Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:56 PM GMT

PDB ID	:	4GMG
Title	:	NADP+ bound structure of a Thiazolinyl Imine Reductase from Yersinia enterocolitica (Irp3)
Authors	:	Lamb, A.L.; Meneely, K.M.
Deposited on	:	2012-08-15
Resolution	:	2.31 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:

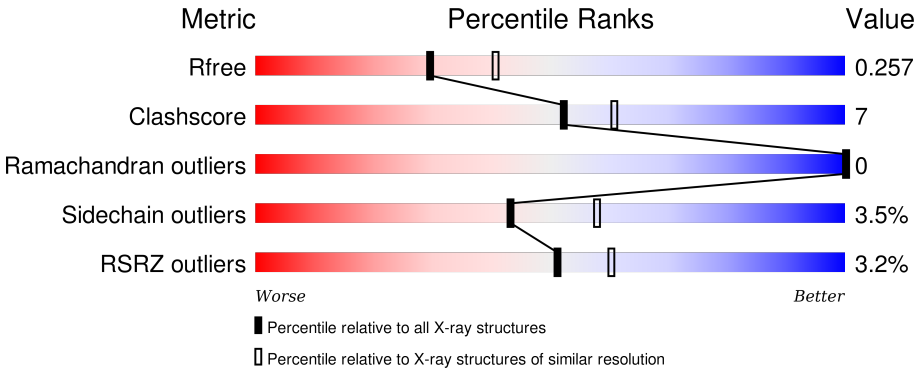
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.31 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	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (2.34-2.30)

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	385	4% 76% 16% • 7%
1	B	385	2% 71% 16% • 10%
1	C	385	2% 70% 15% • 13%
1	D	385	4% 74% 14% • 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11156 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 Yersiniabactin biosynthetic protein YbtU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2806	1784	511	495	16			
1	B	345	Total	C	N	O	S	0	0	0
			2715	1728	493	479	15			
1	C	336	Total	C	N	O	S	0	0	0
			2636	1679	476	466	15			
1	D	343	Total	C	N	O	S	0	0	0
			2699	1719	489	476	15			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP A1JTG0
A	-18	GLY	-	EXPRESSION TAG	UNP A1JTG0
A	-17	SER	-	EXPRESSION TAG	UNP A1JTG0
A	-16	SER	-	EXPRESSION TAG	UNP A1JTG0
A	-15	HIS	-	EXPRESSION TAG	UNP A1JTG0
A	-14	HIS	-	EXPRESSION TAG	UNP A1JTG0
A	-13	HIS	-	EXPRESSION TAG	UNP A1JTG0
A	-12	HIS	-	EXPRESSION TAG	UNP A1JTG0
A	-11	HIS	-	EXPRESSION TAG	UNP A1JTG0
A	-10	HIS	-	EXPRESSION TAG	UNP A1JTG0
A	-9	SER	-	EXPRESSION TAG	UNP A1JTG0
A	-8	SER	-	EXPRESSION TAG	UNP A1JTG0
A	-7	GLY	-	EXPRESSION TAG	UNP A1JTG0
A	-6	LEU	-	EXPRESSION TAG	UNP A1JTG0
A	-5	VAL	-	EXPRESSION TAG	UNP A1JTG0
A	-4	PRO	-	EXPRESSION TAG	UNP A1JTG0
A	-3	ARG	-	EXPRESSION TAG	UNP A1JTG0
A	-2	GLY	-	EXPRESSION TAG	UNP A1JTG0
A	-1	SER	-	EXPRESSION TAG	UNP A1JTG0
A	0	HIS	-	EXPRESSION TAG	UNP A1JTG0
B	-19	MET	-	EXPRESSION TAG	UNP A1JTG0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	EXPRESSION TAG	UNP A1JTG0
B	-17	SER	-	EXPRESSION TAG	UNP A1JTG0
B	-16	SER	-	EXPRESSION TAG	UNP A1JTG0
B	-15	HIS	-	EXPRESSION TAG	UNP A1JTG0
B	-14	HIS	-	EXPRESSION TAG	UNP A1JTG0
B	-13	HIS	-	EXPRESSION TAG	UNP A1JTG0
B	-12	HIS	-	EXPRESSION TAG	UNP A1JTG0
B	-11	HIS	-	EXPRESSION TAG	UNP A1JTG0
B	-10	HIS	-	EXPRESSION TAG	UNP A1JTG0
B	-9	SER	-	EXPRESSION TAG	UNP A1JTG0
B	-8	SER	-	EXPRESSION TAG	UNP A1JTG0
B	-7	GLY	-	EXPRESSION TAG	UNP A1JTG0
B	-6	LEU	-	EXPRESSION TAG	UNP A1JTG0
B	-5	VAL	-	EXPRESSION TAG	UNP A1JTG0
B	-4	PRO	-	EXPRESSION TAG	UNP A1JTG0
B	-3	ARG	-	EXPRESSION TAG	UNP A1JTG0
B	-2	GLY	-	EXPRESSION TAG	UNP A1JTG0
B	-1	SER	-	EXPRESSION TAG	UNP A1JTG0
B	0	HIS	-	EXPRESSION TAG	UNP A1JTG0
C	-19	MET	-	EXPRESSION TAG	UNP A1JTG0
C	-18	GLY	-	EXPRESSION TAG	UNP A1JTG0
C	-17	SER	-	EXPRESSION TAG	UNP A1JTG0
C	-16	SER	-	EXPRESSION TAG	UNP A1JTG0
C	-15	HIS	-	EXPRESSION TAG	UNP A1JTG0
C	-14	HIS	-	EXPRESSION TAG	UNP A1JTG0
C	-13	HIS	-	EXPRESSION TAG	UNP A1JTG0
C	-12	HIS	-	EXPRESSION TAG	UNP A1JTG0
C	-11	HIS	-	EXPRESSION TAG	UNP A1JTG0
C	-10	HIS	-	EXPRESSION TAG	UNP A1JTG0
C	-9	SER	-	EXPRESSION TAG	UNP A1JTG0
C	-8	SER	-	EXPRESSION TAG	UNP A1JTG0
C	-7	GLY	-	EXPRESSION TAG	UNP A1JTG0
C	-6	LEU	-	EXPRESSION TAG	UNP A1JTG0
C	-5	VAL	-	EXPRESSION TAG	UNP A1JTG0
C	-4	PRO	-	EXPRESSION TAG	UNP A1JTG0
C	-3	ARG	-	EXPRESSION TAG	UNP A1JTG0
C	-2	GLY	-	EXPRESSION TAG	UNP A1JTG0
C	-1	SER	-	EXPRESSION TAG	UNP A1JTG0
C	0	HIS	-	EXPRESSION TAG	UNP A1JTG0
D	-19	MET	-	EXPRESSION TAG	UNP A1JTG0
D	-18	GLY	-	EXPRESSION TAG	UNP A1JTG0
D	-17	SER	-	EXPRESSION TAG	UNP A1JTG0

