



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:42 AM GMT

PDB ID : 3FOE
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

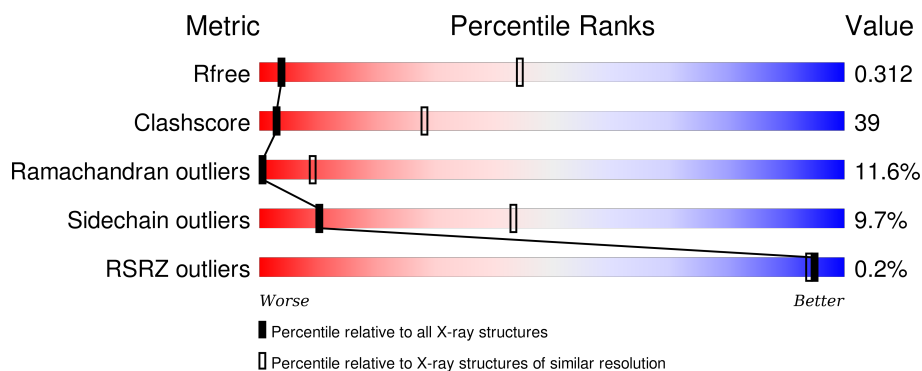
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



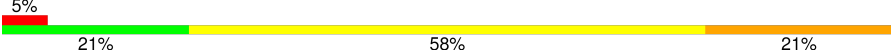

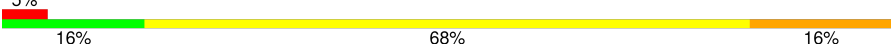
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	496	
1	B	496	
2	C	268	
2	D	268	
3	E	15	

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Mol	Chain	Length	Quality of chain
4	F	19	
5	G	15	
6	H	19	

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	NFX	F	0	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8367 atoms, of which 26 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	0
			2426	1483	471	470	2			
1	B	433	Total	C	N	O	S	0	0	0
			2410	1471	473	465	1			

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
2	C	196	Total	C	N	O	0	0	0
			1039	628	203	208			
2	D	198	Total	C	N	O	0	0	0
			1042	630	204	208			

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
3	E	15	Total	C	N	O	P	0	0	0
			306	144	60	87	15			

- 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
4	F	19	Total	C	N	O	P	0	0	0
			381	179	66	117	19			

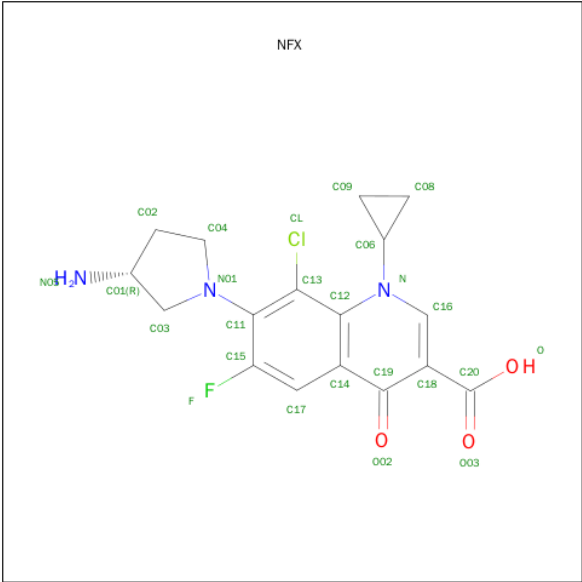
- Molecule 5 is a DNA chain called DNA (5'-D(P*CP*TP*GP*TP*TP*TP*TP*AP*CP*GP*TP*GP*CP*AP*T)-3').

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

- 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
6	H	19	Total	C	N	O	P	0	0	0
			389	183	78	109	19			

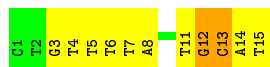
- Molecule 7 is 7-[(3R)-3-AMINOPYRROLIDIN-1-YL]-8-CHLORO-1-CYCLOPROPYL-6-FLUORO-4-OXO-1,4-DIHYDROQUINOLINE-3-CARBOXYLIC ACID (three-letter code: NFX) (formula: C₁₇H₁₇ClFN₃O₃).




Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
7	F	1	Total	C	Cl	F	H	N	O	0	0
			38	17	1	1	13	3	3		
7	H	1	Total	C	Cl	F	H	N	O	0	0
			38	17	1	1	13	3	3		

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

Chain G:  27% 60% 13%



- 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:  5% 16% 68% 16%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	121.68Å 121.68Å 179.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.10 – 4.00 36.10 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (36.10-4.00) 97.1 (36.10-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 3.56Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.258 , 0.313 0.258 , 0.312	Depositor DCC
R_{free} test set	2521 reflections (11.26%)	DCC
Wilson B-factor (Å ²)	171.7	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 299.8	EDS
Estimated twinning fraction	0.410 for -h,-k,l 0.048 for h,-h-k,-l 0.043 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 33366 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8367	wwPDB-VP
Average B, all atoms (Å ²)	202.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.35	0/2455	0.50	0/3397
1	B	0.35	0/2439	0.49	0/3380
2	C	0.30	0/1042	0.47	0/1439
2	D	0.27	0/1046	0.43	0/1446
3	E	0.60	0/344	1.51	4/527 (0.8%)
4	F	0.60	0/426	1.44	6/652 (0.9%)
5	G	0.60	0/332	1.67	5/507 (1.0%)
6	H	0.61	0/438	1.66	10/672 (1.5%)
All	All	0.40	0/8522	0.82	25/12020 (0.2%)

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

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

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	12	DG	O4'-C4'-C3'	-17.31	95.61	106.00
3	E	12	DG	O4'-C4'-C3'	-14.89	97.06	106.00
6	H	9	DA	O4'-C1'-N9	-10.58	100.60	108.00
6	H	6	DT	O4'-C1'-N1	10.18	115.13	108.00
6	H	6	DT	O4'-C4'-C3'	-9.29	100.43	106.00
6	H	8	DC	O4'-C4'-C3'	-8.22	101.07	106.00
6	H	10	DC	O4'-C1'-N1	7.92	113.55	108.00
5	G	13	DC	C1'-O4'-C4'	-7.69	102.41	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	13	DA	C1'-O4'-C4'	-7.43	102.67	110.10
6	H	10	DC	C1'-O4'-C4'	-7.41	102.69	110.10
6	H	8	DC	O4'-C1'-N1	6.81	112.77	108.00
3	E	12	DG	C4'-C3'-C2'	-6.52	97.24	103.10
4	F	8	DC	C1'-O4'-C4'	-6.40	103.70	110.10
6	H	10	DC	O4'-C4'-C3'	-6.30	101.98	104.50
4	F	15	DT	N3-C4-O4	5.99	123.49	119.90
6	H	8	DC	C1'-O4'-C4'	-5.90	104.20	110.10
5	G	12	DG	C4'-C3'-C2'	-5.89	97.80	103.10
5	G	11	DT	O4'-C1'-N1	5.88	112.11	108.00
4	F	10	DT	C1'-O4'-C4'	-5.83	104.27	110.10
6	H	8	DC	P-O3'-C3'	5.60	126.42	119.70
5	G	7	DT	N3-C4-O4	5.56	123.23	119.90
4	F	15	DT	C5-C4-O4	-5.38	121.13	124.90
3	E	11	DT	O4'-C1'-N1	5.26	111.68	108.00
4	F	8	DC	O4'-C1'-N1	5.19	111.64	108.00
4	F	6	DT	O4'-C1'-N1	5.04	111.53	108.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	507	ALA	Peptide

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	2426	0	1390	144	0
1	B	2410	0	1366	131	0
2	C	1039	0	595	74	0
2	D	1042	0	590	65	0
3	E	306	0	160	27	0
4	F	381	0	196	22	0
5	G	298	0	152	27	0
6	H	389	0	204	25	0
7	F	25	13	15	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	25	13	15	6	0
All	All	8341	26	4683	512	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 39.

