Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:31 PM GMT

PDB ID	:	4TM4
Title	:	Kutzneria sp. 744 ornithine N-hydroxylase, KtzI-FADox-red-NADP+-Br
Authors	:	Setser, J.W.; Drennan, C.L.
Deposited on	:	2014-05-30
Resolution	:	2.63 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

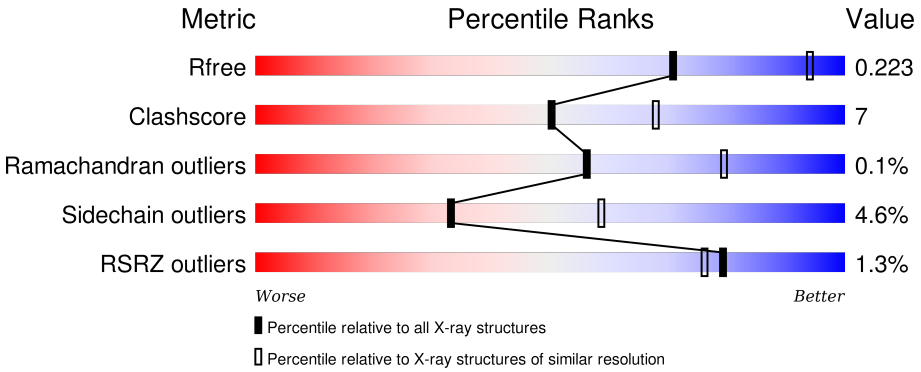
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.63 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	3377 (2.68-2.60)
Clashscore	102246	3781 (2.68-2.60)
Ramachandran outliers	100387	3722 (2.68-2.60)
Sidechain outliers	100360	3722 (2.68-2.60)
RSRZ outliers	91569	3388 (2.68-2.60)

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 <=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	443	77% 15% • 7%
1	B	443	78% 15% • 6%
1	C	443	79% 12% • 7%
1	D	443	80% 13% • 7%

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
4	BR	A	506	-	-	X	-
4	BR	D	509	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13418 atoms, of which 0 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 KtzI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3189	2007	568	604	10			
1	B	415	Total	C	N	O	S	0	0	0
			3193	2009	569	605	10			
1	C	414	Total	C	N	O	S	0	0	0
			3153	1987	558	598	10			
1	D	414	Total	C	N	O	S	0	0	0
			3190	2007	573	600	10			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP A8CF85
A	-17	GLY	-	expression tag	UNP A8CF85
A	-16	SER	-	expression tag	UNP A8CF85
A	-15	SER	-	expression tag	UNP A8CF85
A	-14	HIS	-	expression tag	UNP A8CF85
A	-13	HIS	-	expression tag	UNP A8CF85
A	-12	HIS	-	expression tag	UNP A8CF85
A	-11	HIS	-	expression tag	UNP A8CF85
A	-10	HIS	-	expression tag	UNP A8CF85
A	-9	HIS	-	expression tag	UNP A8CF85
A	-8	SER	-	expression tag	UNP A8CF85
A	-7	SER	-	expression tag	UNP A8CF85
A	-6	GLY	-	expression tag	UNP A8CF85
A	-5	LEU	-	expression tag	UNP A8CF85
A	-4	VAL	-	expression tag	UNP A8CF85
A	-3	PRO	-	expression tag	UNP A8CF85
A	-2	ARG	-	expression tag	UNP A8CF85
A	-1	GLY	-	expression tag	UNP A8CF85
A	0	SER	-	expression tag	UNP A8CF85
A	1	HIS	-	expression tag	UNP A8CF85
A	2	MET	-	expression tag	UNP A8CF85

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	MET	-	initiating methionine	UNP A8CF85
B	-17	GLY	-	expression tag	UNP A8CF85
B	-16	SER	-	expression tag	UNP A8CF85
B	-15	SER	-	expression tag	UNP A8CF85
B	-14	HIS	-	expression tag	UNP A8CF85
B	-13	HIS	-	expression tag	UNP A8CF85
B	-12	HIS	-	expression tag	UNP A8CF85
B	-11	HIS	-	expression tag	UNP A8CF85
B	-10	HIS	-	expression tag	UNP A8CF85
B	-9	HIS	-	expression tag	UNP A8CF85
B	-8	SER	-	expression tag	UNP A8CF85
B	-7	SER	-	expression tag	UNP A8CF85
B	-6	GLY	-	expression tag	UNP A8CF85
B	-5	LEU	-	expression tag	UNP A8CF85
B	-4	VAL	-	expression tag	UNP A8CF85
B	-3	PRO	-	expression tag	UNP A8CF85
B	-2	ARG	-	expression tag	UNP A8CF85
B	-1	GLY	-	expression tag	UNP A8CF85
B	0	SER	-	expression tag	UNP A8CF85
B	1	HIS	-	expression tag	UNP A8CF85
B	2	MET	-	expression tag	UNP A8CF85
C	-18	MET	-	initiating methionine	UNP A8CF85
C	-17	GLY	-	expression tag	UNP A8CF85
C	-16	SER	-	expression tag	UNP A8CF85
C	-15	SER	-	expression tag	UNP A8CF85
C	-14	HIS	-	expression tag	UNP A8CF85
C	-13	HIS	-	expression tag	UNP A8CF85
C	-12	HIS	-	expression tag	UNP A8CF85
C	-11	HIS	-	expression tag	UNP A8CF85
C	-10	HIS	-	expression tag	UNP A8CF85
C	-9	HIS	-	expression tag	UNP A8CF85
C	-8	SER	-	expression tag	UNP A8CF85
C	-7	SER	-	expression tag	UNP A8CF85
C	-6	GLY	-	expression tag	UNP A8CF85
C	-5	LEU	-	expression tag	UNP A8CF85
C	-4	VAL	-	expression tag	UNP A8CF85
C	-3	PRO	-	expression tag	UNP A8CF85
C	-2	ARG	-	expression tag	UNP A8CF85
C	-1	GLY	-	expression tag	UNP A8CF85
C	0	SER	-	expression tag	UNP A8CF85
C	1	HIS	-	expression tag	UNP A8CF85
C	2	MET	-	expression tag	UNP A8CF85

