



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:24 pm GMT

PDB ID : 3JQ8
Title : Crystal structure of pteridine reductase 1 (PTR1) from Trypanosoma brucei in ternary complex with cofactor (NADP+) and inhibitor 6,7,7-trimethyl-7,8-dihydropteridine-2,4-diamine (DX3)
Authors : Tulloch, L.B.; Hunter, W.N.
Deposited on : 2009-09-06
Resolution : 1.95 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

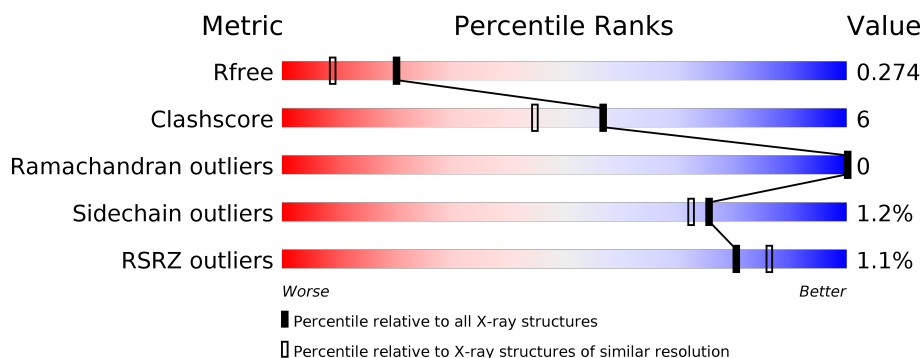
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	100719	2004 (1.96-1.96)
Clashscore	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)
RSRZ outliers	101464	2018 (1.96-1.96)

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	288	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>16%</div> <div>14%</div> </div> </div>
2	B	288	<div> <div>75%</div> <div>10%</div> <div>14%</div> </div>
2	C	288	<div> <div>71%</div> <div>14%</div> <div>16%</div> </div>
2	D	288	<div> <div>%</div> <div>79%</div> <div>7%</div> <div>14%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DX3	B	270	-	-	-	X
4	DX3	C	270	-	-	-	X
4	DX3	D	270[A]	-	-	X	X
4	DX3	D	270[B]	-	-	-	X
5	DTT	C	271	X	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8785 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 Pteridine reductase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	11	0
			1892	1193	332	355	12			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q581W1
A	-18	GLY	-	EXPRESSION TAG	UNP Q581W1
A	-17	SER	-	EXPRESSION TAG	UNP Q581W1
A	-16	SER	-	EXPRESSION TAG	UNP Q581W1
A	-15	HIS	-	EXPRESSION TAG	UNP Q581W1
A	-14	HIS	-	EXPRESSION TAG	UNP Q581W1
A	-13	HIS	-	EXPRESSION TAG	UNP Q581W1
A	-12	HIS	-	EXPRESSION TAG	UNP Q581W1
A	-11	HIS	-	EXPRESSION TAG	UNP Q581W1
A	-10	HIS	-	EXPRESSION TAG	UNP Q581W1
A	-9	SER	-	EXPRESSION TAG	UNP Q581W1
A	-8	SER	-	EXPRESSION TAG	UNP Q581W1
A	-7	GLY	-	EXPRESSION TAG	UNP Q581W1
A	-6	LEU	-	EXPRESSION TAG	UNP Q581W1
A	-5	VAL	-	EXPRESSION TAG	UNP Q581W1
A	-4	PRO	-	EXPRESSION TAG	UNP Q581W1
A	-3	ARG	-	EXPRESSION TAG	UNP Q581W1
A	-2	GLY	-	EXPRESSION TAG	UNP Q581W1
A	-1	SER	-	EXPRESSION TAG	UNP Q581W1
A	0	HIS	-	EXPRESSION TAG	UNP Q581W1

- Molecule 2 is a protein called Pteridine reductase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	248	Total	C	N	O	S	0	13	0
			1893	1192	330	360	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	243	Total	C	N	O	S	0	11	0
			1835	1156	322	347	10			
2	D	249	Total	C	N	O	S	0	13	0
			1899	1199	332	356	12			

There are 60 discrepancies between the modelled and reference sequences:

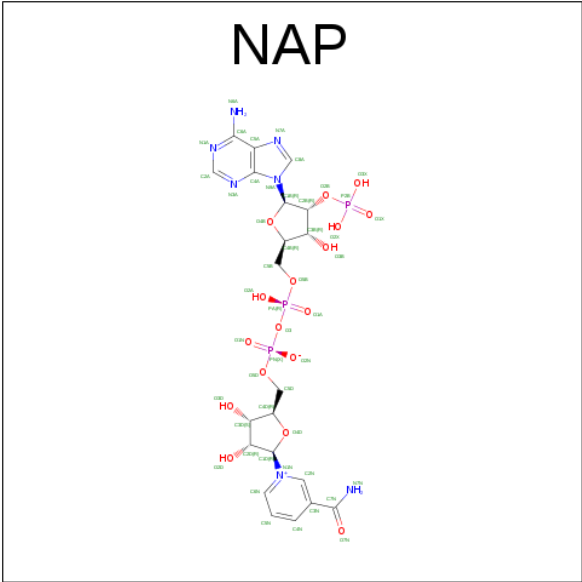
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	EXPRESSION TAG	UNP Q581W1
B	-18	GLY	-	EXPRESSION TAG	UNP Q581W1
B	-17	SER	-	EXPRESSION TAG	UNP Q581W1
B	-16	SER	-	EXPRESSION TAG	UNP Q581W1
B	-15	HIS	-	EXPRESSION TAG	UNP Q581W1
B	-14	HIS	-	EXPRESSION TAG	UNP Q581W1
B	-13	HIS	-	EXPRESSION TAG	UNP Q581W1
B	-12	HIS	-	EXPRESSION TAG	UNP Q581W1
B	-11	HIS	-	EXPRESSION TAG	UNP Q581W1
B	-10	HIS	-	EXPRESSION TAG	UNP Q581W1
B	-9	SER	-	EXPRESSION TAG	UNP Q581W1
B	-8	SER	-	EXPRESSION TAG	UNP Q581W1
B	-7	GLY	-	EXPRESSION TAG	UNP Q581W1
B	-6	LEU	-	EXPRESSION TAG	UNP Q581W1
B	-5	VAL	-	EXPRESSION TAG	UNP Q581W1
B	-4	PRO	-	EXPRESSION TAG	UNP Q581W1
B	-3	ARG	-	EXPRESSION TAG	UNP Q581W1
B	-2	GLY	-	EXPRESSION TAG	UNP Q581W1
B	-1	SER	-	EXPRESSION TAG	UNP Q581W1
B	0	HIS	-	EXPRESSION TAG	UNP Q581W1
C	-19	MET	-	EXPRESSION TAG	UNP Q581W1
C	-18	GLY	-	EXPRESSION TAG	UNP Q581W1
C	-17	SER	-	EXPRESSION TAG	UNP Q581W1
C	-16	SER	-	EXPRESSION TAG	UNP Q581W1
C	-15	HIS	-	EXPRESSION TAG	UNP Q581W1
C	-14	HIS	-	EXPRESSION TAG	UNP Q581W1
C	-13	HIS	-	EXPRESSION TAG	UNP Q581W1
C	-12	HIS	-	EXPRESSION TAG	UNP Q581W1
C	-11	HIS	-	EXPRESSION TAG	UNP Q581W1
C	-10	HIS	-	EXPRESSION TAG	UNP Q581W1
C	-9	SER	-	EXPRESSION TAG	UNP Q581W1
C	-8	SER	-	EXPRESSION TAG	UNP Q581W1
C	-7	GLY	-	EXPRESSION TAG	UNP Q581W1
C	-6	LEU	-	EXPRESSION TAG	UNP Q581W1