All (512) 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)
5:G:12:DG:H5'	5:G:12:DG:C8	1.84	1.12
1:B:130:LEU:HA	1:B:157:ALA:HA	1.33	1.11
2:C:527:ARG:HB2	2:C:527:ARG:NH1	1.66	1.09
1:A:130:LEU:HA	1:A:157:ALA:HA	1.34	1.09
2:C:527:ARG:HB2	2:C:527:ARG:HH11	1.14	1.08
2:D:512:ALA:O	2:D:514:ILE:N	1.88	1.07
2:C:592:TRP:HA	2:C:595:THR:CB	1.87	1.04
2:D:527:ARG:NH1	2:D:527:ARG:HB2	1.72	1.04
2:C:512:ALA:O	2:C:514:ILE:N	1.91	1.03
1:B:79:SER:O	1:B:83:ASP:HB2	1.58	1.01
1:A:79:SER:O	1:A:83:ASP:HB2	1.62	0.98
2:C:621:LEU:O	2:C:623:GLY:N	1.97	0.97
2:D:592:TRP:HA	2:D:595:THR:CB	1.95	0.97
2:C:524:ARG:NH1	2:C:524:ARG:HB3	1.80	0.96
2:D:524:ARG:HB3	2:D:524:ARG:NH1	1.81	0.95
2:D:527:ARG:HB2	2:D:527:ARG:HH11	1.22	0.94
5:G:12:DG:H5'	5:G:12:DG:H8	1.33	0.94
1:B:13:MET:O	1:B:17:PHE:CD1	2.23	0.92
1:A:46:TYR:CD2	1:A:152:PRO:HG2	2.06	0.90
1:A:13:MET:O	1:A:17:PHE:CD1	2.24	0.89
1:A:62:SER:O	1:A:64:LYS:N	2.05	0.89
1:A:363:PHE:O	1:A:366:GLU:N	2.07	0.87
1:B:46:TYR:CD2	1:B:152:PRO:HG2	2.08	0.87
1:A:358:LEU:O	1:A:362:ARG:HG2	1.75	0.87
1:B:358:LEU:O	1:B:362:ARG:HG2	1.73	0.86
1:B:82:TYR:O	1:B:85:MET:N	2.09	0.85
1:A:86:VAL:O	1:A:89:SER:N	2.08	0.85
1:B:62:SER:O	1:B:64:LYS:N	2.10	0.85
1:B:363:PHE:O	1:B:366:GLU:N	2.09	0.84
1:A:82:TYR:O	1:A:85:MET:N	2.11	0.84
2:C:512:ALA:O	2:C:515:GLN:N	2.11	0.83
4:F:11:DG:H2'	4:F:12:DA:C8	2.13	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ALA:HA	1:A:362:ARG:CG	2.09	0.82
1:B:15:GLU:O	1:B:19:ARG:HG2	1.79	0.82
1:A:237:VAL:HA	1:A:324:ASN:O	1.80	0.82
1:A:124:SER:O	1:A:127:ALA:HB3	1.81	0.81
1:B:407:VAL:O	1:B:409:TYR:N	2.13	0.80
1:B:359:ALA:HA	1:B:362:ARG:CG	2.12	0.80
1:A:15:GLU:O	1:A:19:ARG:HG2	1.81	0.79
1:A:23:TYR:CD1	2:C:513:HIS:HB2	2.18	0.79
2:C:444:GLY:O	2:C:446:ASP:N	2.16	0.78
1:B:180:PRO:HB2	1:B:212:ASP:O	1.82	0.78
1:B:412:THR:H	1:B:415:GLN:CB	1.96	0.78
2:C:462:THR:HG21	2:C:521:PHE:HA	1.66	0.78
1:B:181:HIS:HA	1:B:212:ASP:H	1.47	0.78
2:D:512:ALA:O	2:D:515:GLN:N	2.15	0.78
2:D:444:GLY:O	2:D:446:ASP:N	2.15	0.77
1:A:407:VAL:O	1:A:409:TYR:N	2.16	0.77
2:C:618:VAL:O	2:C:618:VAL:HG12	1.85	0.77
5:G:12:DG:C5'	5:G:12:DG:C8	2.67	0.76
1:A:423:GLN:HA	1:B:423:GLN:HA	1.66	0.76
1:B:86:VAL:O	1:B:89:SER:N	2.14	0.76
1:A:62:SER:O	1:A:65:SER:N	2.19	0.76
2:C:508:ASP:O	2:C:511:GLY:N	2.18	0.76
2:D:462:THR:HG21	2:D:521:PHE:HA	1.66	0.76
1:B:124:SER:O	1:B:127:ALA:HB3	1.85	0.76
2:C:611:LEU:O	2:C:613:ARG:N	2.19	0.76
2:C:623:GLY:O	2:C:624:ASP:O	2.04	0.75
2:C:524:ARG:HB3	2:C:524:ARG:CZ	2.15	0.75
1:A:412:THR:H	1:A:415:GLN:CB	1.98	0.75
2:D:524:ARG:CZ	2:D:524:ARG:HB3	2.15	0.74
1:B:29:ALA:HB1	1:B:39:PRO:HG2	1.69	0.74
1:A:341:GLY:H	1:A:344:PRO:HG2	1.51	0.74
1:B:341:GLY:H	1:B:344:PRO:HG2	1.52	0.74
2:D:508:ASP:O	2:D:511:GLY:N	2.21	0.74
1:B:62:SER:O	1:B:65:SER:N	2.20	0.74
2:C:527:ARG:CB	2:C:527:ARG:HH11	1.97	0.73
1:A:180:PRO:HB2	1:A:212:ASP:O	1.88	0.73
1:A:181:HIS:HA	1:A:212:ASP:H	1.53	0.73
1:B:79:SER:O	1:B:83:ASP:CB	2.34	0.73
2:C:621:LEU:O	2:C:622:MET:C	2.28	0.72
1:A:359:ALA:HA	1:A:362:ARG:HG2	1.71	0.72
3:E:5:DA:C4	3:E:6:DG:C8	2.77	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:536:TYR:CB	2:D:603:LEU:O	2.38	0.72
1:A:375:VAL:O	1:A:378:LEU:N	2.23	0.71
2:D:608:ILE:O	2:D:609:GLU:O	2.09	0.71
1:A:29:ALA:HB1	1:A:39:PRO:HG2	1.73	0.70
1:B:412:THR:O	1:B:416:ALA:N	2.24	0.70
5:G:14:DA:C2	5:G:15:DT:C4	2.79	0.70
1:A:28:ARG:HG2	1:A:28:ARG:O	1.91	0.70
2:C:611:LEU:C	2:C:613:ARG:H	1.93	0.70
2:D:611:LEU:O	2:D:613:ARG:N	2.24	0.70
1:B:31:PRO:O	1:B:331:ALA:HB1	1.92	0.70
3:E:6:DG:N2	4:F:15:DT:C2	2.60	0.70
2:D:530:VAL:O	2:D:533:GLY:N	2.25	0.70
2:D:527:ARG:CB	2:D:527:ARG:HH11	2.03	0.69
2:C:536:TYR:CB	2:C:603:LEU:O	2.40	0.69
1:B:375:VAL:O	1:B:378:LEU:N	2.25	0.69
1:B:23:TYR:CD1	2:D:513:HIS:HB2	2.26	0.69
1:B:359:ALA:HA	1:B:362:ARG:HG2	1.74	0.69
6:H:12:DT:H2''	6:H:13:DA:N7	2.07	0.69
1:A:128:GLY:O	1:A:129:TYR:C	2.29	0.68
6:H:11:DG:H2'	6:H:12:DT:C6	2.28	0.68
1:B:84:ALA:O	1:B:87:ARG:HB3	1.93	0.68
1:A:349:TYR:O	1:A:353:ARG:HB2	1.93	0.68
1:A:359:ALA:HA	1:A:362:ARG:HG3	1.76	0.68
5:G:13:DC:C2	5:G:14:DA:N7	2.62	0.68
3:E:4:DA:C2	4:F:17:DG:C2	2.82	0.68
1:A:31:PRO:O	1:A:331:ALA:HB1	1.93	0.67
1:B:128:GLY:O	1:B:129:TYR:C	2.32	0.67
4:F:10:DT:H2''	4:F:11:DG:C8	2.29	0.67
1:B:471:LYS:O	1:B:475:ALA:HA	1.94	0.67
1:A:46:TYR:CE2	1:A:152:PRO:CG	2.76	0.67
6:H:9:DA:H2''	6:H:10:DC:C6	2.30	0.67
1:B:20:TYR:O	1:B:20:TYR:CD2	2.48	0.67
1:B:46:TYR:CE2	1:B:152:PRO:CG	2.77	0.67
1:A:79:SER:O	1:A:83:ASP:CB	2.39	0.67
1:B:46:TYR:CE2	1:B:152:PRO:HG2	2.29	0.67
3:E:12:DG:H5''	3:E:12:DG:C8	2.30	0.67
2:C:477:ASN:OD1	2:C:478:THR:N	2.28	0.67
1:A:403:GLU:O	1:A:405:LEU:N	2.28	0.67
3:E:12:DG:C5'	3:E:12:DG:C8	2.78	0.67
1:A:20:TYR:CD2	1:A:20:TYR:O	2.47	0.66
2:D:611:LEU:C	2:D:613:ARG:H	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:GLU:O	1:A:443:ARG:HB2	1.96	0.66
1:A:28:ARG:CG	1:A:28:ARG:O	2.44	0.66
2:D:523:TYR:OH	2:D:614:ALA:HB2	1.97	0.65
1:B:471:LYS:O	1:B:475:ALA:HB2	1.96	0.65
1:B:41:GLN:O	1:B:44:ILE:N	2.29	0.65
2:C:624:ASP:CB	2:C:628:PRO:HG2	2.26	0.65
1:A:471:LYS:O	1:A:475:ALA:HB2	1.97	0.65
1:B:130:LEU:CA	1:B:157:ALA:HA	2.20	0.65
1:B:359:ALA:HA	1:B:362:ARG:HG3	1.78	0.65
2:C:530:VAL:O	2:C:533:GLY:N	2.29	0.65
1:A:46:TYR:CE2	1:A:152:PRO:HG2	2.32	0.64
2:C:608:ILE:O	2:C:609:GLU:O	2.14	0.64
