Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:30 PM GMT

PDB ID	:	4TLX
Title	:	Kutzneria sp. 744 ornithine N-hydroxylase, KtzI-FADred-NADP+-L-orn
Authors	:	Setser, J.W.; Drennan, C.L.
Deposited on	:	2014-05-30
Resolution	:	2.23 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:

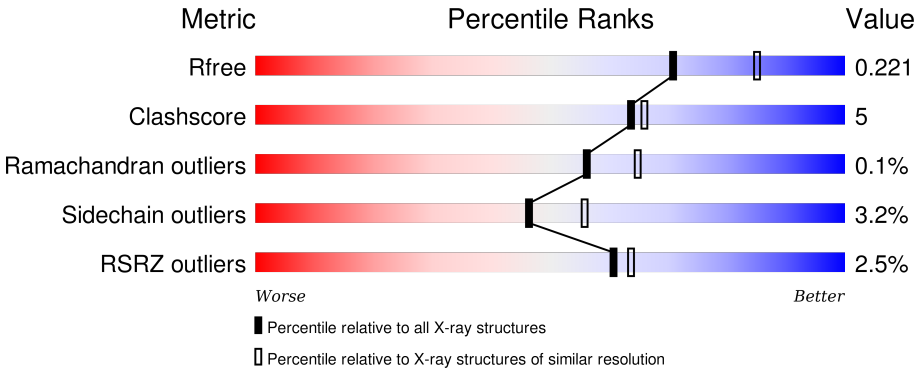
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.23 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	1611 (2.26-2.22)
Clashscore	102246	1764 (2.26-2.22)
Ramachandran outliers	100387	1724 (2.26-2.22)
Sidechain outliers	100360	1724 (2.26-2.22)
RSRZ outliers	91569	1616 (2.26-2.22)

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	2% 83% 10% • 6%
1	B	443	% 82% 11% 6%
1	C	443	5% 81% 13% 6%
1	D	443	% 83% 10% • 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13862 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	415	Total	C	N	O	S	0	0	0
			3210	2016	571	613	10			
1	B	415	Total	C	N	O	S	0	0	0
			3220	2022	577	611	10			
1	C	415	Total	C	N	O	S	0	0	0
			3179	2001	563	605	10			
1	D	415	Total	C	N	O	S	0	0	0
			3215	2019	576	610	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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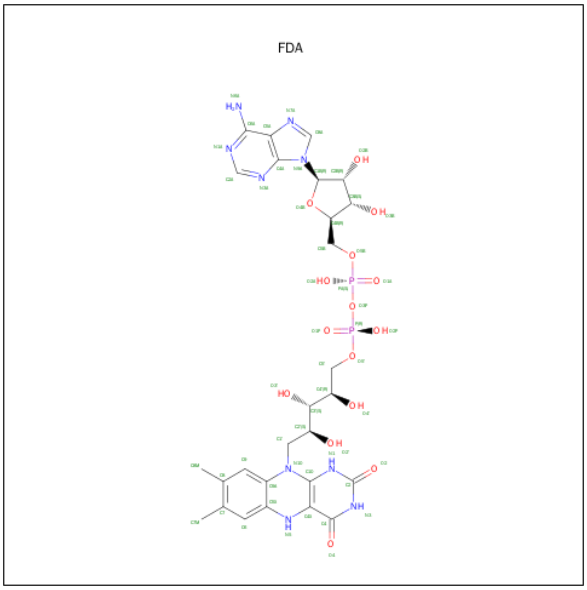
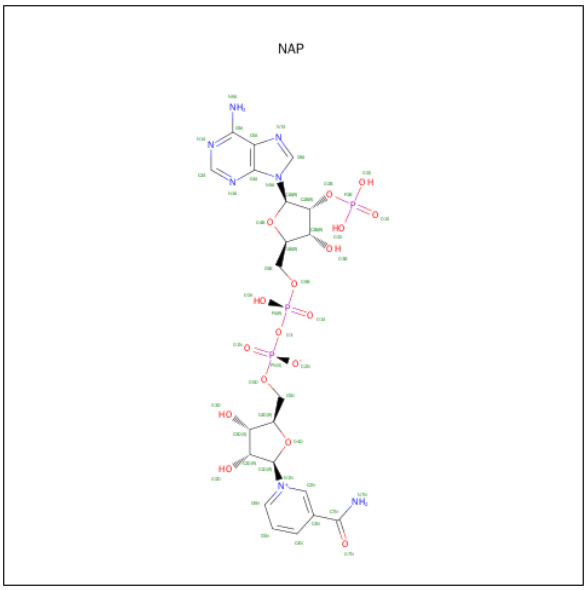
Chain	Residue	Modelled	Actual	Comment	Reference
D	-18	MET	-	initiating methionine	UNP A8CF85
D	-17	GLY	-	expression tag	UNP A8CF85
D	-16	SER	-	expression tag	UNP A8CF85
D	-15	SER	-	expression tag	UNP A8CF85
D	-14	HIS	-	expression tag	UNP A8CF85
D	-13	HIS	-	expression tag	UNP A8CF85
D	-12	HIS	-	expression 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: $C_{27}H_{35}N_9O_{15}P_2$).



