Full wwPDB X-ray Structure Validation Report (i)

Oct 25, 2023 – 02:52 PM EDT

PDB ID	:	3FOF
Title	:	Structural insight into the quinolone-DNA cleavage complex of type IIA topoisomerases
Authors	:	Laponogov, I.; Sohi, M.K.; Veselkov, D.A.; Pan, X.-S.; Sawhney, R.; Thompson, A.W.; McAuley, K.E.; Fisher, L.M.; Sanderson, M.R.
Deposited on	:	2008-12-30
Resolution	:	4.00 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:

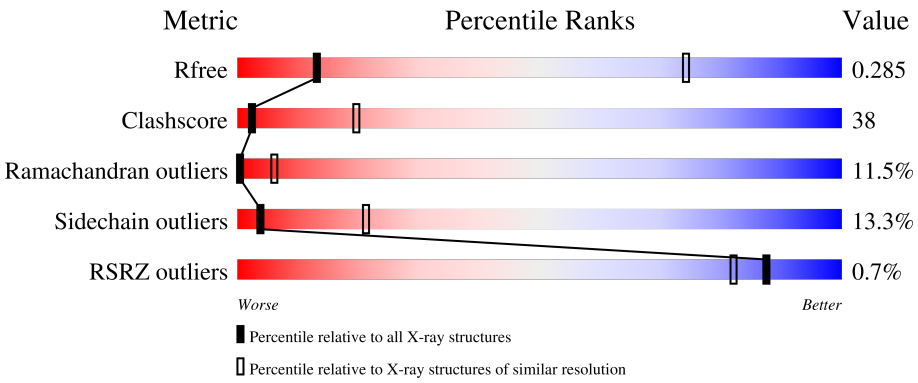
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.00 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	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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	52% 28% 7% 12%
1	B	496	54% 26% 7% 13%
2	C	268	41% 27% • 27%
2	D	268	44% 25% 5% 26%

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Mol	Chain	Length	Quality of chain
3	E	15	7% 33% 60% 7%
4	F	19	11% 21% 68% 11%
5	G	15	7% 40% 40% 20%
6	H	19	11% 21% 63% 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	MFX	F	0	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8498 atoms, of which 46 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	435	2482	1520	483	477	2	0	0	0
1	B	432	2439	1494	476	467	2	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	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			
2	C	196	1040	630	202	208	0	0	0
2	D	199	1059	639	208	212	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	380	MET	-	initiating methionine	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
D	380	MET	-	initiating methionine	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	E	15	306	144	60	87	15	0	0	0

- Molecule 4 is a DNA chain called DNA (5'-D(P*AP*GP*TP*CP*AP*TP*TP*CP*AP*TP*GP*AP*CP*CP*TP*TP*GP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	F	19	381	179	66	117	19	0	0	0

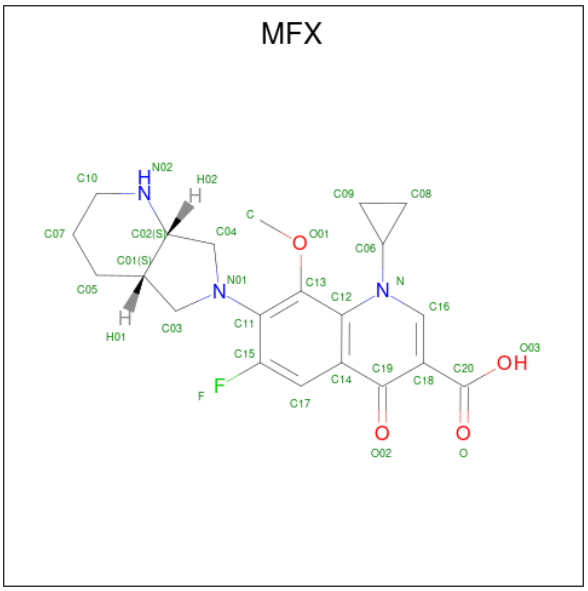
- Molecule 5 is a DNA chain called DNA (5'-D(P*CP*TP*GP*TP*TP*TP*TP*AP*CP*GP*TP*GP*CP*AP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
5	G	15	298	140	48	95	15	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
6	H	19	389	183	78	109	19	0	0	0

- Molecule 7 is 1-cyclopropyl-6-fluoro-8-methoxy-7-[(4aS,7aS)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo-1,4-dihydroquinoline-3-carboxylic acid (three-letter code: MFX) (formula: $C_{21}H_{24}FN_3O_4$).



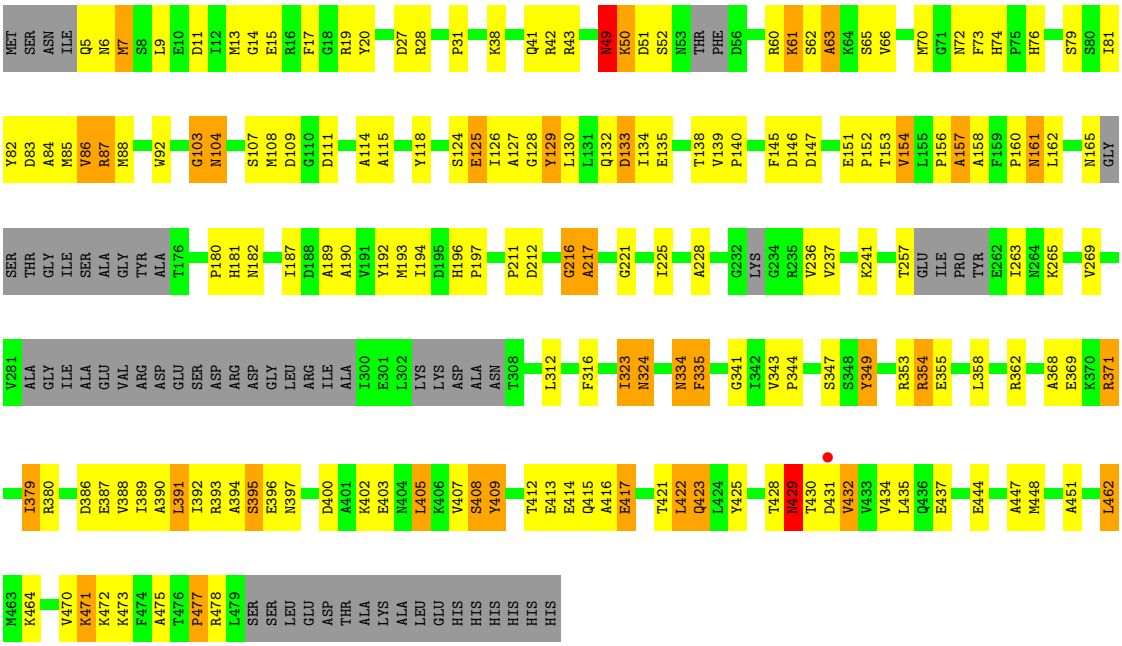
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	F	1	Total	C	F	H	N	O	0	0
			52	21	1	23	3	4		
7	H	1	Total	C	F	H	N	O	0	0
			52	21	1	23	3	4		

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.

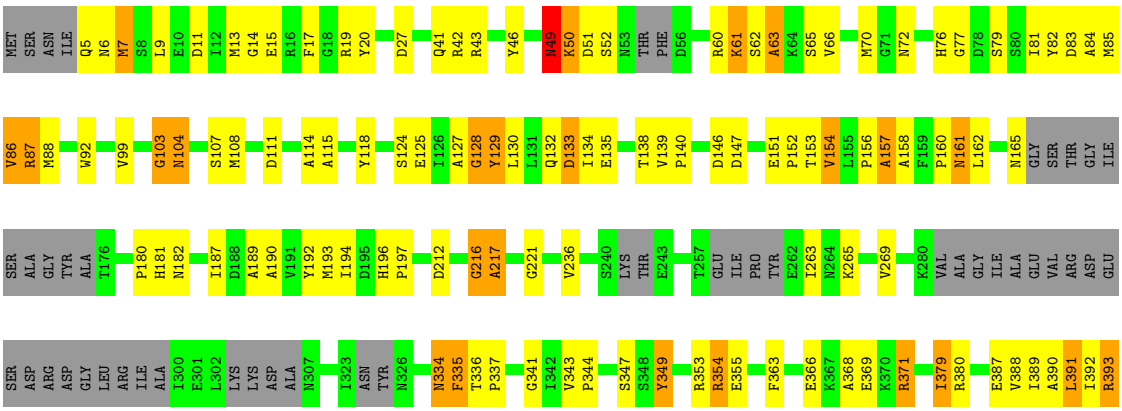
• Molecule 1: DNA topoisomerase 4 subunit A