1:A:412:THR:O	1:A:416:ALA:N	2.26	0.64
1:A:471:LYS:O	1:A:475:ALA:HA	1.97	0.64
1:B:395:SER:O	1:B:396:GLU:CB	2.45	0.64
5:G:13:DC:C2	5:G:14:DA:C8	2.86	0.64
5:G:13:DC:H2''	5:G:14:DA:O5'	1.98	0.64
1:A:158:ALA:O	1:A:349:TYR:OH	2.16	0.64
1:A:130:LEU:CA	1:A:157:ALA:HA	2.22	0.64
1:B:471:LYS:O	1:B:475:ALA:CA	2.46	0.64
2:C:484:GLY:O	2:C:486:GLY:N	2.31	0.64
1:A:141:PHE:CZ	1:A:152:PRO:HD3	2.33	0.64
2:C:609:GLU:O	2:C:610:ASP:CB	2.46	0.64
1:B:349:TYR:O	1:B:353:ARG:HB2	1.97	0.64
1:A:341:GLY:N	1:A:344:PRO:HG2	2.13	0.63
2:C:508:ASP:C	2:C:511:GLY:H	2.02	0.63
1:B:439:GLU:O	1:B:443:ARG:HB2	1.98	0.63
5:G:12:DG:H2''	5:G:13:DC:OP2	1.99	0.63
2:C:474:GLU:O	2:C:477:ASN:OD1	2.17	0.63
2:C:445:ARG:C	2:C:447:ARG:H	2.00	0.63
1:B:403:GLU:O	1:B:405:LEU:N	2.32	0.63
1:A:39:PRO:O	1:A:41:GLN:N	2.31	0.63
1:B:434:VAL:O	1:B:437:GLU:N	2.32	0.63
2:C:523:TYR:OH	2:C:614:ALA:HB2	1.99	0.62
1:B:11:ASP:O	1:B:15:GLU:N	2.31	0.62
1:A:41:GLN:O	1:A:44:ILE:N	2.32	0.62
1:A:395:SER:O	1:A:396:GLU:CB	2.47	0.62
1:B:38:LYS:O	1:B:41:GLN:N	2.28	0.62
1:B:472:LYS:O	1:B:473:LYS:C	2.36	0.62
2:D:445:ARG:C	2:D:447:ARG:H	2.01	0.62
1:A:11:ASP:O	1:A:15:GLU:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:VAL:O	1:A:69:ILE:N	2.33	0.62
1:A:86:VAL:O	1:A:87:ARG:C	2.38	0.62
1:A:66:VAL:O	1:A:67:GLY:C	2.38	0.62
1:A:472:LYS:O	1:A:473:LYS:C	2.38	0.62
2:C:502:ILE:HA	2:C:536:TYR:O	2.00	0.62
2:D:484:GLY:O	2:D:486:GLY:N	2.32	0.62
2:D:609:GLU:O	2:D:610:ASP:CB	2.48	0.62
2:D:512:ALA:C	2:D:514:ILE:N	2.54	0.61
1:A:85:MET:O	1:A:86:VAL:C	2.38	0.61
6:H:12:DT:H2''	6:H:13:DA:C8	2.35	0.61
2:C:512:ALA:C	2:C:514:ILE:N	2.54	0.61
1:A:107:SER:H	1:A:111:ASP:CB	2.13	0.61
1:A:434:VAL:O	1:A:437:GLU:N	2.33	0.61
1:B:86:VAL:O	1:B:87:ARG:C	2.39	0.61
1:B:39:PRO:O	1:B:41:GLN:N	2.34	0.61
2:D:508:ASP:C	2:D:511:GLY:H	2.03	0.61
5:G:13:DC:N4	5:G:14:DA:H62	1.99	0.60
1:B:85:MET:O	1:B:86:VAL:C	2.40	0.60
5:G:5:DT:C2	5:G:6:DT:C6	2.89	0.60
1:B:101:MET:CB	1:B:121:ALA:HB2	2.31	0.60
1:A:62:SER:O	1:A:63:ALA:C	2.39	0.60
5:G:5:DT:C4	5:G:6:DT:C4	2.90	0.60
1:A:132:GLN:O	1:A:133:ASP:CB	2.50	0.60
4:F:1:DA:H5'	7:F:0:NFX:H17	1.82	0.60
1:B:158:ALA:O	1:B:349:TYR:OH	2.20	0.60
3:E:6:DG:H2''	3:E:7:DG:H8	1.67	0.60
1:B:471:LYS:O	1:B:475:ALA:CB	2.50	0.60
1:B:66:VAL:O	1:B:67:GLY:C	2.39	0.60
5:G:13:DC:N4	5:G:14:DA:N6	2.49	0.59
1:B:107:SER:H	1:B:111:ASP:CB	2.15	0.59
1:B:341:GLY:N	1:B:344:PRO:HG2	2.16	0.59
1:A:341:GLY:C	1:A:344:PRO:HD2	2.22	0.59
2:D:621:LEU:O	2:D:622:MET:C	2.41	0.59
6:H:1:DG:H1'	6:H:2:DA:C8	2.37	0.59
2:C:512:ALA:C	2:C:514:ILE:H	2.06	0.59
1:B:11:ASP:C	1:B:14:GLY:H	2.07	0.58
1:B:341:GLY:C	1:B:344:PRO:HD2	2.24	0.58
2:D:502:ILE:HA	2:D:536:TYR:O	2.02	0.58
1:A:471:LYS:O	1:A:475:ALA:CA	2.51	0.58
1:B:132:GLN:O	1:B:133:ASP:CB	2.50	0.58
2:C:508:ASP:CB	2:C:511:GLY:H	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:VAL:O	1:B:69:ILE:N	2.36	0.58
1:B:39:PRO:C	1:B:41:GLN:N	2.57	0.58
3:E:5:DA:C2	3:E:6:DG:C4	2.90	0.58
1:A:471:LYS:O	1:A:475:ALA:CB	2.51	0.58
7:F:0:NFX:CL	7:F:0:NFX:C06	2.88	0.58
1:B:46:TYR:HD2	1:B:152:PRO:HG2	1.65	0.58
2:D:512:ALA:O	2:D:513:HIS:C	2.41	0.58
1:A:23:TYR:CE1	2:C:513:HIS:HB2	2.38	0.58
1:B:81:ILE:O	1:B:84:ALA:HB3	2.04	0.58
2:C:590:GLN:O	2:C:593:GLU:N	2.28	0.58
1:B:413:GLU:O	1:B:416:ALA:N	2.37	0.58
1:B:153:THR:O	1:B:154:VAL:CB	2.51	0.58
1:B:46:TYR:CD1	1:B:46:TYR:O	2.57	0.57
1:A:101:MET:CB	1:A:121:ALA:HB2	2.34	0.57
1:A:46:TYR:HD2	1:A:152:PRO:HG2	1.61	0.57
1:A:128:GLY:O	1:A:131:LEU:N	2.36	0.57
1:B:62:SER:O	1:B:63:ALA:C	2.42	0.57
2:C:618:VAL:CG1	2:C:618:VAL:O	2.53	0.57
1:A:153:THR:O	1:A:154:VAL:CB	2.53	0.57
2:D:433:GLU:O	2:D:437:ALA:HB3	2.04	0.57
1:B:158:ALA:HA	1:B:353:ARG:NH2	2.19	0.56
1:A:6:ASN:O	1:A:7:MET:O	2.24	0.56
1:B:49:ASN:O	1:B:51:ASP:N	2.38	0.56
7:H:0:NFX:C06	7:H:0:NFX:CL	2.90	0.56
1:B:375:VAL:O	1:B:377:GLY:N	2.39	0.56
3:E:13:DA:C4	3:E:14:DA:N7	2.74	0.56
2:C:433:GLU:O	2:C:437:ALA:HB3	2.04	0.56
5:G:14:DA:H2''	5:G:15:DT:H5'	1.88	0.56
1:A:11:ASP:C	1:A:14:GLY:H	2.08	0.56
1:B:412:THR:N	1:B:415:GLN:CB	2.67	0.56
1:A:49:ASN:O	1:A:50:LYS:C	2.43	0.56
2:D:503:ILE:HG23	2:D:537:ILE:HA	1.87	0.56
1:B:128:GLY:O	1:B:131:LEU:N	2.33	0.56
2:D:512:ALA:C	2:D:514:ILE:H	2.09	0.56
6:H:10:DC:H2'	6:H:11:DG:C8	2.41	0.56
1:B:13:MET:O	1:B:17:PHE:CE1	2.59	0.56
1:B:159:PHE:O	1:B:161:ASN:N	2.39	0.56
1:A:39:PRO:C	1:A:41:GLN:N	2.57	0.56
6:H:7:DG:C5	6:H:8:DC:C4	2.94	0.56
1:B:55:PHE:O	1:B:122:ARG:NH1	2.39	0.56
5:G:14:DA:H2'	5:G:15:DT:C6	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:PRO:O	1:A:162:LEU:N	2.39	0.55
2:C:592:TRP:CA	2:C:595:THR:CB	2.74	0.55
1:B:160:PRO:O	1:B:162:LEU:N	2.39	0.55
1:A:158:ALA:HA	1:A:353:ARG:NH2	2.22	0.55
1:B:49:ASN:O	1:B:50:LYS:C	2.45	0.55
1:A:49:ASN:O	1:A:51:ASP:N	2.40	0.55
1:B:341:GLY:H	1:B:344:PRO:CG	2.19	0.55
2:D:627:GLU:N	2:D:628:PRO:CD	2.70	0.55
1:A:341:GLY:H	1:A:344:PRO:CG	2.19	0.54
1:B:82:TYR:O	1:B:85:MET:HB3	2.06	0.54
3:E:13:DA:N6	3:E:14:DA:N6	2.56	0.54
1:A:76:HIS:CD2	1:A:76:HIS:H	2.24	0.54
2:D:524:ARG:HH11	2:D:524:ARG:HB3	1.70	0.54
6:H:10:DC:C2'	6:H:11:DG:C8	2.91	0.54
3:E:12:DG:C6	3:E:13:DA:N6	2.75	0.54
1:B:6:ASN:O	1:B:7:MET:O	2.26	0.54
2:C:512:ALA:O	2:C:513:HIS:C	2.46	0.54
1:A:412:THR:N	1:A:415:GLN:CB	2.70	0.54
1:A:343:VAL:N	1:A:344:PRO:CD	2.70	0.54
5:G:6:DT:O2	6:H:15:DA:C2	2.60	0.54
1:A:13:MET:O	1:A:17:PHE:CE1	2.60	0.54