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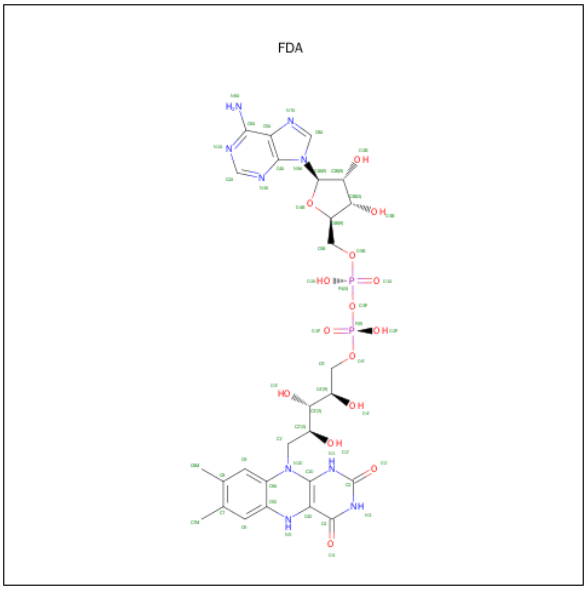
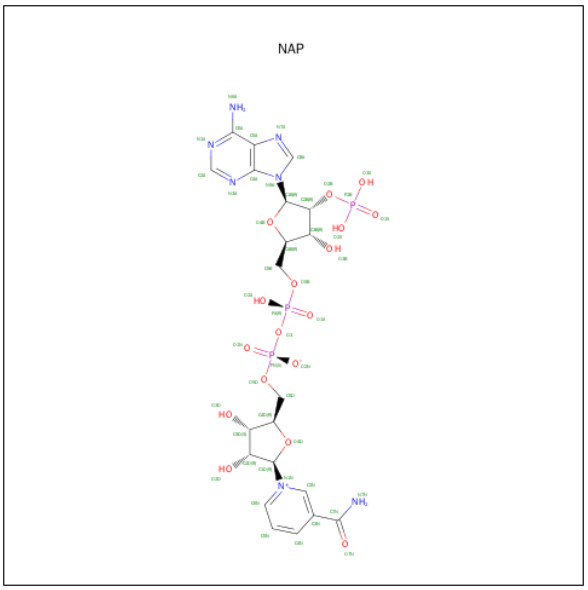
Chain	Residue	Modelled	Actual	Comment	Reference
D	-18	MET	-	initiating methionine	UNP A8CF85
D	-17	GLY	-	expression tag	UNP A8CF85
D	-16	SER	-	expression tag	UNP A8CF85
D	-15	SER	-	expression tag	UNP A8CF85
D	-14	HIS	-	expression tag	UNP A8CF85
D	-13	HIS	-	expression tag	UNP A8CF85
D	-12	HIS	-	expression tag	UNP A8CF85
D	-11	HIS	-	expression tag	UNP A8CF85
D	-10	HIS	-	expression tag	UNP A8CF85
D	-9	HIS	-	expression tag	UNP A8CF85
D	-8	SER	-	expression tag	UNP A8CF85
D	-7	SER	-	expression tag	UNP A8CF85
D	-6	GLY	-	expression tag	UNP A8CF85
D	-5	LEU	-	expression tag	UNP A8CF85
D	-4	VAL	-	expression tag	UNP A8CF85
D	-3	PRO	-	expression tag	UNP A8CF85
D	-2	ARG	-	expression tag	UNP A8CF85
D	-1	GLY	-	expression tag	UNP A8CF85
D	0	SER	-	expression tag	UNP A8CF85
D	1	HIS	-	expression tag	UNP A8CF85
D	2	MET	-	expression tag	UNP A8CF85

- Molecule 2 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (three-letter code: FDA) (formula: $C_{27}H_{35}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	6	Total	Br	0	0
			6	6		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	10	Total Br 10 10	0	0
4	D	7	Total Br 7 7	0	0
4	C	8	Total Br 8 8	0	0

- Molecule 5 is water.

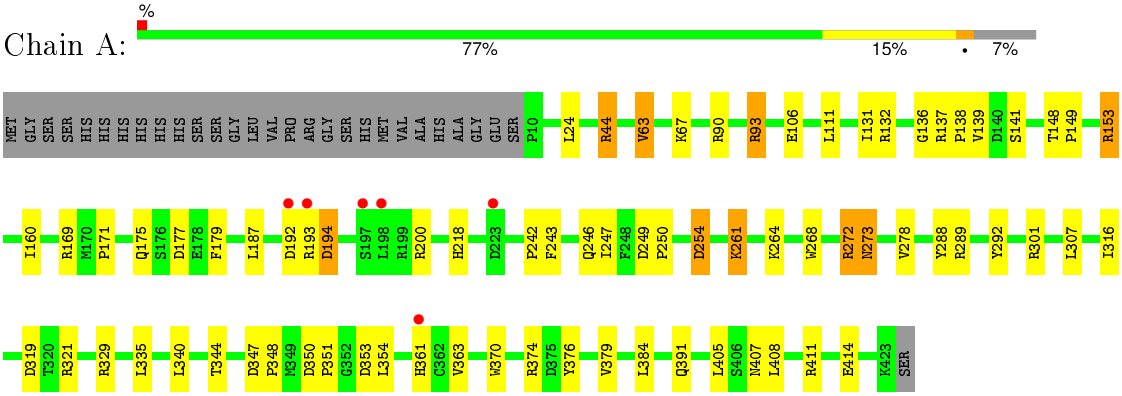
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	68	Total O 68 68	0	0
5	B	68	Total O 68 68	0	0
5	C	59	Total O 59 59	0	0
5	D	63	Total O 63 63	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

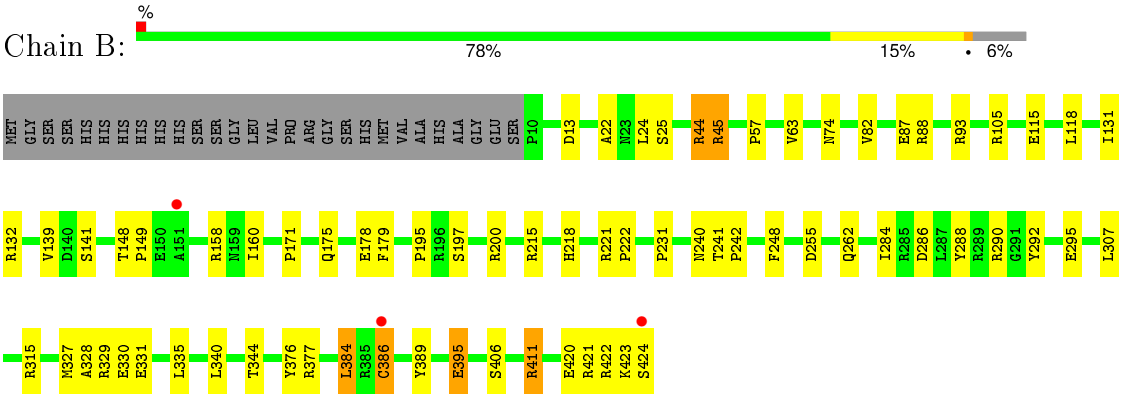
- Molecule 1: KtzI

Chain A:



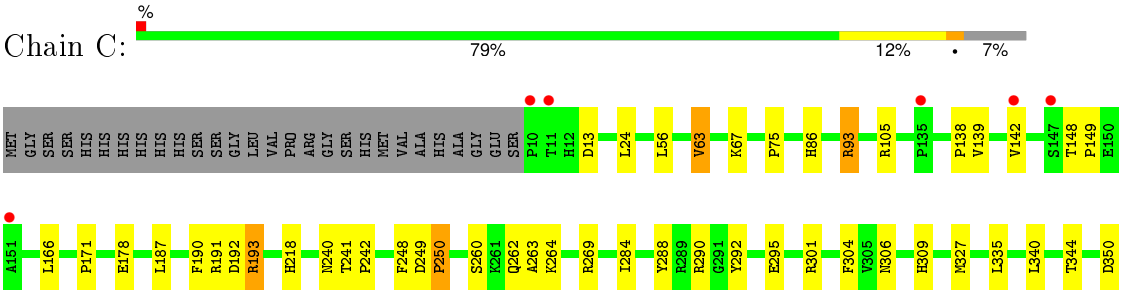
- Molecule 1: KtzI

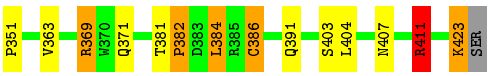
Chain B:



- Molecule 1: KtzI

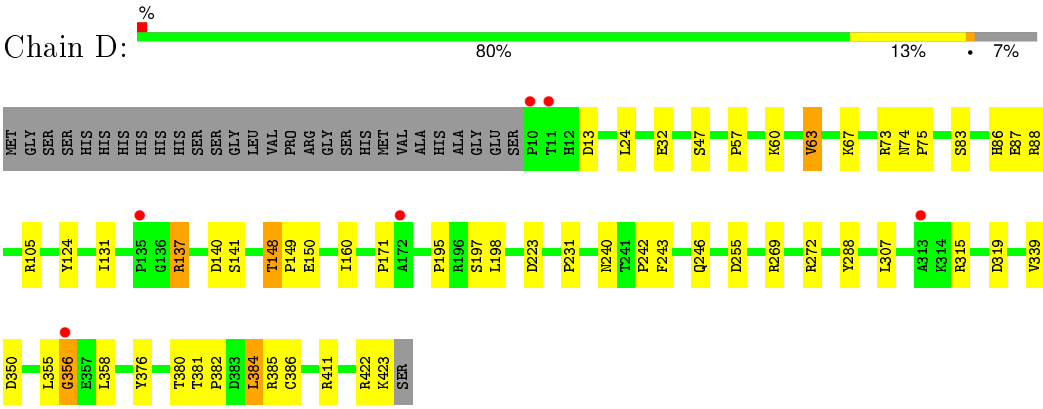
Chain C:





• Molecule 1: KtzI

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	82.39Å 151.96Å 163.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.12 – 2.63 48.38 – 2.63	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.12-2.63) 98.9 (48.38-2.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.193 , 0.223 0.201 , 0.223	Depositor DCC
R_{free} test set	3067 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	43.2	Xtriage
Anisotropy	0.781	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 31.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 61004 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13418	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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, 0.375 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: FDA, NAP, BR

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	0.76	0/3268	0.68	3/4455 (0.1%)
1	B	0.75	1/3271 (0.0%)	0.67	3/4459 (0.1%)
1	C	0.83	5/3231 (0.2%)	0.74	4/4410 (0.1%)
1	D	0.80	3/3269 (0.1%)	0.75	6/4456 (0.1%)
All	All	0.78	9/13039 (0.1%)	0.71	16/17780 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	411	ARG	CZ-NH1	-5.58	1.25	1.33
1	C	411	ARG	CZ-NH1	-5.42	1.26	1.33
1	C	250	PRO	N-CD	5.25	1.55	1.47
1	C	382	PRO	N-CD	5.24	1.55	1.47
1	D	149	PRO	N-CD	5.21	1.55	1.47
1	D	195	PRO	N-CD	5.21	1.55	1.47
1	C	351	PRO	N-CD	5.12	1.55	1.47
1	D	382	PRO	N-CD	5.11	1.54	1.47
1	C	386	CYS	CB-SG	-5.09	1.73	1.81

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	138	PRO	CB-CA-C	-5.98	97.06	112.00
1	A	254	ASP	CB-CG-OD1	5.93	123.64	118.30
1	B	221	ARG	C-N-CD	5.92	140.82	128.40
1	D	350	ASP	C-N-CD	5.77	140.51	128.40
1	D	356	GLY	N-CA-C	5.74	127.44	113.10
1	B	74	ASN	C-N-CD	5.66	140.29	128.40
1	D	148	THR	C-N-CD	5.64	140.24	128.40
1	D	381	THR	C-N-CD	5.56	140.08	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	350	ASP	C-N-CD	5.51	139.97	128.40
1	D	74	ASN	C-N-CD	5.50	139.94	128.40
1	A	350	ASP	C-N-CD	5.35	139.64	128.40
1	B	255	ASP	CB-CG-OD1	5.29	123.06	118.30
1	C	381	THR	C-N-CD	5.26	139.45	128.40
1	C	249	ASP	C-N-CD	5.18	139.28	128.40
1	A	353	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	D	99	ASP	CB-CG-OD1	5.04	122.84	118.30

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	3189	0	3015	53	0
1	B	3193	0	3016	51	0
1	C	3153	0	2953	46	0
1	D	3190	0	3020	47	0
2	A	53	0	29	4	0
2	B	53	0	30	3	0
2	C	53	0	30	0	0
2	D	53	0	30	0	0
3	A	48	0	25	0	0
3	B	48	0	25	1	0
3	C	48	0	25	0	0
3	D	48	0	25	0	0
4	A	10	0	0	4	0
4	B	6	0	0	1	0
4	C	8	0	0	0	0
4	D	7	0	0	4	0
5	A	68	0	0	2	0
5	B	68	0	0	2	0
5	C	59	0	0	3	0
5	D	63	0	0	3	0
All	All	13418	0	12223	177	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 7.