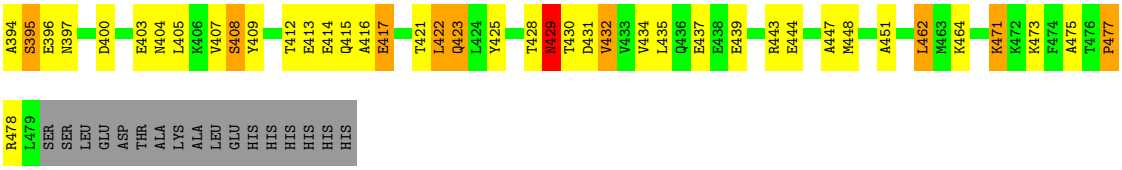
Chain A: 52% 28% 7% 12%



• Molecule 1: DNA topoisomerase 4 subunit A

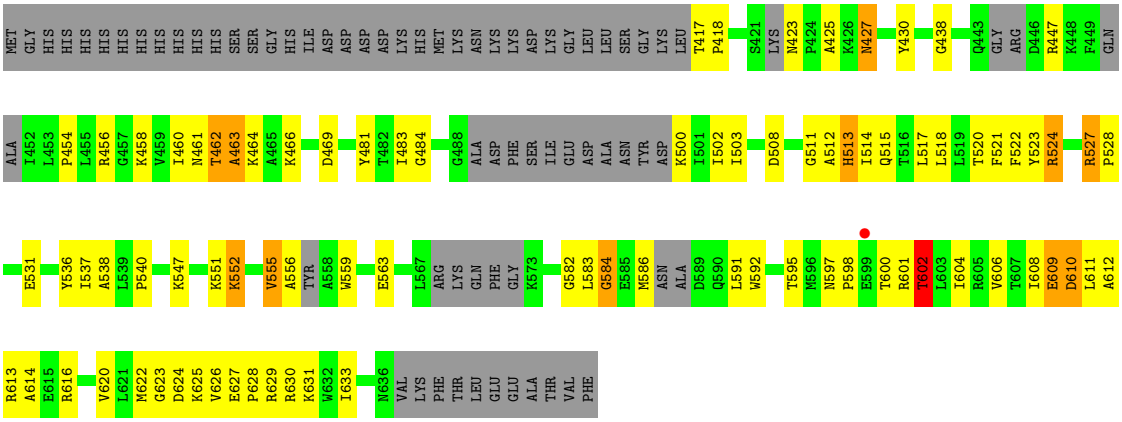
Chain B: 54% 26% 7% 13%





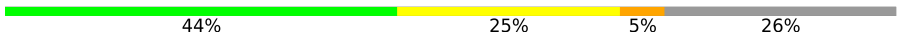
• Molecule 2: DNA topoisomerase 4 subunit B

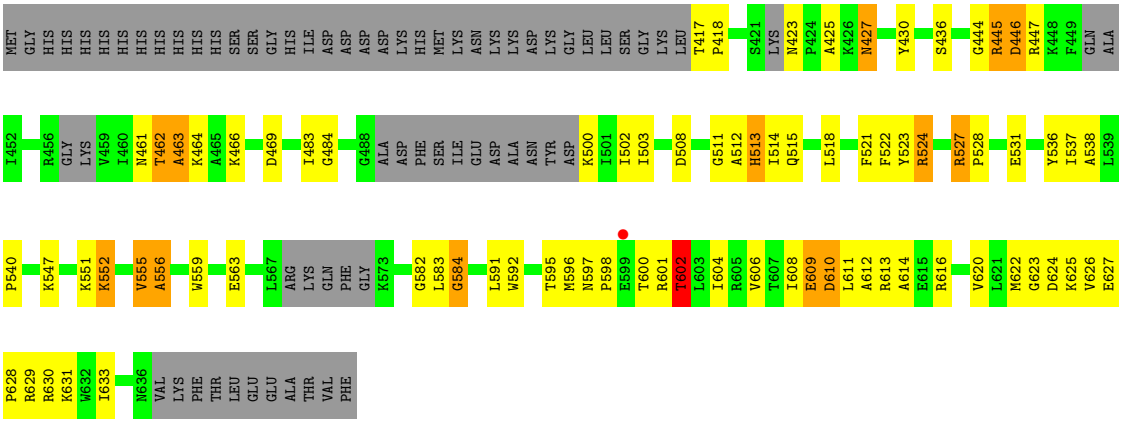
Chain C:



• Molecule 2: DNA topoisomerase 4 subunit B

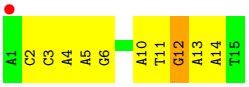
Chain D:



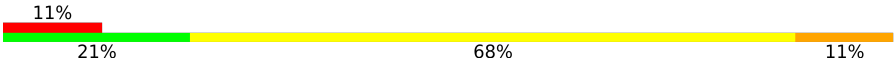


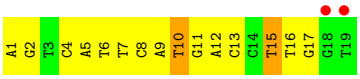
• Molecule 3: DNA (5'-D(P*AP*CP*CP*AP*AP*GP*GP*TP*CP*AP*TP*GP*AP*AP*T)-3')

Chain E:



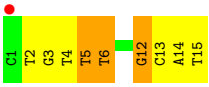
• Molecule 4: DNA (5'-D(P*AP*GP*TP*CP*AP*TP*TP*CP*AP*TP*GP*AP*CP*CP*TP*T P*GP*GP*T)-3')

Chain F: 

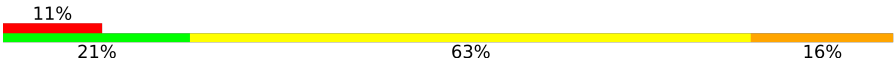


• Molecule 5: DNA (5'-D(P*CP*TP*GP*TP*TP*TP*TP*AP*CP*GP*TP*GP*CP*AP*T)-3')

Chain G:



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

Chain H: 

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	121.60Å 121.60Å 178.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.07 – 4.00 34.07 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.9 (34.07-4.00) 89.8 (34.07-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.239 , 0.289 0.233 , 0.285	Depositor DCC
R_{free} test set	4398 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å^2)	168.4	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.20 , 210.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.428 for -h,-k,l 0.049 for h,-h-k,-l 0.046 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8498	wwPDB-VP
Average B, all atoms (Å^2)	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% 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: MFX

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	0.44	1/2516 (0.0%)	0.55	2/3479 (0.1%)
1	B	0.43	1/2471 (0.0%)	0.52	1/3419 (0.0%)
2	C	0.36	0/1042	0.53	0/1438
2	D	0.37	0/1064	0.51	0/1471
3	E	0.55	0/344	1.45	1/527 (0.2%)
4	F	0.57	0/426	1.39	3/652 (0.5%)
5	G	0.53	0/332	1.54	5/507 (1.0%)
6	H	0.54	0/438	1.43	4/672 (0.6%)
All	All	0.44	2/8633 (0.0%)	0.80	16/12165 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	429	ASN	CB-CG	5.83	1.64	1.51
1	A	429	ASN	CB-CG	5.64	1.64	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	12	DG	O4'-C4'-C3'	-14.72	97.17	106.00
3	E	12	DG	O4'-C4'-C3'	-14.03	97.58	106.00
6	H	8	DC	O4'-C4'-C3'	-7.72	101.37	106.00
6	H	10	DC	C1'-O4'-C4'	-7.53	102.57	110.10
5	G	12	DG	C4'-C3'-C2'	-6.69	97.08	103.10
4	F	15	DT	N3-C4-O4	6.27	123.66	119.90
4	F	15	DT	C5-C4-O4	-6.04	120.67	124.90
1	A	28	ARG	CA-CB-CG	5.97	126.54	113.40
4	F	10	DT	C1'-O4'-C4'	-5.67	104.43	110.10
5	G	5	DT	N3-C4-O4	5.56	123.24	119.90
5	G	6	DT	N3-C4-O4	5.37	123.12	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	393	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	405	LEU	CA-CB-CG	5.26	127.39	115.30
5	G	5	DT	C5-C4-O4	-5.21	121.25	124.90
6	H	8	DC	O4'-C1'-N1	5.17	111.62	108.00
6	H	6	DT	O4'-C1'-N1	5.13	111.59	108.00

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	2482	0	1460	150	0
1	B	2439	0	1420	143	0
2	C	1040	0	602	66	0
2	D	1059	0	608	70	0
3	E	306	0	160	19	0
4	F	381	0	196	27	0
5	G	298	0	152	13	0
6	H	389	0	204	31	0
7	F	29	23	24	10	0
7	H	29	23	24	8	0
All	All	8452	46	4850	504	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 38.