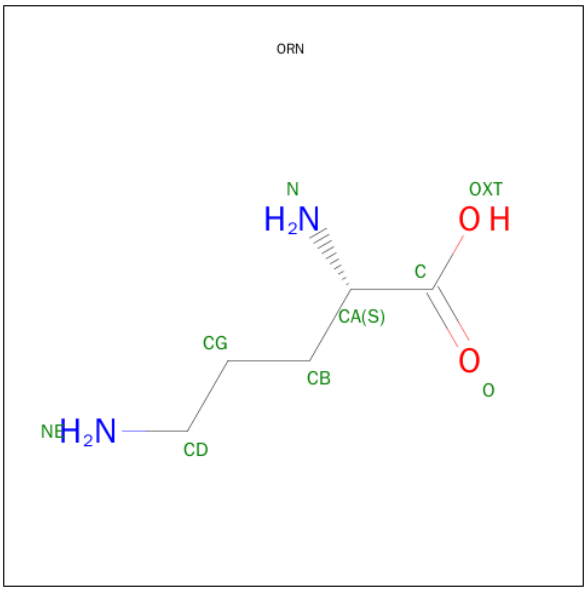
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- 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 L-ornithine (three-letter code: ORN) (formula: $C_5H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 9 5 2 2	0	0
4	B	1	Total C N O 9 5 2 2	0	0
4	C	1	Total C N O 9 5 2 2	0	0
4	D	1	Total C N O 9 5 2 2	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total K 2 2	0	0
5	A	3	Total K 3 3	0	0
5	D	2	Total K 2 2	0	0
5	C	2	Total K 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	171	Total O 171 171	0	0

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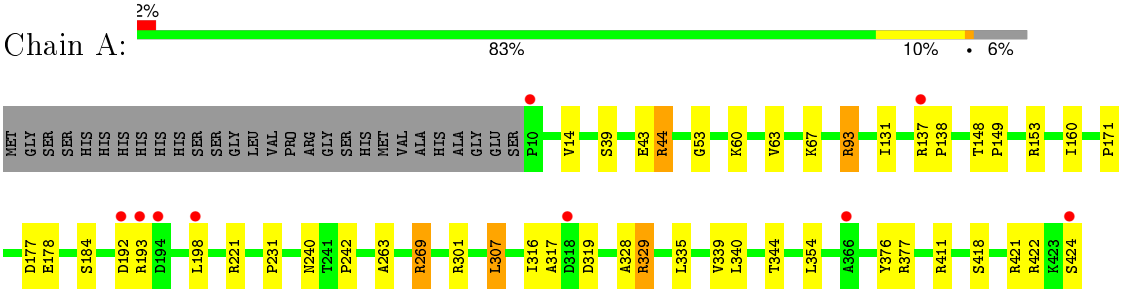
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	147	Total O 147 147	0	0
6	C	125	Total O 125 125	0	0
6	D	146	Total O 146 146	0	0

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.

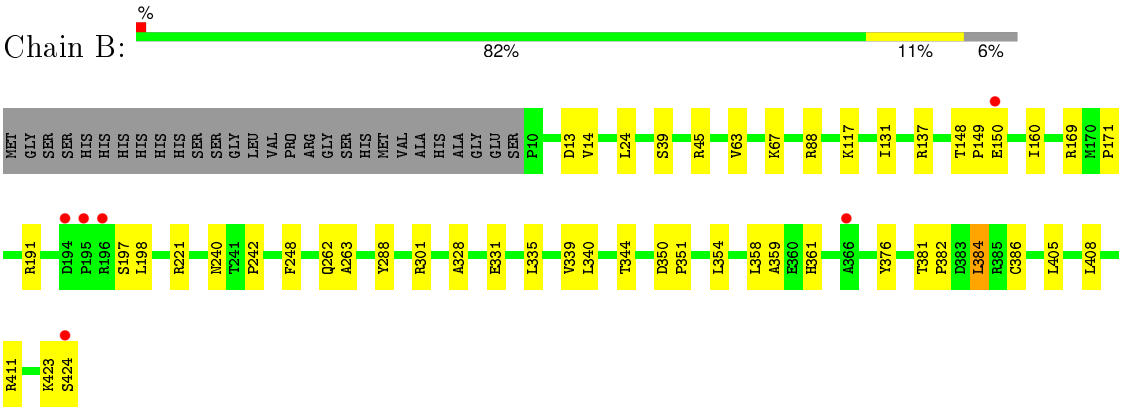
- Molecule 1: KtzI

Chain A:



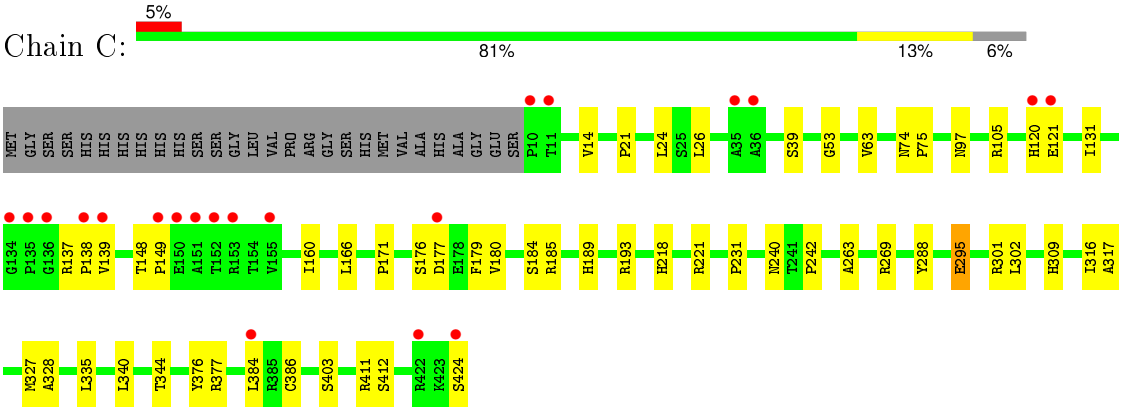
- Molecule 1: KtzI

Chain B:



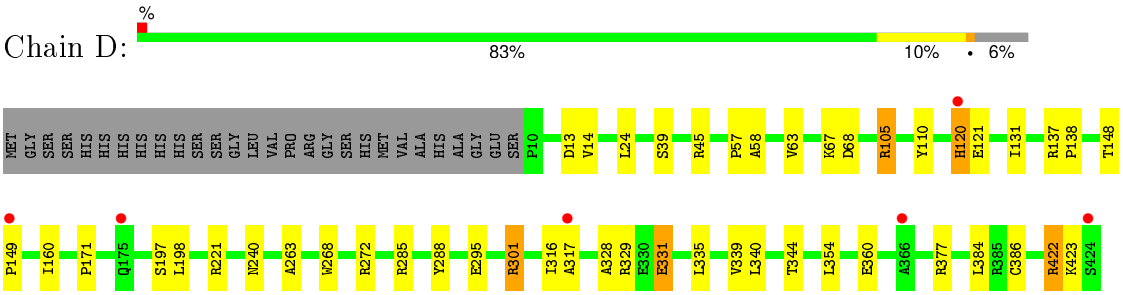
- Molecule 1: KtzI

Chain C:



- Molecule 1: KtzI

Chain D:


%
83%
10%
6%
MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET VAL ALA HIS ALA GLY GLU SER P10 D13 V14 L24 S39 R45 P57 A58 V63 K67 D68 R105 Y110 H120 E121 I131 R137 P138 T148
P149 I160 P171 Q175 S197 L198 R221 N240 A263 W268 R272 R285 Y288 E295 R301 I316 A317 A328 R329 E330 E331 L335 V339 L340 T344 L354 E360 A366 R377 L384 R385 C386 R422 K423 S424

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.15Å 156.91Å 163.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.82 – 2.23 49.82 – 2.23	Depositor EDS
% Data completeness (in resolution range)	92.7 (49.82-2.23) 92.7 (49.82-2.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	4.27 (at 2.22Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.186 , 0.214 0.199 , 0.221	Depositor DCC
R_{free} test set	4884 reflections (5.20%)	DCC
Wilson B-factor (Å^2)	29.7	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 29.7	EDS
Estimated twinning fraction	0.010 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 98975 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13862	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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, ORN, K, NAP

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	0.54	0/3289	0.55	0/4483
1	B	0.54	0/3299	0.59	0/4493
1	C	0.48	0/3259	0.54	0/4447
1	D	0.50	0/3295	0.56	1/4490 (0.0%)
All	All	0.52	0/13142	0.56	1/17913 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	301	ARG	NE-CZ-NH2	-5.44	117.58	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3210	0	3029	33	0
1	B	3220	0	3057	36	0
1	C	3179	0	2984	40	0
1	D	3215	0	3042	34	0
2	A	53	0	31	3	0
2	B	53	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	53	0	31	1	0
2	D	53	0	30	0	0
3	A	48	0	25	0	0
3	B	48	0	25	0	0
3	C	48	0	25	0	0
3	D	48	0	25	0	0
4	A	9	0	11	0	0
4	B	9	0	11	1	0
4	C	9	0	11	0	0
4	D	9	0	11	0	0
5	A	3	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	A	171	0	0	2	0
6	B	147	0	0	4	0
6	C	125	0	0	2	0
6	D	146	0	0	7	0
All	All	13862	0	12379	132	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 5.

