



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:02 AM GMT

PDB ID : 3NRR
Title : Co-crystal structure of dihydrofolate reductase-thymidylate synthase from *Babesia bovis* with dUMP, Raltitrexed and NADP
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2010-06-30
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

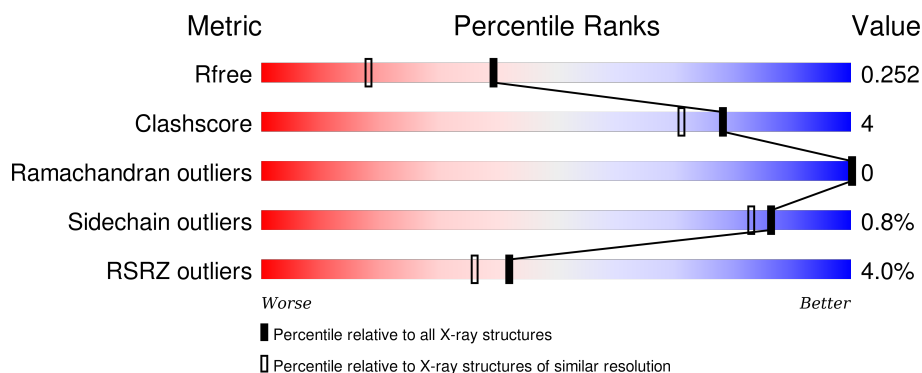
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

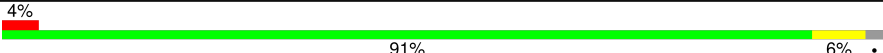
The reported resolution of this entry is 1.80 Å.

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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	515	 4% 91% 6% •
1	B	515	 4% 92% 5% •

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
6	EDO	A	514	-	-	-	X
6	EDO	A	537	-	-	-	X
6	EDO	B	532	-	-	-	X
8	PO4	B	513	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9454 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 Dihydrofolate reductase-thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	503	Total	C	N	O	S	0	3	0
			4013	2578	686	730	19			
1	B	501	Total	C	N	O	S	0	4	0
			3991	2569	678	725	19			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP A7ASX7
A	-2	PRO	-	EXPRESSION TAG	UNP A7ASX7
A	-1	GLY	-	EXPRESSION TAG	UNP A7ASX7
A	0	SER	-	EXPRESSION TAG	UNP A7ASX7
B	-3	GLY	-	EXPRESSION TAG	UNP A7ASX7
B	-2	PRO	-	EXPRESSION TAG	UNP A7ASX7
B	-1	GLY	-	EXPRESSION TAG	UNP A7ASX7
B	0	SER	-	EXPRESSION TAG	UNP A7ASX7

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

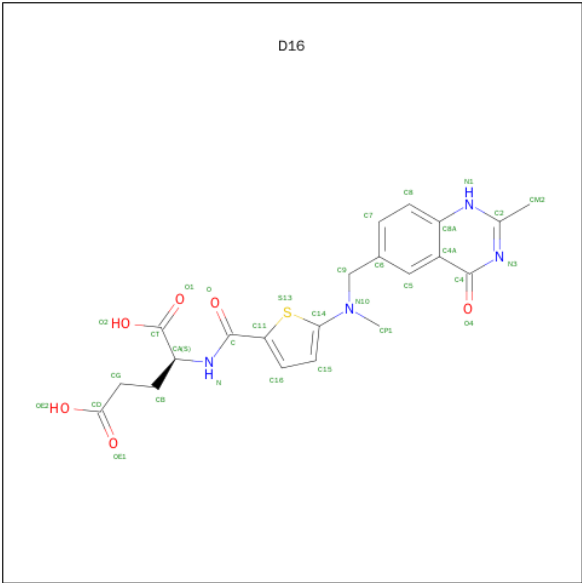
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			96	42	14	34	6		
3	B	1	Total	C	N	O	P	0	1
			96	42	14	34	6		

- Molecule 4 is TOMUDEX (three-letter code: D16) (formula: C₂₁H₂₂N₄O₆S).