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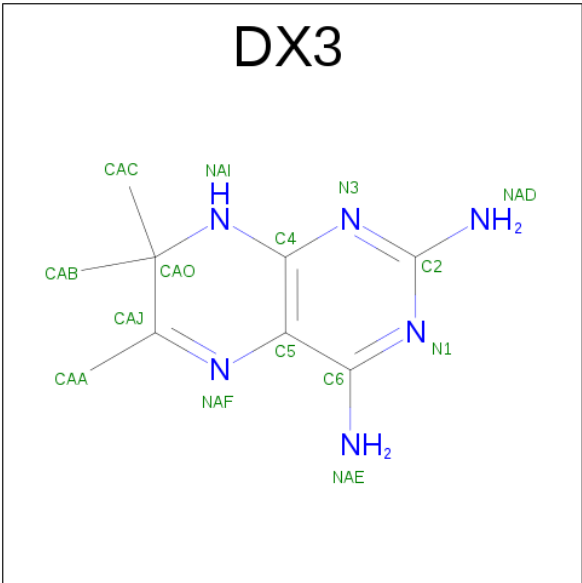
Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	VAL	-	EXPRESSION TAG	UNP Q581W1
C	-4	PRO	-	EXPRESSION TAG	UNP Q581W1
C	-3	ARG	-	EXPRESSION TAG	UNP Q581W1
C	-2	GLY	-	EXPRESSION TAG	UNP Q581W1
C	-1	SER	-	EXPRESSION TAG	UNP Q581W1
C	0	HIS	-	EXPRESSION TAG	UNP Q581W1
D	-19	MET	-	EXPRESSION TAG	UNP Q581W1
D	-18	GLY	-	EXPRESSION TAG	UNP Q581W1
D	-17	SER	-	EXPRESSION TAG	UNP Q581W1
D	-16	SER	-	EXPRESSION TAG	UNP Q581W1
D	-15	HIS	-	EXPRESSION TAG	UNP Q581W1
D	-14	HIS	-	EXPRESSION TAG	UNP Q581W1
D	-13	HIS	-	EXPRESSION TAG	UNP Q581W1
D	-12	HIS	-	EXPRESSION TAG	UNP Q581W1
D	-11	HIS	-	EXPRESSION TAG	UNP Q581W1
D	-10	HIS	-	EXPRESSION TAG	UNP Q581W1
D	-9	SER	-	EXPRESSION TAG	UNP Q581W1
D	-8	SER	-	EXPRESSION TAG	UNP Q581W1
D	-7	GLY	-	EXPRESSION TAG	UNP Q581W1
D	-6	LEU	-	EXPRESSION TAG	UNP Q581W1
D	-5	VAL	-	EXPRESSION TAG	UNP Q581W1
D	-4	PRO	-	EXPRESSION TAG	UNP Q581W1
D	-3	ARG	-	EXPRESSION TAG	UNP Q581W1
D	-2	GLY	-	EXPRESSION TAG	UNP Q581W1
D	-1	SER	-	EXPRESSION TAG	UNP Q581W1
D	0	HIS	-	EXPRESSION TAG	UNP Q581W1

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



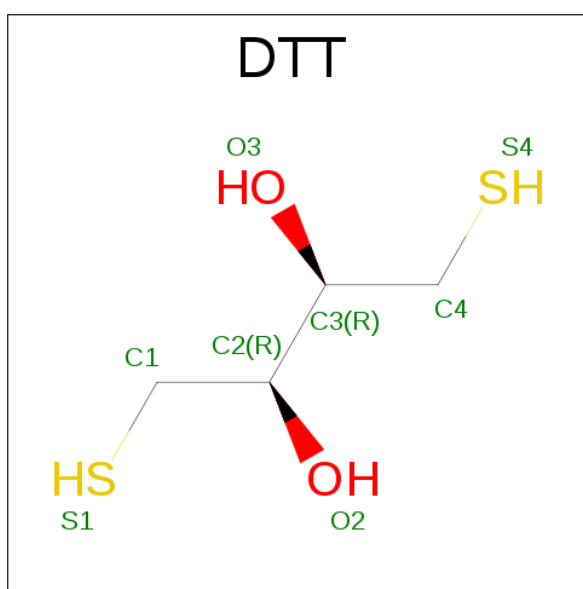
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is 6,7,7-TRIMETHYL-7,8-DIHYDROPTERIDINE-2,4-DIAMINE (three-letter code: DX3) (formula: C₉H₁₄N₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	1
			30	18	12		
4	B	1	Total	C	N	0	0
			15	9	6		
4	C	1	Total	C	N	0	0
			15	9	6		
4	D	1	Total	C	N	0	1
			30	18	12		

