17	0.45
1:A:130:LEU:HD23	1:A:130:LEU:HA	1.76	0.45
1:A:343:VAL:HG12	1:A:344:PRO:N	2.31	0.45
2:D:501:ILE:HD12	2:D:529:LEU:HD11	1.98	0.45
1:A:40:VAL:O	1:A:44:ILE:HG13	2.17	0.45
1:A:51:ASP:O	1:A:60:ARG:NH2	2.49	0.45
1:A:416:ALA:O	1:A:420:VAL:HB	2.17	0.45
1:B:476:THR:HB	1:B:477:PRO:HD2	1.99	0.45
5:G:13:DC:H2"	5:G:14:DA:O5'	2.17	0.45
1:A:90:GLN:HB3	1:A:92:TRP:CH2	2.51	0.45
1:B:194:ILE:HD11	1:B:463:MET:HE3	1.99	0.45
1:B:320:ASP:C	1:B:322:GLN:N	2.69	0.45
2:C:475:GLU:O	2:C:479:MET:HG3	2.17	0.45
2:D:466:LYS:O	2:D:468:ALA:N	2.50	0.44
2:C:430:TYR:CZ	2:C:502:ILE:HD12	2.52	0.44
2:D:491:PHE:HD1	2:D:528:PRO:HG2	1.83	0.44
1:B:61:LYS:HB2	1:B:61:LYS:HE2	1.84	0.44
1:B:70:MET:HE1	1:B:78:ASP:CA	2.47	0.44
1:B:307:ASN:HB3	1:B:310:LEU:HB2	1.99	0.44
1:A:281:VAL:CG2	1:A:310:LEU:CD1	2.96	0.44
1:B:4:ILE:HD11	2:D:605:ARG:CB	2.47	0.44
2:C:423:ASN:C	2:C:425:ALA:H	2.20	0.44
2:D:423:ASN:C	2:D:425:ALA:N	2.71	0.44
2:C:428:GLU:HG2	2:C:500:LYS:HB2	2.00	0.44
2:C:526:MET:HE1	2:C:529:LEU:HD12	1.88	0.44
1:A:132:GLN:O	1:A:133:ASP:HB2	2.18	0.44
1:B:412:THR:HG23	1:B:415:GLN:OE1	2.17	0.44
2:D:462:THR:HG21	2:D:521:PHE:HD2	1.83	0.44
1:A:218:ILE:O	1:A:238:VAL:HA	2.18	0.43
1:B:13:MET:HE2	2:D:520:THR:HG22	2.00	0.43
2:C:519:LEU:HD23	2:C:519:LEU:HA	1.82	0.43
2:D:529:LEU:CD2	2:D:534:HIS:CB	2.96	0.43
1:A:340:VAL:HB	1:A:344:PRO:HG2	2.00	0.43
1:B:210:GLY:HA2	1:B:229:TYR:OH	2.18	0.43
1:A:13:MET:HE1	2:C:520:THR:HG22	2.01	0.43
1:A:144:ASN:O	1:A:146:ASP:N	2.52	0.43
1:A:59:TYR:HB3	1:A:120:GLU:HB3	2.01	0.43
1:B:145:PHE:CD1	1:B:146:ASP:N	2.86	0.43
2:C:451:ALA:O	2:C:452:ILE:HD13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:489:ALA:C	2:C:491:PHE:N	2.70	0.43
2:D:476:ILE:HD12	2:D:476:ILE:HA	1.75	0.43
2:D:526:MET:HE2	2:D:529:LEU:HD12	1.99	0.43
1:A:393:ARG:NH1	1:B:386:ASP:OD1	2.51	0.43
1:B:40:VAL:CG1	1:B:41:GLN:N	2.81	0.43
1:A:316:PHE:CE2	1:A:321:LEU:HD13	2.53	0.43
1:A:462:LEU:HD23	1:A:462:LEU:HA	1.72	0.43
2:C:479:MET:O	2:C:483:ILE:HG13	2.18	0.43
2:D:429:LEU:HA	2:D:429:LEU:HD23	1.78	0.43
2:D:529:LEU:HD22	2:D:534:HIS:HB2	2.01	0.43
1:B:132:GLN:O	1:B:133:ASP:HB2	2.19	0.43
1:B:162:LEU:HA	1:B:162:LEU:HD23	1.64	0.43
1:A:412:THR:OG1	1:A:415:GLN:HG3	2.19	0.43
1:A:463:MET:HE2	1:A:463:MET:HB3	1.76	0.43
1:B:44:ILE:CD1	1:B:88:MET:HE3	2.48	0.43
1:B:111:ASP:HB2	1:B:112:PRO:CD	2.49	0.43
2:D:475:GLU:O	2:D:479:MET:HG3	2.18	0.43
2:D:476:ILE:HG22	2:D:477:ASN:N	2.33	0.43
1:A:40:VAL:CG1	1:A:41:GLN:N	2.81	0.42
1:A:216:GLY:O	1:A:217:ALA:CB	2.61	0.42
1:A:375:VAL:O	1:A:379:ILE:HG13	2.19	0.42
1:B:41:GLN:HA	1:B:88:MET:HE1	2.01	0.42