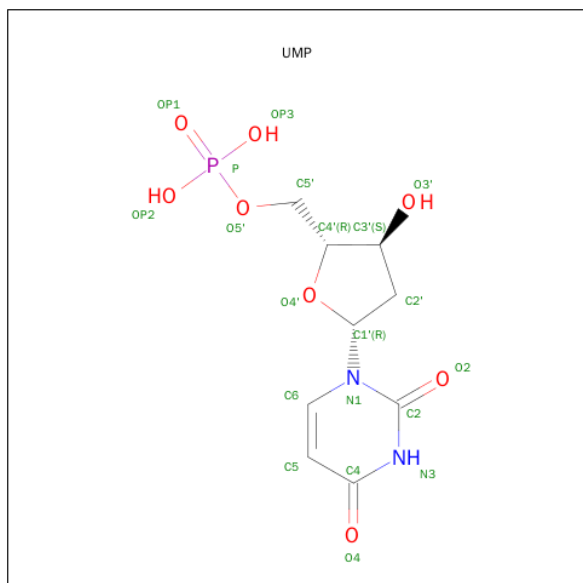
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			32	21	4	6	1		
4	A	1	Total	C	N	O	S	0	0
			32	21	4	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			32	21	4	6	1		
4	B	1	Total	C	N	O	S	0	0
			32	21	4	6	1		

- Molecule 5 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: $C_9H_{13}N_2O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
5	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



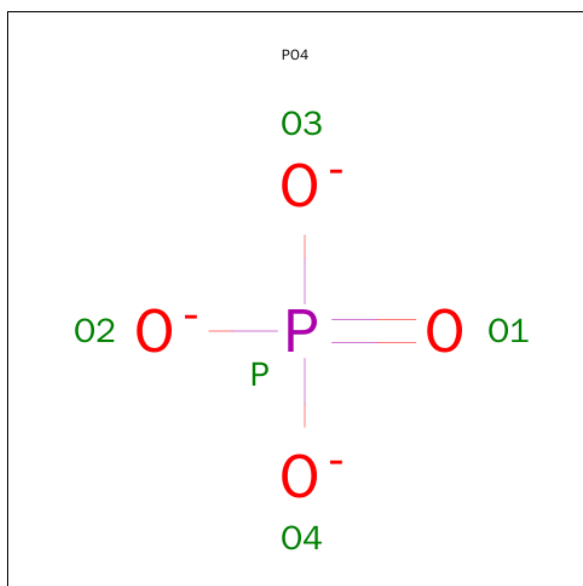
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	O	P	0	0
			5	4	1		

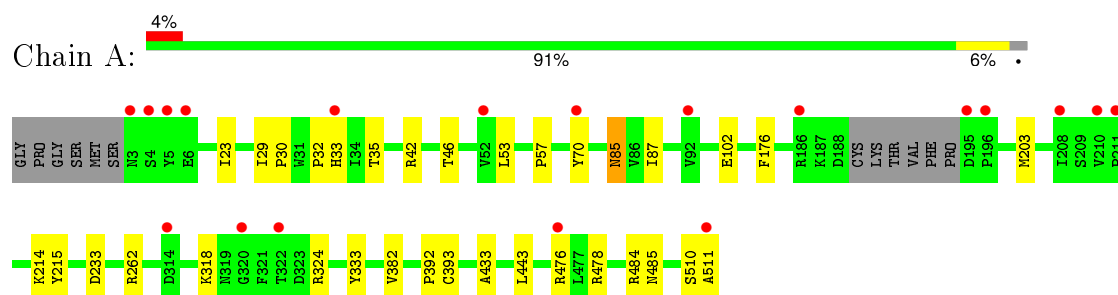
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	537	Total 537	O 537	0	0
9	B	488	Total 488	O 488	0	0