All (504) 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:471:LYS:O	1:A:475:ALA:HB2	1.20	1.35
1:B:471:LYS:O	1:B:475:ALA:HB2	1.19	1.30
1:B:124:SER:O	1:B:127:ALA:HB3	1.35	1.23
1:A:124:SER:O	1:A:127:ALA:HB3	1.36	1.19
1:A:471:LYS:O	1:A:475:ALA:CB	1.95	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:LYS:O	1:B:475:ALA:CB	1.96	1.13
3:E:12:DG:H5'	3:E:12:DG:C8	1.83	1.12
1:A:13:MET:O	1:A:17:PHE:CD1	2.13	1.02
1:A:60:ARG:O	1:A:61:LYS:O	1.78	1.01
2:C:598:PRO:O	2:C:602:THR:HG22	1.61	1.01
1:B:60:ARG:O	1:B:61:LYS:O	1.80	1.00
1:B:180:PRO:HB2	1:B:212:ASP:O	1.62	0.99
1:A:49:ASN:O	1:A:51:ASP:N	1.97	0.98
1:A:180:PRO:HB2	1:A:212:ASP:O	1.63	0.97
1:B:13:MET:O	1:B:17:PHE:CD1	2.18	0.96
2:D:598:PRO:O	2:D:602:THR:HG22	1.65	0.94
1:B:158:ALA:HA	1:B:353:ARG:NH2	1.84	0.93
1:A:79:SER:O	1:A:83:ASP:HB2	1.68	0.93
2:C:527:ARG:HH11	2:C:527:ARG:HB2	1.33	0.93
2:D:527:ARG:HH11	2:D:527:ARG:HB2	1.33	0.92
1:B:79:SER:O	1:B:83:ASP:HB2	1.69	0.92
1:A:341:GLY:O	1:A:344:PRO:HD2	1.70	0.92
1:B:341:GLY:O	1:B:344:PRO:HD2	1.69	0.91
1:B:49:ASN:O	1:B:51:ASP:N	2.04	0.91
1:A:158:ALA:HA	1:A:353:ARG:NH2	1.85	0.90
1:A:387:GLU:O	1:A:390:ALA:HB3	1.72	0.89
2:C:538:ALA:O	2:C:540:PRO:HD3	1.72	0.89
3:E:12:DG:H5'	3:E:12:DG:H8	1.34	0.89
2:D:444:GLY:O	2:D:446:ASP:N	2.07	0.88
2:D:538:ALA:O	2:D:540:PRO:HD3	1.72	0.88
1:B:387:GLU:O	1:B:390:ALA:HB3	1.73	0.88
1:A:434:VAL:O	1:A:437:GLU:N	2.09	0.85
2:C:527:ARG:HB2	2:C:527:ARG:NH1	1.92	0.85
1:A:62:SER:O	1:A:65:SER:N	2.10	0.84
1:B:62:SER:O	1:B:65:SER:N	2.10	0.84
2:C:430:TYR:HA	2:C:502:ILE:HG13	1.59	0.84
1:A:265:LYS:O	1:A:269:VAL:HG23	1.76	0.84
1:B:265:LYS:O	1:B:269:VAL:HG23	1.77	0.84
2:D:430:TYR:HA	2:D:502:ILE:HG13	1.61	0.82
2:D:512:ALA:O	2:D:514:ILE:N	2.11	0.82
2:D:527:ARG:HB2	2:D:527:ARG:NH1	1.92	0.82
1:B:130:LEU:HA	1:B:157:ALA:HA	1.62	0.82
1:B:160:PRO:O	1:B:162:LEU:N	2.13	0.82
4:F:12:DA:H2"	4:F:13:DC:C6	2.15	0.81
5:G:12:DG:C8	5:G:12:DG:H5'	2.16	0.81
6:H:12:DT:H2"	6:H:13:DA:N7	1.96	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:GLY:C	1:B:344:PRO:HD2	2.02	0.80
2:D:463:ALA:HB3	2:D:622:MET:CB	2.10	0.80
1:A:341:GLY:C	1:A:344:PRO:HD2	2.02	0.80
2:C:512:ALA:O	2:C:514:ILE:N	2.15	0.80
1:A:160:PRO:O	1:A:162:LEU:N	2.15	0.80
1:A:11:ASP:O	1:A:14:GLY:N	2.15	0.79
4:F:1:DA:H4'	4:F:2:DG:OP1	1.80	0.79
4:F:11:DG:H2"	4:F:12:DA:C8	2.18	0.79
1:B:11:ASP:O	1:B:14:GLY:N	2.14	0.79
1:B:434:VAL:O	1:B:437:GLU:N	2.16	0.79
1:A:471:LYS:C	1:A:475:ALA:HB2	2.03	0.78
1:B:471:LYS:C	1:B:475:ALA:HB2	2.03	0.78
4:F:1:DA:N6	7:F:0:MFX:HB	1.99	0.78
2:C:524:ARG:NH1	2:C:524:ARG:HB3	1.99	0.77
1:B:124:SER:C	1:B:127:ALA:HB3	2.04	0.77
1:A:130:LEU:HA	1:A:157:ALA:HA	1.67	0.77
1:B:391:LEU:N	1:B:391:LEU:HD23	2.00	0.76
2:D:524:ARG:HB3	2:D:524:ARG:NH1	1.99	0.76
2:C:463:ALA:HB3	2:C:622:MET:CB	2.16	0.76
1:A:334:ASN:O	1:A:335:PHE:CD1	2.39	0.75
2:D:611:LEU:C	2:D:613:ARG:H	1.88	0.75
1:A:124:SER:C	1:A:127:ALA:HB3	2.04	0.75
1:B:79:SER:O	1:B:83:ASP:CB	2.35	0.75
1:B:124:SER:O	1:B:127:ALA:CB	2.28	0.75
2:C:611:LEU:C	2:C:613:ARG:H	1.88	0.75
2:C:466:LYS:O	2:C:469:ASP:CB	2.35	0.75
1:A:423:GLN:HB3	1:B:422:LEU:O	1.87	0.74
2:C:438:GLY:HA3	2:C:454:PRO:HG3	1.69	0.74
1:A:422:LEU:O	1:B:423:GLN:HB3	1.87	0.74
5:G:12:DG:H5'	5:G:12:DG:H8	1.52	0.73
1:A:124:SER:O	1:A:127:ALA:CB	2.28	0.72
5:G:13:DC:H2"	5:G:14:DA:O5'	1.90	0.72
1:B:341:GLY:H	1:B:344:PRO:HG2	1.55	0.71
3:E:12:DG:C8	3:E:12:DG:C5'	2.69	0.71
1:A:49:ASN:O	1:A:52:SER:N	2.23	0.71
1:A:79:SER:O	1:A:83:ASP:CB	2.37	0.71
1:A:341:GLY:H	1:A:344:PRO:HG2	1.55	0.71
1:A:428:THR:O	1:A:430:THR:N	2.24	0.71
1:B:428:THR:O	1:B:430:THR:N	2.23	0.71
1:B:391:LEU:H	1:B:391:LEU:CD2	2.05	0.70
4:F:12:DA:H2"	4:F:13:DC:H6	1.53	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:466:LYS:O	2:D:469:ASP:CB	2.38	0.70
2:D:512:ALA:O	2:D:515:GLN:N	2.25	0.70
1:B:391:LEU:N	1:B:391:LEU:CD2	2.54	0.69
1:B:158:ALA:HA	1:B:353:ARG:HH21	1.54	0.69
2:C:609:GLU:O	2:C:610:ASP:CB	2.41	0.69
2:D:609:GLU:O	2:D:610:ASP:CB	2.40	0.69
1:B:49:ASN:O	1:B:52:SER:N	2.19	0.69
1:A:15:GLU:O	1:A:19:ARG:HG2	1.93	0.68
2:C:611:LEU:O	2:C:613:ARG:N	2.26	0.68
1:A:391:LEU:HD23	1:A:391:LEU:N	2.08	0.68
3:E:12:DG:H2"	3:E:13:DA:OP2	1.93	0.68
1:B:11:ASP:C	1:B:14:GLY:H	1.97	0.67
1:A:391:LEU:N	1:A:391:LEU:CD2	2.59	0.66
2:C:512:ALA:O	2:C:515:GLN:N	2.29	0.66
2:C:592:TRP:HA	2:C:595:THR:CB	2.25	0.66
2:D:611:LEU:O	2:D:613:ARG:N	2.27	0.66
2:D:503:ILE:HG23	2:D:537:ILE:HA	1.77	0.66
1:B:334:ASN:O	1:B:335:PHE:HD1	1.79	0.66
1:B:129:TYR:O	1:B:132:GLN:CB	2.44	0.66
2:D:430:TYR:CB	2:D:502:ILE:HD11	2.26	0.66
1:A:11:ASP:C	1:A:14:GLY:H	1.99	0.65
5:G:12:DG:C8	5:G:12:DG:C5'	2.80	0.65
2:D:555:VAL:O	2:D:556:ALA:HB2	1.97	0.65
6:H:1:DG:O6	7:H:0:MFX:HB	1.97	0.64
2:D:592:TRP:HA	2:D:595:THR:CB	2.27	0.64
1:A:129:TYR:O	1:A:132:GLN:CB	2.46	0.64
2:C:503:ILE:HG23	2:C:537:ILE:HA	1.79	0.64
1:B:158:ALA:O	1:B:349:TYR:OH	2.16	0.64
1:A:391:LEU:CD2	1:A:391:LEU:H	2.11	0.64
1:A:158:ALA:HA	1:A:353:ARG:HH21	1.61	0.64
4:F:1:DA:C2	7:F:0:MFX:H04A	2.33	0.64
2:D:503:ILE:CG2	2:D:537:ILE:HA	2.29	0.63
2:D:528:PRO:HA	2:D:531:GLU:CB	2.28	0.63
1:B:9:LEU:HA	2:D:604:ILE:O	1.99	0.62
4:F:5:DA:H2"	4:F:6:DT:H5'	1.81	0.62
1:A:334:ASN:O	1:A:335:PHE:HD1	1.81	0.62
1:A:388:VAL:C	1:A:390:ALA:H	2.03	0.62
1:B:20:TYR:O	1:B:20:TYR:CD2	2.53	0.61
2:D:445:ARG:C	2:D:447:ARG:H	2.04	0.61
2:D:524:ARG:HB3	2:D:524:ARG:CZ	2.29	0.61
1:B:103:GLY:O	1:B:104:ASN:CB	2.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:LEU:HA	2:C:604:ILE:O	2.00	0.61
2:C:528:PRO:HA	2:C:531:GLU:CB	2.30	0.61
6:H:12:DT:O3'	6:H:13:DA:H8	1.83	0.61
1:B:407:VAL:O	1:B:409:TYR:N	2.33	0.61
2:C:524:ARG:HB3	2:C:524:ARG:CZ	2.31	0.61
2:C:598:PRO:O	2:C:602:THR:CG2	2.44	0.61
1:B:82:TYR:O	1:B:85:MET:HB3	2.00	0.61
1:B:334:ASN:O	1:B:335:PHE:CD1	2.54	0.61
1:B:388:VAL:C	1:B:390:ALA:H	2.04	0.61
1:A:11:ASP:O	1:A:14:GLY:CA	2.49	0.60
1:A:368:ALA:O	1:A:369:GLU:C	2.39	0.60
1:B:11:ASP:O	1:B:14:GLY:CA	2.49	0.60
1:B:160:PRO:HA	1:B:349:TYR:HE1	1.66	0.60
1:A:391:LEU:HD23	1:A:392:ILE:N	2.16	0.60
1:B:216:GLY:O	1:B:217:ALA:HB3	2.01	0.60
6:H:1:DG:C6	7:H:0:MFX:HB	2.36	0.60
1:B:15:GLU:O	1:B:19:ARG:HG2	2.02	0.60
4:F:1:DA:H2"	4:F:2:DG:O5'	2.02	0.60
1:A:132:GLN:O	1:A:133:ASP:CB	2.49	0.59
1:A:158:ALA:O	1:A:349:TYR:OH	2.20	0.59
1:B:368:ALA:O	1:B:371:ARG:N	2.35	0.59
3:E:4:DA:C2	4:F:17:DG:C2	2.89	0.59
2:C:601:ARG:O	2:C:602:THR:O	2.20	0.59
2:D:512:ALA:O	2:D:513:HIS:C	2.40	0.59
1:A:216:GLY:O	1:A:217:ALA:HB3	2.02	0.59
6:H:3:DC:C5'	6:H:3:DC:H6	2.14	0.59
1:B:62:SER:O	1:B:63:ALA:C	2.41	0.59
1:B:160:PRO:HA	1:B:349:TYR:CE1	2.38	0.59
1:B:368:ALA:O	1:B:369:GLU:C	2.41	0.59
7:F:0:MFX:H06	7:F:0:MFX:O01	2.01	0.59
1:B:132:GLN:O	1:B:133:ASP:CB	2.50	0.58
3:E:5:DA:H2"	3:E:6:DG:H8	1.67	0.58
2:C:527:ARG:HH11	2:C:527:ARG:CB	2.13	0.58
2:C:527:ARG:HB3	2:C:528:PRO:HD3	1.84	0.58
7:F:0:MFX:H07	6:H:5:DA:O4'	2.02	0.58
6:H:12:DT:O3'	6:H:13:DA:C8	2.57	0.58
1:B:153:THR:O	1:B:154:VAL:CB	2.52	0.58
1:A:13:MET:O	1:A:17:PHE:HD1	1.81	0.58
7:H:0:MFX:H06	7:H:0:MFX:O01	2.02	0.58
2:D:611:LEU:C	2:D:613:ARG:N	2.55	0.58