1:B:254:ILE:HD13	1:B:312:LEU:HD13	2.01	0.42
1:B:330:VAL:HG12	1:B:331:ALA:N	2.34	0.42
2:C:476:ILE:HD12	2:C:476:ILE:HA	1.69	0.42
2:C:536:TYR:CD2	2:C:536:TYR:N	2.87	0.42
2:D:453:LEU:C	2:D:453:LEU:HD22	2.38	0.42
3:E:12:DG:H2'	3:E:12:DG:O5'	2.19	0.42
1:A:389:ILE:HD11	1:A:427:LEU:HD13	2.01	0.42
1:B:338:ARG:O	1:B:340:VAL:HG13	2.19	0.42
1:A:281:VAL:HG22	1:A:310:LEU:CD1	2.49	0.42
1:B:7:MET:HB3	1:B:12:ILE:HD11	2.00	0.42
1:B:228:ALA:HA	1:B:233:LYS:O	2.20	0.42
1:A:380:ARG:NH2	1:A:409:TYR:O	2.29	0.42
2:D:526:MET:C	2:D:528:PRO:HD2	2.39	0.42
1:B:6:ASN:OD1	1:B:6:ASN:N	2.53	0.42
1:B:45:LEU:HD11	1:B:98:LEU:HD13	2.00	0.42
1:B:290:GLU:HB2	1:B:297:ARG:HG2	2.01	0.42
1:A:95:ARG:HB2	1:A:180:PRO:HB2	2.00	0.42
1:A:167:SER:O	1:A:168:THR:HG22	2.17	0.42
1:A:240:SER:OG	1:A:321:LEU:O	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ALA:O	1:A:150:LYS:HA	2.20	0.42
5:G:9:DC:H2"	5:G:10:DG:C8	2.54	0.42
1:B:336:THR:HG23	1:B:337:PRO:HD2	2.01	0.42
2:C:433:GLU:HB2	2:C:505:THR:HG22	2.02	0.42
2:C:500:LYS:HG2	2:C:536:TYR:CE2	2.54	0.42
6:H:6:DT:H2"	6:H:7:DG:H5'	2.01	0.42
2:C:526:MET:C	2:C:528:PRO:HD2	2.40	0.41
1:A:434:VAL:HG13	1:A:435:LEU:H	1.81	0.41
2:D:483:ILE:HG22	2:D:483:ILE:O	2.19	0.41
1:B:173:GLY:H	6:H:9:DA:H5"	1.85	0.41
1:B:245:GLU:OE2	1:B:297:ARG:NH2	2.53	0.41
2:D:491:PHE:CD1	2:D:528:PRO:HG2	2.55	0.41
1:B:127:ALA:O	1:B:130:LEU:HB2	2.20	0.41
1:B:414:GLU:CD	1:B:414:GLU:H	2.22	0.41
1:A:358:LEU:HD23	1:A:358:LEU:HA	1.85	0.41
1:A:423:GLN:OE1	1:A:425:TYR:HE1	2.02	0.41
1:B:87:ARG:HA	1:B:90:GLN:CG	2.50	0.41
1:B:462:LEU:HA	1:B:462:LEU:HD23	1.68	0.41
2:D:431:LEU:HD13	2:D:479:MET:HE1	2.03	0.41
2:D:491:PHE:HE1	2:D:528:PRO:HB2	1.83	0.41
1:A:44:ILE:HD13	1:A:85:MET:HB2	2.02	0.41
1:B:233:LYS:HG3	1:B:339:GLN:OE1	2.21	0.41
1:A:434:VAL:CG1	1:A:435:LEU:N	2.82	0.41
1:B:60:ARG:HH11	1:B:60:ARG:HB2	1.84	0.41
2:D:597:ASN:HA	2:D:598:PRO:HD3	1.88	0.41
1:B:70:MET:CE	1:B:78:ASP:HA	2.50	0.41
1:A:261:TYR:N	9:A:609:HOH:O	2.54	0.41
1:B:191:VAL:HG13	1:B:464:LYS:HG2	2.03	0.41
1:B:272:ILE:HG22	1:B:287:VAL:HG21	2.03	0.41
1:B:402:LYS:O	1:B:406:LYS:HG3	2.21	0.41
1:A:16:ARG:HD2	1:A:16:ARG:HA	1.86	0.41
1:A:370:LYS:O	1:A:374:ILE:HD13	2.22	0.40
1:B:285:ALA:HB3	1:B:301:GLU:O	2.21	0.40
1:B:316:PHE:CE2	1:B:321:LEU:HD13	2.55	0.40
1:A:389:ILE:CD1	1:A:427:LEU:HD13	2.50	0.40
1:B:24:ILE:HD12	1:B:28:ARG:NH2	2.37	0.40
1:A:190:ALA:O	1:A:194:ILE:HG13	2.22	0.40
1:A:55:PHE:HA	1:A:122:ARG:HD2	2.03	0.40
1:A:87:ARG:C	1:A:89:SER:H	2.24	0.40
2:C:581:LYS:N	2:C:585:GLU:OE1	2.50	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:ARG:NH2	1:B:279:ASN:O[4_545]	2.10	0.10