1:B:343:VAL:N	1:B:344:PRO:CD	2.71	0.54
5:G:3:DG:C4	5:G:4:DT:C5	2.95	0.54
2:D:590:GLN:O	2:D:593:GLU:N	2.30	0.54
4:F:1:DA:H2''	4:F:2:DG:O5'	2.08	0.54
4:F:5:DA:H1'	4:F:6:DT:H5''	1.90	0.54
1:B:23:TYR:CE1	2:D:513:HIS:HB2	2.42	0.53
1:A:82:TYR:O	1:A:85:MET:HB3	2.08	0.53
1:B:189:ALA:O	1:B:192:TYR:N	2.41	0.53
1:A:82:TYR:O	1:A:83:ASP:C	2.47	0.53
3:E:12:DG:H5'	3:E:12:DG:C8	2.43	0.53
1:B:434:VAL:O	1:B:435:LEU:C	2.46	0.53
1:A:72:ASN:O	1:A:73:PHE:CD1	2.61	0.53
4:F:10:DT:H2''	4:F:11:DG:H8	1.74	0.53
2:C:503:ILE:HG23	2:C:537:ILE:HA	1.90	0.53
4:F:10:DT:C2'	4:F:11:DG:C8	2.91	0.53
1:B:39:PRO:C	1:B:41:GLN:H	2.11	0.53
2:C:627:GLU:N	2:C:628:PRO:CD	2.72	0.52
6:H:1:DG:N2	6:H:2:DA:C2	2.77	0.52
1:A:62:SER:C	1:A:64:LYS:N	2.62	0.52
1:B:125:GLU:O	1:B:126:ILE:C	2.47	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:11:DG:C2'	4:F:12:DA:C8	2.91	0.52
7:H:0:NFX:C04	7:H:0:NFX:CL	2.95	0.52
1:A:85:MET:O	1:A:88:MET:N	2.41	0.52
1:B:82:TYR:O	1:B:83:ASP:C	2.48	0.52
4:F:4:DC:N3	7:H:0:NFX:H04	2.25	0.52
1:B:23:TYR:O	1:B:23:TYR:CD2	2.64	0.51
2:C:524:ARG:HB3	2:C:524:ARG:HH11	1.69	0.51
1:A:46:TYR:O	1:A:46:TYR:CD1	2.64	0.51
3:E:12:DG:H5'	3:E:12:DG:H8	1.74	0.51
1:A:159:PHE:O	1:A:161:ASN:N	2.40	0.51
4:F:7:DT:C4	4:F:8:DC:N4	2.78	0.51
1:A:375:VAL:O	1:A:377:GLY:N	2.44	0.51
1:A:125:GLU:O	1:A:126:ILE:C	2.48	0.51
2:C:620:VAL:O	2:C:621:LEU:O	2.29	0.51
1:A:75:PRO:O	1:A:76:HIS:O	2.29	0.51
2:D:611:LEU:C	2:D:613:ARG:N	2.62	0.51
1:A:391:LEU:HD23	1:A:391:LEU:C	2.31	0.51
1:A:189:ALA:O	1:A:192:TYR:N	2.43	0.51
1:A:434:VAL:O	1:A:435:LEU:C	2.49	0.51
1:A:359:ALA:CA	1:A:362:ARG:HG2	2.40	0.50
4:F:16:DT:C2	4:F:17:DG:N7	2.79	0.50
1:B:62:SER:C	1:B:64:LYS:N	2.64	0.50
1:A:41:GLN:O	1:A:42:ARG:C	2.50	0.50
2:D:623:GLY:O	2:D:624:ASP:C	2.50	0.50
1:A:72:ASN:C	1:A:73:PHE:CD1	2.85	0.50
4:F:7:DT:C4	4:F:8:DC:C4	2.99	0.50
2:D:508:ASP:CB	2:D:511:GLY:H	2.24	0.50
6:H:17:DC:H2'	6:H:18:DA:C8	2.47	0.50
2:D:417:THR:N	2:D:418:PRO:CD	2.75	0.50
2:C:506:ASP:O	2:C:507:ALA:HB2	2.12	0.50
1:A:38:LYS:O	1:A:41:GLN:N	2.30	0.50
1:B:359:ALA:CA	1:B:362:ARG:HG2	2.42	0.49
1:A:39:PRO:C	1:A:41:GLN:H	2.14	0.49
6:H:12:DT:O3'	6:H:13:DA:H8	1.94	0.49
7:F:0:NFX:C03	7:F:0:NFX:CL	2.97	0.49
4:F:1:DA:C8	7:F:0:NFX:C17	2.96	0.49
5:G:8:DA:C2	6:H:13:DA:C2	3.00	0.49
1:A:182:ASN:O	1:A:184:ALA:N	2.45	0.49
2:C:445:ARG:C	2:C:447:ARG:N	2.66	0.49
2:C:417:THR:N	2:C:418:PRO:CD	2.75	0.49
2:C:508:ASP:HB2	2:C:511:GLY:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ARG:NE	1:A:338:ARG:HA	2.27	0.49
4:F:3:DT:H2'	4:F:4:DC:O4'	2.13	0.49
1:A:81:ILE:O	1:A:84:ALA:HB3	2.13	0.49
5:G:5:DT:H2''	5:G:6:DT:H6	1.78	0.48
1:B:391:LEU:C	1:B:391:LEU:HD23	2.33	0.48
6:H:10:DC:H2'	6:H:11:DG:H8	1.78	0.48
3:E:13:DA:H2''	3:E:14:DA:H8	1.77	0.48
1:B:416:ALA:O	1:B:417:GLU:C	2.52	0.48
2:D:599:GLU:CB	2:D:602:THR:CB	2.91	0.48
2:C:599:GLU:CB	2:C:602:THR:CB	2.92	0.48
1:B:85:MET:O	1:B:88:MET:N	2.46	0.48
1:B:101:MET:HA	1:B:121:ALA:HB2	1.95	0.48
1:A:23:TYR:O	1:A:23:TYR:CD2	2.66	0.48
1:B:349:TYR:C	1:B:349:TYR:CD2	2.87	0.48
1:A:101:MET:HA	1:A:121:ALA:HB2	1.96	0.48
1:A:109:ASP:O	1:A:111:ASP:N	2.46	0.48
1:A:417:GLU:O	1:A:420:VAL:N	2.45	0.48
6:H:7:DG:C8	6:H:8:DC:C5	3.02	0.48
2:D:445:ARG:C	2:D:447:ARG:N	2.67	0.48
7:H:0:NFX:CL	7:H:0:NFX:H06	2.49	0.48
2:D:500:LYS:HA	2:D:534:HIS:O	2.14	0.48
2:D:461:ASN:O	2:D:462:THR:C	2.53	0.47
1:B:363:PHE:O	1:B:364:ASP:C	2.53	0.47
2:D:621:LEU:O	2:D:623:GLY:N	2.47	0.47
6:H:8:DC:H2''	6:H:9:DA:O5'	2.15	0.47
1:B:76:HIS:H	1:B:76:HIS:CD2	2.31	0.47
1:A:363:PHE:O	1:A:364:ASP:C	2.53	0.47
5:G:14:DA:N3	5:G:15:DT:C5	2.83	0.47
1:A:416:ALA:O	1:A:417:GLU:C	2.52	0.47
1:B:109:ASP:O	1:B:111:ASP:N	2.47	0.47
1:B:75:PRO:O	1:B:76:HIS:O	2.32	0.47
2:C:629:ARG:C	2:C:631:LYS:H	2.18	0.47
2:D:584:GLY:O	2:D:585:GLU:C	2.53	0.47
1:A:130:LEU:O	1:A:156:PRO:HD2	2.14	0.47
1:A:413:GLU:O	1:A:416:ALA:N	2.48	0.47
2:C:500:LYS:HA	2:C:534:HIS:O	2.14	0.47
2:D:506:ASP:O	2:D:507:ALA:HB2	2.15	0.47
2:D:528:PRO:O	2:D:529:LEU:C	2.52	0.47
1:B:417:GLU:O	1:B:420:VAL:N	2.46	0.47
6:H:2:DA:C4	6:H:3:DC:C5	3.03	0.47
1:A:60:ARG:O	1:A:61:LYS:O	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:TYR:CD1	1:B:46:TYR:C	2.88	0.47
2:C:524:ARG:NH1	2:C:524:ARG:CB	2.66	0.46
1:B:375:VAL:O	1:B:376:GLU:C	2.53	0.46
2:D:624:ASP:CB	2:D:628:PRO:HG2	2.45	0.46
1:B:55:PHE:O	1:B:56:ASP:C	2.54	0.46
7:F:0:NFX:CL	7:F:0:NFX:H06	2.51	0.46
2:C:508:ASP:O	2:C:511:GLY:CA	2.63	0.46
1:B:41:GLN:O	1:B:42:ARG:C	2.54	0.46
4:F:1:DA:H1'	4:F:2:DG:C8	2.51	0.46
2:C:528:PRO:O	2:C:529:LEU:C	2.52	0.46
1:A:46:TYR:C	1:A:46:TYR:CD1	2.89	0.46
6:H:16:DA:C4	6:H:17:DC:C5	3.03	0.46
2:D:608:ILE:O	2:D:609:GLU:C	2.54	0.46
2:C:507:ALA:O	2:C:508:ASP:C	2.54	0.46
3:E:5:DA:C6	3:E:6:DG:C5	3.04	0.46
3:E:13:DA:C6	3:E:14:DA:N6	2.83	0.46
3:E:13:DA:H2''	3:E:14:DA:O5'	2.16	0.46
1:A:133:ASP:O	1:A:138:THR:CB	2.64	0.46
3:E:3:DC:C2	3:E:4:DA:N7	2.84	0.45
3:E:12:DG:C6	3:E:13:DA:C6	3.04	0.45
1:B:101:MET:HA	1:B:121:ALA:CB	2.46	0.45
2:D:590:GLN:O	2:D:591:LEU:C	2.54	0.45
2:C:625:LYS:O	2:C:626:VAL:CB	2.63	0.45
2:D:527:ARG:HB3	2:D:528:PRO:HD3	1.99	0.45
2:D:508:ASP:O	2:D:511:GLY:CA	2.64	0.45
1:A:349:TYR:CD2	1:A:349:TYR:C	2.89	0.45
1:B:60:ARG:O	1:B:61:LYS:O	2.34	0.45
1:B:87:ARG:NH1	5:G:12:DG:OP1	2.49	0.45
1:A:379:ILE:O	1:A:382:ILE:N	2.50	0.45
5:G:14:DA:C4	5:G:15:DT:C5	3.04	0.45