All (132) 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:C:177:ASP:OD2	1:C:180:VAL:HB	1.40	1.18
1:B:149:PRO:HG2	1:B:150:GLU:OE2	1.51	1.09
1:D:384:LEU:HD11	1:D:386:CYS:SG	1.94	1.05
1:B:384:LEU:CD2	1:B:386:CYS:SG	2.47	1.03
1:B:384:LEU:HD22	1:B:386:CYS:SG	2.07	0.93
1:D:105:ARG:HD2	6:D:720:HOH:O	1.68	0.92
1:C:148:THR:HB	1:C:149:PRO:HD2	1.53	0.88
1:B:148:THR:HB	1:B:149:PRO:HD2	1.56	0.88
1:A:148:THR:HB	1:A:149:PRO:HD2	1.55	0.87
1:D:148:THR:HB	1:D:149:PRO:HD2	1.56	0.87
1:B:384:LEU:HD21	1:B:386:CYS:SG	2.20	0.82
1:C:179:PHE:CD1	1:C:193:ARG:NH2	2.48	0.82
1:C:177:ASP:OD2	1:C:180:VAL:CB	2.26	0.78
1:D:384:LEU:CD1	1:D:386:CYS:SG	2.72	0.75
1:D:45:ARG:HD2	6:D:717:HOH:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ARG:NH2	1:A:329:ARG:HG3	2.04	0.73
1:B:150:GLU:N	1:B:150:GLU:OE2	2.23	0.72
1:C:179:PHE:HD1	1:C:193:ARG:HH22	1.35	0.72
1:A:329:ARG:HH21	1:A:329:ARG:HG3	1.54	0.72
1:C:218:HIS:HD2	1:C:302:LEU:HD13	1.54	0.72
1:D:422:ARG:HD3	6:D:693:HOH:O	1.90	0.72
1:B:45:ARG:NH1	6:B:719:HOH:O	2.22	0.71
1:D:57:PRO:O	1:D:58:ALA:HB3	1.91	0.70
1:A:377:ARG:NH1	1:A:422:ARG:NH1	2.40	0.70
1:C:218:HIS:HD2	1:C:302:LEU:CD1	2.06	0.68
1:B:149:PRO:CG	1:B:150:GLU:OE2	2.34	0.68
1:C:139:VAL:HB	1:C:384:LEU:HD23	1.76	0.67
1:D:285:ARG:HG2	6:D:697:HOH:O	1.98	0.64
1:A:329:ARG:HH21	1:A:329:ARG:CG	2.14	0.59
1:C:384:LEU:HD22	1:C:386:CYS:SG	2.42	0.59
1:C:177:ASP:N	1:C:177:ASP:OD2	2.36	0.58
1:A:269:ARG:HH11	1:A:269:ARG:CG	2.16	0.58
1:B:361:HIS:HB2	1:B:384:LEU:HD12	1.85	0.58
1:C:120:HIS:HD2	1:C:121:GLU:H	1.52	0.58
1:A:178:GLU:O	1:A:193:ARG:NH2	2.37	0.57
1:C:218:HIS:CD2	1:C:302:LEU:HD13	2.37	0.57
1:A:171:PRO:HG3	1:A:344:THR:HG21	1.86	0.57
1:C:97:ASN:HB3	6:C:652:HOH:O	2.05	0.56
1:A:44:ARG:HG2	2:A:501:FDA:C4A	2.36	0.55
1:C:148:THR:HB	1:C:149:PRO:CD	2.34	0.55
1:B:131:ILE:HD13	1:B:160:ILE:HD13	1.89	0.55
1:B:117:LYS:HD2	6:B:602:HOH:O	2.07	0.54
1:D:57:PRO:O	1:D:58:ALA:CB	2.55	0.54
1:C:131:ILE:HD13	1:C:160:ILE:HD13	1.90	0.54
1:D:105:ARG:CD	6:D:720:HOH:O	2.41	0.53
1:B:242:PRO:HB2	1:C:288:TYR:CD1	2.44	0.53
1:B:358:LEU:O	1:B:359:ALA:C	2.46	0.52
1:D:131:ILE:HD13	1:D:160:ILE:HD13	1.91	0.52
1:C:179:PHE:CE1	1:C:193:ARG:NH2	2.78	0.52
1:B:169:ARG:NH1	1:B:344:THR:O	2.43	0.52
1:A:137:ARG:HA	1:A:138:PRO:C	2.30	0.51
1:A:421:ARG:O	1:A:424:SER:HB2	2.10	0.51
1:C:218:HIS:CD2	1:C:302:LEU:CD1	2.90	0.51
1:D:377:ARG:NH2	6:D:693:HOH:O	2.27	0.51
1:B:381:THR:HB	1:B:382:PRO:HD2	1.93	0.50
1:D:171:PRO:HG3	1:D:344:THR:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ILE:HD13	1:A:160:ILE:HD13	1.94	0.49
1:A:221:ARG:O	1:A:301:ARG:NH2	2.45	0.49
1:D:137:ARG:HA	1:D:138:PRO:C	2.33	0.49
1:D:13:ASP:OD1	1:D:423:LYS:HE3	2.12	0.49
1:A:418:SER:O	1:A:422:ARG:HG3	2.13	0.49
1:C:221:ARG:O	1:C:301:ARG:NH2	2.46	0.48
1:D:221:ARG:O	1:D:301:ARG:NH2	2.46	0.48
1:A:148:THR:HB	1:A:149:PRO:CD	2.35	0.48
1:B:191:ARG:NH1	6:B:743:HOH:O	2.45	0.48
1:C:171:PRO:HG3	1:C:344:THR:HG21	1.96	0.47
1:B:242:PRO:HB2	1:C:288:TYR:CG	2.49	0.47
1:D:423:LYS:HG3	6:D:736:HOH:O	2.15	0.47