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%)	451 (94%)	23 (5%)	7 (2%)	10	43
1	B	481/496 (97%)	448 (93%)	29 (6%)	4 (1%)	19	57
2	C	202/268 (75%)	179 (89%)	19 (9%)	4 (2%)	7	37
2	D	204/268 (76%)	186 (91%)	14 (7%)	4 (2%)	7	37
All	All	1368/1528 (90%)	1264 (92%)	85 (6%)	19 (1%)	11	44

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	168	THR
2	D	569	LYS
1	A	168	THR
2	C	424	PRO
2	D	588	ALA
1	A	116	MET
1	A	145	PHE
1	A	217	ALA
2	D	424	PRO
2	D	467	MET
1	A	169	GLY
1	A	248	LYS
1	B	157	ALA
1	B	169	GLY
2	C	490	ASP
2	C	588	ALA

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Mol	Chain	Res	Type
1	B	221	GLY
1	A	221	GLY
2	C	584	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	380/431 (88%)	355 (93%)	25 (7%)	16	49
1	B	376/431 (87%)	351 (93%)	25 (7%)	16	49
2	C	120/224 (54%)	101 (84%)	19 (16%)	2	14
2	D	116/224 (52%)	97 (84%)	19 (16%)	2	12
All	All	992/1310 (76%)	904 (91%)	88 (9%)	9	36

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	24	ILE
1	A	60	ARG
1	A	90	GLN
1	A	93	LYS
1	A	96	GLU
1	A	102	HIS
1	A	111	ASP
1	A	146	ASP
1	A	162	LEU
1	A	168	THR
1	A	208	LEU
1	A	236	VAL
1	A	268	LEU
1	A	279	ASN
1	A	281	VAL
1	A	293	ARG
1	A	308	THR