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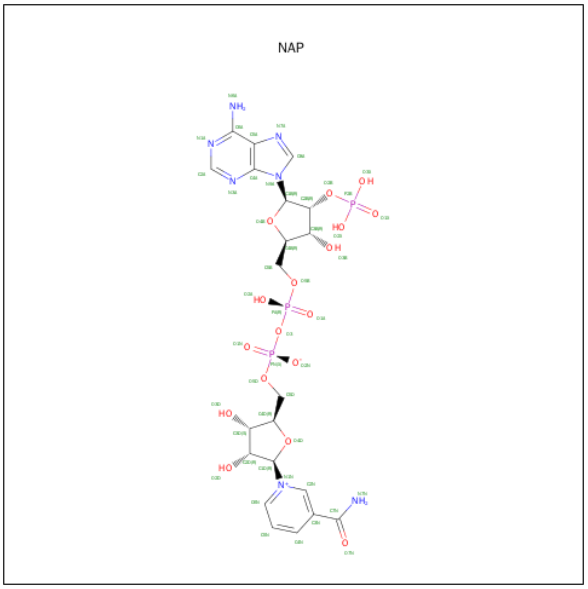
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	EXPRESSION TAG	UNP A1JTG0
D	-15	HIS	-	EXPRESSION TAG	UNP A1JTG0
D	-14	HIS	-	EXPRESSION TAG	UNP A1JTG0
D	-13	HIS	-	EXPRESSION TAG	UNP A1JTG0
D	-12	HIS	-	EXPRESSION TAG	UNP A1JTG0
D	-11	HIS	-	EXPRESSION TAG	UNP A1JTG0
D	-10	HIS	-	EXPRESSION TAG	UNP A1JTG0
D	-9	SER	-	EXPRESSION TAG	UNP A1JTG0
D	-8	SER	-	EXPRESSION TAG	UNP A1JTG0
D	-7	GLY	-	EXPRESSION TAG	UNP A1JTG0
D	-6	LEU	-	EXPRESSION TAG	UNP A1JTG0
D	-5	VAL	-	EXPRESSION TAG	UNP A1JTG0
D	-4	PRO	-	EXPRESSION TAG	UNP A1JTG0
D	-3	ARG	-	EXPRESSION TAG	UNP A1JTG0
D	-2	GLY	-	EXPRESSION TAG	UNP A1JTG0
D	-1	SER	-	EXPRESSION TAG	UNP A1JTG0
D	0	HIS	-	EXPRESSION TAG	UNP A1JTG0

- Molecule 2 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
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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

- Molecule 3 is water.

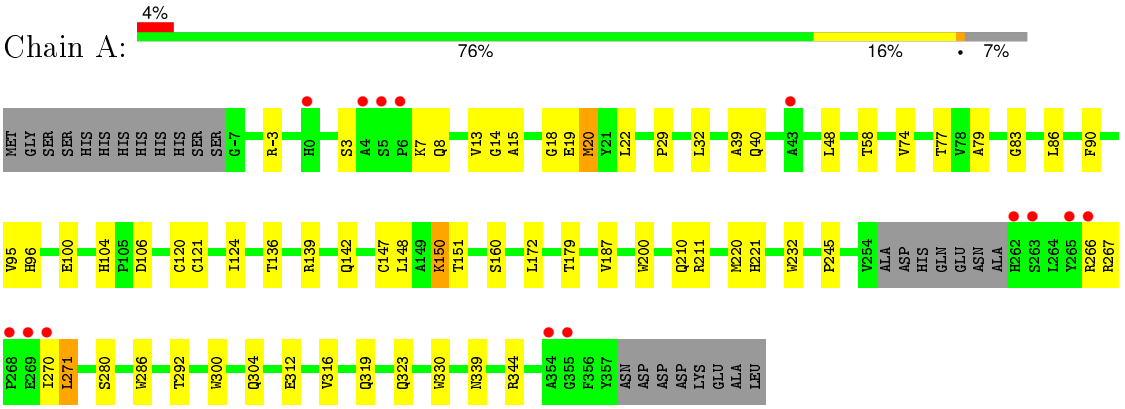
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	29	Total	O	0	0
			29	29		
3	B	34	Total	O	0	0
			34	34		
3	C	23	Total	O	0	0
			23	23		
3	D	22	Total	O	0	0
			22	22		

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.