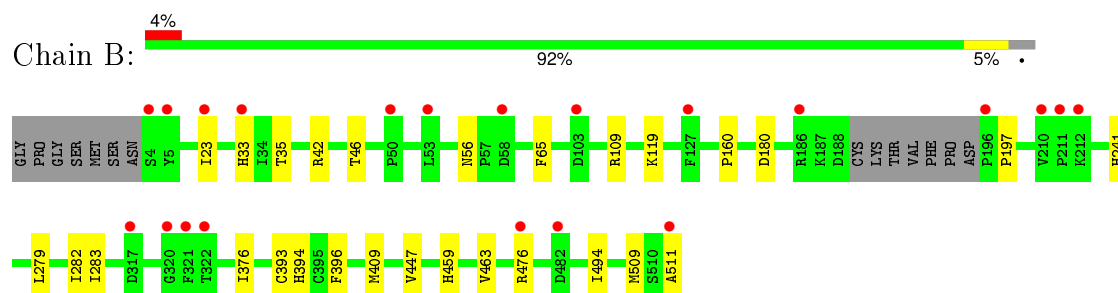
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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: Dihydrofolate reductase-thymidylate synthase



- Molecule 1: Dihydrofolate reductase-thymidylate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.33Å 83.83Å 83.92Å 119.61° 102.04° 90.26°	Depositor
Resolution (Å)	19.94 – 1.80 19.94 – 1.79	Depositor EDS
% Data completeness (in resolution range)	98.5 (19.94-1.80) 81.9 (19.94-1.79)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.194 , 0.236 0.209 , 0.252	Depositor DCC
R_{free} test set	5538 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	17.0	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.7	EDS
Estimated twinning fraction	0.000 for -h,k,-k-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Outliers	0 of 109818 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9454	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, D16, UMP, CL, PO4, EDO, 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	0.72	0/4127	0.78	3/5617 (0.1%)
1	B	0.77	1/4108 (0.0%)	0.78	2/5593 (0.0%)
All	All	0.75	1/8235 (0.0%)	0.78	5/11210 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	394	HIS	C-O	-5.12	1.13	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	MET	CG-SD-CE	-5.96	90.66	100.20
1	B	180	ASP	CB-CG-OD1	5.50	123.25	118.30
1	B	396	PHE	N-CA-CB	-5.35	100.96	110.60
1	A	324	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	233	ASP	CB-CG-OD2	-5.02	113.79	118.30

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	4013	0	3931	29	0
1	B	3991	0	3910	22	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	96	0	50	3	0
3	B	96	0	50	2	0
4	A	64	0	40	4	0
4	B	64	0	40	4	0
5	A	20	0	11	2	0
5	B	20	0	11	2	0
6	A	32	0	48	1	0
6	B	20	0	30	3	0
7	A	6	0	8	0	0
8	B	5	0	0	0	0
9	A	537	0	0	5	0
9	B	488	0	0	5	0
All	All	9454	0	8129	59	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 4.