All (177) 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:63:VAL:HG22	1:A:67:LYS:HD2	1.48	0.93
1:D:137:ARG:HH11	1:D:137:ARG:HG2	1.36	0.91
1:D:380:THR:HG21	1:D:384:LEU:HD12	1.55	0.87
1:A:193:ARG:HH11	1:A:193:ARG:HG2	1.38	0.86
1:C:139:VAL:HB	1:C:384:LEU:HD23	1.54	0.86
1:A:414:GLU:OE1	4:A:506:BR:BR	2.50	0.85
1:C:139:VAL:HB	1:C:384:LEU:CD2	2.06	0.84
1:B:218:HIS:CE1	1:B:290:ARG:HG2	2.21	0.75
1:D:380:THR:CG2	1:D:384:LEU:HD12	2.16	0.75
1:A:194:ASP:OD2	1:A:194:ASP:N	2.18	0.73
1:C:93:ARG:NH2	5:C:648:HOH:O	2.21	0.73
1:A:169:ARG:NH1	1:A:344:THR:O	2.23	0.71
1:A:44:ARG:HG2	2:A:501:FDA:C4A	2.21	0.70
1:B:132:ARG:CB	1:B:132:ARG:HH11	2.04	0.70
1:A:192:ASP:OD1	1:A:193:ARG:NH1	2.24	0.70
1:B:240:ASN:ND2	5:B:663:HOH:O	2.25	0.69
1:D:13:ASP:OD1	1:D:423:LYS:HE2	1.92	0.69
1:B:179:PHE:CD2	1:B:315:ARG:HD3	2.28	0.69
1:D:240:ASN:ND2	5:D:658:HOH:O	2.27	0.67
1:D:380:THR:HG21	1:D:384:LEU:CD1	2.24	0.67
1:B:377:ARG:NH2	1:B:422:ARG:CZ	2.58	0.67
1:D:198:LEU:CD2	1:D:339:VAL:HG23	2.26	0.66
1:C:218:HIS:CD2	1:C:301:ARG:NH1	2.63	0.66
1:A:90:ARG:NH2	1:A:106:GLU:OE2	2.28	0.66
1:B:148:THR:HB	1:B:149:PRO:HD2	1.78	0.66
1:A:273:ASN:HB2	5:A:665:HOH:O	1.95	0.66
1:B:141:SER:HA	1:B:386:CYS:SG	2.36	0.65
1:B:13:ASP:OD1	1:B:423:LYS:NZ	2.29	0.65
1:A:63:VAL:CG2	1:A:67:LYS:HD2	2.25	0.65
1:A:93:ARG:HD2	1:C:292:TYR:HD2	1.61	0.64
1:D:198:LEU:HD22	1:D:339:VAL:CG2	2.27	0.64
1:A:148:THR:HB	1:A:149:PRO:HD2	1.78	0.64
1:A:261:LYS:HE3	1:A:264:LYS:HD2	1.79	0.64
1:B:377:ARG:HH21	1:B:422:ARG:NH2	1.96	0.64
1:B:423:LYS:O	1:B:424:SER:CB	2.46	0.63
1:D:148:THR:OG1	1:D:150:GLU:HG2	1.98	0.63
1:A:218:HIS:CD2	1:A:301:ARG:NH2	2.67	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:THR:HB	1:C:149:PRO:HD2	1.79	0.62
1:B:132:ARG:HB2	1:B:132:ARG:NH1	2.14	0.62
1:A:44:ARG:HD2	2:A:501:FDA:O2B	1.99	0.62
1:A:193:ARG:NH1	1:A:193:ARG:HG2	2.09	0.61
1:B:295:GLU:OE2	1:D:93:ARG:NH1	2.34	0.60
1:B:377:ARG:NH2	1:B:422:ARG:NH2	2.50	0.60
1:D:198:LEU:CD2	1:D:339:VAL:CG2	2.79	0.60
1:C:86:HIS:CG	1:D:75:PRO:HG3	2.37	0.60
1:D:307:LEU:HD12	4:D:508:BR:BR	2.57	0.59
1:D:63:VAL:HG13	1:D:67:LYS:HB2	1.85	0.58
1:A:44:ARG:HG2	2:A:501:FDA:N3A	2.19	0.57
1:A:200:ARG:NH1	1:A:319:ASP:OD1	2.20	0.57
1:A:405:LEU:HD22	1:A:408:LEU:HD11	1.85	0.57
1:D:32:GLU:OE1	1:D:73:ARG:NH2	2.37	0.57
1:B:132:ARG:HB2	1:B:132:ARG:HH11	1.66	0.56
1:D:198:LEU:HD22	1:D:339:VAL:HG23	1.85	0.56
1:B:44:ARG:HD2	2:B:501:FDA:C4A	2.36	0.56
1:C:63:VAL:HG22	1:C:67:LYS:CD	2.36	0.56
1:D:137:ARG:NH1	1:D:137:ARG:HG2	2.11	0.56
1:C:178:GLU:O	1:C:193:ARG:NH1	2.36	0.55
1:B:329:ARG:O	1:B:330:GLU:HB2	2.07	0.54
1:A:131:ILE:HD13	1:A:160:ILE:HD13	1.90	0.54
1:B:242:PRO:HB2	1:C:288:TYR:CD1	2.43	0.54
1:C:363:VAL:O	1:C:371:GLN:HG3	2.08	0.54
1:A:93:ARG:HD2	1:C:292:TYR:CD2	2.42	0.54
1:C:63:VAL:HG22	1:C:67:LYS:HD3	1.91	0.53
1:B:131:ILE:HD13	1:B:160:ILE:HD13	1.90	0.53
1:A:249:ASP:OD2	1:A:250:PRO:HD2	2.09	0.53
1:A:351:PRO:HG2	1:A:370:TRP:CD1	2.43	0.53
1:D:243:PHE:O	1:D:246:GLN:HB2	2.09	0.53
1:B:376:TYR:CE1	1:B:411:ARG:HG3	2.44	0.53
1:D:137:ARG:HH11	1:D:137:ARG:CG	2.13	0.52
1:B:139:VAL:HB	1:B:384:LEU:HD23	1.91	0.52
1:A:179:PHE:HD2	4:A:510:BR:BR	2.47	0.52
1:A:292:TYR:HD2	1:C:93:ARG:HD2	1.75	0.52
1:C:139:VAL:HB	1:C:384:LEU:HD21	1.90	0.51
1:A:363:VAL:HG21	1:A:379:VAL:HG12	1.93	0.51
1:B:44:ARG:HG2	1:B:45:ARG:N	2.25	0.51
1:D:60:LYS:NZ	5:D:641:HOH:O	2.25	0.51
1:B:288:TYR:CG	1:C:242:PRO:HB2	2.46	0.51
1:B:44:ARG:HG2	1:B:45:ARG:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:TYR:CD1	1:C:242:PRO:HB2	2.46	0.50
1:B:292:TYR:HD2	1:D:93:ARG:HG2	1.75	0.50
1:A:171:PRO:HG3	1:A:344:THR:HG21	1.92	0.50
1:C:240:ASN:ND2	5:C:656:HOH:O	2.36	0.50
1:D:231:PRO:O	1:D:307:LEU:HA	2.12	0.50
1:A:132:ARG:NH1	1:A:132:ARG:HB2	2.27	0.50
1:A:273:ASN:O	1:A:278:VAL:HG21	2.12	0.49
1:D:197:SER:O	1:D:198:LEU:HG	2.13	0.49
1:D:57:PRO:HB2	4:D:506:BR:BR	2.68	0.49
1:D:63:VAL:HG22	1:D:67:LYS:HD2	1.95	0.49
1:A:243:PHE:O	1:A:246:GLN:HB2	2.12	0.49
1:C:190:PHE:O	1:C:191:ARG:C	2.50	0.49
1:D:140:ASP:C	1:D:386:CYS:SG	2.91	0.48
1:C:56:LEU:HD23	1:C:187:LEU:HD11	1.94	0.48
1:A:391:GLN:HB3	1:A:411:ARG:HH21	1.77	0.48
1:D:315:ARG:HD2	1:D:319:ASP:O	2.13	0.48
1:C:218:HIS:CE1	1:C:290:ARG:HB3	2.49	0.48