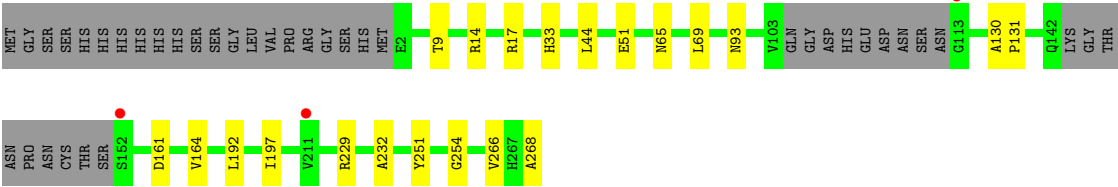
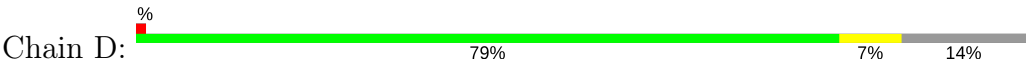
- Molecule 5 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	245	Total	O	0	0
			245	245		
6	B	238	Total	O	0	0
			238	238		
6	C	265	Total	O	0	0
			265	265		
6	D	228	Total	O	0	0
			228	228		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.10Å 89.15Å 84.19Å 90.00° 115.49° 90.00°	Depositor
Resolution (Å)	66.89 – 1.95 66.88 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.7 (66.89-1.95) 97.7 (66.88-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.229 , 0.281 0.226 , 0.274	Depositor DCC
R_{free} test set	3569 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	13.9	Xtriage
Anisotropy	0.616	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8785	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.19% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, DX3, CSX, DTT

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	0.39	2/1945 (0.1%)	0.54	2/2633 (0.1%)
2	B	0.66	2/1930 (0.1%)	0.49	0/2616
2	C	0.34	0/1867	0.49	0/2528
2	D	0.34	0/1942	0.49	0/2630
All	All	0.45	4/7684 (0.1%)	0.50	2/10407 (0.0%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	216[A]	GLU	CG-CD	-17.63	1.25	1.51
2	B	216[B]	GLU	CG-CD	-17.63	1.25	1.51
1	A	53[A]	SER	CB-OG	-5.96	1.34	1.42
1	A	53[B]	SER	CB-OG	-5.96	1.34	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	LEU	C-N-CD	-5.59	108.30	120.60
1	A	209	LEU	C-N-CA	5.20	143.82	122.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	209	LEU	Peptide

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	1892	0	1944	38	0
2	B	1893	0	1918	20	0
2	C	1835	0	1873	28	0
2	D	1899	0	1953	18	0
3	A	48	0	25	2	0
3	B	48	0	25	0	0
3	C	48	0	25	0	0
3	D	48	0	25	0	0
4	A	30	0	28	2	0
4	B	15	0	14	0	0
4	C	15	0	14	0	0
4	D	30	0	28	6	0
5	C	8	0	10	0	0
6	A	245	0	0	4	0
6	B	238	0	0	4	0
6	C	265	0	0	7	0
6	D	228	0	0	1	0
All	All	8785	0	7882	90	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 6.