All (59) 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:393:CYS:SG	5:A:525:UMP:C6	2.39	1.16
1:B:393:CYS:SG	5:B:525:UMP:C6	2.51	1.04
1:B:476[B]:ARG:HH21	1:B:476[B]:ARG:HG2	1.29	0.96
1:A:476[B]:ARG:HH11	1:A:476[B]:ARG:HG2	1.44	0.83
1:A:511:ALA:HB3	9:A:879:HOH:O	1.86	0.76
1:B:511:ALA:HB2	9:B:995:HOH:O	1.89	0.73
1:B:476[B]:ARG:NH2	1:B:476[B]:ARG:HG2	2.03	0.68
1:A:393:CYS:SG	5:A:525:UMP:C5	2.87	0.67
1:B:511:ALA:CB	9:B:995:HOH:O	2.43	0.66
1:A:33:HIS:CE1	1:A:35:THR:HG22	2.30	0.65
4:B:520:D16:HP13	4:B:520:D16:C7	2.27	0.64
4:A:520:D16:HP13	4:A:520:D16:C7	2.27	0.63
1:A:476[B]:ARG:HG2	1:A:476[B]:ARG:NH1	2.09	0.63
1:B:393:CYS:SG	5:B:525:UMP:C5	2.92	0.62
1:B:33:HIS:CE1	1:B:35:THR:HG22	2.36	0.60
1:A:510:SER:O	1:A:511:ALA:CB	2.48	0.60
1:B:476[B]:ARG:HD3	9:B:910:HOH:O	2.02	0.58
1:B:459:HIS:O	1:B:463[A]:VAL:HG22	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:MET:SD	1:B:511:ALA:OXT	2.64	0.55
1:A:23:ILE:O	3:A:515[B]:NAP:H2N	2.07	0.54
1:A:23:ILE:O	3:A:515[A]:NAP:H2N	2.08	0.54
1:A:510:SER:O	1:A:511:ALA:HB3	2.09	0.52
1:A:433:ALA:HA	1:A:443:LEU:HD21	1.92	0.51
1:A:32:PRO:HB2	1:A:176:PHE:CZ	2.46	0.51
1:A:102:GLU:O	3:A:515[B]:NAP:H2A	2.11	0.51
4:B:520:D16:CP1	4:B:520:D16:C7	2.89	0.50
4:A:520:D16:CP1	4:A:520:D16:C7	2.90	0.50
1:B:197:PRO:HG2	9:B:944:HOH:O	2.11	0.50
1:A:215:TYR:HA	6:A:532:EDO:H22	1.93	0.49
1:A:214:LYS:HG2	1:A:215:TYR:CE1	2.47	0.49
1:A:511:ALA:HB1	9:A:666:HOH:O	2.12	0.48
1:A:42:ARG:O	1:A:46:THR:HG23	2.13	0.48
1:B:23:ILE:O	3:B:515[A]:NAP:H2N	2.13	0.48
1:B:23:ILE:O	3:B:515[B]:NAP:H2N	2.13	0.48
1:A:478[A]:ARG:HD3	9:A:786:HOH:O	2.13	0.48
4:A:520:D16:HP13	4:A:520:D16:H7	1.95	0.48
4:B:520:D16:HP13	4:B:520:D16:H7	1.95	0.47
1:A:85:ASN:N	1:A:85:ASN:HD22	2.13	0.47
1:A:33:HIS:HE1	1:A:35:THR:HG22	1.76	0.47
4:B:520:D16:CP1	4:B:520:D16:H7	2.45	0.46
1:A:485:ASN:HB3	9:A:539:HOH:O	2.14	0.46
1:B:109:ARG:NE	6:B:537:EDO:O2	2.45	0.46
1:A:476[B]:ARG:HH11	1:A:476[B]:ARG:CG	2.22	0.46
1:B:376:ILE:O	6:B:532:EDO:H22	2.16	0.45
1:A:70:TYR:CD2	1:A:87:ILE:HD11	2.52	0.45
4:A:520:D16:CP1	4:A:520:D16:H7	2.48	0.43
1:A:53:LEU:O	1:A:57:PRO:HA	2.18	0.43
1:B:42:ARG:O	1:B:46:THR:HG23	2.18	0.43
1:B:409:MET:HA	1:B:447:VAL:O	2.19	0.42
1:A:511:ALA:HB2	9:A:994:HOH:O	2.19	0.42
1:B:283:ILE:HG23	1:B:494:ILE:HD13	2.03	0.41
1:B:476[B]:ARG:CG	1:B:476[B]:ARG:HH21	2.16	0.41
1:B:279:LEU:HA	1:B:282:ILE:HD12	2.01	0.41
1:A:214:LYS:HG2	1:A:215:TYR:CD1	2.55	0.41
1:A:333:TYR:CE1	1:A:392:PRO:HB3	2.56	0.41
1:A:29:ILE:HA	1:A:30:PRO:HD3	1.92	0.41
1:A:382:VAL:HG13	6:B:532:EDO:H11	2.03	0.40
1:B:119:LYS:HG3	1:B:119:LYS:HZ2	1.72	0.40
1:B:241:HIS:HD2	9:B:603:HOH:O	2.05	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	502/515 (98%)	492 (98%)	10 (2%)	0	100	100
1	B	501/515 (97%)	489 (98%)	12 (2%)	0	100	100
All	All	1003/1030 (97%)	981 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	440/460 (96%)	436 (99%)	4 (1%)	84	80
1	B	437/460 (95%)	434 (99%)	3 (1%)	88	86
All	All	877/920 (95%)	870 (99%)	7 (1%)	86	83