2:C:508:ASP:CB	2:C:511:GLY:N	2.79	0.45
2:C:584:GLY:O	2:C:585:GLU:C	2.54	0.45
2:D:524:ARG:CB	2:D:524:ARG:NH1	2.67	0.45
1:A:448:MET:O	1:A:451:ALA:HB3	2.16	0.45
2:C:590:GLN:O	2:C:591:LEU:C	2.54	0.45
3:E:14:DA:H2'	3:E:15:DT:C6	2.51	0.45
1:A:72:ASN:O	1:A:73:PHE:CG	2.69	0.45
1:A:381:VAL:O	1:A:382:ILE:C	2.55	0.45
1:A:158:ALA:O	1:A:160:PRO:HD3	2.17	0.45
2:C:508:ASP:HB2	2:C:511:GLY:H	1.81	0.45
5:G:13:DC:C4	5:G:14:DA:N7	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:VAL:O	1:A:376:GLU:C	2.55	0.44
1:A:182:ASN:O	1:A:183:LEU:C	2.55	0.44
1:B:448:MET:O	1:B:451:ALA:HB3	2.17	0.44
5:G:13:DC:N3	5:G:14:DA:N7	2.64	0.44
2:C:523:TYR:HD2	2:C:524:ARG:HG2	1.82	0.44
3:E:12:DG:H2'	3:E:12:DG:H5'	1.69	0.44
2:C:417:THR:HG23	2:C:418:PRO:HD3	2.00	0.44
2:D:523:TYR:HD2	2:D:524:ARG:HG2	1.82	0.44
3:E:6:DG:H2''	3:E:7:DG:C8	2.49	0.44
1:B:412:THR:O	1:B:415:GLN:CB	2.66	0.44
1:B:349:TYR:O	1:B:349:TYR:CD2	2.69	0.44
4:F:9:DA:C5	4:F:10:DT:C4	3.06	0.44
4:F:9:DA:H2''	4:F:10:DT:C6	2.52	0.44
1:A:22:LYS:O	1:A:25:ILE:HG12	2.17	0.44
2:C:590:GLN:O	2:C:592:TRP:N	2.51	0.44
3:E:13:DA:C5	3:E:14:DA:N7	2.85	0.44
1:B:379:ILE:O	1:B:382:ILE:N	2.50	0.44
2:C:629:ARG:C	2:C:631:LYS:N	2.71	0.43
2:C:461:ASN:O	2:C:462:THR:C	2.56	0.43
1:A:101:MET:HA	1:A:121:ALA:CB	2.48	0.43
1:A:379:ILE:O	1:A:381:VAL:N	2.50	0.43
1:B:182:ASN:O	1:B:184:ALA:N	2.51	0.43
2:C:608:ILE:O	2:C:609:GLU:C	2.56	0.43
5:G:5:DT:C2	5:G:6:DT:C5	3.07	0.43
1:B:379:ILE:O	1:B:381:VAL:N	2.51	0.43
1:A:334:ASN:O	1:A:334:ASN:ND2	2.52	0.43
4:F:11:DG:H2'	4:F:12:DA:N7	2.32	0.43
1:B:38:LYS:O	1:B:41:GLN:CB	2.67	0.43
5:G:3:DG:C5	5:G:4:DT:C4	3.05	0.43
2:C:503:ILE:CG2	2:C:537:ILE:HA	2.48	0.43
1:A:178:ILE:HA	1:A:179:PRO:HD3	1.78	0.43
1:B:381:VAL:O	1:B:382:ILE:C	2.57	0.43
6:H:12:DT:O3'	6:H:13:DA:C8	2.71	0.43
1:B:128:GLY:O	1:B:130:LEU:N	2.51	0.43
2:D:592:TRP:CA	2:D:595:THR:CB	2.82	0.43
1:A:25:ILE:O	1:A:28:ARG:HB3	2.19	0.43
2:D:629:ARG:C	2:D:631:LYS:N	2.72	0.43
2:D:555:VAL:O	2:D:556:ALA:HB2	2.19	0.43
2:C:527:ARG:HB2	2:C:527:ARG:CZ	2.41	0.43
2:D:625:LYS:O	2:D:626:VAL:CB	2.66	0.43
2:D:463:ALA:HB2	2:D:524:ARG:HE	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:LEU:O	1:B:156:PRO:HD2	2.18	0.42
2:C:527:ARG:HB3	2:C:528:PRO:HD3	2.00	0.42
1:B:6:ASN:C	1:B:7:MET:O	2.58	0.42
1:A:6:ASN:C	1:A:7:MET:O	2.57	0.42
1:A:146:ASP:O	1:A:147:ASP:HB2	2.20	0.42
1:B:21:SER:O	1:B:22:LYS:C	2.58	0.42
1:B:22:LYS:O	1:B:25:ILE:HG12	2.19	0.42
1:A:403:GLU:C	1:A:405:LEU:N	2.73	0.42
6:H:1:DG:C2	6:H:2:DA:C6	3.07	0.42
6:H:3:DC:H2'	6:H:4:DT:C6	2.55	0.42
1:A:141:PHE:CE1	1:A:152:PRO:HG3	2.55	0.42
2:D:430:TYR:HA	2:D:502:ILE:HG13	2.02	0.42
2:D:445:ARG:O	2:D:447:ARG:N	2.52	0.42
1:A:125:GLU:O	1:A:128:GLY:N	2.53	0.42
2:D:461:ASN:O	2:D:463:ALA:N	2.52	0.42
1:A:417:GLU:O	1:A:418:ALA:C	2.56	0.42
6:H:12:DT:C2'	6:H:13:DA:C8	3.03	0.42
2:D:629:ARG:C	2:D:631:LYS:H	2.22	0.42
1:A:128:GLY:O	1:A:130:LEU:N	2.53	0.42
1:A:324:ASN:HA	1:A:325:TYR:HA	1.68	0.42
3:E:2:DC:N4	3:E:3:DC:N4	2.68	0.42
1:B:20:TYR:CD2	1:B:20:TYR:C	2.92	0.42
1:B:46:TYR:CE2	1:B:152:PRO:CD	3.03	0.42
1:A:20:TYR:CD2	1:A:20:TYR:C	2.94	0.42
6:H:7:DG:H2'	6:H:7:DG:O5'	2.20	0.41
1:B:402:LYS:O	1:B:403:GLU:C	2.59	0.41
7:H:0:NFX:CL	7:H:0:NFX:H04A	2.56	0.41
2:D:423:ASN:HA	2:D:424:PRO:HD3	1.84	0.41
2:C:503:ILE:O	2:C:503:ILE:HG23	2.20	0.41
1:B:114:ALA:O	1:B:115:ALA:O	2.38	0.41
1:A:222:ARG:O	1:A:223:ASP:C	2.58	0.41
1:B:407:VAL:C	1:B:409:TYR:N	2.73	0.41
3:E:5:DA:C5	3:E:6:DG:C5	3.07	0.41
3:E:8:DT:H2''	3:E:9:DC:C6	2.56	0.41
1:B:101:MET:CA	1:B:121:ALA:HB2	2.51	0.41
2:D:585:GLU:O	2:D:586:MET:CB	2.69	0.41
6:H:9:DA:C2'	6:H:10:DC:C6	3.03	0.41
1:B:82:TYR:O	1:B:85:MET:CB	2.68	0.41
5:G:14:DA:C2	5:G:15:DT:C5	3.09	0.41
2:C:523:TYR:CD2	2:C:524:ARG:N	2.89	0.41
2:D:462:THR:CG2	2:D:521:PHE:HA	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:GLU:O	1:B:414:GLU:C	2.59	0.41
1:B:139:VAL:HA	1:B:140:PRO:HD3	1.85	0.41
2:C:445:ARG:O	2:C:447:ARG:N	2.51	0.41
1:B:368:ALA:O	1:B:369:GLU:C	2.59	0.41
1:A:86:VAL:O	1:A:88:MET:N	2.53	0.41
4:F:9:DA:C2'	4:F:10:DT:C6	3.04	0.41
1:A:435:LEU:O	1:A:438:GLU:N	2.54	0.41
1:A:103:GLY:HA2	1:A:104:ASN:HA	1.66	0.41
1:A:82:TYR:O	1:A:85:MET:CB	2.69	0.40
2:C:524:ARG:HH11	2:C:524:ARG:CB	2.32	0.40
1:A:22:LYS:O	1:A:25:ILE:CG1	2.70	0.40
2:C:430:TYR:HA	2:C:502:ILE:HG13	2.03	0.40
1:B:417:GLU:O	1:B:418:ALA:C	2.60	0.40
6:H:16:DA:C5	6:H:17:DC:C4	3.10	0.40
3:E:10:DA:C5	3:E:11:DT:C4	3.09	0.40
1:A:413:GLU:O	1:A:414:GLU:C	2.59	0.40
1:A:391:LEU:O	1:A:391:LEU:HD23	2.21	0.40
1:B:182:ASN:C	1:B:184:ALA:N	2.75	0.40
1:A:368:ALA:O	1:A:369:GLU:C	2.59	0.40
5:G:14:DA:N1	5:G:15:DT:C4	2.89	0.40
2:D:523:TYR:C	2:D:525:TYR:N	2.75	0.40
2:C:461:ASN:O	2:C:463:ALA:N	2.55	0.40
1:A:38:LYS:O	1:A:39:PRO:C	2.60	0.40
1:A:160:PRO:C	1:A:162:LEU:H	2.25	0.40
1:B:439:GLU:O	1:B:443:ARG:CB	2.69	0.40
4:F:5:DA:N6	7:H:0:NFX:CL	2.92	0.40
1:A:182:ASN:C	1:A:184:ALA:N	2.73	0.40
1:A:160:PRO:HA	1:A:349:TYR:CE1	2.56	0.40
3:E:14:DA:H2'	3:E:15:DT:H6	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	414/496 (84%)	298 (72%)	72 (17%)	44 (11%)	0	11
1	B	417/496 (84%)	297 (71%)	73 (18%)	47 (11%)	0	10
2	C	182/268 (68%)	116 (64%)	40 (22%)	26 (14%)	0	6
2	D	186/268 (69%)	120 (64%)	44 (24%)	22 (12%)	0	9
All	All	1199/1528 (78%)	831 (69%)	229 (19%)	139 (12%)	0	9