1:D:422:ARG:HG2	1:D:422:ARG:HH11	1.79	0.48
1:D:355:LEU:O	1:D:358:LEU:N	2.47	0.48
1:D:243:PHE:HB2	5:D:601:HOH:O	2.14	0.47
1:B:22:ALA:O	1:B:25:SER:HB3	2.13	0.47
1:C:193:ARG:HG2	1:C:193:ARG:HH21	1.80	0.47
1:B:376:TYR:CZ	1:B:411:ARG:HG3	2.49	0.47
1:A:307:LEU:HD12	4:D:509:BR:BR	2.70	0.47
1:D:131:ILE:HD13	1:D:160:ILE:HD13	1.96	0.47
1:A:218:HIS:CD2	1:A:301:ARG:HH21	2.31	0.47
1:A:242:PRO:HB2	1:D:288:TYR:CG	2.50	0.47
1:C:75:PRO:HD3	1:D:86:HIS:CD2	2.50	0.47
1:C:391:GLN:HB3	1:C:411:ARG:NH1	2.29	0.47
1:B:132:ARG:CB	1:B:132:ARG:NH1	2.73	0.47
1:B:171:PRO:HG3	1:B:344:THR:HG21	1.96	0.47
1:D:223:ASP:OD2	1:D:223:ASP:N	2.48	0.46
1:B:384:LEU:HD22	1:B:386:CYS:H	1.80	0.46
1:B:179:PHE:HD2	1:B:315:ARG:HD3	1.80	0.46
1:C:193:ARG:CG	1:C:193:ARG:HH21	2.29	0.46
1:B:82:VAL:HG23	5:B:602:HOH:O	2.16	0.46
1:B:328:ALA:HA	1:C:263:ALA:HB2	1.98	0.46
1:A:44:ARG:CG	2:A:501:FDA:N3A	2.79	0.46
1:A:153:ARG:NH2	4:A:508:BR:BR	2.94	0.46
1:A:407:ASN:ND2	4:A:506:BR:BR	3.04	0.45
1:B:377:ARG:NH2	1:B:422:ARG:NH1	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:THR:HB	1:C:284:ILE:HG21	1.98	0.45
1:D:83:SER:O	1:D:87:GLU:HG3	2.16	0.45
1:C:304:PHE:HB3	1:C:306:ASN:ND2	2.31	0.45
1:D:198:LEU:HD22	1:D:339:VAL:HG21	1.97	0.45
1:A:316:ILE:HD12	1:A:321:ARG:HD2	1.97	0.45
1:D:137:ARG:NH1	1:D:137:ARG:CG	2.73	0.45
1:A:93:ARG:NE	1:C:295:GLU:OE2	2.41	0.45
1:D:171:PRO:HG3	1:D:344:THR:HG21	1.99	0.45
1:A:361:HIS:CB	1:A:384:LEU:HG	2.47	0.45
1:C:260:SER:O	1:C:264:LYS:HG3	2.18	0.44
1:B:231:PRO:O	1:B:307:LEU:HA	2.18	0.44
1:B:377:ARG:HD3	1:B:389:TYR:CZ	2.52	0.44
1:B:178:GLU:HG2	1:B:179:PHE:CE1	2.53	0.44
1:C:63:VAL:HG22	1:C:67:LYS:HD2	1.99	0.44
1:B:262:GLN:NE2	1:C:327:MET:HG2	2.33	0.44
1:C:171:PRO:HG3	1:C:344:THR:HG21	1.98	0.44
1:B:242:PRO:HB2	1:C:288:TYR:CG	2.53	0.43
1:D:141:SER:N	1:D:386:CYS:SG	2.91	0.43
1:A:139:VAL:CG1	1:A:141:SER:O	2.66	0.43
1:D:376:TYR:CZ	1:D:411:ARG:HG3	2.53	0.43
1:C:369:ARG:HB2	1:C:369:ARG:HE	1.65	0.43
1:C:13:ASP:OD1	1:C:423:LYS:NZ	2.49	0.43
1:B:44:ARG:HD3	2:B:501:FDA:O2B	2.19	0.43
1:B:215:ARG:HD2	1:B:286:ASP:OD2	2.19	0.43
1:C:250:PRO:HG3	1:C:407:ASN:OD1	2.18	0.43
1:A:137:ARG:HA	1:A:138:PRO:C	2.39	0.42
1:D:47:SER:HA	1:D:124:TYR:CD1	2.54	0.42
1:A:193:ARG:NH1	1:A:193:ARG:CG	2.73	0.42
1:B:195:PRO:C	1:B:197:SER:H	2.23	0.42
1:A:169:ARG:NH2	5:A:627:HOH:O	2.53	0.42
1:A:90:ARG:HD2	1:C:295:GLU:HG2	2.01	0.42
1:D:141:SER:CA	1:D:386:CYS:SG	3.08	0.42
1:C:187:LEU:HA	1:C:187:LEU:HD23	1.79	0.42
1:B:284:ILE:HG21	1:C:241:THR:HB	2.02	0.42
1:A:288:TYR:CD1	1:D:242:PRO:HB2	2.55	0.42
2:B:501:FDA:HM73	3:B:502:NAP:C5N	2.50	0.42
1:A:254:ASP:OD1	1:A:374:ARG:NH2	2.51	0.42
1:A:218:HIS:CG	1:A:301:ARG:NH2	2.88	0.41
1:A:268:TRP:O	1:A:272:ARG:HB3	2.19	0.41
1:C:142:VAL:HG13	1:C:386:CYS:SG	2.60	0.41
1:A:347:ASP:HA	1:A:348:PRO:HD3	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:ARG:NH1	5:C:618:HOH:O	2.53	0.41
1:B:248:PHE:HB3	1:B:406:SER:HB2	2.02	0.41
1:B:115:GLU:O	1:B:118:LEU:HB2	2.20	0.41
1:A:376:TYR:CE2	1:A:411:ARG:HD2	2.54	0.41
1:D:255:ASP:HB3	4:D:509:BR:BR	2.75	0.41
1:D:422:ARG:HG2	1:D:422:ARG:NH1	2.36	0.41
1:A:24:LEU:HD23	1:A:111:LEU:HD22	2.03	0.41
1:D:198:LEU:CD2	1:D:339:VAL:HG21	2.49	0.40
1:B:292:TYR:CD2	1:D:93:ARG:HG2	2.55	0.40
1:B:395:GLU:HG2	1:B:395:GLU:H	1.54	0.40
1:A:187:LEU:HA	1:A:187:LEU:HD23	1.75	0.40
1:B:158:ARG:O	1:B:386:CYS:SG	2.77	0.40
1:C:166:LEU:HD21	1:C:403:SER:HB2	2.02	0.40
1:B:57:PRO:HB2	4:B:504:BR:BR	2.77	0.40
1:C:248:PHE:CE1	1:C:404:LEU:HD12	2.57	0.40
1:C:63:VAL:CG2	1:C:67:LYS:HD3	2.52	0.40
1:B:327:MET:HG2	1:C:262:GLN:NE2	2.36	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	412/443 (93%)	391 (95%)	20 (5%)	1 (0%)	52 76
1	B	413/443 (93%)	396 (96%)	17 (4%)	0	100 100
1	C	412/443 (93%)	389 (94%)	23 (6%)	0	100 100
1	D	412/443 (93%)	390 (95%)	21 (5%)	1 (0%)	52 76
All	All	1649/1772 (93%)	1566 (95%)	81 (5%)	2 (0%)	56 79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	GLY
1	D	356	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	332/372 (89%)	316 (95%)	16 (5%)	31	56
1	B	331/372 (89%)	312 (94%)	19 (6%)	25	47
1	C	323/372 (87%)	308 (95%)	15 (5%)	33	59
1	D	331/372 (89%)	321 (97%)	10 (3%)	48	75
All	All	1317/1488 (88%)	1257 (95%)	60 (5%)	33	59