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	262	ARG
1	A	318	LYS
1	A	484	ARG
1	B	56	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	65	PHE
1	B	160	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	241	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 2 are monoatomic - leaving 25 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	$\# Z > 2$
6	EDO	A	514	-	3,3,3	0.48	0	2,2,2	0.38	0
3	NAP	A	515[A]	-	42,52,52	0.84	1 (2%)	54,80,80	1.77	8 (14%)
3	NAP	A	515[B]	-	42,52,52	0.79	1 (2%)	54,80,80	1.66	8 (14%)
4	D16	A	520	-	25,34,34	1.64	4 (16%)	22,48,48	1.86	7 (31%)
5	UMP	A	525	-	16,21,21	1.13	3 (18%)	23,31,31	2.17	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	D16	A	530	-	25,34,34	1.67	4 (16%)	22,48,48	1.65	3 (13%)
6	EDO	A	531	-	3,3,3	0.74	0	2,2,2	0.53	0
6	EDO	A	532	-	3,3,3	0.60	0	2,2,2	0.20	0
6	EDO	A	533	-	3,3,3	0.53	0	2,2,2	0.13	0
6	EDO	A	534	-	3,3,3	0.67	0	2,2,2	0.15	0
6	EDO	A	535	-	3,3,3	0.44	0	2,2,2	0.42	0
6	EDO	A	536	-	3,3,3	0.45	0	2,2,2	0.27	0
6	EDO	A	537	-	3,3,3	0.47	0	2,2,2	0.23	0
7	GOL	A	540	-	5,5,5	0.14	0	5,5,5	0.56	0
8	PO4	B	513	-	4,4,4	0.43	0	6,6,6	0.26	0
3	NAP	B	515[A]	-	42,52,52	0.80	1 (2%)	54,80,80	1.74	9 (16%)
3	NAP	B	515[B]	-	42,52,52	0.84	2 (4%)	54,80,80	1.62	6 (11%)
4	D16	B	520	-	25,34,34	1.63	5 (20%)	22,48,48	1.79	7 (31%)
5	UMP	B	525	-	16,21,21	1.37	3 (18%)	23,31,31	2.57	2 (8%)
4	D16	B	530	-	25,34,34	1.54	4 (16%)	22,48,48	1.77	6 (27%)
6	EDO	B	532	-	3,3,3	0.61	0	2,2,2	0.29	0
6	EDO	B	533	-	3,3,3	0.38	0	2,2,2	0.54	0
6	EDO	B	534	-	3,3,3	0.48	0	2,2,2	0.38	0
6	EDO	B	537	-	3,3,3	0.46	0	2,2,2	0.40	0
6	EDO	B	539	-	3,3,3	0.56	0	2,2,2	0.30	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
6	EDO	A	514	-	-	0/1/1/1	0/0/0/0
3	NAP	A	515[A]	-	-	0/27/67/67	0/5/5/5
3	NAP	A	515[B]	-	-	0/27/67/67	0/5/5/5
4	D16	A	520	-	-	0/13/25/25	0/3/3/3
5	UMP	A	525	-	-	0/6/22/22	0/2/2/2
4	D16	A	530	-	-	0/13/25/25	0/3/3/3
6	EDO	A	531	-	-	0/1/1/1	0/0/0/0
6	EDO	A	532	-	-	0/1/1/1	0/0/0/0
6	EDO	A	533	-	-	0/1/1/1	0/0/0/0
6	EDO	A	534	-	-	0/1/1/1	0/0/0/0
6	EDO	A	535	-	-	0/1/1/1	0/0/0/0
6	EDO	A	536	-	-	0/1/1/1	0/0/0/0
6	EDO	A	537	-	-	0/1/1/1	0/0/0/0
7	GOL	A	540	-	-	0/4/4/4	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PO4	B	513	-	-	0/0/0/0	0/0/0/0
3	NAP	B	515[A]	-	-	0/27/67/67	0/5/5/5
3	NAP	B	515[B]	-	-	0/27/67/67	0/5/5/5
4	D16	B	520	-	-	0/13/25/25	0/3/3/3
5	UMP	B	525	-	-	0/6/22/22	0/2/2/2
4	D16	B	530	-	-	0/13/25/25	0/3/3/3
6	EDO	B	532	-	-	0/1/1/1	0/0/0/0
6	EDO	B	533	-	-	0/1/1/1	0/0/0/0
6	EDO	B	534	-	-	0/1/1/1	0/0/0/0
6	EDO	B	537	-	-	0/1/1/1	0/0/0/0
6	EDO	B	539	-	-	0/1/1/1	0/0/0/0