All (90) 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:28:TYR:HE2	6:A:789:HOH:O	1.33	1.12
1:A:88:ASP:HB2	6:A:789:HOH:O	1.65	0.96
1:A:209:LEU:HB3	1:A:210:PRO:C	2.02	0.80
2:D:14[A]:ARG:HH22	4:D:270[A]:DX3:CAC	2.00	0.75
1:A:9:THR:HA	1:A:33:HIS:HB3	1.76	0.68
2:D:14[A]:ARG:HH22	4:D:270[A]:DX3:HACA	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:TRP:HA	1:A:224:LYS:HD2	1.78	0.65
1:A:206:VAL:HG12	4:A:270[B]:DX3:HAB	1.78	0.65
2:C:244:LEU:HG	6:C:747:HOH:O	1.99	0.63
2:D:14[A]:ARG:NH2	4:D:270[A]:DX3:CAC	2.63	0.61
1:A:65:ASN:HA	1:A:69:LEU:HD22	1.82	0.61
2:B:163:MET:HG3	6:B:511:HOH:O	2.00	0.60
2:D:9:THR:HA	2:D:33:HIS:HB3	1.84	0.60
2:C:206:VAL:HG23	2:C:263:LEU:HD22	1.82	0.60
1:A:14:ARG:NH1	1:A:209:LEU:O	2.22	0.59
2:D:14[A]:ARG:NH2	4:D:270[A]:DX3:HACA	2.16	0.59
2:B:17:ARG:HG3	2:B:44:LEU:HD22	1.85	0.58
1:A:210:PRO:HA	1:A:212:ALA:HA	1.85	0.58
2:B:65:ASN:HA	2:B:69:LEU:HD22	1.86	0.56
2:C:9:THR:HA	2:C:33:HIS:HB3	1.89	0.55
1:A:266:VAL:HB	2:D:268:ALA:HB2	1.89	0.55
2:C:17:ARG:HG3	2:C:44:LEU:HD22	1.89	0.54
2:C:243:PHE:HD2	6:C:747:HOH:O	1.90	0.54
1:A:215:GLU:HA	1:A:218:LYS:HD3	1.89	0.54
2:D:17:ARG:HG3	2:D:44:LEU:HD22	1.89	0.54
1:A:172[A]:SER:HG	2:B:132:PHE:HE1	1.55	0.54
1:A:210:PRO:HG2	4:A:270[A]:DX3:HABB	1.90	0.53
2:B:216[A]:GLU:HG3	2:B:217:GLU:N	2.24	0.53
2:D:65:ASN:HA	2:D:69:LEU:HD22	1.91	0.53
1:A:258[A]:LYS:HE3	6:A:318:HOH:O	2.10	0.52
2:D:14[A]:ARG:HH22	4:D:270[A]:DX3:HACB	1.73	0.52
2:C:65:ASN:HA	2:C:69:LEU:HD22	1.90	0.52
2:B:247:GLY:O	2:B:250:GLN:HG2	2.10	0.51
2:C:29:ARG:HG2	2:C:55:THR:HG22	1.93	0.51
1:A:257:ILE:HG12	2:C:257:ILE:HG12	1.93	0.50
2:B:235[A]:GLU:HG3	6:B:552:HOH:O	2.12	0.49
2:D:14[A]:ARG:NH2	4:D:270[A]:DX3:HACB	2.28	0.49
2:C:138:PHE:O	2:C:142:GLN:HG2	2.12	0.48
2:D:192:LEU:HB3	2:D:197:ILE:HB	1.95	0.48
1:A:247:GLY:HA2	1:A:250[B]:GLN:HE21	1.78	0.48
2:B:216[B]:GLU:CD	2:B:217:GLU:H	2.17	0.48
1:A:206:VAL:HG13	1:A:263:LEU:HD22	1.96	0.48
2:D:161:ASP:HB3	2:D:164:VAL:HG13	1.95	0.48
2:C:243:PHE:HB3	6:C:747:HOH:O	2.14	0.48
2:B:161:ASP:HB3	2:B:164:VAL:HG13	1.96	0.48
1:A:268:ALA:HB2	2:D:266:VAL:HB	1.96	0.48
1:A:160:CYS:HB3	6:A:292:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:117:GLU:HA	6:D:804:HOH:O	2.13	0.47
2:C:161:ASP:HB3	2:C:164:VAL:HG13	1.96	0.47
1:A:232:ALA:HB2	2:C:251:TYR:CE2	2.50	0.47