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	63	VAL
1	A	93	ARG
1	A	153	ARG
1	A	175	GLN
1	A	177	ASP
1	A	194	ASP
1	A	247	ILE
1	A	261	LYS
1	A	272	ARG
1	A	273	ASN
1	A	289	ARG
1	A	329	ARG
1	A	335	LEU
1	A	340	LEU
1	A	354	LEU
1	B	24	LEU
1	B	44	ARG
1	B	45	ARG
1	B	63	VAL

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Mol	Chain	Res	Type
1	B	87	GLU
1	B	88	ARG
1	B	93	ARG
1	B	105	ARG
1	B	175	GLN
1	B	200	ARG
1	B	222	PRO
1	B	331	GLU
1	B	335	LEU
1	B	340	LEU
1	B	384	LEU
1	B	386	CYS
1	B	395	GLU
1	B	420	GLU
1	B	421	ARG
1	C	24	LEU
1	C	63	VAL
1	C	93	ARG
1	C	105	ARG
1	C	192	ASP
1	C	193	ARG
1	C	269	ARG
1	C	309	HIS
1	C	335	LEU
1	C	340	LEU
1	C	369	ARG
1	C	382	PRO
1	C	384	LEU
1	C	411	ARG
1	C	423	LYS
1	D	24	LEU
1	D	63	VAL
1	D	88	ARG
1	D	105	ARG
1	D	137	ARG
1	D	269	ARG
1	D	272	ARG
1	D	340	LEU
1	D	384	LEU
1	D	385	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	240	ASN
1	A	273	ASN
1	A	306	ASN
1	B	189	HIS
1	B	240	ASN
1	B	262	GLN
1	B	306	ASN
1	D	240	ASN
1	D	246	GLN
1	D	361	HIS

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 39 ligands modelled in this entry, 31 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FDA	A	501	-	48,58,58	2.40	16 (33%)	54,89,89	2.39	11 (20%)
3	NAP	A	502	-	42,52,52	1.40	5 (11%)	54,80,80	1.99	9 (16%)
2	FDA	B	501	-	48,58,58	2.25	16 (33%)	54,89,89	2.65	20 (37%)
3	NAP	B	502	-	42,52,52	1.44	5 (11%)	54,80,80	2.31	11 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	FDA	C	501	-	48,58,58	2.41	17 (35%)	54,89,89	2.69	17 (31%)
3	NAP	C	502	-	42,52,52	1.44	6 (14%)	54,80,80	1.80	12 (22%)
2	FDA	D	501	-	48,58,58	2.20	15 (31%)	54,89,89	2.14	12 (22%)
3	NAP	D	502	-	42,52,52	1.32	5 (11%)	54,80,80	2.32	12 (22%)

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
2	FDA	A	501	-	-	0/30/50/50	0/6/6/6
3	NAP	A	502	-	-	0/27/67/67	0/5/5/5
2	FDA	B	501	-	-	0/30/50/50	0/6/6/6
3	NAP	B	502	-	-	0/27/67/67	0/5/5/5
2	FDA	C	501	-	-	0/30/50/50	0/6/6/6
3	NAP	C	502	-	-	0/27/67/67	0/5/5/5
2	FDA	D	501	-	-	0/30/50/50	0/6/6/6
3	NAP	D	502	-	-	0/27/67/67	0/5/5/5

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	FDA	O2B-C2B	-5.70	1.29	1.43
2	A	501	FDA	O2B-C2B	-5.70	1.29	1.43
2	D	501	FDA	O2B-C2B	-5.33	1.30	1.43
2	B	501	FDA	O2B-C2B	-5.29	1.30	1.43
3	B	502	NAP	C3B-C2B	-4.42	1.43	1.53
2	A	501	FDA	O4B-C1B	-4.03	1.36	1.41
3	D	502	NAP	C2D-C3D	-3.96	1.42	1.53
2	C	501	FDA	C2B-C3B	-3.81	1.43	1.53
2	D	501	FDA	C2B-C3B	-3.80	1.43	1.53
3	A	502	NAP	C3B-C2B	-3.80	1.44	1.53
3	B	502	NAP	C2D-C3D	-3.78	1.43	1.53
2	C	501	FDA	O4B-C1B	-3.75	1.36	1.41
2	B	501	FDA	O3'-C3'	-3.71	1.34	1.43
2	A	501	FDA	C2B-C3B	-3.66	1.43	1.53
3	C	502	NAP	C3B-C2B	-3.63	1.44	1.53
2	D	501	FDA	O3'-C3'	-3.54	1.34	1.43
3	C	502	NAP	C2D-C3D	-3.52	1.43	1.53
2	B	501	FDA	C2B-C3B	-3.50	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	FDA	C9A-N10	-3.48	1.34	1.38
2	A	501	FDA	C9A-N10	-3.45	1.34	1.38
2	D	501	FDA	O4B-C1B	-3.41	1.36	1.41
2	C	501	FDA	O3'-C3'	-3.34	1.35	1.43
2	A	501	FDA	O2'-C2'	-3.25	1.36	1.43
3	A	502	NAP	C2D-C3D	-3.22	1.44	1.53
3	D	502	NAP	C3B-C2B	-3.19	1.45	1.53
2	A	501	FDA	O3'-C3'	-3.16	1.35	1.43
2	C	501	FDA	O2'-C2'	-3.10	1.36	1.43
2	B	501	FDA	O4B-C1B	-3.04	1.37	1.41
2	D	501	FDA	O4'-C4'	-3.03	1.36	1.43
2	B	501	FDA	O2'-C2'	-2.98	1.36	1.43
2	A	501	FDA	O4'-C4'	-2.91	1.36	1.43
2	C	501	FDA	O4'-C4'	-2.85	1.37	1.43
2	C	501	FDA	C9A-N10	-2.84	1.34	1.38
2	D	501	FDA	O2'-C2'	-2.79	1.37	1.43
2	B	501	FDA	O4'-C4'	-2.65	1.37	1.43
3	C	502	NAP	O4D-C4D	-2.64	1.38	1.45
2	B	501	FDA	C9A-N10	-2.59	1.35	1.38
2	C	501	FDA	C9A-C5X	-2.21	1.38	1.42
2	A	501	FDA	C9A-C5X	-2.20	1.38	1.42
3	A	502	NAP	O4D-C4D	-2.17	1.40	1.45
2	B	501	FDA	C9A-C5X	-2.12	1.38	1.42
2	D	501	FDA	C9A-C5X	-2.07	1.38	1.42
3	D	502	NAP	O4D-C4D	-2.04	1.40	1.45
2	C	501	FDA	C2A-N3A	2.02	1.35	1.32
2	C	501	FDA	C5'-C4'	2.07	1.54	1.51
2	D	501	FDA	PA-O1A	2.09	1.58	1.51
2	A	501	FDA	C2A-N3A	2.09	1.35	1.32
2	B	501	FDA	C2A-N3A	2.11	1.35	1.32
3	B	502	NAP	O4D-C1D	2.28	1.44	1.41
2	A	501	FDA	PA-O1A	2.30	1.59	1.51
2	A	501	FDA	C4X-N5	2.33	1.37	1.33
2	B	501	FDA	C4X-N5	2.34	1.37	1.33
3	C	502	NAP	O4D-C1D	2.36	1.44	1.41
2	C	501	FDA	C4X-N5	2.43	1.37	1.33
2	D	501	FDA	C4X-N5	2.69	1.37	1.33
2	C	501	FDA	PA-O1A	2.86	1.61	1.51
2	B	501	FDA	PA-O1A	3.11	1.62	1.51
2	D	501	FDA	C4-C4X	3.13	1.47	1.41
3	C	502	NAP	C6A-N6A	3.14	1.44	1.34
3	D	502	NAP	C7N-N7N	3.15	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	FDA	C1'-N10	3.45	1.52	1.48
3	B	502	NAP	C7N-N7N	3.54	1.40	1.33
2	C	501	FDA	C4-C4X	3.55	1.48	1.41
3	B	502	NAP	C6A-N6A	3.59	1.46	1.34
3	D	502	NAP	C6A-N6A	3.64	1.46	1.34
3	A	502	NAP	C7N-N7N	3.66	1.40	1.33
3	A	502	NAP	C6A-N6A	3.72	1.46	1.34
2	B	501	FDA	C4-C4X	3.74	1.48	1.41
2	A	501	FDA	C4-C4X	3.87	1.49	1.41
2	B	501	FDA	C4-N3	4.13	1.40	1.33
3	C	502	NAP	C7N-N7N	4.13	1.41	1.33
2	D	501	FDA	C6A-N6A	4.24	1.48	1.34
2	B	501	FDA	C6A-N6A	4.40	1.48	1.34
2	C	501	FDA	C6A-N6A	4.41	1.48	1.34
2	A	501	FDA	C6A-N6A	4.42	1.48	1.34
2	D	501	FDA	C4-N3	4.66	1.41	1.33
2	B	501	FDA	C1'-N10	4.70	1.53	1.48
2	A	501	FDA	C4-N3	4.82	1.42	1.33
2	C	501	FDA	C4-N3	4.91	1.42	1.33
2	A	501	FDA	C10-N1	5.10	1.44	1.35
2	D	501	FDA	C10-N1	5.42	1.44	1.35
2	C	501	FDA	C10-N1	5.48	1.44	1.35
2	B	501	FDA	C10-N1	5.51	1.44	1.35
2	C	501	FDA	C1'-N10	5.98	1.54	1.48
2	A	501	FDA	C1'-N10	6.48	1.55	1.48