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	515[A]	NAP	C7N-N7N	-2.95	1.27	1.33
3	A	515[B]	NAP	C7N-N7N	-2.87	1.27	1.33
3	B	515[B]	NAP	C7N-N7N	-2.52	1.27	1.33
3	B	515[A]	NAP	C7N-N7N	-2.52	1.27	1.33
5	B	525	UMP	P-OP2	-2.19	1.46	1.54
5	A	525	UMP	P-OP3	-2.04	1.47	1.54
4	B	530	D16	C2-N1	2.08	1.37	1.34
4	B	520	D16	C9-N10	2.09	1.50	1.47
3	B	515[B]	NAP	O4B-C1B	2.12	1.43	1.41
5	A	525	UMP	C6-N1	2.15	1.38	1.35
5	B	525	UMP	C4-N3	2.17	1.37	1.33
4	A	530	D16	C4A-C8A	2.25	1.46	1.41
5	A	525	UMP	C4-N3	2.53	1.37	1.33
5	B	525	UMP	C6-N1	2.77	1.39	1.35
4	B	530	D16	O4-C4	2.89	1.31	1.24
4	B	520	D16	C4A-C8A	3.00	1.48	1.41
4	A	520	D16	C14-N10	3.12	1.46	1.36
4	A	520	D16	C4A-C8A	3.14	1.48	1.41
4	A	530	D16	O4-C4	3.26	1.32	1.24
4	B	520	D16	C14-N10	3.28	1.47	1.36
4	B	530	D16	C14-N10	3.39	1.47	1.36
4	B	520	D16	C4-C4A	3.51	1.47	1.41
4	A	530	D16	C14-N10	3.83	1.48	1.36
4	A	520	D16	O4-C4	3.88	1.34	1.24
4	A	530	D16	C4-C4A	4.00	1.48	1.41
4	A	520	D16	C4-C4A	4.01	1.48	1.41
4	B	530	D16	C4-C4A	4.09	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	520	D16	O4-C4	4.17	1.34	1.24