2:D:9:THR:O	2:D:93:ASN:HB3	2.14	0.47
1:A:192:LEU:HB3	1:A:197:ILE:HB	1.97	0.46
2:C:115:THR:O	2:C:119:GLN:HG3	2.15	0.46
2:C:100:THR:HB	6:C:823:HOH:O	2.15	0.46
1:A:138:PHE:O	1:A:142:GLN:HG2	2.16	0.46
2:B:9:THR:O	2:B:93:ASN:HB3	2.15	0.46
2:B:262:GLY:HA2	6:B:291:HOH:O	2.17	0.45
1:A:160:CYS:O	3:A:269:NAP:H6N	2.16	0.45
2:D:130:ALA:HB3	2:D:131:PRO:HD3	1.99	0.45
2:B:266:VAL:HG11	6:B:782:HOH:O	2.15	0.45
2:B:232:ALA:HB2	2:D:251:TYR:CE2	2.52	0.45
2:B:265:LEU:HD11	2:D:254:GLY:HA3	1.99	0.45
2:C:160:CYS:HB3	6:C:282:HOH:O	2.18	0.44
1:A:251:TYR:CE2	2:C:232:ALA:HB2	2.53	0.44
2:C:130:ALA:HB3	2:C:131:PRO:HD3	1.98	0.44
1:A:254:GLY:HA3	2:C:265:LEU:HD11	1.99	0.44
1:A:35:HIS:HB2	3:A:269:NAP:C2A	2.47	0.44
2:C:78:ASN:HB3	6:C:497:HOH:O	2.18	0.44
1:A:250[A]:GLN:HG3	2:C:236:GLN:HE21	1.82	0.43
1:A:232:ALA:HB2	2:C:251:TYR:CD2	2.54	0.43
2:B:130:ALA:HB3	2:B:131:PRO:HD3	1.99	0.43
2:B:268:ALA:HB2	2:C:266:VAL:HB	2.00	0.43
1:A:9:THR:O	1:A:93:ASN:HB3	2.18	0.43
2:B:251:TYR:CE2	2:D:232:ALA:HB2	2.54	0.43
1:A:153:ASN:CG	1:A:250[B]:GLN:HE22	2.22	0.42
2:B:9:THR:HA	2:B:33:HIS:HB3	2.01	0.42
1:A:265:LEU:HD11	2:C:254:GLY:HA3	2.01	0.42
2:B:230:ARG:HD3	2:B:231:GLU:OE2	2.19	0.42
1:A:61:ALA:HB3	1:A:76:ILE:HD11	2.02	0.42
2:C:247:GLY:HA2	2:C:250:GLN:HG3	2.00	0.42
1:A:210:PRO:O	1:A:218:LYS:HD2	2.20	0.41
1:A:161:ASP:HB3	1:A:164:VAL:HG13	2.02	0.41
1:A:123:LEU:HD22	1:A:174:TYR:HB2	2.03	0.41
1:A:210:PRO:HB3	1:A:213:MET:HB2	2.03	0.41
1:A:3:ALA:HA	1:A:4:PRO:HD3	1.95	0.41
2:C:240:ALA:O	6:C:747:HOH:O	2.22	0.41
2:C:3:ALA:HA	2:C:4:PRO:HD3	1.93	0.41
2:C:9:THR:O	2:C:93:ASN:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:LEU:CB	1:A:210:PRO:C	2.83	0.40
2:B:22:LYS:HD2	2:B:242:ILE:HG13	2.04	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	249/288 (86%)	239 (96%)	10 (4%)	0	100	100
2	B	250/288 (87%)	241 (96%)	9 (4%)	0	100	100
2	C	239/288 (83%)	231 (97%)	8 (3%)	0	100	100
2	D	250/288 (87%)	240 (96%)	10 (4%)	0	100	100
All	All	988/1152 (86%)	951 (96%)	37 (4%)	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	205/231 (89%)	203 (99%)	2 (1%)	80	78
2	B	202/230 (88%)	199 (98%)	3 (2%)	70	65
2	C	196/230 (85%)	194 (99%)	2 (1%)	80	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	204/230 (89%)	202 (99%)	2 (1%)	80	78
All	All	807/921 (88%)	798 (99%)	9 (1%)	75	75