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Mol	Chain	Res	Type
1	A	321	LEU
1	A	336	THR
1	A	342	ILE
1	A	385	LEU
1	A	414	GLU
1	A	430	THR
1	A	462	LEU
1	B	6	ASN
1	B	12	ILE
1	B	60	ARG
1	B	90	GLN
1	B	96	GLU
1	B	139	VAL
1	B	162	LEU
1	B	167	SER
1	B	168	THR
1	B	183	LEU
1	B	208	LEU
1	B	236	VAL
1	B	268	LEU
1	B	293	ARG
1	B	308	THR
1	B	310	LEU
1	B	321	LEU
1	B	342	ILE
1	B	361	SER
1	B	372	LEU
1	B	381	VAL
1	B	385	LEU
1	B	414	GLU
1	B	431	ASP
1	B	462	LEU
2	C	416	LEU
2	C	429	LEU
2	C	445	ARG
2	C	453	LEU
2	C	456	ARG
2	C	475	GLU
2	C	476	ILE
2	C	514	ILE
2	C	516	THR
2	C	520	THR

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Mol	Chain	Res	Type
2	C	524	ARG
2	C	534	HIS
2	C	563	GLU
2	C	564	LEU
2	C	595	THR
2	C	603	LEU
2	C	605	ARG
2	C	611	LEU
2	C	617	ARG
2	D	416	LEU
2	D	429	LEU
2	D	436	SER
2	D	445	ARG
2	D	453	LEU
2	D	475	GLU
2	D	476	ILE
2	D	478	THR
2	D	499	ASP
2	D	514	ILE
2	D	516	THR
2	D	520	THR
2	D	524	ARG
2	D	529	LEU
2	D	564	LEU
2	D	591	LEU
2	D	603	LEU
2	D	611	LEU
2	D	617	ARG

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

Mol	Chain	Res	Type
1	B	53	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	AF5	H	101	7	28,31,31	1.34	5 (17%)	33,48,48	3.55	10 (30%)
8	AF5	F	101	7	28,31,31	1.43	5 (17%)	33,48,48	3.23	11 (33%)

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	AF5	H	101	7	-	4/8/33/33	0/5/5/5
8	AF5	F	101	7	-	0/8/33/33	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	101	AF5	C12-C10	-3.28	1.41	1.48
8	H	101	AF5	C12-C10	-3.27	1.41	1.48
8	F	101	AF5	C14-C15	3.20	1.49	1.46
8	H	101	AF5	C14-C15	2.76	1.48	1.46
8	F	101	AF5	C06-C10	-2.64	1.38	1.44
8	F	101	AF5	O08-C07	-2.57	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	101	AF5	C06-C10	-2.55	1.38	1.44
8	H	101	AF5	C21-C22	-2.18	1.49	1.53
8	F	101	AF5	C21-C22	-2.08	1.50	1.53
8	H	101	AF5	C02-N01	-2.02	1.43	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	101	AF5	C04-C02-N01	13.98	140.98	118.87
8	F	101	AF5	C04-C02-N01	13.75	140.62	118.87
8	H	101	AF5	C24-C14-C15	-9.59	114.03	122.98
8	F	101	AF5	C24-C14-C15	-7.15	116.30	122.98
8	H	101	AF5	C03-C02-N01	-5.81	109.68	118.87
8	H	101	AF5	C22-C18-N19	4.07	103.28	100.63
8	F	101	AF5	C02-N01-C05	-3.84	114.11	119.74
8	H	101	AF5	C02-N01-C05	-3.70	114.32	119.74
8	F	101	AF5	C03-C02-N01	-3.59	113.19	118.87
8	F	101	AF5	C13-N01-C02	3.33	125.84	122.35
8	F	101	AF5	O09-C07-C06	-3.14	116.17	122.67
8	H	101	AF5	C13-C14-C24	2.88	122.38	115.70
8	H	101	AF5	C13-N01-C02	2.83	125.31	122.35
8	F	101	AF5	O08-C07-C06	2.72	122.05	115.69
8	F	101	AF5	C13-C14-C24	2.54	121.59	115.70
8	H	101	AF5	C17-C18-C22	2.50	120.88	114.66
8	F	101	AF5	C27-C25-C24	-2.38	119.80	123.34
8	H	101	AF5	C21-C20-N19	2.22	106.03	104.15
8	F	101	AF5	C07-C06-C10	2.11	124.74	121.61
8	F	101	AF5	C17-C18-C22	2.07	119.83	114.66
8	H	101	AF5	C27-C25-C24	-2.05	120.29	123.34