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	515[A]	NAP	N3A-C2A-N1A	-9.67	121.49	128.89
3	B	515[A]	NAP	N3A-C2A-N1A	-9.26	121.81	128.89
3	A	515[B]	NAP	N3A-C2A-N1A	-8.96	122.03	128.89
3	B	515[B]	NAP	N3A-C2A-N1A	-8.82	122.14	128.89
4	A	530	D16	C6-C9-N10	-4.07	107.87	113.03
4	A	520	D16	C6-C5-C4A	-3.64	116.11	122.65
4	B	520	D16	C6-C5-C4A	-3.49	116.37	122.65
4	A	520	D16	C7-C8-C8A	-3.31	117.28	120.88
3	B	515[A]	NAP	O7N-C7N-C3N	-3.07	116.23	119.59
3	B	515[B]	NAP	O7N-C7N-C3N	-3.06	116.25	119.59
3	A	515[A]	NAP	O7N-C7N-C3N	-2.99	116.32	119.59
3	A	515[A]	NAP	O2B-P2B-O1X	-2.97	99.70	107.11
4	B	530	D16	C4-C4A-C8A	-2.91	115.70	118.54
3	A	515[B]	NAP	O7N-C7N-C3N	-2.88	116.45	119.59
3	B	515[B]	NAP	O4D-C1D-N1N	-2.62	105.25	108.13
4	B	520	D16	C7-C8-C8A	-2.62	118.04	120.88
3	B	515[A]	NAP	O4D-C1D-N1N	-2.55	105.32	108.13
3	B	515[A]	NAP	C4A-C5A-N7A	-2.52	107.16	109.48
4	B	530	D16	C6-C9-N10	-2.43	109.95	113.03
3	B	515[A]	NAP	C1B-N9A-C4A	-2.40	123.32	126.94
3	A	515[B]	NAP	O3-PA-O5B	-2.40	96.58	102.94
4	A	520	D16	C6-C9-N10	-2.39	110.01	113.03
3	A	515[B]	NAP	C4A-C5A-N7A	-2.33	107.34	109.48
4	B	520	D16	C4-C4A-C8A	-2.30	116.30	118.54
4	B	530	D16	N1-C2-N3	-2.30	121.06	125.58
3	A	515[A]	NAP	O3-PA-O5B	-2.28	96.88	102.94
3	A	515[A]	NAP	O4D-C1D-N1N	-2.28	105.63	108.13
4	B	520	D16	C6-C9-N10	-2.28	110.15	113.03
3	A	515[B]	NAP	O2B-P2B-O1X	-2.17	101.68	107.11
3	B	515[A]	NAP	O2B-P2B-O1X	-2.08	101.91	107.11
3	A	515[B]	NAP	O4D-C1D-N1N	-2.06	105.86	108.13
3	B	515[B]	NAP	O2X-P2B-O1X	2.02	117.07	110.58
3	A	515[A]	NAP	O2X-P2B-O1X	2.04	117.15	110.58
4	B	520	D16	C7-C6-C5	2.08	122.21	118.82
3	B	515[A]	NAP	O2X-P2B-O1X	2.18	117.59	110.58
3	A	515[B]	NAP	O3X-P2B-O2X	2.22	115.83	107.38
5	A	525	UMP	OP3-P-OP2	2.23	115.88	107.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	530	D16	C5-C4A-C8A	2.27	120.85	118.14
3	A	515[A]	NAP	O3X-P2B-O2X	2.32	116.21	107.38
3	B	515[B]	NAP	O3X-P2B-O2X	2.47	116.79	107.38
3	B	515[A]	NAP	O3X-P2B-O2X	2.52	116.98	107.38
3	A	515[B]	NAP	C3N-C7N-N7N	2.55	120.61	117.82
3	A	515[A]	NAP	C3N-C7N-N7N	2.55	120.61	117.82
4	B	530	D16	C8-C8A-N1	2.60	122.86	118.73
5	B	525	UMP	C2'-C1'-N1	2.74	120.82	114.16
4	A	520	D16	C7-C6-C5	2.75	123.29	118.82
4	A	520	D16	O-C-N	2.76	127.43	122.44
4	A	530	D16	C8-C8A-N1	2.78	123.14	118.73
3	B	515[B]	NAP	C3N-C7N-N7N	2.90	121.00	117.82
3	B	515[A]	NAP	C3N-C7N-N7N	2.90	121.00	117.82
4	A	520	D16	C5-C4A-C8A	2.98	121.70	118.14
4	A	520	D16	C2-N1-C8A	3.00	119.24	115.86
4	B	520	D16	C5-C4A-C8A	3.07	121.80	118.14
4	B	520	D16	C2-N1-C8A	3.27	119.54	115.86
5	A	525	UMP	C2'-C1'-N1	3.84	123.49	114.16
4	A	530	D16	C2-N1-C8A	4.29	120.69	115.86
4	B	530	D16	C2-N1-C8A	5.04	121.54	115.86