1:A:341:GLY:N	1:A:344:PRO:HG2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:GLY:O	1:A:104:ASN:CB	2.52	0.57
2:D:527:ARG:HB3	2:D:528:PRO:HD3	1.86	0.57
2:C:430:TYR:CB	2:C:502:ILE:HD11	2.34	0.57
2:D:444:GLY:C	2:D:446:ASP:H	2.03	0.57
2:D:518:LEU:O	2:D:522:PHE:N	2.37	0.57
1:A:386:ASP:OD1	1:B:393:ARG:NH2	2.34	0.57
2:C:508:ASP:O	2:C:511:GLY:N	2.38	0.57
1:B:77:GLY:HA3	7:F:0:MFX:O03	2.04	0.57
5:G:5:DT:C4	5:G:6:DT:C4	2.93	0.57
1:B:84:ALA:O	1:B:87:ARG:HB3	2.05	0.57
6:H:6:DT:H2"	6:H:7:DG:OP2	2.04	0.57
2:D:601:ARG:O	2:D:602:THR:O	2.22	0.56
1:A:84:ALA:O	1:A:87:ARG:HB3	2.05	0.56
1:A:413:GLU:O	1:A:416:ALA:N	2.39	0.56
1:B:448:MET:O	1:B:451:ALA:N	2.36	0.56
2:C:611:LEU:C	2:C:613:ARG:N	2.56	0.56
2:D:512:ALA:C	2:D:514:ILE:N	2.57	0.56
6:H:10:DC:H2"	6:H:11:DG:H8	1.71	0.56
1:A:124:SER:H	1:A:127:ALA:CB	2.19	0.56
1:B:397:ASN:H	1:B:400:ASP:CB	2.19	0.56
6:H:10:DC:H2"	6:H:11:DG:C8	2.41	0.56
1:B:334:ASN:C	1:B:335:PHE:CD1	2.79	0.56
5:G:14:DA:H2"	5:G:15:DT:H5'	1.87	0.56
1:A:17:PHE:CZ	2:C:616:ARG:CB	2.89	0.56
1:A:448:MET:O	1:A:451:ALA:N	2.38	0.56
1:A:368:ALA:O	1:A:371:ARG:N	2.35	0.56
1:B:391:LEU:HD23	1:B:392:ILE:N	2.21	0.56
1:B:128:GLY:O	1:B:129:TYR:C	2.44	0.56
1:B:353:ARG:O	1:B:354:ARG:C	2.43	0.56
1:A:107:SER:H	1:A:111:ASP:CB	2.19	0.55
1:A:146:ASP:O	1:A:147:ASP:HB2	2.06	0.55
2:C:512:ALA:O	2:C:513:HIS:C	2.43	0.55
2:D:508:ASP:O	2:D:511:GLY:N	2.40	0.55
6:H:7:DG:H2'	6:H:7:DG:O5'	2.06	0.55
1:A:41:GLN:O	1:A:42:ARG:C	2.44	0.55
1:B:391:LEU:H	1:B:391:LEU:HD22	1.71	0.55
2:D:598:PRO:O	2:D:602:THR:CG2	2.47	0.55
1:A:153:THR:O	1:A:154:VAL:CB	2.54	0.55
2:C:625:LYS:O	2:C:626:VAL:CB	2.54	0.55
1:A:397:ASN:H	1:A:400:ASP:CB	2.19	0.55
4:F:7:DT:C4	4:F:8:DC:N4	2.74	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:GLN:O	1:B:42:ARG:C	2.44	0.55
1:B:161:ASN:O	1:B:165:ASN:HB2	2.07	0.55
1:B:341:GLY:N	1:B:344:PRO:HG2	2.19	0.55
1:B:413:GLU:O	1:B:416:ALA:N	2.40	0.55
6:H:16:DA:C4	6:H:17:DC:C5	2.94	0.55
1:B:17:PHE:CZ	2:D:616:ARG:CB	2.90	0.54
1:B:431:ASP:O	1:B:432:VAL:C	2.45	0.54
2:D:436:SER:CB	4:F:1:DA:OP2	2.55	0.54
6:H:1:DG:C2	7:H:0:MFX:H04A	2.42	0.54
2:C:555:VAL:O	2:C:556:ALA:HB2	2.07	0.54
3:E:6:DG:N2	4:F:15:DT:C2	2.75	0.54
2:C:508:ASP:HB2	2:C:511:GLY:H	1.73	0.54
2:C:518:LEU:O	2:C:522:PHE:N	2.40	0.54
1:B:124:SER:H	1:B:127:ALA:CB	2.20	0.54
1:B:349:TYR:CD2	1:B:349:TYR:O	2.61	0.54
1:B:444:GLU:O	1:B:447:ALA:HB3	2.08	0.54
2:C:512:ALA:C	2:C:514:ILE:N	2.59	0.54
2:D:625:LYS:O	2:D:626:VAL:CB	2.55	0.54
1:A:17:PHE:HZ	2:C:616:ARG:CB	2.21	0.54
2:C:503:ILE:CG2	2:C:537:ILE:HA	2.36	0.54
1:A:20:TYR:CD2	1:A:20:TYR:O	2.61	0.54
2:D:462:THR:C	2:D:464:LYS:H	2.11	0.54
1:B:107:SER:H	1:B:111:ASP:CB	2.21	0.53
1:A:62:SER:O	1:A:63:ALA:C	2.46	0.53
1:A:128:GLY:O	1:A:129:TYR:C	2.46	0.53
1:A:160:PRO:HA	1:A:349:TYR:CE1	2.44	0.53
1:B:146:ASP:O	1:B:147:ASP:HB2	2.09	0.53
1:B:181:HIS:O	1:B:182:ASN:HB3	2.07	0.53
2:D:523:TYR:OH	2:D:614:ALA:HB2	2.07	0.53
1:A:391:LEU:H	1:A:391:LEU:HD22	1.73	0.53
1:A:87:ARG:O	1:A:87:ARG:HD3	2.08	0.53
1:B:17:PHE:HZ	2:D:616:ARG:CB	2.21	0.53
1:B:387:GLU:O	1:B:390:ALA:CB	2.53	0.53
1:A:160:PRO:C	1:A:162:LEU:H	2.13	0.53
1:A:388:VAL:C	1:A:390:ALA:N	2.62	0.53
1:B:471:LYS:O	1:B:475:ALA:HB1	2.05	0.53
2:D:430:TYR:CB	2:D:502:ILE:CD1	2.86	0.53
6:H:3:DC:H6	6:H:3:DC:H5"	1.73	0.53
1:A:423:GLN:HA	1:B:423:GLN:HA	1.91	0.52
1:B:49:ASN:O	1:B:50:LYS:C	2.47	0.52
1:B:344:PRO:O	1:B:347:SER:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:ARG:C	1:B:395:SER:H	2.12	0.52
1:A:181:HIS:O	1:A:182:ASN:HB3	2.08	0.52
1:A:387:GLU:O	1:A:390:ALA:CB	2.53	0.52
1:A:431:ASP:O	1:A:432:VAL:C	2.46	0.52
1:A:334:ASN:C	1:A:335:PHE:CD1	2.82	0.52
6:H:12:DT:H2"	6:H:13:DA:C8	2.44	0.52
1:A:421:THR:O	1:A:422:LEU:O	2.27	0.52
2:D:503:ILE:HG23	2:D:503:ILE:O	2.09	0.52
1:B:160:PRO:C	1:B:162:LEU:H	2.13	0.52
1:A:241:LYS:O	1:A:257:THR:HG23	2.10	0.52
1:B:388:VAL:C	1:B:390:ALA:N	2.62	0.52
5:G:3:DG:C4	5:G:4:DT:C5	2.99	0.51
6:H:7:DG:C5	6:H:8:DC:C4	2.98	0.51
2:C:523:TYR:CD2	2:C:524:ARG:N	2.78	0.51
2:D:508:ASP:HB2	2:D:511:GLY:H	1.75	0.51
3:E:5:DA:C2	3:E:6:DG:C4	2.98	0.51
7:F:0:MFX:H05A	6:H:5:DA:C5	2.46	0.51
1:A:49:ASN:O	1:A:50:LYS:C	2.47	0.51
1:B:353:ARG:O	1:B:355:GLU:N	2.42	0.51
2:C:417:THR:N	2:C:418:PRO:CD	2.73	0.51
2:C:462:THR:C	2:C:464:LYS:H	2.14	0.51
4:F:6:DT:H2"	4:F:7:DT:OP2	2.10	0.51
1:A:49:ASN:C	1:A:51:ASP:N	2.63	0.51
1:A:82:TYR:O	1:A:85:MET:HB3	2.11	0.51
2:C:582:GLY:O	2:C:584:GLY:N	2.43	0.51
5:G:3:DG:C2	5:G:4:DT:C2	2.99	0.51
2:C:597:ASN:CB	2:C:600:THR:CB	2.88	0.51
2:D:608:ILE:O	2:D:609:GLU:O	2.29	0.51
1:A:448:MET:O	1:A:451:ALA:HB3	2.11	0.51
2:C:559:TRP:O	2:C:563:GLU:CB	2.59	0.51
1:A:407:VAL:O	1:A:409:TYR:N	2.43	0.50
1:B:46:TYR:CD2	1:B:152:PRO:HG2	2.46	0.50
1:B:349:TYR:CD2	1:B:349:TYR:C	2.85	0.50
2:D:445:ARG:C	2:D:447:ARG:N	2.65	0.50
2:D:627:GLU:CB	2:D:628:PRO:HD3	2.41	0.50
1:B:49:ASN:C	1:B:51:ASP:N	2.65	0.50
2:C:503:ILE:HG23	2:C:503:ILE:O	2.11	0.50
2:D:417:THR:N	2:D:418:PRO:CD	2.74	0.50
2:D:527:ARG:HH11	2:D:527:ARG:CB	2.13	0.50
1:A:391:LEU:HD23	1:A:392:ILE:H	1.76	0.50
1:A:124:SER:N	1:A:127:ALA:CB	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:PRO:HA	1:A:349:TYR:HE1	1.77	0.50
2:C:503:ILE:HG22	2:C:536:TYR:O	2.12	0.50
1:A:353:ARG:O	1:A:354:ARG:C	2.47	0.50
1:B:11:ASP:O	1:B:15:GLU:N	2.39	0.50
7:F:0:MFX:H05A	6:H:5:DA:C4	2.47	0.50
1:A:161:ASN:O	1:A:165:ASN:HB2	2.12	0.50
1:A:393:ARG:C	1:A:395:SER:H	2.15	0.50
4:F:10:DT:H2"	4:F:11:DG:C8	2.47	0.50
2:C:608:ILE:O	2:C:609:GLU:O	2.30	0.49
7:F:0:MFX:H05A	6:H:5:DA:C8	2.47	0.49
6:H:7:DG:C5	6:H:8:DC:N4	2.80	0.49
1:A:11:ASP:O	1:A:15:GLU:N	2.42	0.49
1:B:5:GLN:O	1:B:7:MET:N	2.39	0.49
2:C:523:TYR:OH	2:C:614:ALA:HB2	2.12	0.49
2:C:427:ASN:CB	2:C:500:LYS:N	2.75	0.49
2:D:503:ILE:HG22	2:D:536:TYR:O	2.13	0.49
1:B:187:ILE:HA	1:B:190:ALA:HB3	1.94	0.49
1:B:379:ILE:O	1:B:380:ARG:C	2.50	0.49
1:A:5:GLN:O	1:A:7:MET:N	2.42	0.49
1:A:416:ALA:O	1:A:417:GLU:C	2.51	0.49
2:C:461:ASN:CB	2:C:464:LYS:CB	2.91	0.49
1:A:85:MET:O	1:A:86:VAL:C	2.51	0.49
1:A:193:MET:O	1:A:196:HIS:O	2.31	0.49
1:A:434:VAL:O	1:A:435:LEU:C	2.51	0.49
1:B:87:ARG:O	1:B:87:ARG:HD3	2.12	0.49
3:E:13:DA:H2"	3:E:14:DA:O5'	2.13	0.49
1:A:353:ARG:O	1:A:355:GLU:N	2.45	0.48
1:A:87:ARG:HD3	1:A:87:ARG:C	2.33	0.48
1:A:189:ALA:O	1:A:192:TYR:N	2.47	0.48
1:B:124:SER:N	1:B:127:ALA:CB	2.76	0.48
1:B:391:LEU:HD23	1:B:392:ILE:H	1.78	0.48
4:F:9:DA:C5	4:F:10:DT:C4	3.00	0.48
2:D:508:ASP:HB2	2:D:511:GLY:N	2.29	0.48
1:B:85:MET:O	1:B:86:VAL:C	2.51	0.48
2:C:461:ASN:O	2:C:463:ALA:N	2.46	0.48
1:B:193:MET:O	1:B:196:HIS:O	2.31	0.48
2:C:538:ALA:C	2:C:540:PRO:HD3	2.34	0.48
3:E:12:DG:C6	3:E:13:DA:N6	2.81	0.48
5:G:5:DT:C2	5:G:6:DT:C6	3.01	0.48
1:B:448:MET:O	1:B:451:ALA:HB3	2.12	0.48
2:C:512:ALA:C	2:C:514:ILE:H	2.18	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:508:ASP:C	2:D:511:GLY:H	2.18	0.48
2:D:512:ALA:C	2:D:514:ILE:H	2.16	0.48
1:A:92:TRP:CH2	1:A:108:MET:HA	2.49	0.47
2:D:582:GLY:O	2:D:584:GLY:N	2.46	0.47
1:A:344:PRO:O	1:A:347:SER:N	2.46	0.47
2:D:555:VAL:O	2:D:556:ALA:CB	2.63	0.47