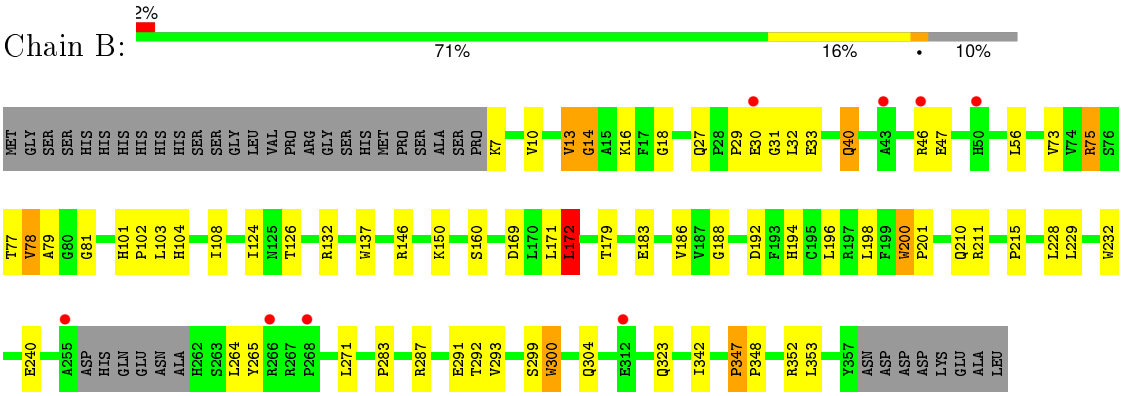
- Molecule 1: Yersiniabactin biosynthetic protein YbtU

Chain A:



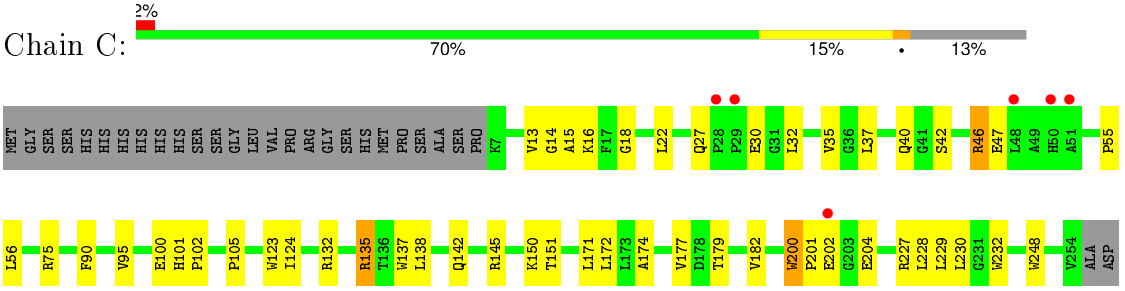
- Molecule 1: Yersiniabactin biosynthetic protein YbtU

Chain B:



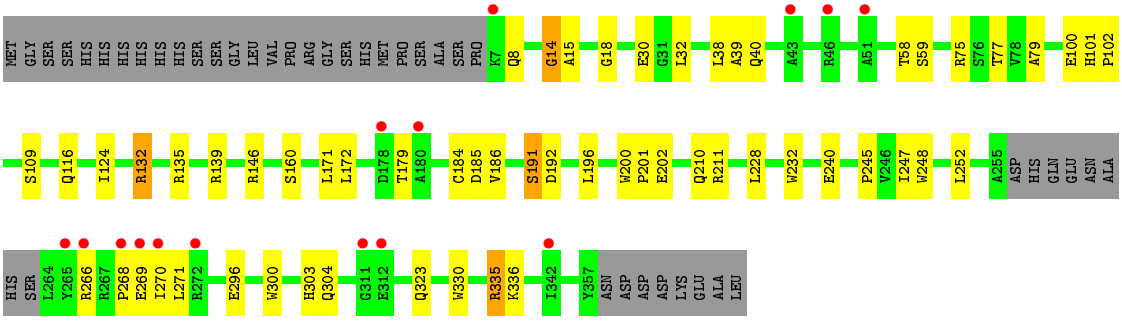
- Molecule 1: Yersiniabactin biosynthetic protein YbtU

Chain C:



• Molecule 1: Yersiniabactin biosynthetic protein YbtU

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	83.42Å 93.82Å 181.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.89 – 2.31 39.89 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.89-2.31) 99.5 (39.89-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.39	Depositor
$< I/\sigma(I) >$ [1]	2.95 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.197 , 0.260 0.196 , 0.257	Depositor DCC
R_{free} test set	3214 reflections (5.36%)	DCC
Wilson B-factor (Å^2)	29.6	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 35.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	6 of 63389 reflections (0.009%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11156	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.76 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.5938e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: 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	0.92	4/2885 (0.1%)	0.92	3/3933 (0.1%)
1	B	0.89	4/2790 (0.1%)	0.91	4/3803 (0.1%)
1	C	0.94	6/2708 (0.2%)	0.94	7/3692 (0.2%)
1	D	0.84	3/2773 (0.1%)	0.88	1/3780 (0.0%)
All	All	0.90	17/11156 (0.2%)	0.91	15/15208 (0.1%)