All (139) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	MET
1	A	61	LYS
1	A	63	ALA
1	A	76	HIS
1	A	86	VAL
1	A	133	ASP
1	A	138	THR
1	A	194	ILE
1	A	323	ILE
1	A	396	GLU
1	A	408	SER
1	A	417	GLU
1	B	7	MET
1	B	61	LYS
1	B	63	ALA
1	B	76	HIS
1	B	86	VAL
1	B	104	ASN
1	B	133	ASP
1	B	138	THR
1	B	194	ILE
1	B	396	GLU
1	B	408	SER
1	B	417	GLU
2	C	445	ARG
2	C	462	THR
2	C	507	ALA
2	C	513	HIS
2	C	585	GLU
2	C	606	VAL
2	C	609	GLU
2	C	612	ALA
2	C	621	LEU

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Mol	Chain	Res	Type
2	C	622	MET
2	C	624	ASP
2	D	445	ARG
2	D	462	THR
2	D	507	ALA
2	D	513	HIS
2	D	585	GLU
2	D	606	VAL
2	D	609	GLU
2	D	612	ALA
1	A	40	VAL
1	A	50	LYS
1	A	67	GLY
1	A	110	GLY
1	A	115	ALA
1	A	154	VAL
1	A	157	ALA
1	A	375	VAL
1	A	376	GLU
1	A	404	ASN
1	A	423	GLN
1	B	40	VAL
1	B	50	LYS
1	B	56	ASP
1	B	67	GLY
1	B	110	GLY
1	B	115	ALA
1	B	154	VAL
1	B	375	VAL
1	B	376	GLU
1	B	404	ASN
1	B	423	GLN
1	B	434	VAL
2	C	446	ASP
2	C	463	ALA
2	C	485	ALA
2	C	512	ALA
2	C	610	ASP
2	D	446	ASP
2	D	485	ALA
2	D	512	ALA
2	D	610	ASP