1:B:434:VAL:O	1:B:435:LEU:C	2.52	0.47
2:C:508:ASP:HB2	2:C:511:GLY:N	2.30	0.47
4:F:10:DT:H2"	4:F:11:DG:H8	1.80	0.47
1:A:114:ALA:HB1	1:A:118:TYR:CD2	2.49	0.47
1:A:187:ILE:HA	1:A:190:ALA:HB3	1.96	0.47
1:A:444:GLU:O	1:A:447:ALA:HB3	2.15	0.47
1:B:421:THR:O	1:B:422:LEU:O	2.33	0.47
2:D:423:ASN:O	2:D:425:ALA:N	2.46	0.47
2:D:523:TYR:CD2	2:D:524:ARG:N	2.83	0.47
6:H:9:DA:C5	6:H:10:DC:C4	3.02	0.47
1:B:158:ALA:CA	1:B:353:ARG:HH21	2.26	0.47
4:F:12:DA:C2'	4:F:13:DC:C6	2.94	0.47
1:B:407:VAL:O	1:B:408:SER:C	2.52	0.47
2:D:518:LEU:O	2:D:521:PHE:N	2.48	0.47
6:H:16:DA:C5	6:H:17:DC:C4	3.03	0.47
1:B:160:PRO:C	1:B:162:LEU:N	2.68	0.47
2:D:427:ASN:CB	2:D:500:LYS:N	2.78	0.47
1:B:156:PRO:O	1:B:157:ALA:HB3	2.16	0.46
2:C:629:ARG:C	2:C:631:LYS:N	2.68	0.46
2:D:461:ASN:CB	2:D:464:LYS:CB	2.93	0.46
1:A:124:SER:N	1:A:127:ALA:HB3	2.30	0.46
1:A:462:LEU:O	1:A:464:LYS:N	2.48	0.46
1:B:114:ALA:HB1	1:B:118:TYR:CD2	2.51	0.46
4:F:4:DC:C4	7:H:0:MFX:C	2.99	0.46
1:B:129:TYR:O	1:B:132:GLN:N	2.48	0.46
1:B:92:TRP:CH2	1:B:108:MET:HA	2.51	0.46
1:B:343:VAL:N	1:B:344:PRO:CD	2.79	0.46
1:B:416:ALA:O	1:B:417:GLU:C	2.54	0.46
2:C:508:ASP:CB	2:C:511:GLY:H	2.29	0.46
1:B:353:ARG:C	1:B:355:GLU:N	2.70	0.46
2:D:462:THR:HG21	2:D:521:PHE:HA	1.97	0.46
6:H:7:DG:C4	6:H:8:DC:C4	3.04	0.46
1:A:60:ARG:C	1:A:61:LYS:O	2.52	0.45
1:A:312:LEU:O	1:A:316:PHE:HB2	2.17	0.45
1:A:379:ILE:O	1:A:380:ARG:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:ARG:HD3	1:B:87:ARG:C	2.37	0.45
6:H:2:DA:H2"	6:H:3:DC:O5'	2.16	0.45
2:C:584:GLY:C	2:C:586:MET:H	2.19	0.45
3:E:2:DC:H2"	3:E:3:DC:O4'	2.17	0.45
1:B:82:TYR:O	1:B:85:MET:N	2.50	0.45
1:A:156:PRO:O	1:A:157:ALA:HB3	2.16	0.45
1:A:412:THR:H	1:A:415:GLN:CB	2.30	0.45
3:E:6:DG:N2	4:F:15:DT:O2	2.50	0.45
2:C:462:THR:HG21	2:C:521:PHE:HA	1.99	0.45
2:D:461:ASN:O	2:D:463:ALA:N	2.50	0.45
1:B:41:GLN:O	1:B:43:ARG:N	2.49	0.45
2:D:597:ASN:CB	2:D:600:THR:CB	2.94	0.45
2:D:629:ARG:C	2:D:631:LYS:N	2.70	0.45
1:A:471:LYS:O	1:A:475:ALA:HB1	2.03	0.45
1:B:412:THR:CB	1:B:414:GLU:OE1	2.65	0.45
2:C:423:ASN:O	2:C:425:ALA:N	2.46	0.45
1:B:462:LEU:O	1:B:464:LYS:N	2.49	0.45
2:C:508:ASP:C	2:C:511:GLY:H	2.20	0.45
2:C:518:LEU:O	2:C:521:PHE:N	2.50	0.45
3:E:5:DA:C4	3:E:6:DG:C8	3.05	0.45
1:A:49:ASN:HB3	1:A:50:LYS:H	1.63	0.45
1:A:139:VAL:HA	1:A:140:PRO:HD3	1.74	0.45
1:B:20:TYR:CD2	1:B:20:TYR:C	2.90	0.45
1:A:129:TYR:O	1:A:132:GLN:N	2.50	0.44
1:B:124:SER:N	1:B:127:ALA:HB3	2.32	0.44
3:E:5:DA:C5	3:E:6:DG:C5	3.05	0.44
1:A:358:LEU:O	1:A:362:ARG:HG3	2.17	0.44
6:H:8:DC:H2"	6:H:9:DA:O5'	2.17	0.44
1:A:343:VAL:N	1:A:344:PRO:CD	2.80	0.44
1:B:151:GLU:HA	1:B:152:PRO:HD3	1.82	0.44
1:A:341:GLY:H	1:A:344:PRO:CG	2.27	0.44
1:B:403:GLU:O	1:B:405:LEU:N	2.50	0.44
6:H:11:DG:H2"	6:H:12:DT:C6	2.51	0.44
6:H:12:DT:C2'	6:H:13:DA:N7	2.76	0.44
1:A:407:VAL:O	1:A:408:SER:C	2.56	0.44
1:A:189:ALA:O	1:A:190:ALA:C	2.56	0.44
1:A:353:ARG:C	1:A:355:GLU:N	2.71	0.44
1:A:412:THR:CB	1:A:414:GLU:OE1	2.65	0.44
2:D:508:ASP:CB	2:D:511:GLY:H	2.29	0.44
2:D:538:ALA:C	2:D:540:PRO:HD3	2.34	0.44
1:A:74:HIS:N	1:A:145:PHE:HE2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:TYR:C	1:A:349:TYR:CD2	2.91	0.44
3:E:11:DT:H2"	3:E:12:DG:H5"	1.98	0.44
1:A:41:GLN:O	1:A:43:ARG:N	2.50	0.44
1:A:125:GLU:O	1:A:128:GLY:N	2.51	0.44
1:A:72:ASN:HB3	1:A:73:PHE:CE1	2.53	0.43
1:A:237:VAL:HA	1:A:324:ASN:O	2.17	0.43
1:B:139:VAL:HA	1:B:140:PRO:HD3	1.74	0.43
3:E:5:DA:C6	3:E:6:DG:C6	3.06	0.43
1:A:134:ILE:O	1:A:135:GLU:C	2.56	0.43
1:B:134:ILE:O	1:B:135:GLU:C	2.57	0.43
1:B:216:GLY:O	1:B:217:ALA:CB	2.67	0.43
2:C:627:GLU:CB	2:C:628:PRO:HD3	2.48	0.43
4:F:12:DA:C2	4:F:13:DC:C2	3.06	0.43
1:B:85:MET:O	1:B:88:MET:N	2.51	0.43
3:E:5:DA:H2"	3:E:6:DG:C8	2.50	0.43
3:E:10:DA:H2"	3:E:11:DT:C6	2.53	0.43
1:A:349:TYR:CD2	1:A:349:TYR:O	2.72	0.43
1:A:477:PRO:HB2	1:A:478:ARG:H	1.56	0.43
1:B:335:PHE:CD1	1:B:335:PHE:N	2.85	0.43
1:A:49:ASN:C	1:A:51:ASP:H	2.19	0.43
4:F:5:DA:N9	7:H:0:MFX:H05A	2.33	0.43
1:A:180:PRO:O	1:A:211:PRO:HB3	2.19	0.43
1:B:72:ASN:HD22	1:B:72:ASN:HA	1.60	0.43
1:B:341:GLY:H	1:B:344:PRO:CG	2.26	0.43
1:B:189:ALA:O	1:B:192:TYR:N	2.52	0.43
1:B:49:ASN:HB3	1:B:50:LYS:H	1.69	0.42
2:C:629:ARG:O	2:C:630:ARG:C	2.57	0.42
4:F:1:DA:H61	7:F:0:MFX:HB	1.82	0.42
1:B:66:VAL:O	1:B:70:MET:N	2.51	0.42
2:D:629:ARG:O	2:D:630:ARG:C	2.55	0.42
4:F:4:DC:N3	7:H:0:MFX:C	2.82	0.42
3:E:2:DC:H2'	3:E:3:DC:C6	2.54	0.42
2:D:559:TRP:O	2:D:563:GLU:CB	2.67	0.42
5:G:3:DG:H2"	5:G:4:DT:H6	1.84	0.42
5:G:12:DG:H5'	5:G:12:DG:H2'	1.71	0.42
1:B:13:MET:O	1:B:17:PHE:HD1	1.87	0.42
6:H:3:DC:H2'	6:H:4:DT:O4'	2.19	0.42
1:A:49:ASN:HD22	1:A:49:ASN:HA	1.55	0.42
1:A:82:TYR:O	1:A:85:MET:N	2.52	0.42
4:F:1:DA:H2"	4:F:2:DG:C8	2.54	0.42
1:A:85:MET:O	1:A:88:MET:N	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:GLU:C	1:A:127:ALA:N	2.73	0.41
2:C:517:LEU:O	2:C:520:THR:N	2.53	0.41
2:C:591:LEU:O	2:C:595:THR:CB	2.68	0.41
1:A:403:GLU:O	1:A:405:LEU:N	2.53	0.41
2:C:460:ILE:HA	4:F:7:DT:OP1	2.20	0.41
1:A:422:LEU:O	1:B:423:GLN:CB	2.65	0.41
1:B:388:VAL:O	1:B:390:ALA:N	2.54	0.41
2:C:430:TYR:CB	2:C:502:ILE:CD1	2.98	0.41
5:G:3:DG:C5	5:G:4:DT:C4	3.07	0.41
1:A:31:PRO:HD3	1:A:38:LYS:CB	2.51	0.41
1:A:107:SER:C	1:A:109:ASP:H	2.24	0.41
1:B:160:PRO:O	1:B:161:ASN:C	2.58	0.41
1:B:336:THR:HA	1:B:337:PRO:HD3	1.80	0.41
1:A:66:VAL:O	1:A:70:MET:N	2.54	0.41
7:F:0:MFX:H03	6:H:5:DA:C6	2.55	0.41
5:G:2:DT:H2"	5:G:3:DG:O4'	2.21	0.41
1:A:225:ILE:O	1:A:228:ALA:N	2.53	0.41
1:B:19:ARG:HB3	2:D:512:ALA:HB1	2.02	0.41
1:A:124:SER:C	1:A:127:ALA:CB	2.84	0.41
1:A:421:THR:C	1:A:422:LEU:O	2.58	0.41
6:H:6:DT:C2'	6:H:7:DG:OP2	2.67	0.41
1:A:323:ILE:O	1:A:324:ASN:O	2.39	0.41
1:A:470:VAL:O	1:A:471:LYS:C	2.58	0.41
1:B:412:THR:H	1:B:415:GLN:CB	2.34	0.41
4:F:16:DT:C2	4:F:17:DG:C8	3.09	0.41
1:A:20:TYR:CD2	1:A:20:TYR:C	2.94	0.41
1:A:151:GLU:HA	1:A:152:PRO:HD3	1.78	0.41
1:A:402:LYS:O	1:A:405:LEU:HB2	2.20	0.41
1:A:470:VAL:O	1:A:472:LYS:N	2.54	0.41
2:C:551:LYS:O	2:C:552:LYS:O	2.39	0.41
1:A:124:SER:CA	1:A:127:ALA:HB3	2.51	0.41
1:B:421:THR:C	1:B:422:LEU:O	2.60	0.41
1:B:477:PRO:HB2	1:B:478:ARG:H	1.56	0.41
2:C:523:TYR:HD2	2:C:524:ARG:N	2.19	0.41
1:B:124:SER:CA	1:B:127:ALA:HB3	2.50	0.40
1:B:363:PHE:O	1:B:366:GLU:N	2.54	0.40
1:B:412:THR:O	1:B:416:ALA:N	2.43	0.40
6:H:12:DT:C2'	6:H:13:DA:C8	3.04	0.40
1:A:82:TYR:O	1:A:83:ASP:C	2.60	0.40
1:B:60:ARG:C	1:B:61:LYS:O	2.54	0.40
4:F:5:DA:C4	7:H:0:MFX:H05A	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:445:ARG:O	2:D:447:ARG:N	2.54	0.40
2:D:551:LYS:O	2:D:552:LYS:O	2.38	0.40
1:B:49:ASN:C	1:B:51:ASP:H	2.23	0.40
2:D:591:LEU:O	2:D:595:THR:CB	2.69	0.40
1:A:412:THR:O	1:A:416:ALA:N	2.44	0.40
1:B:439:GLU:O	1:B:443:ARG:HB2	2.21	0.40
2:D:446:ASP:CB	2:D:596:MET:CB	3.00	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	421/496 (85%)	278 (66%)	97 (23%)	46 (11%)	0 7
1	B	416/496 (84%)	276 (66%)	95 (23%)	45 (11%)	0 7
2	C	180/268 (67%)	114 (63%)	42 (23%)	24 (13%)	0 4
2	D	187/268 (70%)	122 (65%)	42 (22%)	23 (12%)	0 5
All	All	1204/1528 (79%)	790 (66%)	276 (23%)	138 (12%)	0 6