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
1	A	0	1
1	B	0	2
1	D	0	1
All	All	0	4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	200	TRP	CD2-CE2	6.57	1.49	1.41
1	C	123	TRP	CD2-CE2	6.46	1.49	1.41
1	C	200	TRP	CD2-CE2	6.44	1.49	1.41
1	D	232	TRP	CD2-CE2	6.27	1.48	1.41
1	C	248	TRP	CD2-CE2	6.26	1.48	1.41
1	B	200	TRP	CD2-CE2	5.81	1.48	1.41
1	A	232	TRP	CD2-CE2	5.81	1.48	1.41
1	C	300	TRP	CD2-CE2	5.78	1.48	1.41
1	D	248	TRP	CD2-CE2	5.75	1.48	1.41
1	D	330	TRP	CD2-CE2	5.71	1.48	1.41
1	B	137	TRP	CD2-CE2	5.71	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	232	TRP	CD2-CE2	5.57	1.48	1.41
1	B	232	TRP	CD2-CE2	5.42	1.47	1.41
1	A	286	TRP	CD2-CE2	5.17	1.47	1.41
1	C	137	TRP	CD2-CE2	5.13	1.47	1.41
1	A	330	TRP	CD2-CE2	5.08	1.47	1.41
1	B	300	TRP	CD2-CE2	5.08	1.47	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	75	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	B	172	LEU	CA-CB-CG	-7.78	97.42	115.30
1	C	135	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	B	103	LEU	CA-CB-CG	6.45	130.14	115.30
1	B	81	GLY	N-CA-C	5.94	127.95	113.10
1	C	227	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	C	132	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	211	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	C	13	VAL	CA-C-N	5.22	126.65	116.20
1	D	15	ALA	N-CA-C	5.21	125.06	111.00
1	C	271	LEU	CA-CB-CG	5.16	127.17	115.30
1	B	240	GLU	OE1-CD-OE2	-5.05	117.24	123.30
1	A	-3	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	C	32	LEU	CA-CB-CG	5.02	126.85	115.30
1	A	15	ALA	N-CA-C	5.02	124.55	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	VAL	Peptide
1	B	13	VAL	Peptide
1	B	14	GLY	Peptide
1	D	14	GLY	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	2806	0	2785	41	1
1	B	2715	0	2691	40	0
1	C	2636	0	2615	34	1
1	D	2699	0	2679	39	0
2	A	48	0	25	3	0
2	B	48	0	25	4	0
2	C	48	0	25	4	0
2	D	48	0	25	4	0
3	A	29	0	0	0	0
3	B	34	0	0	1	0
3	C	23	0	0	0	0
3	D	22	0	0	1	0
All	All	11156	0	10870	146	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (146) 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:151:THR:HG21	1:C:202:GLU:OE1	1.36	1.23
1:C:151:THR:CG2	1:C:202:GLU:OE1	1.94	1.15
1:A:40:GLN:O	2:A:401:NAP:O1X	1.77	1.00
1:D:171:LEU:HD13	1:D:228:LEU:HD23	1.49	0.95
1:A:124:ILE:H	1:A:323:GLN:HE22	1.14	0.93
1:A:172:LEU:CD2	1:A:179:THR:HG23	1.99	0.93
1:D:132:ARG:HH11	1:D:132:ARG:HG2	1.38	0.89
1:D:172:LEU:HD13	1:D:179:THR:HG23	1.58	0.85
1:A:104:HIS:HD2	1:A:106:ASP:H	1.27	0.83
1:B:40:GLN:O	2:B:401:NAP:O3X	1.98	0.81
1:A:172:LEU:HD22	1:A:179:THR:HG23	1.60	0.81
1:B:124:ILE:H	1:B:323:GLN:HE22	1.30	0.80
1:D:184:CYS:O	1:D:336:LYS:HE2	1.82	0.79
1:A:96:HIS:HD2	1:A:121:CYS:H	1.27	0.79
1:D:124:ILE:H	1:D:323:GLN:HE22	1.32	0.78
1:B:171:LEU:HD13	1:B:228:LEU:HD23	1.66	0.77
1:C:124:ILE:H	1:C:323:GLN:HE22	1.31	0.77
1:C:172:LEU:HD22	1:C:179:THR:HG23	1.70	0.74
1:A:8:GLN:HB2	1:A:32:LEU:HD23	1.70	0.73
1:D:132:ARG:HG2	1:D:132:ARG:NH1	2.04	0.72
1:A:74:VAL:HG21	1:A:86:LEU:HD12	1.71	0.71
1:C:105:PRO:HD3	1:C:327:SER:OG	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:LYS:HB3	2:B:401:NAP:O2N	1.93	0.67
1:B:7:LYS:HE2	1:B:31:GLY:HA2	1.76	0.67
1:D:171:LEU:CD1	1:D:228:LEU:HD23	2.24	0.67
1:C:142:GLN:HG2	1:C:145:ARG:NH2	2.10	0.67
1:B:27:GLN:HE21	1:D:335:ARG:HE	1.41	0.66
1:A:104:HIS:CD2	1:A:106:ASP:H	2.11	0.65
1:D:75:ARG:HB3	1:D:79:ALA:HB3	1.79	0.64
1:D:8:GLN:HB2	1:D:32:LEU:HD23	1.79	0.64
1:D:270:ILE:O	1:D:271:LEU:HB2	1.97	0.63
1:C:307:SER:HB3	1:C:312:GLU:HG3	1.83	0.60
1:C:100:GLU:HG3	2:C:401:NAP:H1D	1.84	0.60
1:A:266:ARG:HG3	1:B:47:GLU:OE1	2.01	0.60
1:A:172:LEU:HD23	1:A:179:THR:HG23	1.83	0.59
1:D:40:GLN:O	2:D:401:NAP:O2X	2.19	0.59
1:A:312:GLU:HA	1:A:312:GLU:OE1	2.04	0.58
1:C:151:THR:HG23	1:C:202:GLU:OE1	1.98	0.56
1:A:96:HIS:CD2	1:A:120:CYS:HB2	2.40	0.56
1:B:29:PRO:HG2	1:B:32:LEU:HD13	1.88	0.55
1:D:200:TRP:HB2	1:D:201:PRO:HD2	1.88	0.55
1:B:172:LEU:HD22	1:B:179:THR:OG1	2.05	0.55
1:B:186:VAL:HA	1:B:196:LEU:HD23	1.89	0.55
1:B:46:ARG:HG2	1:B:56:LEU:HD22	1.89	0.55
1:C:16:LYS:HE2	2:C:401:NAP:H51A	1.89	0.55
1:B:108:ILE:HG12	1:B:124:ILE:HD11	1.87	0.54
1:D:132:ARG:CG	1:D:132:ARG:HH11	2.17	0.54
1:C:172:LEU:HD21	1:C:182:VAL:HG21	1.90	0.54
1:A:187:VAL:CG1	1:B:188:GLY:HA3	2.37	0.54