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Mol	Chain	Res	Type
2	D	624	ASP
1	A	85	MET
1	A	129	TYR
1	A	161	ASN
1	A	183	LEU
1	A	197	PRO
1	A	380	ARG
1	A	413	GLU
1	A	434	VAL
1	B	129	TYR
1	B	157	ALA
1	B	161	ASN
1	B	197	PRO
1	B	380	ARG
1	B	413	GLU
2	C	422	LYS
2	C	483	ILE
2	C	508	ASP
2	D	422	LYS
2	D	447	ARG
2	D	463	ALA
2	D	483	ILE
2	D	508	ASP
1	A	49	ASN
1	A	71	GLY
1	A	126	ILE
1	A	347	SER
1	A	430	THR
1	B	49	ASN
1	B	54	THR
1	B	71	GLY
1	B	73	PHE
1	B	85	MET
1	B	183	LEU
1	B	407	VAL
1	B	430	THR
2	C	447	ARG
2	D	548	GLY
1	A	66	VAL
1	A	83	ASP
1	A	407	VAL
1	B	66	VAL

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Mol	Chain	Res	Type
1	B	126	ILE
1	B	347	SER
1	B	363	PHE
1	B	379	ILE
2	C	464	LYS
2	C	524	ARG
2	C	548	GLY
2	C	598	PRO
2	D	598	PRO
1	A	73	PHE
1	A	379	ILE
1	B	83	ASP
2	C	434	GLY
1	B	160	PRO
2	C	633	ILE
2	D	633	ILE
2	D	434	GLY
1	A	103	GLY
1	A	160	PRO
1	A	330	VAL
1	B	236	VAL
1	B	330	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	68/431 (16%)	63 (93%)	5 (7%)	17	56
1	B	63/431 (15%)	57 (90%)	6 (10%)	11	45
2	C	23/224 (10%)	20 (87%)	3 (13%)	5	31
2	D	21/224 (9%)	18 (86%)	3 (14%)	4	28
All	All	175/1310 (13%)	158 (90%)	17 (10%)	10	43