1:D:316:ILE:O	1:D:317:ALA:HB3	2.13	0.47
1:A:316:ILE:O	1:A:317:ALA:HB3	2.14	0.47
1:D:148:THR:HB	1:D:149:PRO:CD	2.37	0.47
1:A:319:ASP:OD2	6:A:601:HOH:O	2.20	0.47
1:C:185:ARG:O	1:C:189:HIS:HD2	1.96	0.47
1:B:221:ARG:O	1:B:301:ARG:NH2	2.48	0.47
1:D:329:ARG:O	1:D:331:GLU:HG2	2.15	0.47
1:D:14:VAL:O	1:D:39:SER:HA	2.15	0.46
1:B:14:VAL:O	1:B:39:SER:HA	2.16	0.46
1:D:422:ARG:O	1:D:423:LYS:C	2.52	0.46
1:C:316:ILE:O	1:C:317:ALA:HB3	2.15	0.46
1:D:120:HIS:ND1	1:D:121:GLU:N	2.63	0.46
1:B:171:PRO:HG3	1:B:344:THR:HG21	1.96	0.46
1:B:137:ARG:HD2	1:B:137:ARG:HA	1.75	0.46
1:A:14:VAL:O	1:A:39:SER:HA	2.16	0.46
1:A:43:GLU:OE2	2:A:501:FDA:O2B	2.34	0.45
1:B:288:TYR:CD1	1:C:242:PRO:HB2	2.52	0.45
1:B:381:THR:HB	1:B:382:PRO:CD	2.47	0.45
1:A:377:ARG:NH1	1:A:422:ARG:CZ	2.79	0.45
1:C:74:ASN:HA	1:C:75:PRO:HD2	1.87	0.45
1:C:376:TYR:CE1	1:C:411:ARG:HG3	2.52	0.44
1:C:120:HIS:CD2	1:C:121:GLU:N	2.85	0.44
1:C:120:HIS:HD2	1:C:121:GLU:N	2.14	0.44
6:C:700:HOH:O	1:D:67:LYS:HE3	2.18	0.44
1:D:68:ASP:HB2	1:D:110:TYR:OH	2.18	0.44
1:C:137:ARG:HA	1:C:138:PRO:C	2.36	0.44
1:B:13:ASP:OD1	1:B:423:LYS:HE3	2.18	0.44
1:B:263:ALA:HB2	1:C:328:ALA:HA	1.98	0.44
1:C:14:VAL:O	1:C:39:SER:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:GLY:HA3	1:A:184:SER:O	2.17	0.44
1:A:269:ARG:CG	1:A:269:ARG:NH1	2.80	0.43
1:A:67:LYS:HE3	6:A:665:HOH:O	2.17	0.43
1:A:198:LEU:HD22	1:A:339:VAL:HG23	2.00	0.43
1:D:354:LEU:HD12	1:D:354:LEU:HA	1.70	0.43
1:A:242:PRO:HB2	1:D:288:TYR:CG	2.53	0.43
1:B:376:TYR:CE1	1:B:411:ARG:HG3	2.54	0.43
1:B:198:LEU:HD22	1:B:339:VAL:HG23	2.00	0.43
2:A:501:FDA:H1'2	2:A:501:FDA:HN1	1.71	0.43
1:A:93:ARG:NH2	1:C:295:GLU:HB2	2.34	0.42
1:B:148:THR:HB	1:B:149:PRO:CD	2.37	0.42
1:A:60:LYS:HB3	1:A:60:LYS:HE2	1.72	0.42
1:C:26:LEU:HA	1:C:412:SER:HB2	2.02	0.42
1:A:263:ALA:HB2	1:D:328:ALA:HA	2.00	0.42
1:D:197:SER:O	1:D:198:LEU:HD23	2.19	0.42
1:A:376:TYR:CE1	1:A:411:ARG:HG3	2.55	0.42
1:B:248:PHE:CE2	4:B:503:ORN:HA	2.55	0.42
1:B:405:LEU:HD22	1:B:408:LEU:HD11	2.02	0.41
1:A:354:LEU:HA	1:A:354:LEU:HD12	1.66	0.41
1:A:242:PRO:HB2	1:D:288:TYR:CD1	2.55	0.41
1:B:197:SER:O	1:B:198:LEU:HD23	2.20	0.41
1:A:328:ALA:HA	1:D:263:ALA:HB2	2.02	0.41
1:B:328:ALA:HA	1:C:263:ALA:HB2	2.02	0.41
1:B:288:TYR:CG	1:C:242:PRO:HB2	2.55	0.41
1:B:350:ASP:HA	1:B:351:PRO:HD2	1.79	0.41
1:C:166:LEU:HD21	1:C:403:SER:HB2	2.01	0.41
1:A:231:PRO:O	1:A:307:LEU:HD12	2.20	0.41
1:D:384:LEU:HD11	1:D:386:CYS:HG	1.79	0.41
1:D:268:TRP:O	1:D:272:ARG:HB2	2.20	0.41
1:B:262:GLN:NE2	1:C:327:MET:HG2	2.36	0.41
1:D:198:LEU:HD22	1:D:339:VAL:HG23	2.02	0.40
1:C:231:PRO:HB3	1:C:309:HIS:CE1	2.56	0.40
1:B:67:LYS:HE3	6:B:622:HOH:O	2.20	0.40
1:C:53:GLY:HA3	1:C:184:SER:O	2.22	0.40
1:C:21:PRO:HD2	2:C:501:FDA:O2A	2.22	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	413/443 (93%)	396 (96%)	17 (4%)	0	100	100
1	B	413/443 (93%)	399 (97%)	14 (3%)	0	100	100
1	C	413/443 (93%)	398 (96%)	15 (4%)	0	100	100
1	D	413/443 (93%)	395 (96%)	17 (4%)	1 (0%)	52	60
All	All	1652/1772 (93%)	1588 (96%)	63 (4%)	1 (0%)	56	65