1:D:300:TRP:O	1:D:304:GLN:HG2	2.08	0.53
1:A:3:SER:HB2	1:A:7:LYS:HE2	1.89	0.53
1:B:46:ARG:HG2	1:B:56:LEU:CD2	2.39	0.52
1:B:75:ARG:HG2	1:B:79:ALA:HB1	1.90	0.52
1:A:19:GLU:HA	1:A:22:LEU:HD12	1.91	0.52
1:A:100:GLU:HG3	2:A:401:NAP:H1D	1.91	0.51
1:D:135:ARG:NH2	1:D:296:GLU:OE1	2.44	0.50
1:C:30:GLU:O	1:C:303:HIS:HE1	1.94	0.50
1:B:126:THR:OG1	1:B:169:ASP:OD2	2.19	0.50
1:B:75:ARG:HD3	2:B:401:NAP:O2A	2.12	0.50
1:D:269:GLU:CD	1:D:269:GLU:H	2.16	0.50
1:B:132:ARG:NH2	1:D:185:ASP:OD2	2.45	0.49
1:D:101:HIS:HB2	1:D:102:PRO:HA	1.94	0.49
1:D:160:SER:HA	1:D:210:GLN:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:LEU:C	1:C:229:LEU:HD23	2.33	0.49
1:A:74:VAL:CG2	1:A:83:GLY:HA2	2.43	0.49
1:A:245:PRO:HA	1:A:280:SER:O	2.12	0.49
1:A:14:GLY:O	1:A:18:GLY:HA3	2.12	0.48
1:B:14:GLY:O	1:B:18:GLY:HA3	2.13	0.48
1:C:138:LEU:O	1:C:142:GLN:HG3	2.14	0.48
1:A:136:THR:HG21	1:A:280:SER:HB2	1.94	0.48
1:D:240:GLU:HB2	1:D:245:PRO:HD2	1.96	0.48
1:A:74:VAL:HG23	1:A:83:GLY:CA	2.44	0.47
1:D:75:ARG:HG3	2:D:401:NAP:O2A	2.14	0.47
1:C:101:HIS:HB2	1:C:102:PRO:HA	1.97	0.47
1:B:229:LEU:C	1:B:229:LEU:HD23	2.35	0.47
1:A:147:CYS:HB3	1:B:352:ARG:O	2.15	0.47
1:C:15:ALA:HB2	1:C:37:LEU:HD21	1.96	0.47
1:A:270:ILE:O	1:A:271:LEU:HB2	2.14	0.46
1:A:150:LYS:HA	1:A:150:LYS:HE3	1.97	0.46
1:A:74:VAL:HG23	1:A:83:GLY:HA2	1.97	0.46
1:B:77:THR:O	1:B:79:ALA:O	2.33	0.46
1:C:200:TRP:HB2	1:C:201:PRO:HD2	1.97	0.46
1:B:291:GLU:O	1:D:335:ARG:NH1	2.49	0.46
1:C:287:ARG:O	1:C:291:GLU:HG3	2.16	0.46
1:C:47:GLU:OE1	1:D:266:ARG:HG3	2.15	0.46
1:A:100:GLU:CG	2:A:401:NAP:H1D	2.47	0.45
1:D:39:ALA:O	1:D:58:THR:HA	2.15	0.45
1:D:100:GLU:HG3	2:D:401:NAP:H1D	1.98	0.45
1:B:215:PRO:CD	1:B:342:ILE:HG23	2.47	0.45
1:C:174:ALA:HB1	1:C:230:LEU:HD11	1.98	0.45
1:C:151:THR:HG21	1:C:202:GLU:CD	2.26	0.45
1:D:200:TRP:HB2	1:D:201:PRO:CD	2.47	0.45
1:C:171:LEU:HD13	1:C:228:LEU:HD23	1.99	0.45
1:A:300:TRP:O	1:A:304:GLN:HG2	2.17	0.45
1:B:29:PRO:HG2	1:B:32:LEU:CD1	2.47	0.45
1:A:29:PRO:HG2	1:A:32:LEU:HD12	1.98	0.44
1:D:14:GLY:HA2	1:D:38:LEU:O	2.16	0.44
1:A:77:THR:O	1:A:79:ALA:O	2.36	0.44
1:B:78:VAL:HG22	1:B:104:HIS:HB2	1.98	0.44
1:C:270:ILE:HG12	1:C:271:LEU:N	2.32	0.44
1:C:172:LEU:CD2	1:C:179:THR:HG23	2.44	0.44
1:A:39:ALA:O	1:A:58:THR:HA	2.18	0.44
1:C:22:LEU:HD11	1:C:37:LEU:HD22	1.98	0.44
1:D:14:GLY:O	1:D:18:GLY:HA3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:VAL:HA	1:D:196:LEU:HD23	2.00	0.44
1:C:46:ARG:HA	1:C:56:LEU:HD22	1.99	0.43
1:B:283:PRO:HG3	1:B:293:VAL:HG21	2.00	0.43
1:D:266:ARG:C	1:D:268:PRO:HD3	2.39	0.43
1:B:13:VAL:O	1:B:73:VAL:N	2.36	0.43
1:C:14:GLY:O	1:C:18:GLY:HA3	2.18	0.43
1:D:192:ASP:C	1:D:211:ARG:HG2	2.38	0.43
1:A:22:LEU:CD1	1:A:48:LEU:HD13	2.48	0.43
1:C:46:ARG:HA	1:C:56:LEU:CD2	2.49	0.42
1:D:146:ARG:NH1	3:D:501:HOH:O	2.51	0.42
1:A:8:GLN:HB2	1:A:32:LEU:CD2	2.43	0.42
1:D:77:THR:O	1:D:79:ALA:O	2.37	0.42
1:B:192:ASP:O	1:B:211:ARG:HG2	2.18	0.42
1:B:101:HIS:HB2	1:B:102:PRO:HA	2.01	0.42
1:C:90:PHE:HB3	1:C:95:VAL:HB	2.01	0.42
1:B:194:HIS:HD2	3:B:512:HOH:O	2.02	0.42
1:B:183:GLU:O	1:B:198:LEU:HA	2.19	0.42
1:A:220:MET:O	1:A:221:HIS:HB2	2.19	0.42
1:A:267:ARG:O	1:A:270:ILE:HG22	2.20	0.42
1:D:40:GLN:C	2:D:401:NAP:O2X	2.58	0.42
1:B:160:SER:HA	1:B:210:GLN:HB3	2.02	0.41
1:C:42:SER:OG	2:C:401:NAP:O1X	2.28	0.41
1:B:200:TRP:HB2	1:B:201:PRO:HD2	2.03	0.41
1:C:135:ARG:NH2	1:C:296:GLU:OE1	2.41	0.41
1:B:300:TRP:O	1:B:304:GLN:HG2	2.20	0.41
1:D:30:GLU:HB2	1:D:303:HIS:CD2	2.54	0.41
1:A:319:GLN:O	1:A:323:GLN:HG3	2.21	0.41
1:A:148:LEU:HD21	1:B:353:LEU:HD21	2.03	0.41
1:A:160:SER:HA	1:A:210:GLN:HB3	2.03	0.41
1:A:104:HIS:CD2	1:A:106:ASP:HB2	2.54	0.41
1:C:35:VAL:O	1:C:55:PRO:HG2	2.20	0.41
1:B:347:PRO:HA	1:B:348:PRO:HD3	1.88	0.41
1:C:171:LEU:CD1	1:C:228:LEU:HD23	2.50	0.41
1:B:40:GLN:C	2:B:401:NAP:O3X	2.58	0.41
1:C:204:GLU:OE2	1:D:191:SER:N	2.48	0.41
1:A:90:PHE:HB3	1:A:95:VAL:HB	2.03	0.40
1:D:240:GLU:HG3	1:D:247:ILE:HD12	2.03	0.40
1:B:171:LEU:HA	1:B:171:LEU:HD12	1.82	0.40
1:A:20:MET:HE3	1:A:20:MET:HB2	1.98	0.40
1:D:200:TRP:CD1	1:D:202:GLU:HG2	2.56	0.40
2:C:401:NAP:H2D	2:C:401:NAP:H6N	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:VAL:N	1:B:33:GLU:O	2.48	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ASN:OD1	1:C:27:GLN:NE2[1_655]	2.17	0.03