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	TYR
1	A	49	ASN
1	A	143	TRP
1	A	334	ASN
1	A	353	ARG
1	B	46	TYR
1	B	49	ASN
1	B	72	ASN
1	B	143	TRP
1	B	334	ASN
1	B	353	ARG
2	C	503	ILE
2	C	524	ARG
2	C	527	ARG
2	D	503	ILE
2	D	524	ARG
2	D	527	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	72	ASN
1	A	74	HIS
1	A	334	ASN
1	A	423	GLN
1	B	49	ASN
1	B	72	ASN
1	B	74	HIS
1	B	334	ASN
1	B	423	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	NFX	F	0	-	21,28,28	6.12	14 (66%)	22,43,43	2.68	3 (13%)
7	NFX	H	0	-	21,28,28	5.21	14 (66%)	22,43,43	2.69	3 (13%)

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	NFX	F	0	-	-	0/4/23/23	0/3/4/4
7	NFX	H	0	-	-	0/4/23/23	0/3/4/4

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	0	NFX	C14-C12	-10.80	1.33	1.41
7	H	0	NFX	C14-C12	-8.36	1.35	1.41
7	F	0	NFX	C02-C01	-4.73	1.44	1.53
7	H	0	NFX	C02-C01	-3.78	1.46	1.53
7	F	0	NFX	C01-N05	-3.38	1.37	1.47
7	H	0	NFX	C01-N05	-3.23	1.38	1.47
7	H	0	NFX	C03-C01	-3.02	1.47	1.52
7	H	0	NFX	C04-N01	-2.96	1.42	1.47
7	F	0	NFX	C03-C01	-2.76	1.47	1.52
7	F	0	NFX	C04-N01	-2.49	1.43	1.47
7	H	0	NFX	C16-C18	-2.15	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	0	NFX	C11-N01	2.48	1.48	1.40
7	F	0	NFX	C09-C06	2.52	1.53	1.48
7	H	0	NFX	C08-C06	2.56	1.53	1.48
7	H	0	NFX	C09-C06	2.56	1.53	1.48
7	F	0	NFX	C08-C06	2.59	1.53	1.48
7	H	0	NFX	C11-N01	2.67	1.48	1.40
7	F	0	NFX	C17-C15	3.42	1.39	1.35
7	H	0	NFX	C19-C14	7.87	1.52	1.41
7	H	0	NFX	C17-C14	8.18	1.57	1.41
7	H	0	NFX	C13-C12	8.78	1.59	1.43
7	F	0	NFX	C17-C14	8.89	1.59	1.41
7	H	0	NFX	C11-C15	9.54	1.55	1.39
7	F	0	NFX	C11-C15	9.81	1.56	1.39
7	F	0	NFX	C19-C14	9.82	1.55	1.41
7	F	0	NFX	C13-C12	10.49	1.62	1.43
7	H	0	NFX	C16-N	11.45	1.52	1.35
7	F	0	NFX	C16-N	14.24	1.56	1.35

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
7	F	0	NFX	C02-C01-C03	-11.20	85.52	102.03
7	H	0	NFX	C02-C01-C03	-11.16	85.58	102.03
7	F	0	NFX	C17-C15-C11	-2.35	119.97	123.29
7	F	0	NFX	C02-C04-N01	-2.34	100.30	103.35
7	H	0	NFX	C17-C15-C11	-2.01	120.45	123.29
7	H	0	NFX	C01-C03-N01	3.28	108.60	102.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	0	NFX	5	0
7	H	0	NFX	6	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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	432/496 (87%)	-1.10	0 100 100	66, 174, 275, 370	0
1	B	433/496 (87%)	-1.11	0 100 100	72, 173, 275, 372	0
2	C	196/268 (73%)	-0.98	0 100 100	97, 176, 290, 370	0
2	D	198/268 (73%)	-0.99	0 100 100	97, 178, 292, 371	0
3	E	15/15 (100%)	-0.70	0 100 100	132, 294, 394, 554	0
4	F	19/19 (100%)	-0.39	1 (5%) 30 22	145, 231, 588, 600	0
5	G	15/15 (100%)	-0.66	0 100 100	119, 277, 378, 526	0
6	H	19/19 (100%)	-0.55	1 (5%) 30 22	148, 229, 556, 566	0
All	All	1327/1596 (83%)	-1.04	2 (0%) 95 94	66, 177, 302, 600	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	19	DT	4.4
6	H	19	DG	2.3

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
7	NFX	F	0	25/25	0.85	0.24	2.05	372,383,454,472	0
7	NFX	H	0	25/25	0.90	0.16	0.16	250,266,316,356	0

6.5 Other polymers [i](#)

There are no such residues in this entry.