All (138) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	LYS
1	A	61	LYS
1	A	125	GLU
1	A	129	TYR
1	A	133	ASP
1	A	161	ASN
1	A	323	ILE
1	A	396	GLU

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Mol	Chain	Res	Type
1	A	408	SER
1	A	417	GLU
1	A	422	LEU
1	A	429	ASN
1	A	477	PRO
1	B	50	LYS
1	B	61	LYS
1	B	125	GLU
1	B	129	TYR
1	B	133	ASP
1	B	161	ASN
1	B	396	GLU
1	B	408	SER
1	B	417	GLU
1	B	429	ASN
1	B	477	PRO
2	C	447	ARG
2	C	456	ARG
2	C	583	LEU
2	C	602	THR
2	C	606	VAL
2	C	609	GLU
2	C	610	ASP
2	C	612	ALA
2	C	620	VAL
2	D	445	ARG
2	D	556	ALA
2	D	583	LEU
2	D	602	THR
2	D	606	VAL
2	D	609	GLU
2	D	610	ASP
2	D	612	ALA
2	D	620	VAL
1	A	49	ASN
1	A	104	ASN
1	A	115	ALA
1	A	154	VAL
1	A	395	SER
1	B	49	ASN
1	B	104	ASN
1	B	138	THR

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Mol	Chain	Res	Type
1	B	154	VAL
1	B	197	PRO
1	B	216	GLY
1	B	395	SER
1	B	422	LEU
2	C	462	THR
2	C	513	HIS
2	C	552	LYS
2	C	555	VAL
2	D	446	ASP
2	D	462	THR
2	D	463	ALA
2	D	513	HIS
2	D	552	LYS
2	D	555	VAL
2	D	624	ASP
1	A	6	ASN
1	A	7	MET
1	A	63	ALA
1	A	76	HIS
1	A	138	THR
1	A	157	ALA
1	A	197	PRO
1	A	216	GLY
1	A	217	ALA
1	A	221	GLY
1	A	354	ARG
1	A	473	LYS
1	B	6	ASN
1	B	63	ALA
1	B	76	HIS
1	B	115	ALA
1	B	194	ILE
1	B	217	ALA
1	B	221	GLY
1	B	354	ARG
1	B	394	ALA
1	B	473	LYS
2	C	463	ALA
2	C	624	ASP
1	A	194	ILE
1	A	394	ALA