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	354/385 (92%)	341 (96%)	13 (4%)	0	100	100
1	B	341/385 (89%)	329 (96%)	12 (4%)	0	100	100
1	C	332/385 (86%)	321 (97%)	11 (3%)	0	100	100
1	D	339/385 (88%)	329 (97%)	10 (3%)	0	100	100
All	All	1366/1540 (89%)	1320 (97%)	46 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	302/325 (93%)	293 (97%)	9 (3%)	48 65
1	B	291/325 (90%)	277 (95%)	14 (5%)	31 42
1	C	283/325 (87%)	273 (96%)	10 (4%)	43 58
1	D	289/325 (89%)	281 (97%)	8 (3%)	51 67
All	All	1165/1300 (90%)	1124 (96%)	41 (4%)	43 58

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	MET
1	A	139	ARG
1	A	142	GLN
1	A	150	LYS
1	A	151	THR
1	A	271	LEU
1	A	292	THR
1	A	316	VAL
1	A	344	ARG
1	B	30	GLU
1	B	40	GLN
1	B	75	ARG
1	B	78	VAL
1	B	146	ARG
1	B	150	LYS
1	B	172	LEU
1	B	264	LEU
1	B	265	TYR
1	B	271	LEU
1	B	287	ARG
1	B	292	THR
1	B	299	SER
1	B	347	PRO
1	C	40	GLN
1	C	46	ARG
1	C	150	LYS
1	C	177	VAL
1	C	270	ILE
1	C	272	ARG
1	C	287	ARG
1	C	319	GLN
1	C	331	GLN
1	C	351	ASP