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	120	HIS

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	336/372 (90%)	324 (96%)	12 (4%)	42	50
1	B	338/372 (91%)	328 (97%)	10 (3%)	48	58
1	C	330/372 (89%)	319 (97%)	11 (3%)	45	54
1	D	337/372 (91%)	327 (97%)	10 (3%)	48	58
All	All	1341/1488 (90%)	1298 (97%)	43 (3%)	46	56

All (43) 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	177	ASP
1	A	192	ASP
1	A	240	ASN
1	A	269	ARG
1	A	307	LEU
1	A	329	ARG
1	A	335	LEU
1	A	340	LEU
1	B	24	LEU
1	B	63	VAL
1	B	88	ARG
1	B	240	ASN
1	B	331	GLU
1	B	335	LEU
1	B	340	LEU
1	B	354	LEU
1	B	384	LEU
1	B	424	SER
1	C	24	LEU
1	C	63	VAL
1	C	105	ARG
1	C	176	SER
1	C	240	ASN
1	C	269	ARG
1	C	295	GLU
1	C	335	LEU
1	C	340	LEU
1	C	377	ARG
1	C	424	SER
1	D	24	LEU
1	D	63	VAL
1	D	105	ARG
1	D	240	ASN
1	D	295	GLU
1	D	331	GLU
1	D	335	LEU
1	D	340	LEU
1	D	360	GLU
1	D	422	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	GLN
1	A	189	HIS
1	A	240	ASN
1	A	246	GLN
1	A	306	ASN
1	A	309	HIS
1	B	240	ASN
1	B	306	ASN
1	B	309	HIS
1	C	120	HIS
1	C	189	HIS
1	C	240	ASN
1	C	246	GLN
1	C	306	ASN
1	C	309	HIS
1	D	175	GLN
1	D	240	ASN
1	D	246	GLN
1	D	306	ASN
1	D	309	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 21 ligands modelled in this entry, 9 are monoatomic - leaving 12 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	2.30	17 (35%)	54,89,89	2.52	13 (24%)
3	NAP	A	502	-	42,52,52	1.43	6 (14%)	54,80,80	1.84	9 (16%)
4	ORN	A	503	-	5,8,8	0.44	0	3,9,9	0.70	0
2	FDA	B	501	-	48,58,58	2.22	16 (33%)	54,89,89	2.23	10 (18%)
3	NAP	B	502	-	42,52,52	1.36	4 (9%)	54,80,80	2.05	8 (14%)
4	ORN	B	503	-	5,8,8	0.59	0	3,9,9	0.96	0
2	FDA	C	501	-	48,58,58	2.34	17 (35%)	54,89,89	2.75	19 (35%)
3	NAP	C	502	-	42,52,52	1.48	6 (14%)	54,80,80	2.01	9 (16%)
4	ORN	C	503	-	5,8,8	0.58	0	3,9,9	0.41	0
2	FDA	D	501	-	48,58,58	2.27	16 (33%)	54,89,89	2.30	14 (25%)
3	NAP	D	502	-	42,52,52	1.45	5 (11%)	54,80,80	2.04	6 (11%)
4	ORN	D	503	-	5,8,8	0.57	0	3,9,9	0.58	0

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
4	ORN	A	503	-	-	0/4/8/8	0/0/0/0
2	FDA	B	501	-	-	0/30/50/50	0/6/6/6
3	NAP	B	502	-	-	0/27/67/67	0/5/5/5
4	ORN	B	503	-	-	0/4/8/8	0/0/0/0
2	FDA	C	501	-	-	0/30/50/50	0/6/6/6
3	NAP	C	502	-	-	0/27/67/67	0/5/5/5
4	ORN	C	503	-	-	0/4/8/8	0/0/0/0
2	FDA	D	501	-	-	0/30/50/50	0/6/6/6
3	NAP	D	502	-	-	0/27/67/67	0/5/5/5
4	ORN	D	503	-	-	0/4/8/8	0/0/0/0