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	230	ARG
2	B	141	ARG
2	B	166	GLN
2	B	208	LEU
2	C	22	LYS
2	C	219	ASP
2	D	51	GLU
2	D	229	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	78	ASN
1	A	119	GLN
1	A	166	GLN
1	A	175	ASN
2	B	67	ASN
2	B	166	GLN
2	C	25	GLN
2	C	54	ASN
2	C	67	ASN
2	C	236	GLN
2	C	250	GLN
2	D	166	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	CSX	B	168	2	4,6,7	0.61	0	2,6,8	1.44	0
2	CSX	C	168	2	4,6,7	0.57	0	2,6,8	1.28	0
2	CSX	D	168	2	4,6,7	0.60	0	2,6,8	1.31	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	CSX	B	168	2	-	0/1/5/7	0/0/0/0
2	CSX	C	168	2	-	0/1/5/7	0/0/0/0
2	CSX	D	168	2	-	0/1/5/7	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

11 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	$\# Z > 2$
3	NAP	A	269	-	44,52,52	1.61	3 (6%)	51,80,80	1.73	2 (3%)
4	DX3	A	270[A]	-	14,16,16	1.14	1 (7%)	17,25,25	1.87	5 (29%)
4	DX3	A	270[B]	-	14,16,16	1.07	1 (7%)	17,25,25	1.87	4 (23%)
3	NAP	B	269	-	44,52,52	1.62	3 (6%)	51,80,80	1.77	2 (3%)
4	DX3	B	270	-	14,16,16	1.11	1 (7%)	17,25,25	1.93	5 (29%)
3	NAP	C	269	-	44,52,52	1.62	3 (6%)	51,80,80	1.72	2 (3%)
4	DX3	C	270	-	14,16,16	1.26	2 (14%)	17,25,25	2.00	4 (23%)
5	DTT	C	271	-	7,7,7	0.46	0	4,8,8	0.25	0
3	NAP	D	269	-	44,52,52	1.38	4 (9%)	51,80,80	1.76	3 (5%)
4	DX3	D	270[A]	-	14,16,16	1.10	1 (7%)	17,25,25	1.85	6 (35%)
4	DX3	D	270[B]	-	14,16,16	1.11	1 (7%)	17,25,25	1.89	4 (23%)

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
3	NAP	A	269	-	-	0/27/67/67	0/5/5/5
4	DX3	A	270[A]	-	-	0/0/15/15	0/2/2/2
4	DX3	A	270[B]	-	-	0/0/15/15	0/2/2/2
3	NAP	B	269	-	-	0/27/67/67	0/5/5/5
4	DX3	B	270	-	-	0/0/15/15	0/2/2/2
3	NAP	C	269	-	-	0/27/67/67	0/5/5/5
4	DX3	C	270	-	-	0/0/15/15	0/2/2/2
5	DTT	C	271	-	1/1/2/2	0/8/8/8	0/0/0/0
3	NAP	D	269	-	-	0/27/67/67	0/5/5/5
4	DX3	D	270[A]	-	-	0/0/15/15	0/2/2/2
4	DX3	D	270[B]	-	-	0/0/15/15	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	270	DX3	CAO-NAI	2.26	1.49	1.47
3	A	269	NAP	C2A-N1A	2.47	1.38	1.33
3	B	269	NAP	C2A-N1A	2.59	1.38	1.33
3	D	269	NAP	C2A-N1A	2.59	1.38	1.33
3	C	269	NAP	C2A-N1A	2.61	1.38	1.33
4	B	270	DX3	CAA-CAJ	2.97	1.53	1.49
4	D	270[A]	DX3	CAA-CAJ	3.03	1.54	1.49
4	A	270[A]	DX3	CAA-CAJ	3.13	1.54	1.49
4	D	270[B]	DX3	CAA-CAJ	3.16	1.54	1.49
4	A	270[B]	DX3	CAA-CAJ	3.18	1.54	1.49
4	C	270	DX3	CAA-CAJ	3.41	1.54	1.49
3	A	269	NAP	C2A-N3A	3.71	1.38	1.32
3	D	269	NAP	C2A-N3A	3.73	1.38	1.32
3	B	269	NAP	C2A-N3A	3.83	1.38	1.32
3	C	269	NAP	C2A-N3A	3.98	1.38	1.32
3	D	269	NAP	C7N-N7N	4.49	1.41	1.33
3	D	269	NAP	O7N-C7N	4.50	1.33	1.24
3	C	269	NAP	O7N-C7N	8.39	1.41	1.24
3	A	269	NAP	O7N-C7N	8.44	1.41	1.24
3	B	269	NAP	O7N-C7N	8.47	1.41	1.24