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	NAP	N3A-C2A-N1A	-10.79	120.63	128.89
3	A	502	NAP	N3A-C2A-N1A	-10.58	120.80	128.89
3	D	502	NAP	N3A-C2A-N1A	-9.83	121.37	128.89
2	A	501	FDA	N3A-C2A-N1A	-9.74	121.43	128.89
2	C	501	FDA	N3A-C2A-N1A	-9.20	121.85	128.89
2	D	501	FDA	N3A-C2A-N1A	-8.81	122.15	128.89
2	B	501	FDA	O5'-P-O1P	-8.61	76.18	109.62
3	D	502	NAP	O3-PA-O5B	-8.60	80.12	102.94
2	B	501	FDA	N3A-C2A-N1A	-8.04	122.73	128.89
2	A	501	FDA	O5'-P-O1P	-7.64	79.96	109.62
2	C	501	FDA	O5'-P-O1P	-7.50	80.49	109.62
3	C	502	NAP	N3A-C2A-N1A	-7.35	123.26	128.89
2	C	501	FDA	O3P-PA-O5B	-6.11	86.71	102.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	FDA	O2P-P-O5'	-5.00	83.23	108.46
2	C	501	FDA	O3P-P-O5'	-4.69	90.50	102.94
2	B	501	FDA	O2A-PA-O3P	-4.60	84.24	105.09
2	B	501	FDA	O3P-PA-O5B	-4.58	90.77	102.94
2	A	501	FDA	O3P-P-O5'	-4.40	91.25	102.94
2	A	501	FDA	O2P-P-O5'	-4.32	86.67	108.46
2	B	501	FDA	O3P-P-O5'	-4.22	91.73	102.94
3	D	502	NAP	O2A-PA-O3	-4.20	86.02	105.09
2	D	501	FDA	C4X-C10-N10	-4.20	118.05	120.52
2	B	501	FDA	O2P-P-O5'	-4.11	87.72	108.46
2	C	501	FDA	C4X-C10-N10	-3.54	118.44	120.52
3	C	502	NAP	O7N-C7N-C3N	-3.36	115.92	119.59
2	C	501	FDA	O2A-PA-O3P	-3.35	89.88	105.09
2	A	501	FDA	P-O3P-PA	-3.25	123.60	132.73
2	D	501	FDA	C4X-C4-N3	-3.25	119.15	123.59
3	B	502	NAP	C4B-O4B-C1B	-3.25	106.15	109.72
2	D	501	FDA	C4B-O4B-C1B	-3.21	106.19	109.72
2	B	501	FDA	C4X-C4-N3	-3.14	119.29	123.59
3	C	502	NAP	PN-O3-PA	-3.11	124.00	132.73
2	C	501	FDA	O3'-C3'-C2'	-3.09	100.97	108.75
2	B	501	FDA	C4X-C10-N10	-2.98	118.77	120.52
2	A	501	FDA	C4X-C4-N3	-2.94	119.56	123.59
2	C	501	FDA	C4A-C5A-N7A	-2.75	106.95	109.48
3	A	502	NAP	O7N-C7N-C3N	-2.75	116.59	119.59
3	D	502	NAP	C4A-C5A-N7A	-2.67	107.03	109.48
3	A	502	NAP	C1B-N9A-C4A	-2.59	123.03	126.94
3	A	502	NAP	PN-O3-PA	-2.57	125.51	132.73
2	C	501	FDA	C4X-C4-N3	-2.57	120.07	123.59
2	B	501	FDA	C4A-C5A-N7A	-2.54	107.14	109.48
3	B	502	NAP	C1B-N9A-C4A	-2.53	123.13	126.94
2	D	501	FDA	C1B-N9A-C4A	-2.49	123.18	126.94
2	B	501	FDA	O3B-C3B-C4B	-2.48	103.60	111.05
2	D	501	FDA	O2'-C2'-C1'	-2.47	103.86	109.94
3	B	502	NAP	PN-O3-PA	-2.45	125.85	132.73
2	B	501	FDA	C1B-N9A-C4A	-2.45	123.25	126.94
2	C	501	FDA	C1B-N9A-C4A	-2.43	123.28	126.94
2	B	501	FDA	C4B-O4B-C1B	-2.40	107.09	109.72
3	C	502	NAP	C4B-O4B-C1B	-2.32	107.17	109.72
3	A	502	NAP	C4B-O4B-C1B	-2.31	107.18	109.72
2	D	501	FDA	C4A-C5A-N7A	-2.29	107.37	109.48
3	C	502	NAP	C4A-C5A-N7A	-2.27	107.39	109.48
3	B	502	NAP	C5N-C4N-C3N	-2.25	117.51	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	NAP	C4A-C5A-N7A	-2.21	107.45	109.48
3	C	502	NAP	C5N-C4N-C3N	-2.05	117.75	120.33
2	A	501	FDA	C4A-C5A-N7A	-2.04	107.60	109.48
3	C	502	NAP	O3-PA-O5B	2.01	108.27	102.94
2	D	501	FDA	C1'-N10-C9A	2.03	121.14	118.86
3	B	502	NAP	O5D-C5D-C4D	2.06	116.72	109.12
2	D	501	FDA	O4B-C4B-C5B	2.08	116.77	109.32
3	C	502	NAP	O5D-C5D-C4D	2.19	117.19	109.12
2	B	501	FDA	C5X-C9A-N10	2.22	119.31	117.62
2	B	501	FDA	C4-C4X-N5	2.27	121.47	118.72
3	C	502	NAP	O3-PN-O5D	2.29	109.00	102.94
3	B	502	NAP	O3-PN-O5D	2.30	109.03	102.94
3	D	502	NAP	O3-PN-O5D	2.31	109.06	102.94
2	A	501	FDA	O2P-P-O3P	2.35	115.77	105.09
3	D	502	NAP	O4B-C1B-N9A	2.38	113.08	108.10
3	D	502	NAP	O2A-PA-O5B	2.39	120.50	108.46
3	A	502	NAP	C2N-C3N-C4N	2.39	120.95	118.29
3	B	502	NAP	O3-PA-O5B	2.40	109.29	102.94
2	B	501	FDA	C1'-C2'-C3'	2.40	116.68	109.82
2	B	501	FDA	O5B-C5B-C4B	2.46	118.20	109.12
2	C	501	FDA	O5B-C5B-C4B	2.47	118.22	109.12
2	A	501	FDA	O3P-PA-O5B	2.56	109.73	102.94
3	D	502	NAP	C2N-C3N-C4N	2.59	121.17	118.29
3	B	502	NAP	O4B-C4B-C5B	2.60	118.64	109.32
3	D	502	NAP	O2B-P2B-O1X	2.74	113.95	107.11
3	D	502	NAP	O5B-C5B-C4B	2.75	119.27	109.12
2	C	501	FDA	O3'-C3'-C4'	2.82	115.86	108.75
3	D	502	NAP	O5B-PA-O1A	2.87	120.75	109.62
2	B	501	FDA	O5B-PA-O1A	2.88	120.78	109.62