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FDA	O2B-C2B	-5.61	1.29	1.43
2	B	501	FDA	O2B-C2B	-5.30	1.30	1.43
2	D	501	FDA	O2B-C2B	-5.27	1.30	1.43
2	C	501	FDA	O2B-C2B	-5.22	1.30	1.43
3	A	502	NAP	C2D-C3D	-4.13	1.42	1.53
3	A	502	NAP	C3B-C2B	-4.12	1.43	1.53
3	C	502	NAP	C3B-C2B	-4.00	1.44	1.53
2	D	501	FDA	C2B-C3B	-3.96	1.42	1.53
2	C	501	FDA	C2B-C3B	-3.86	1.42	1.53
2	A	501	FDA	C2B-C3B	-3.84	1.42	1.53
3	B	502	NAP	C3B-C2B	-3.81	1.44	1.53
3	D	502	NAP	C2D-C3D	-3.76	1.43	1.53
2	D	501	FDA	O3'-C3'	-3.73	1.34	1.43
2	B	501	FDA	C2B-C3B	-3.71	1.43	1.53
3	D	502	NAP	C3B-C2B	-3.69	1.44	1.53
3	C	502	NAP	C2D-C3D	-3.67	1.43	1.53
2	A	501	FDA	O3'-C3'	-3.62	1.34	1.43
2	A	501	FDA	O4B-C1B	-3.60	1.36	1.41
3	B	502	NAP	C2D-C3D	-3.50	1.43	1.53
2	B	501	FDA	O3'-C3'	-3.40	1.34	1.43
2	B	501	FDA	C9A-N10	-3.26	1.34	1.38
2	C	501	FDA	O4B-C1B	-3.20	1.37	1.41
2	D	501	FDA	O2'-C2'	-3.08	1.36	1.43
2	C	501	FDA	O3'-C3'	-3.08	1.35	1.43
2	A	501	FDA	C10-N10	-2.99	1.35	1.39
2	B	501	FDA	O4B-C1B	-2.87	1.37	1.41
2	C	501	FDA	O2'-C2'	-2.87	1.36	1.43
2	C	501	FDA	C9A-N10	-2.84	1.34	1.38
2	D	501	FDA	O4'-C4'	-2.82	1.37	1.43
2	D	501	FDA	C9A-N10	-2.69	1.35	1.38
2	A	501	FDA	O2'-C2'	-2.47	1.37	1.43
2	C	501	FDA	O4'-C4'	-2.47	1.37	1.43
2	B	501	FDA	O2'-C2'	-2.44	1.37	1.43
2	B	501	FDA	O4'-C4'	-2.38	1.38	1.43
2	A	501	FDA	C9A-N10	-2.37	1.35	1.38
2	A	501	FDA	O4'-C4'	-2.26	1.38	1.43
2	C	501	FDA	C9A-C5X	-2.21	1.38	1.42
2	D	501	FDA	C9A-C5X	-2.15	1.38	1.42
2	C	501	FDA	C10-N10	-2.09	1.36	1.39
3	D	502	NAP	O4B-C1B	-2.06	1.38	1.41
2	D	501	FDA	O4B-C1B	-2.06	1.38	1.41
3	A	502	NAP	O4D-C4D	-2.02	1.40	1.45
2	B	501	FDA	C2A-N3A	2.04	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	FDA	O3B-C3B	2.10	1.48	1.43
2	B	501	FDA	O3B-C3B	2.19	1.48	1.43
3	A	502	NAP	C2A-N3A	2.20	1.36	1.32
3	C	502	NAP	O4D-C1D	2.20	1.44	1.41
2	A	501	FDA	C2A-N3A	2.22	1.36	1.32
3	C	502	NAP	C2A-N3A	2.22	1.36	1.32
2	B	501	FDA	PA-O1A	2.32	1.59	1.51
2	A	501	FDA	C5'-C4'	2.33	1.55	1.51
2	D	501	FDA	PA-O1A	2.42	1.60	1.51
2	B	501	FDA	C4X-N5	2.46	1.37	1.33
2	C	501	FDA	PA-O1A	2.57	1.60	1.51
2	A	501	FDA	PA-O1A	2.62	1.60	1.51
2	C	501	FDA	C5'-C4'	2.91	1.56	1.51
2	D	501	FDA	C4X-N5	3.26	1.38	1.33
2	C	501	FDA	C4X-N5	3.34	1.38	1.33
2	A	501	FDA	C4-C4X	3.37	1.48	1.41
3	D	502	NAP	C7N-N7N	3.49	1.40	1.33
2	B	501	FDA	C4-C4X	3.51	1.48	1.41
2	A	501	FDA	C4X-N5	3.52	1.38	1.33
3	A	502	NAP	C7N-N7N	3.52	1.40	1.33
3	C	502	NAP	C7N-N7N	3.67	1.40	1.33
3	B	502	NAP	C7N-N7N	3.70	1.40	1.33
3	B	502	NAP	C6A-N6A	3.71	1.46	1.34
2	C	501	FDA	C4-C4X	3.78	1.48	1.41
3	D	502	NAP	C6A-N6A	3.87	1.46	1.34
3	A	502	NAP	C6A-N6A	3.92	1.47	1.34
3	C	502	NAP	C6A-N6A	3.96	1.47	1.34
2	D	501	FDA	C4-C4X	3.99	1.49	1.41
2	A	501	FDA	C6A-N6A	4.08	1.47	1.34
2	D	501	FDA	C1'-N10	4.21	1.52	1.48
2	B	501	FDA	C6A-N6A	4.22	1.48	1.34
2	C	501	FDA	C6A-N6A	4.32	1.48	1.34
2	D	501	FDA	C6A-N6A	4.35	1.48	1.34
2	C	501	FDA	C1'-N10	4.55	1.53	1.48
2	A	501	FDA	C4-N3	4.62	1.41	1.33
2	B	501	FDA	C10-N1	4.86	1.43	1.35
2	D	501	FDA	C4-N3	4.92	1.42	1.33
2	B	501	FDA	C1'-N10	4.95	1.53	1.48
2	A	501	FDA	C10-N1	4.96	1.43	1.35
2	C	501	FDA	C10-N1	5.12	1.44	1.35
2	B	501	FDA	C4-N3	5.14	1.42	1.33
2	A	501	FDA	C1'-N10	5.22	1.53	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	FDA	C10-N1	5.60	1.44	1.35
2	C	501	FDA	C4-N3	5.66	1.43	1.33