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Mol	Chain	Res	Type
1	D	59	SER
1	D	109	SER
1	D	116	GLN
1	D	132	ARG
1	D	139	ARG
1	D	191	SER
1	D	252	LEU
1	D	335	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	104	HIS
1	A	130	HIS
1	A	156	HIS
1	A	323	GLN
1	A	331	GLN
1	B	194	HIS
1	B	323	GLN
1	B	350	HIS
1	C	303	HIS
1	C	319	GLN
1	C	323	GLN
1	C	332	GLN
1	C	350	HIS
1	D	303	HIS
1	D	323	GLN
1	D	339	ASN

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)

4 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	$\#\|Z\| > 2$
2	NAP	A	401	-	42,52,52	1.86	10 (23%)	54,80,80	1.79	7 (12%)
2	NAP	B	401	-	42,52,52	1.07	3 (7%)	54,80,80	2.18	11 (20%)
2	NAP	C	401	-	42,52,52	1.71	11 (26%)	54,80,80	1.65	8 (14%)
2	NAP	D	401	-	42,52,52	1.65	9 (21%)	54,80,80	1.36	7 (12%)

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	NAP	A	401	-	-	0/27/67/67	0/5/5/5
2	NAP	B	401	-	-	0/27/67/67	0/5/5/5
2	NAP	C	401	-	-	0/27/67/67	0/5/5/5
2	NAP	D	401	-	-	0/27/67/67	0/5/5/5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAP	PA-O2A	-3.83	1.38	1.54
2	C	401	NAP	PN-O1N	-3.71	1.37	1.51
2	D	401	NAP	P2B-O2X	-3.56	1.41	1.54
2	A	401	NAP	P2B-O2X	-3.48	1.42	1.54
2	C	401	NAP	P2B-O2X	-3.37	1.42	1.54
2	A	401	NAP	P2B-O3X	-3.28	1.42	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	NAP	PN-O2N	-3.16	1.41	1.54
2	A	401	NAP	PN-O1N	-3.11	1.39	1.51
2	D	401	NAP	P2B-O3X	-3.09	1.43	1.54
2	A	401	NAP	PN-O2N	-3.08	1.41	1.54
2	C	401	NAP	P2B-O3X	-3.01	1.43	1.54
2	C	401	NAP	PA-O2A	-2.94	1.42	1.54
2	A	401	NAP	P2B-O1X	-2.94	1.41	1.51
2	C	401	NAP	C5A-N7A	-2.89	1.29	1.39
2	A	401	NAP	O4D-C4D	-2.83	1.38	1.45
2	A	401	NAP	PA-O1A	-2.82	1.40	1.51
2	A	401	NAP	C5A-N7A	-2.81	1.29	1.39
2	D	401	NAP	O7N-C7N	-2.75	1.18	1.24
2	D	401	NAP	PN-O2N	-2.60	1.43	1.54
2	D	401	NAP	PA-O2A	-2.57	1.44	1.54
2	D	401	NAP	C4A-N3A	-2.49	1.31	1.35
2	D	401	NAP	C5A-N7A	-2.45	1.31	1.39
2	C	401	NAP	O4D-C4D	-2.45	1.39	1.45
2	D	401	NAP	PA-O1A	-2.45	1.42	1.51
2	D	401	NAP	O2D-C2D	-2.20	1.37	1.43
2	C	401	NAP	C2N-C3N	-2.09	1.35	1.39
2	C	401	NAP	O7N-C7N	-2.08	1.19	1.24
2	C	401	NAP	P2B-O1X	-2.08	1.44	1.51
2	C	401	NAP	PN-O5D	-2.04	1.49	1.59
2	A	401	NAP	O7N-C7N	-2.00	1.19	1.24
2	B	401	NAP	O4D-C1D	2.22	1.44	1.41
2	B	401	NAP	C5A-C4A	3.53	1.48	1.40
2	B	401	NAP	O4B-C1B	3.59	1.45	1.41