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	H	101	AF5	C10-C06-C07-O09
8	H	101	AF5	C10-C06-C07-O08
8	H	101	AF5	C05-C06-C07-O08
8	H	101	AF5	C05-C06-C07-O09

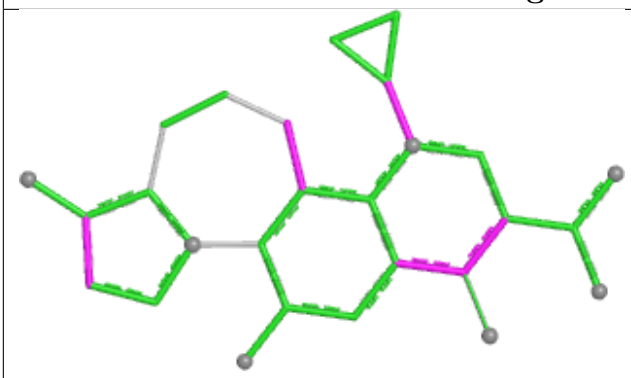
There are no ring outliers.

2 monomers are involved in 11 short contacts:

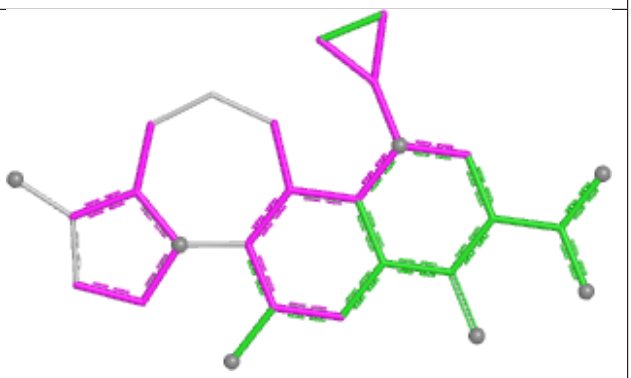
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	H	101	AF5	5	0
8	F	101	AF5	6	0