3	C	502	NAP	C3N-C7N-N7N	2.94	121.03	117.82
2	B	501	FDA	O2P-P-O3P	2.98	118.59	105.09
2	A	501	FDA	C5X-C9A-N10	3.09	119.97	117.62
3	C	502	NAP	C2N-C3N-C4N	3.19	121.84	118.29
2	B	501	FDA	C1'-N10-C9A	3.29	122.56	118.86
3	B	502	NAP	C2N-C3N-C4N	3.31	121.98	118.29
2	D	501	FDA	C5X-C9A-N10	3.47	120.25	117.62
2	C	501	FDA	O5B-PA-O1A	3.59	123.55	109.62
3	A	502	NAP	O4D-C1D-N1N	3.60	112.08	108.13
3	D	502	NAP	O4D-C1D-N1N	3.60	112.09	108.13
2	C	501	FDA	O2P-P-O3P	3.81	122.36	105.09
3	A	502	NAP	C3N-C7N-N7N	3.96	122.15	117.82
2	C	501	FDA	C5X-C9A-N10	4.10	120.73	117.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	FDA	O3P-P-O5'	4.44	114.71	102.94
2	C	501	FDA	C4-N3-C2	4.75	119.36	115.25
3	C	502	NAP	O4D-C1D-N1N	5.03	113.66	108.13
2	A	501	FDA	C4-N3-C2	5.07	119.63	115.25
2	B	501	FDA	C4-N3-C2	6.17	120.58	115.25
2	D	501	FDA	C4-N3-C2	6.47	120.84	115.25
3	B	502	NAP	O4D-C1D-N1N	8.44	117.41	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FDA	4	0
2	B	501	FDA	3	0
3	B	502	NAP	1	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	414/443 (93%)	-0.08	6 (1%)	78	74	18, 31, 58, 83	0
1	B	415/443 (93%)	-0.06	3 (0%)	89	87	20, 32, 61, 82	0
1	C	414/443 (93%)	0.02	6 (1%)	78	74	16, 32, 63, 83	0
1	D	414/443 (93%)	-0.04	6 (1%)	78	74	22, 33, 64, 98	0
All	All	1657/1772 (93%)	-0.04	21 (1%)	79	76	16, 32, 62, 98	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	135	PRO	3.4
1	D	356	GLY	3.1
1	C	151	ALA	2.8
1	D	313	ALA	2.8
1	C	147	SER	2.7
1	A	192	ASP	2.4
1	A	223	ASP	2.4
1	B	424	SER	2.3
1	B	386	CYS	2.3
1	A	361	HIS	2.2
1	A	198	LEU	2.2
1	C	11	THR	2.2
1	B	151	ALA	2.2
1	C	142	VAL	2.2
1	C	10	PRO	2.1
1	C	135	PRO	2.1
1	D	10	PRO	2.1
1	D	172	ALA	2.1
1	A	197	SER	2.0
1	D	11	THR	2.0
1	A	193	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no 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, 95^{th} 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(Å^2)	Q<0.9
2	FDA	A	501	53/53	0.97	0.14	-0.11	18,24,34,36	0
2	FDA	C	501	53/53	0.96	0.16	-0.31	19,27,40,43	0
3	NAP	C	502	48/48	0.97	0.15	-0.35	16,22,29,37	0
2	FDA	D	501	53/53	0.96	0.13	-0.42	23,28,33,40	0
2	FDA	B	501	53/53	0.96	0.14	-0.73	21,27,33,36	0
3	NAP	A	502	48/48	0.98	0.12	-0.83	18,23,30,33	0
3	NAP	D	502	48/48	0.97	0.13	-0.99	21,27,36,43	0
3	NAP	B	502	48/48	0.98	0.13	-1.01	17,28,36,43	0
4	BR	B	506	1/1	0.99	0.12	-1.51	33,33,33,33	1
4	BR	C	507	1/1	0.99	0.10	-1.74	32,32,32,32	1
4	BR	A	510	1/1	0.91	0.13	-1.86	51,51,51,51	1
4	BR	D	504	1/1	0.98	0.14	-2.29	26,26,26,26	1
4	BR	A	511	1/1	0.98	0.14	-2.49	32,32,32,32	1
4	BR	D	503	1/1	0.98	0.08	-2.58	36,36,36,36	1
4	BR	A	507	1/1	0.99	0.09	-2.65	24,24,24,24	1
4	BR	C	503	1/1	0.95	0.13	-2.89	39,39,39,39	1
4	BR	C	508	1/1	0.98	0.05	-2.92	39,39,39,39	1
4	BR	C	509	1/1	0.98	0.06	-3.21	33,33,33,33	1
4	BR	A	506	1/1	0.99	0.07	-3.30	27,27,27,27	1
4	BR	A	503	1/1	0.97	0.10	-3.35	37,37,37,37	1
4	BR	A	509	1/1	0.96	0.06	-3.37	31,31,31,31	1
4	BR	A	504	1/1	0.99	0.11	-3.40	20,20,20,20	1
4	BR	B	503	1/1	0.99	0.12	-3.88	27,27,27,27	1
4	BR	B	504	1/1	0.97	0.07	-4.20	37,37,37,37	1
4	BR	B	507	1/1	0.97	0.06	-4.29	38,38,38,38	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	BR	C	506	1/1	0.98	0.07	-4.62	42,42,42,42	1
4	BR	C	504	1/1	0.99	0.10	-5.36	31,31,31,31	1
4	BR	D	507	1/1	0.98	0.04	-7.01	37,37,37,37	1
4	BR	C	505	1/1	0.99	0.09	-	45,45,45,45	1
4	BR	D	505	1/1	0.98	0.09	-	29,29,29,29	1
4	BR	B	505	1/1	1.00	0.08	-	28,28,28,28	1
4	BR	A	508	1/1	0.90	0.20	-	56,56,56,56	1
4	BR	C	510	1/1	0.97	0.19	-	33,33,33,33	1
4	BR	A	512	1/1	0.90	0.13	-	60,60,60,60	1
4	BR	D	508	1/1	0.99	0.04	-	55,55,55,55	1
4	BR	D	506	1/1	0.91	0.12	-	47,47,47,47	1
4	BR	A	505	1/1	0.99	0.04	-	34,34,34,34	1
4	BR	B	508	1/1	0.96	0.05	-	39,39,39,39	1
4	BR	D	509	1/1	0.98	0.15	-	51,51,51,51	1

6.5 Other polymers (i)

There are no such residues in this entry.