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	FDA	N3A-C2A-N1A	-11.73	119.91	128.89
3	D	502	NAP	N3A-C2A-N1A	-11.48	120.10	128.89
2	C	501	FDA	N3A-C2A-N1A	-11.15	120.36	128.89
2	B	501	FDA	N3A-C2A-N1A	-10.76	120.66	128.89
3	B	502	NAP	N3A-C2A-N1A	-10.71	120.69	128.89
3	C	502	NAP	N3A-C2A-N1A	-10.64	120.75	128.89
2	D	501	FDA	N3A-C2A-N1A	-10.33	120.98	128.89
3	A	502	NAP	N3A-C2A-N1A	-9.33	121.75	128.89
2	C	501	FDA	O5'-P-O1P	-7.51	80.48	109.62
2	C	501	FDA	O3P-PA-O5B	-6.30	86.21	102.94
2	C	501	FDA	O2P-P-O5'	-4.65	85.03	108.46
2	D	501	FDA	C4X-C4-N3	-3.55	118.74	123.59
2	D	501	FDA	C4X-C10-N10	-3.46	118.48	120.52
2	B	501	FDA	C4X-C4-N3	-3.29	119.08	123.59
2	C	501	FDA	O2A-PA-O3P	-3.28	90.20	105.09
2	A	501	FDA	C4-C4X-C10	-3.22	117.88	119.94
3	A	502	NAP	C4B-O4B-C1B	-3.11	106.31	109.72
2	C	501	FDA	C4X-C10-N10	-3.11	118.69	120.52
2	C	501	FDA	O3P-P-O5'	-3.09	94.73	102.94
3	B	502	NAP	C4B-O4B-C1B	-3.00	106.42	109.72
2	A	501	FDA	C4X-C4-N3	-2.99	119.50	123.59
2	B	501	FDA	P-O3P-PA	-2.93	124.49	132.73
2	D	501	FDA	C1B-N9A-C4A	-2.93	122.52	126.94
3	C	502	NAP	PN-O3-PA	-2.85	124.73	132.73
2	C	501	FDA	O2'-C2'-C1'	-2.84	102.96	109.94
3	A	502	NAP	C4A-C5A-N7A	-2.84	106.86	109.48
2	C	501	FDA	C1B-N9A-C4A	-2.79	122.73	126.94
2	A	501	FDA	C4A-C5A-N7A	-2.76	106.94	109.48
2	D	501	FDA	P-O3P-PA	-2.75	125.00	132.73
3	A	502	NAP	PN-O3-PA	-2.68	125.20	132.73
2	A	501	FDA	C4X-C10-N10	-2.65	118.95	120.52
3	B	502	NAP	C4A-C5A-N7A	-2.52	107.16	109.48
2	B	501	FDA	C4B-O4B-C1B	-2.48	106.99	109.72
2	C	501	FDA	C4X-C4-N3	-2.48	120.20	123.59
3	D	502	NAP	PN-O3-PA	-2.40	125.98	132.73
3	C	502	NAP	C4B-O4B-C1B	-2.39	107.09	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	502	NAP	C4A-C5A-N7A	-2.38	107.29	109.48
2	D	501	FDA	C4B-O4B-C1B	-2.38	107.11	109.72
2	C	501	FDA	C4B-O4B-C1B	-2.35	107.13	109.72
3	C	502	NAP	O7N-C7N-N7N	-2.31	119.34	122.59
3	B	502	NAP	PN-O3-PA	-2.14	126.73	132.73
3	A	502	NAP	C1B-N9A-C4A	-2.12	123.74	126.94
2	D	501	FDA	C4A-C5A-N7A	-2.12	107.53	109.48
2	A	501	FDA	C1B-N9A-C4A	-2.06	123.84	126.94
2	C	501	FDA	O5B-C5B-C4B	2.01	116.52	109.12
3	D	502	NAP	O5D-C5D-C4D	2.03	116.60	109.12
2	C	501	FDA	O2A-PA-O1A	2.05	123.64	112.53
3	C	502	NAP	O4B-C1B-N9A	2.06	112.41	108.10
2	D	501	FDA	O4B-C4B-C5B	2.07	116.72	109.32
3	A	502	NAP	C3N-C7N-N7N	2.14	120.16	117.82
2	A	501	FDA	O2P-P-O3P	2.16	114.89	105.09
3	B	502	NAP	C2N-C3N-C4N	2.20	120.73	118.29
3	D	502	NAP	O2B-P2B-O1X	2.31	112.87	107.11
3	C	502	NAP	O4B-C4B-C5B	2.34	117.68	109.32
3	D	502	NAP	O3-PN-O5D	2.35	109.16	102.94
2	D	501	FDA	C1'-N10-C9A	2.35	121.50	118.86
2	B	501	FDA	C5X-C9A-N10	2.38	119.42	117.62
2	B	501	FDA	C4-C4X-N5	2.39	121.62	118.72
3	A	502	NAP	O4B-C4B-C5B	2.41	117.94	109.32
3	A	502	NAP	C2N-C3N-C4N	2.44	121.00	118.29
2	C	501	FDA	O5B-PA-O1A	2.46	119.15	109.62
2	C	501	FDA	C2B-C1B-N9A	2.49	118.10	114.29
2	D	501	FDA	O2P-P-O3P	2.51	116.50	105.09
2	A	501	FDA	C4-C4X-N5	2.65	121.94	118.72
2	D	501	FDA	C5X-C9A-N10	2.67	119.65	117.62
2	D	501	FDA	C4-C4X-N5	2.69	121.98	118.72
2	B	501	FDA	O2P-P-O3P	2.76	117.60	105.09
2	A	501	FDA	C2B-C1B-N9A	2.76	118.50	114.29
2	B	501	FDA	O4B-C4B-C5B	2.76	119.21	109.32
2	C	501	FDA	C4-C4X-N5	2.94	122.28	118.72
2	C	501	FDA	C5X-C9A-N10	2.95	119.86	117.62
2	C	501	FDA	O2P-P-O3P	2.96	118.53	105.09
3	B	502	NAP	C3N-C7N-N7N	3.14	121.26	117.82
3	B	502	NAP	O3-PN-O5D	3.18	111.36	102.94
2	B	501	FDA	O3P-P-O5'	3.30	111.70	102.94
3	C	502	NAP	C3N-C7N-N7N	3.49	121.63	117.82
2	A	501	FDA	C1'-N10-C9A	3.80	123.13	118.86
2	D	501	FDA	O3P-P-O5'	3.96	113.45	102.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	FDA	O3P-P-O5'	4.36	114.49	102.94
3	A	502	NAP	O4D-C1D-N1N	4.36	112.92	108.13
3	C	502	NAP	O4D-C1D-N1N	4.46	113.03	108.13
2	A	501	FDA	C5X-C9A-N10	4.62	121.13	117.62
2	C	501	FDA	C4-N3-C2	5.01	119.58	115.25
3	B	502	NAP	O4D-C1D-N1N	5.26	113.91	108.13
3	D	502	NAP	O4D-C1D-N1N	5.61	114.30	108.13
2	B	501	FDA	C4-N3-C2	6.62	120.97	115.25
2	D	501	FDA	C4-N3-C2	6.92	121.23	115.25
2	A	501	FDA	C4-N3-C2	7.35	121.60	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FDA	3	0
4	B	503	ORN	1	0
2	C	501	FDA	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	415/443 (93%)	-0.12	9 (2%) 65 68	19, 28, 50, 76	0
1	B	415/443 (93%)	0.00	6 (1%) 78 80	20, 30, 53, 70	0
1	C	415/443 (93%)	0.20	21 (5%) 32 33	21, 35, 63, 76	0
1	D	415/443 (93%)	-0.08	6 (1%) 78 80	21, 33, 54, 68	0
All	All	1660/1772 (93%)	-0.00	42 (2%) 61 64	19, 32, 57, 76	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	424	SER	6.3
1	C	177	ASP	4.4
1	C	134	GLY	4.4
1	D	424	SER	4.1
1	C	135	PRO	4.0
1	C	36	ALA	3.9
1	A	10	PRO	3.8
1	B	366	ALA	3.8
1	A	194	ASP	3.6
1	C	151	ALA	3.6
1	D	366	ALA	3.6
1	A	193	ARG	3.5
1	C	149	PRO	3.4
1	B	424	SER	3.1
1	C	384	LEU	2.9
1	C	120	HIS	2.8
1	A	318	ASP	2.7
1	C	10	PRO	2.7
1	D	120	HIS	2.6
1	C	155	VAL	2.6
1	B	150	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	196	ARG	2.5
1	C	152	THR	2.5
1	D	149	PRO	2.4
1	B	195	PRO	2.4
1	C	153	ARG	2.4
1	C	136	GLY	2.4
1	C	11	THR	2.4
1	A	424	SER	2.3
1	C	138	PRO	2.3
1	B	194	ASP	2.2
1	D	317	ALA	2.2
1	A	192	ASP	2.2
1	A	137	ARG	2.2
1	A	366	ALA	2.2
1	C	150	GLU	2.1
1	A	198	LEU	2.1
1	C	422	ARG	2.1
1	D	175	GLN	2.1
1	C	121	GLU	2.1
1	C	139	VAL	2.1
1	C	35	ALA	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
4	ORN	B	503	9/9	0.95	0.17	1.16	25,30,31,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	ORN	D	503	9/9	0.92	0.15	0.14	27,30,34,34	0
4	ORN	C	503	9/9	0.94	0.17	0.08	28,31,33,34	0
3	NAP	B	502	48/48	0.97	0.13	-0.00	19,25,29,38	0
5	K	A	504	1/1	0.94	0.10	-0.04	44,44,44,44	0
2	FDA	A	501	53/53	0.97	0.12	-0.21	19,23,26,27	0
2	FDA	B	501	53/53	0.96	0.12	-0.25	16,23,29,31	0
2	FDA	C	501	53/53	0.94	0.13	-0.29	19,28,42,44	0
3	NAP	C	502	48/48	0.97	0.12	-0.37	21,26,33,42	0
3	NAP	A	502	48/48	0.98	0.12	-0.39	15,24,30,42	0
3	NAP	D	502	48/48	0.97	0.11	-0.50	21,26,31,36	0
2	FDA	D	501	53/53	0.96	0.10	-0.87	22,28,33,34	0
5	K	C	504	1/1	0.88	0.11	-0.97	58,58,58,58	0
5	K	D	504	1/1	0.96	0.08	-1.12	46,46,46,46	0
4	ORN	A	503	9/9	0.96	0.13	-1.13	22,26,29,30	0
5	K	D	505	1/1	0.89	0.07	-1.32	51,51,51,51	0
5	K	C	505	1/1	0.93	0.08	-1.79	57,57,57,57	0
5	K	A	505	1/1	0.98	0.07	-1.90	45,45,45,45	0
5	K	B	504	1/1	0.94	0.09	-2.12	49,49,49,49	0
5	K	B	505	1/1	0.94	0.08	-2.23	54,54,54,54	0
5	K	A	506	1/1	0.83	0.08	-	58,58,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.