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

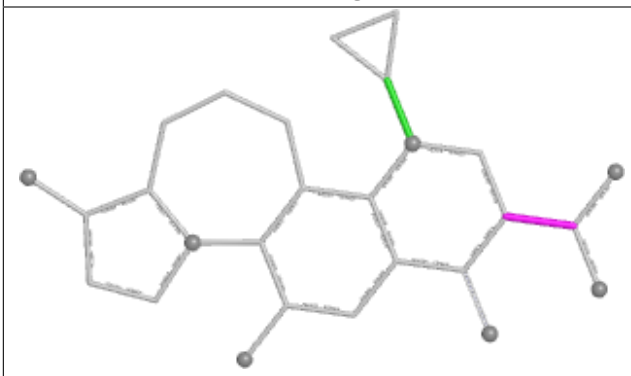
Ligand AF5 H 101



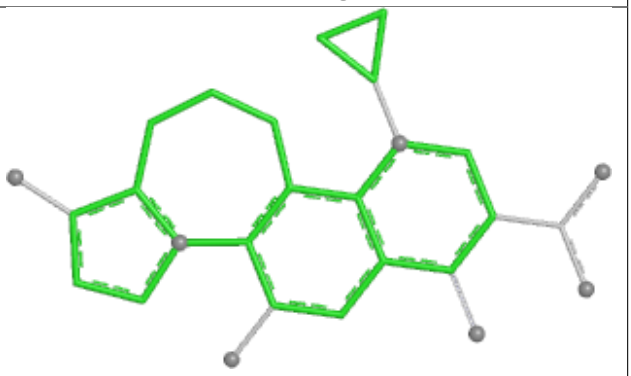
Bond lengths



Bond angles

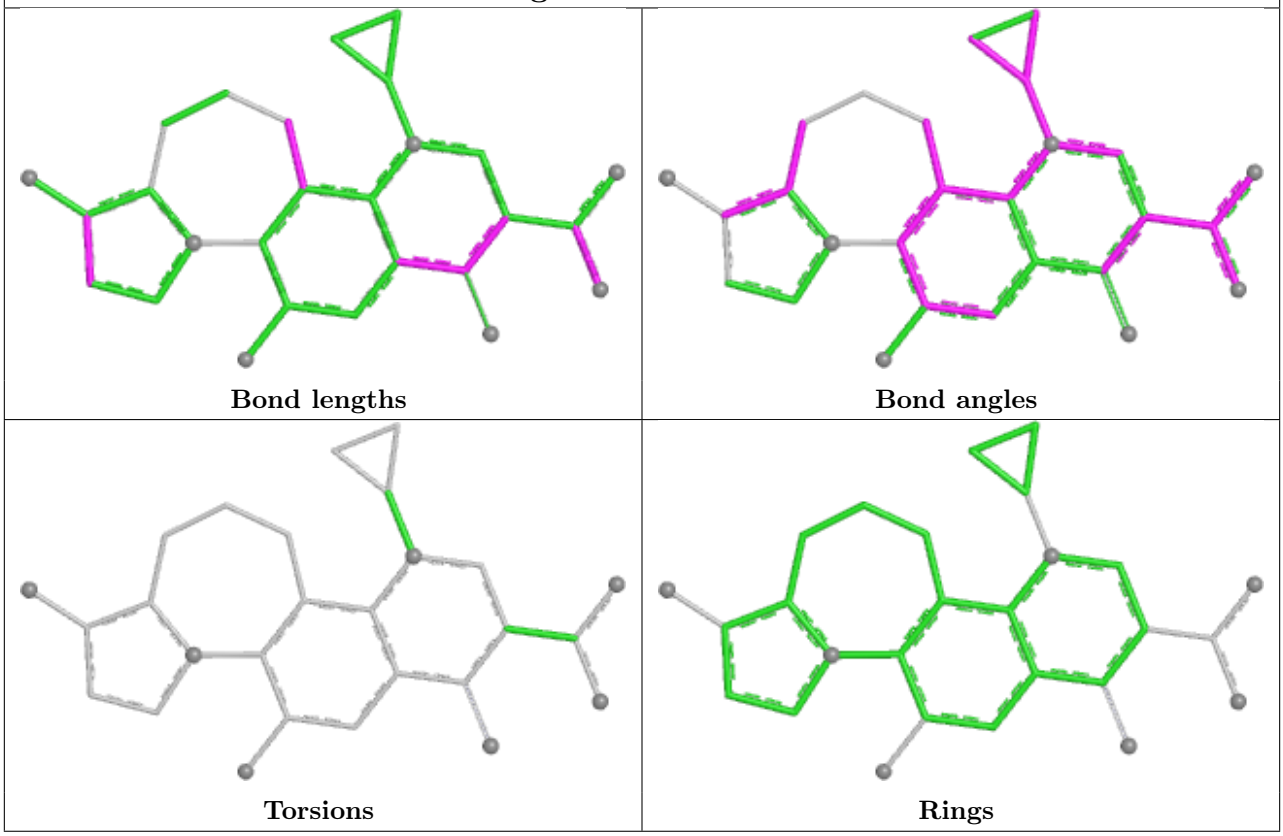


Torsions



Rings

Ligand AF5 F 101



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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	28, 45, 78, 109	0
1	B	482/496 (97%)	-0.62	0	100	100	26, 44, 73, 100	0
2	C	208/268 (77%)	-0.18	3 (1%)	75	72	49, 78, 113, 150	0
2	D	210/268 (78%)	-0.15	5 (2%)	59	57	49, 81, 118, 153	0
3	E	7/7 (100%)	-0.47	0	100	100	48, 53, 80, 110	0
4	F	11/11 (100%)	-0.34	0	100	100	54, 64, 80, 97	0
5	G	7/7 (100%)	-0.21	0	100	100	45, 51, 82, 100	0
6	H	11/11 (100%)	-0.16	0	100	100	55, 64, 73, 94	0
All	All	1418/1564 (90%)	-0.47	8 (0%)	89	87	26, 52, 100, 153	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	556	ALA	3.1
2	D	570	GLN	2.9
2	D	557	TYR	2.7
2	C	561	ASP	2.6
2	C	564	LEU	2.5
2	C	556	ALA	2.3
2	D	543	TYR	2.2
2	D	564	LEU	2.1

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 monosaccharides in this entry.