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	NAP	N3A-C2A-N1A	-8.99	122.01	128.89
2	B	401	NAP	N3A-C2A-N1A	-8.78	122.17	128.89
2	C	401	NAP	N3A-C2A-N1A	-7.73	122.97	128.89
2	B	401	NAP	C4A-C5A-N7A	-4.99	104.89	109.48
2	D	401	NAP	N3A-C2A-N1A	-4.85	125.18	128.89
2	A	401	NAP	O2B-P2B-O1X	-4.45	96.00	107.11
2	B	401	NAP	C5D-C4D-C3D	-4.41	97.70	115.21
2	C	401	NAP	C4A-C5A-N7A	-3.20	106.54	109.48
2	A	401	NAP	C4A-C5A-N7A	-3.10	106.62	109.48
2	B	401	NAP	O2N-PN-O5D	-2.95	93.59	108.46
2	C	401	NAP	C1B-N9A-C4A	-2.68	122.90	126.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	NAP	C1B-N9A-C4A	-2.67	122.92	126.94
2	D	401	NAP	C4A-C5A-N7A	-2.59	107.10	109.48
2	B	401	NAP	C5N-C4N-C3N	-2.31	117.43	120.33
2	C	401	NAP	O3-PN-O5D	2.11	108.55	102.94
2	A	401	NAP	O2N-PN-O3	2.14	114.81	105.09
2	C	401	NAP	C2A-N1A-C6A	2.17	122.65	118.77
2	D	401	NAP	C2N-C3N-C4N	2.19	120.73	118.29
2	C	401	NAP	C2B-C3B-C4B	2.24	107.15	101.85
2	B	401	NAP	O2X-P2B-O1X	2.27	117.89	110.58
2	C	401	NAP	P2B-O2B-C2B	2.29	127.05	121.56
2	D	401	NAP	O4D-C1D-N1N	2.36	110.72	108.13
2	A	401	NAP	O3X-P2B-O2X	2.43	116.62	107.38
2	D	401	NAP	O2A-PA-O3	2.44	116.16	105.09
2	D	401	NAP	C4D-O4D-C1D	2.52	112.49	109.72
2	B	401	NAP	C2N-C3N-C4N	2.53	121.11	118.29
2	B	401	NAP	C2A-N1A-C6A	2.65	123.50	118.77
2	A	401	NAP	C2A-N1A-C6A	2.72	123.63	118.77
2	A	401	NAP	P2B-O2B-C2B	3.15	129.12	121.56
2	C	401	NAP	O2N-PN-O3	3.31	120.10	105.09
2	B	401	NAP	O2N-PN-O3	3.32	120.16	105.09
2	B	401	NAP	O3-PN-O5D	3.91	113.32	102.94
2	B	401	NAP	O4D-C1D-N1N	6.35	115.10	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAP	3	0
2	B	401	NAP	4	0
2	C	401	NAP	4	0
2	D	401	NAP	4	0

5.7 Other polymers (i)

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	358/385 (92%)	-0.04	14 (3%) 43 52	13, 24, 49, 98	0
1	B	345/385 (89%)	0.01	8 (2%) 64 72	12, 25, 48, 67	0
1	C	336/385 (87%)	-0.09	7 (2%) 67 74	14, 26, 44, 67	0
1	D	343/385 (89%)	0.11	15 (4%) 38 47	13, 28, 52, 86	0
All	All	1382/1540 (89%)	-0.00	44 (3%) 51 60	12, 26, 49, 98	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	268	PRO	6.8
1	D	268	PRO	4.3
1	D	43	ALA	4.3
1	A	265	TYR	4.3
1	A	266	ARG	3.9
1	A	4	ALA	3.8
1	D	269	GLU	3.8
1	D	342	ILE	3.7
1	C	28	PRO	3.6
1	D	265	TYR	3.5
1	D	311	GLY	3.5
1	A	262	HIS	3.5
1	A	270	ILE	3.5
1	A	263	SER	3.4
1	B	43	ALA	3.3
1	D	270	ILE	3.3
1	A	269	GLU	3.2
1	B	255	ALA	3.1
1	D	266	ARG	2.9
1	B	50	HIS	2.9
1	B	46	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	355	GLY	2.8
1	D	180	ALA	2.8
1	C	50	HIS	2.7
1	A	0	HIS	2.7
1	D	46	ARG	2.6
1	D	178	ASP	2.5
1	C	202	GLU	2.5
1	C	48	LEU	2.5
1	A	6	PRO	2.4
1	D	312	GLU	2.4
1	B	268	PRO	2.3
1	D	7	LYS	2.2
1	C	51	ALA	2.2
1	D	51	ALA	2.2
1	C	29	PRO	2.1
1	A	354	ALA	2.1
1	C	272	ARG	2.1
1	B	312	GLU	2.1
1	B	266	ARG	2.1
1	B	30	GLU	2.1
1	A	43	ALA	2.1
1	A	5	SER	2.0
1	D	272	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	NAP	A	401	48/48	0.94	0.12	-0.52	24,28,52,54	0
2	NAP	C	401	48/48	0.96	0.10	-0.81	26,31,49,50	0
2	NAP	B	401	48/48	0.95	0.10	-0.82	29,35,43,45	0
2	NAP	D	401	48/48	0.95	0.10	-1.14	25,35,42,52	0

6.5 Other polymers (i)

There are no such residues in this entry.