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Mol	Chain	Res	Type
1	A	425	TYR
1	A	471	LYS
1	B	7	MET
1	B	157	ALA
1	B	389	ILE
1	B	425	TYR
1	B	462	LEU
1	B	471	LYS
2	C	427	ASN
2	C	483	ILE
2	C	484	GLY
2	D	427	ASN
2	D	483	ILE
2	D	484	GLY
1	A	324	ASN
1	A	409	TYR
1	A	462	LEU
1	B	81	ILE
1	B	236	VAL
1	B	379	ILE
1	B	404	ASN
2	C	481	TYR
2	C	547	LYS
2	D	547	LYS
1	A	236	VAL
1	A	389	ILE
1	B	263	ILE
1	B	432	VAL
2	C	458	LYS
2	C	633	ILE
2	D	633	ILE
1	A	263	ILE
1	A	379	ILE
1	A	432	VAL
2	C	623	GLY
2	D	623	GLY
1	A	81	ILE
1	A	86	VAL
1	B	128	GLY
2	C	584	GLY
1	B	86	VAL
1	B	103	GLY

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Mol	Chain	Res	Type
1	A	103	GLY
1	A	126	ILE
1	B	99	VAL
2	D	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	76/431 (18%)	66 (87%)	10 (13%)	4 21
1	B	71/431 (16%)	61 (86%)	10 (14%)	3 19
2	C	24/224 (11%)	21 (88%)	3 (12%)	4 22
2	D	24/224 (11%)	21 (88%)	3 (12%)	4 22
All	All	195/1310 (15%)	169 (87%)	26 (13%)	4 21

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASP
1	A	49	ASN
1	A	87	ARG
1	A	334	ASN
1	A	335	PHE
1	A	349	TYR
1	A	371	ARG
1	A	391	LEU
1	A	423	GLN
1	A	429	ASN
1	B	27	ASP
1	B	49	ASN
1	B	87	ARG
1	B	334	ASN
1	B	335	PHE
1	B	349	TYR
1	B	371	ARG

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Mol	Chain	Res	Type
1	B	391	LEU
1	B	423	GLN
1	B	429	ASN
2	C	524	ARG
2	C	527	ARG
2	C	602	THR
2	D	524	ARG
2	D	527	ARG
2	D	602	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	72	ASN
1	A	76	HIS
1	A	334	ASN
1	B	49	ASN
1	B	72	ASN
1	B	76	HIS
1	B	334	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)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	MFX	F	0	-	33,33,33	5.40	14 (42%)	46,50,50	1.86	8 (17%)
7	MFX	H	0	-	33,33,33	5.43	14 (42%)	46,50,50	1.81	10 (21%)

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
7	MFX	F	0	-	-	5/14/35/35	0/5/5/5
7	MFX	H	0	-	-	7/14/35/35	0/5/5/5

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	0	MFX	C12-N	16.20	1.60	1.40
7	F	0	MFX	C12-N	16.08	1.60	1.40
7	H	0	MFX	C17-C14	13.90	1.61	1.39
7	F	0	MFX	C17-C14	13.79	1.61	1.39
7	H	0	MFX	C12-C13	13.38	1.64	1.40
7	F	0	MFX	C12-C13	13.32	1.64	1.40
7	H	0	MFX	C16-N	11.41	1.52	1.34
7	F	0	MFX	C16-N	11.41	1.52	1.34
7	F	0	MFX	C11-C15	7.92	1.56	1.39
7	H	0	MFX	C11-C15	7.91	1.56	1.39
7	H	0	MFX	C14-C19	5.86	1.59	1.48
7	F	0	MFX	C14-C19	5.75	1.59	1.48
7	H	0	MFX	C14-C12	-5.07	1.33	1.40
7	F	0	MFX	C14-C12	-4.99	1.34	1.40
7	F	0	MFX	C18-C19	3.94	1.54	1.44
7	H	0	MFX	C18-C19	3.92	1.53	1.44
7	H	0	MFX	O03-C20	3.54	1.41	1.30
7	F	0	MFX	O03-C20	3.49	1.40	1.30
7	F	0	MFX	C18-C20	3.39	1.54	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	0	MFX	C18-C20	3.36	1.54	1.48
7	H	0	MFX	C11-N01	3.04	1.49	1.40
7	F	0	MFX	C11-N01	2.99	1.49	1.40
7	H	0	MFX	C09-C06	2.82	1.55	1.48
7	F	0	MFX	C02-N02	2.80	1.51	1.47
7	F	0	MFX	C09-C06	2.78	1.54	1.48
7	H	0	MFX	C02-N02	2.73	1.51	1.47
7	F	0	MFX	C08-C06	2.62	1.54	1.48
7	H	0	MFX	C08-C06	2.58	1.54	1.48

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	F	0	MFX	C10-N02-C02	6.18	115.48	111.62
7	H	0	MFX	C10-N02-C02	5.23	114.88	111.62
7	F	0	MFX	C13-C11-C15	4.36	119.71	116.02
7	H	0	MFX	C13-C11-C15	3.89	119.31	116.02
7	H	0	MFX	C18-C16-N	-3.72	120.32	124.49
7	F	0	MFX	C18-C16-N	-3.48	120.59	124.49
7	H	0	MFX	C14-C19-C18	3.42	119.94	115.59
7	F	0	MFX	C04-N01-C03	-3.41	107.18	111.67
7	H	0	MFX	C03-N01-C11	3.37	129.45	123.04
7	F	0	MFX	C14-C19-C18	3.34	119.83	115.59
7	H	0	MFX	C04-N01-C03	-3.30	107.31	111.67
7	F	0	MFX	C03-N01-C11	3.27	129.26	123.04
7	H	0	MFX	O02-C19-C18	-2.31	119.35	123.22
7	H	0	MFX	C07-C05-C01	2.29	115.84	111.93
7	F	0	MFX	C-O01-C13	2.22	120.86	114.78
7	F	0	MFX	O02-C19-C18	-2.18	119.56	123.22
7	H	0	MFX	C-O01-C13	2.06	120.42	114.78
7	H	0	MFX	C08-C06-N	-2.01	115.82	118.84

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	F	0	MFX	C13-C11-N01-C04
7	F	0	MFX	C16-C18-C20-O03
7	F	0	MFX	C16-C18-C20-O
7	F	0	MFX	C19-C18-C20-O03
7	F	0	MFX	C19-C18-C20-O
7	H	0	MFX	C15-C11-N01-C04

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Mol	Chain	Res	Type	Atoms
7	H	0	MFX	C16-C18-C20-O03
7	H	0	MFX	C16-C18-C20-O
7	H	0	MFX	C19-C18-C20-O03
7	H	0	MFX	C19-C18-C20-O
7	H	0	MFX	C13-C11-N01-C04
7	H	0	MFX	C13-C11-N01-C03

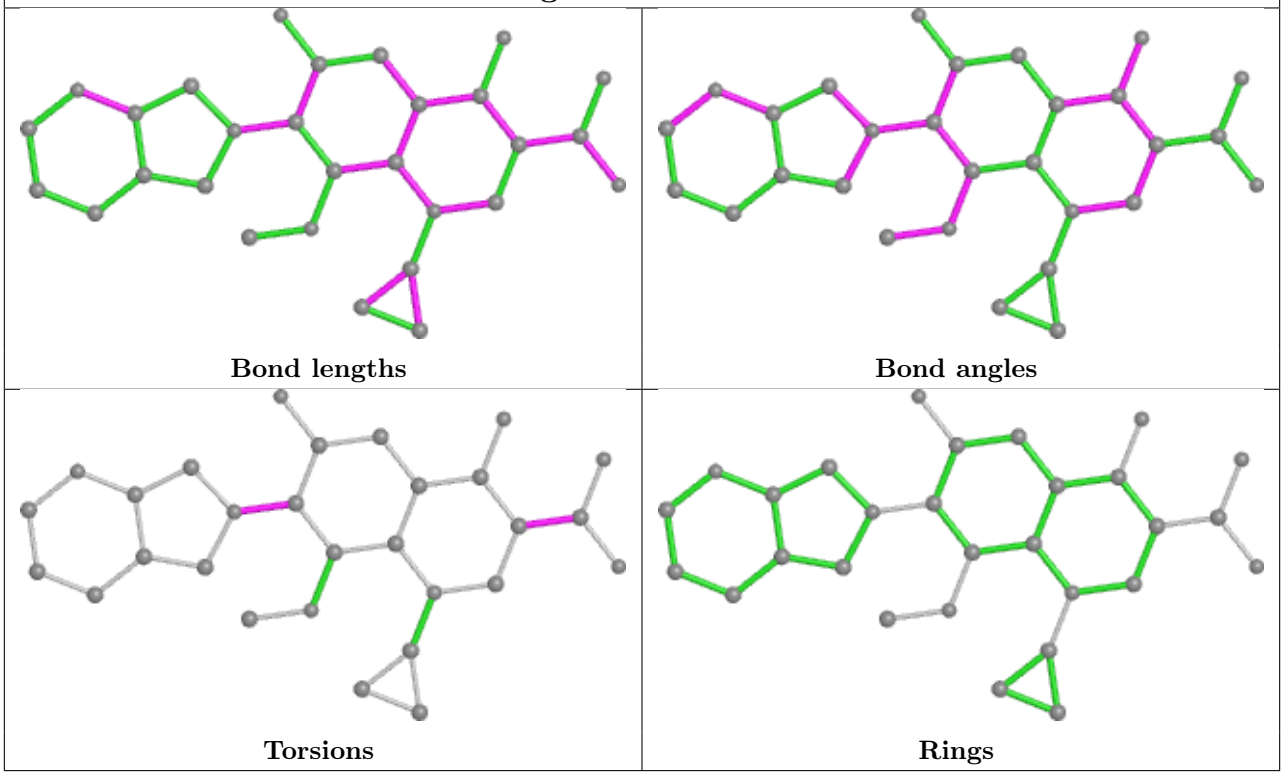
There are no ring outliers.