6.4 Ligands (i)

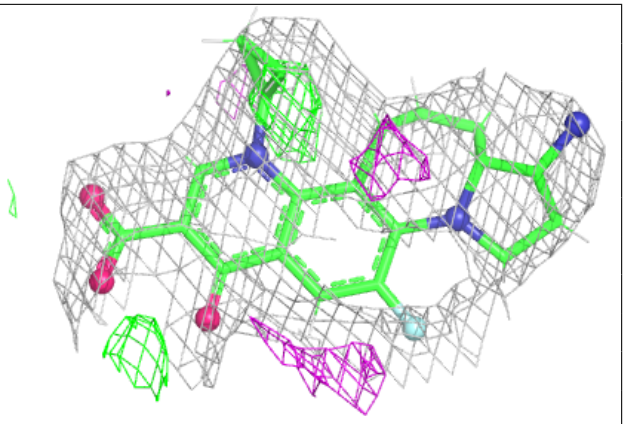
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

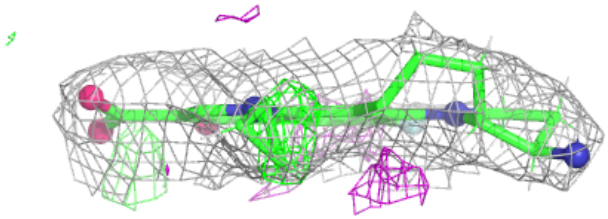
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	MG	B	501	1/1	0.88	0.14	54,54,54,54	0
7	MG	A	501	1/1	0.91	0.11	43,43,43,43	0
7	MG	A	502	1/1	0.92	0.28	53,53,53,53	0
8	AF5	H	101	27/27	0.92	0.24	66,92,133,155	0
8	AF5	F	101	27/27	0.94	0.23	51,71,87,90	0
7	MG	C	701	1/1	0.94	0.41	59,59,59,59	0
7	MG	D	701	1/1	0.96	0.67	52,52,52,52	0
7	MG	B	502	1/1	0.97	0.39	64,64,64,64	0

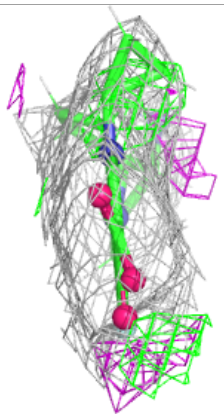
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AF5 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)

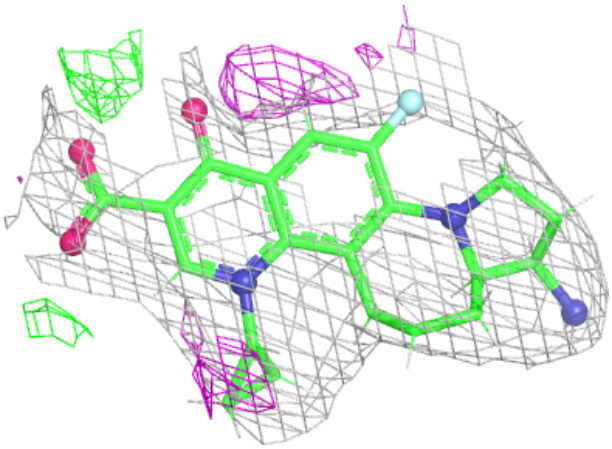


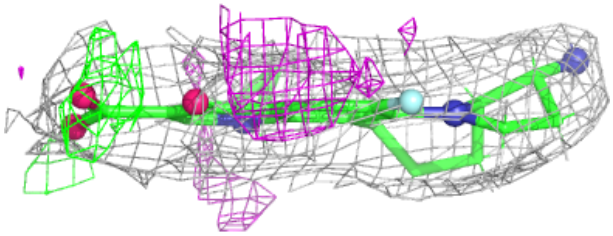


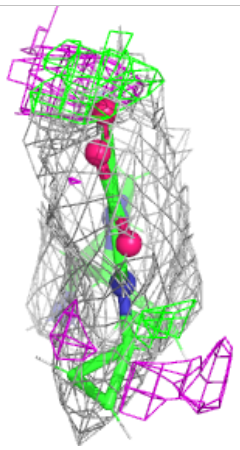


Electron density around AF5 F 101:

$2mF_o$-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.