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	269	NAP	N3A-C2A-N1A	-10.99	119.29	128.86
3	D	269	NAP	N3A-C2A-N1A	-10.88	119.38	128.86
3	A	269	NAP	N3A-C2A-N1A	-10.86	119.40	128.86
3	C	269	NAP	N3A-C2A-N1A	-10.79	119.46	128.86
3	B	269	NAP	C4B-O4B-C1B	-4.13	105.37	109.77
3	A	269	NAP	C4B-O4B-C1B	-3.92	105.60	109.77
3	C	269	NAP	C4B-O4B-C1B	-3.50	106.05	109.77
3	D	269	NAP	C4B-O4B-C1B	-3.34	106.22	109.77
4	C	270	DX3	N3-C2-N1	-3.03	120.54	125.45
4	A	270[A]	DX3	N3-C2-N1	-2.87	120.79	125.45
4	D	270[B]	DX3	N3-C2-N1	-2.81	120.89	125.45
4	B	270	DX3	N3-C2-N1	-2.80	120.92	125.45
4	D	270[A]	DX3	N3-C2-N1	-2.76	120.97	125.45
4	A	270[B]	DX3	N3-C2-N1	-2.75	120.99	125.45
4	A	270[A]	DX3	NAE-C6-N1	2.07	120.06	117.00
4	D	270[A]	DX3	NAD-C2-N1	2.08	120.57	117.24
3	D	269	NAP	C3N-C7N-N7N	2.14	120.22	117.77
4	B	270	DX3	NAE-C6-N1	2.15	120.18	117.00
4	D	270[A]	DX3	NAE-C6-N1	2.21	120.27	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	270[B]	DX3	C2-N3-C4	2.58	120.33	114.51
4	D	270[B]	DX3	C2-N3-C4	2.63	120.43	114.51
4	B	270	DX3	C2-N3-C4	2.71	120.63	114.51
4	C	270	DX3	C2-N3-C4	2.74	120.68	114.51
4	D	270[A]	DX3	C2-N3-C4	2.83	120.89	114.51
4	A	270[A]	DX3	C2-N3-C4	2.85	120.93	114.51
4	D	270[A]	DX3	C2-N1-C6	3.05	120.38	116.99
4	A	270[A]	DX3	C2-N1-C6	3.30	120.66	116.99
4	A	270[B]	DX3	C2-N1-C6	3.48	120.85	116.99
4	B	270	DX3	C2-N1-C6	3.51	120.89	116.99
4	D	270[B]	DX3	C2-N1-C6	3.57	120.95	116.99
4	C	270	DX3	C2-N1-C6	3.92	121.34	116.99
4	A	270[A]	DX3	C6-C5-C4	3.95	118.41	114.81
4	D	270[A]	DX3	C6-C5-C4	3.96	118.42	114.81
4	A	270[B]	DX3	C6-C5-C4	4.04	118.49	114.81
4	D	270[B]	DX3	C6-C5-C4	4.16	118.61	114.81
4	C	270	DX3	C6-C5-C4	4.23	118.67	114.81
4	B	270	DX3	C6-C5-C4	4.28	118.71	114.81

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	271	DTT	C3

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	269	NAP	2	0
4	A	270[A]	DX3	1	0
4	A	270[B]	DX3	1	0
4	D	270[A]	DX3	6	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	248/288 (86%)	0.11	6 (2%)	59	69	6, 13, 25, 40	3 (1%)
2	B	247/288 (85%)	0.04	1 (0%)	92	95	7, 13, 24, 27	1 (0%)
2	C	242/288 (84%)	0.06	1 (0%)	92	95	7, 14, 26, 33	2 (0%)
2	D	248/288 (86%)	0.02	3 (1%)	79	85	7, 13, 21, 24	2 (0%)
All	All	985/1152 (85%)	0.06	11 (1%)	80	86	6, 13, 24, 40	8 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	210	PRO	6.0
1	A	113	GLY	5.7
1	A	209	LEU	3.6
1	A	152	SER	3.4
2	D	113	GLY	3.4
2	D	152	SER	3.2
2	C	113	GLY	2.7
2	D	211	VAL	2.6
1	A	195	TYR	2.4
2	B	113	GLY	2.3
1	A	103	VAL	2.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CSX	B	168	7/8	0.89	0.12	-	15,16,18,19	0
2	CSX	D	168	7/8	0.89	0.11	-	14,14,15,15	1
2	CSX	C	168	7/8	0.87	0.12	-	14,14,14,16	1

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	DTT	C	271	8/8	0.60	0.35	5.19	33,33,34,34	8
4	DX3	C	270	15/15	0.64	0.25	4.64	40,41,41,41	0
4	DX3	D	270[B]	15/15	0.78	0.22	4.40	19,19,19,19	15
4	DX3	D	270[A]	15/15	0.78	0.22	3.94	11,12,12,12	15
4	DX3	B	270	15/15	0.71	0.19	2.59	33,33,34,34	0
4	DX3	A	270[B]	15/15	0.81	0.19	0.41	19,19,19,19	15
4	DX3	A	270[A]	15/15	0.81	0.19	0.28	18,18,18,18	15
3	NAP	B	269	48/48	0.96	0.10	-0.36	8,11,13,14	0
3	NAP	D	269	48/48	0.96	0.10	-0.38	9,11,14,15	0
3	NAP	A	269	48/48	0.95	0.10	-0.40	9,11,13,14	0
3	NAP	C	269	48/48	0.96	0.09	-0.71	9,11,13,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.