5	A	525	UMP	C4-N3-C2	8.69	122.74	114.14
5	B	525	UMP	C4-N3-C2	11.27	125.30	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	515[A]	NAP	1	0
3	A	515[B]	NAP	2	0
4	A	520	D16	4	0
5	A	525	UMP	2	0
6	A	532	EDO	1	0
3	B	515[A]	NAP	1	0
3	B	515[B]	NAP	1	0
4	B	520	D16	4	0
5	B	525	UMP	2	0
6	B	532	EDO	2	0
6	B	537	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	503/515 (97%)	0.26	19 (3%) 44 38	8, 16, 41, 79	0
1	B	501/515 (97%)	0.22	21 (4%) 40 34	7, 16, 39, 82	0
All	All	1004/1030 (97%)	0.24	40 (3%) 42 36	7, 16, 40, 82	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	511	ALA	7.7
1	B	511	ALA	7.1
1	A	211	PRO	5.9
1	B	210	VAL	5.0
1	A	210	VAL	4.8
1	B	211	PRO	4.7
1	A	33	HIS	3.8
1	B	322	THR	3.7
1	A	196	PRO	3.4
1	A	208	ILE	3.3
1	B	196	PRO	3.3
1	A	4	SER	3.3
1	A	3	ASN	3.3
1	B	4	SER	3.2
1	B	317	ASP	3.1
1	A	92	VAL	3.0
1	A	322	THR	2.9
1	A	320	GLY	2.8
1	B	5	TYR	2.7
1	B	320	GLY	2.7
1	A	476[A]	ARG	2.6
1	B	476[A]	ARG	2.6
1	B	50	PRO	2.5
1	A	314	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	23	ILE	2.3
1	A	5	TYR	2.3
1	A	6	GLU	2.3
1	B	53	LEU	2.3
1	B	58	ASP	2.2
1	B	127	PHE	2.2
1	B	482	ASP	2.2
1	A	186	ARG	2.2
1	A	52	VAL	2.2
1	B	103	ASP	2.2
1	A	70	TYR	2.2
1	B	212	LYS	2.1
1	A	195	ASP	2.1
1	B	321	PHE	2.1
1	B	186	ARG	2.0
1	B	33	HIS	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
8	PO4	B	513	5/5	0.86	0.27	5.34	47,51,52,53	0
6	EDO	B	532	4/4	0.87	0.18	3.35	28,29,30,30	0
6	EDO	A	514	4/4	0.82	0.18	2.75	31,32,33,35	0
6	EDO	A	537	4/4	0.61	0.25	2.74	34,35,37,39	0
6	EDO	A	536	4/4	0.84	0.16	1.46	35,39,40,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	EDO	A	534	4/4	0.60	0.18	1.37	45,46,46,46	0
4	D16	B	520	32/32	0.85	0.17	1.37	14,23,40,41	0
6	EDO	A	532	4/4	0.65	0.16	1.29	37,38,39,42	0
6	EDO	B	539	4/4	0.81	0.15	1.24	28,32,34,35	0
4	D16	A	520	32/32	0.82	0.18	0.96	16,25,48,50	0
6	EDO	A	531	4/4	0.85	0.12	0.91	25,25,27,31	0
6	EDO	A	535	4/4	0.80	0.12	0.58	34,38,38,42	0
6	EDO	B	534	4/4	0.81	0.12	-0.01	40,41,42,42	0
4	D16	B	530	32/32	0.93	0.12	-0.12	10,14,32,35	0
4	D16	A	530	32/32	0.93	0.11	-0.26	10,14,30,31	0
5	UMP	A	525	20/20	0.97	0.09	-0.31	9,10,14,15	0
3	NAP	B	515[B]	48/48	0.95	0.11	-0.32	11,18,28,29	48
6	EDO	A	533	4/4	0.93	0.10	-0.37	35,36,38,40	0
3	NAP	A	515[A]	48/48	0.94	0.11	-0.39	13,19,30,30	48
5	UMP	B	525	20/20	0.97	0.09	-0.41	7,11,15,17	0
3	NAP	B	515[A]	48/48	0.95	0.11	-0.43	11,18,26,27	48
3	NAP	A	515[B]	48/48	0.94	0.11	-0.50	13,20,30,32	48
2	CL	A	513	1/1	0.96	0.09	-0.78	28,28,28,28	0
6	EDO	B	533	4/4	0.94	0.09	-	35,35,36,38	0
2	CL	B	514	1/1	0.88	0.14	-	54,54,54,54	0
6	EDO	B	537	4/4	0.74	0.17	-	48,50,50,51	0
7	GOL	A	540	6/6	0.68	0.27	-	40,43,44,45	0

6.5 Other polymers

There are no such residues in this entry.