2 monomers are involved in 18 short contacts:

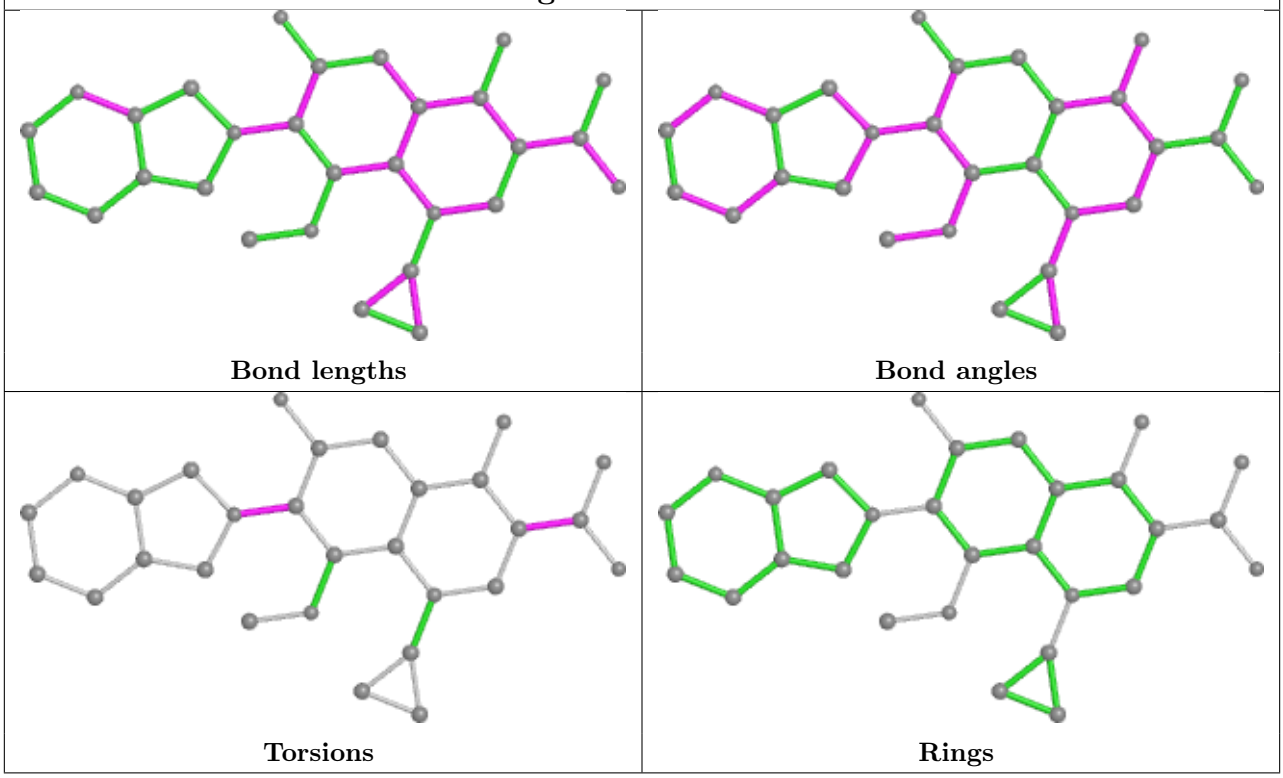
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	0	MFX	10	0
7	H	0	MFX	8	0

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

Ligand MFX F 0



Ligand MFX H 0



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	435/496 (87%)	-1.00	1 (0%) 95 93	91, 178, 258, 361	0
1	B	432/496 (87%)	-1.00	0 100 100	91, 178, 255, 355	0
2	C	196/268 (73%)	-0.88	1 (0%) 91 85	114, 180, 291, 395	0
2	D	199/268 (74%)	-0.87	1 (0%) 91 85	107, 182, 292, 386	0
3	E	15/15 (100%)	-0.03	1 (6%) 17 14	143, 263, 436, 512	0
4	F	19/19 (100%)	0.06	2 (10%) 6 6	148, 232, 469, 484	0
5	G	15/15 (100%)	-0.12	1 (6%) 17 14	141, 253, 368, 479	0
6	H	19/19 (100%)	0.04	2 (10%) 6 6	155, 209, 445, 475	0
All	All	1330/1596 (83%)	-0.91	9 (0%) 87 82	91, 181, 282, 512	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	19	DT	4.9
6	H	18	DA	3.3
4	F	18	DG	3.3
2	D	599	GLU	3.1
6	H	19	DG	2.8
3	E	1	DA	2.7
5	G	1	DC	2.6
2	C	599	GLU	2.5
1	A	431	ASP	2.2

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)

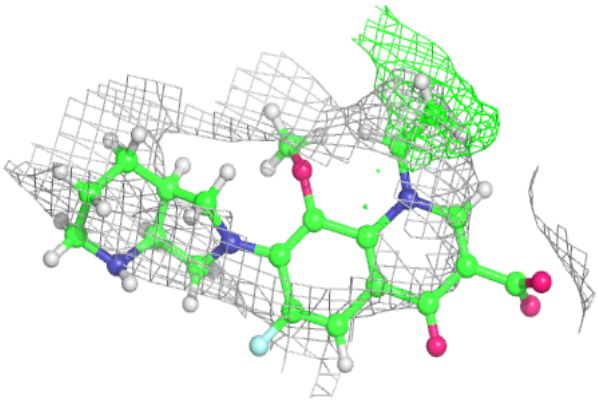
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

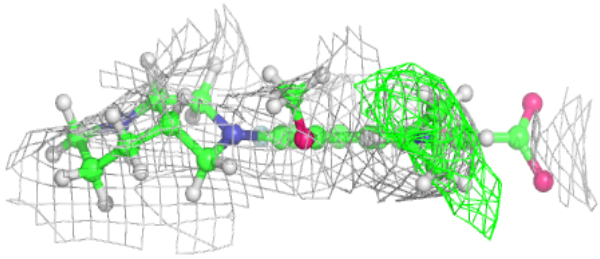
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	MFX	F	0	29/29	0.83	0.29	229,278,346,350	0
7	MFX	H	0	29/29	0.84	0.31	224,270,369,415	0

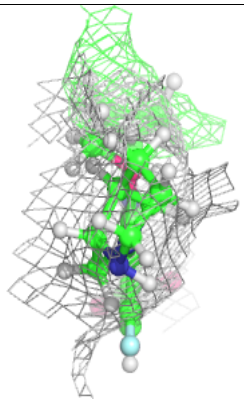
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MFX F 0:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

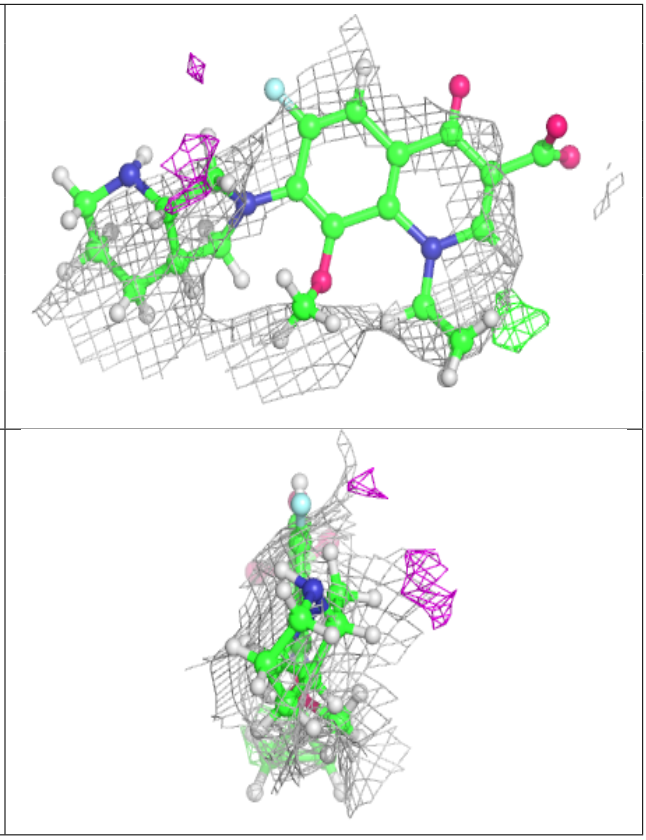






Electron density around MFX H 0:

$2mF_o$-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.