



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:48 AM GMT

PDB ID : 3JQC  
Title : Crystal structure of pteridine reductase 1 (PTR1) from Trypanosoma brucei in ternary complex with cofactor (NADP+) and inhibitor 2-amino-6-bromo-4-oxo-4,7-dihydro-3H-pyrrolo[2,3-d]pyrimidine-5-carbonitrile (JU2)  
Authors : Tulloch, L.B.; Hunter, W.N.  
Deposited on : 2009-09-06  
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](mailto: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.

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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

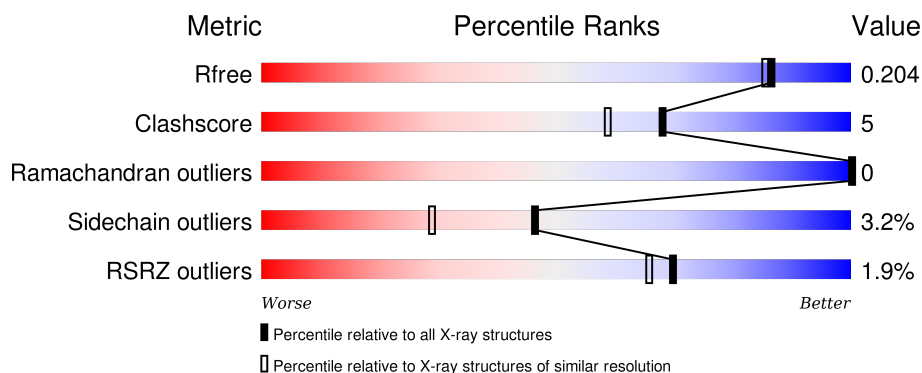
# 1 Overall quality at a glance

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  $\geq 3$ , 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>79% 7% • 14%</div> </div>
1	B	288	<div> <div>2%</div> <div>74% 11% • 13%</div> </div>
1	C	288	<div> <div>2%</div> <div>75% 10% • 13%</div> </div>
1	D	288	<div> <div>2%</div> <div>76% 10% • 14%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8546 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	249	Total	C	N	O	S	0	6	0
			1871	1179	328	353	11			
1	B	250	Total	C	N	O	S	0	12	0
			1901	1196	334	360	11			
1	C	250	Total	C	N	O	S	0	14	0
			1907	1199	334	362	12			
1	D	249	Total	C	N	O	S	0	11	0
			1888	1188	333	356	11			

There are 80 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
B	-19	MET	-	EXPRESSION TAG	UNP Q581W1

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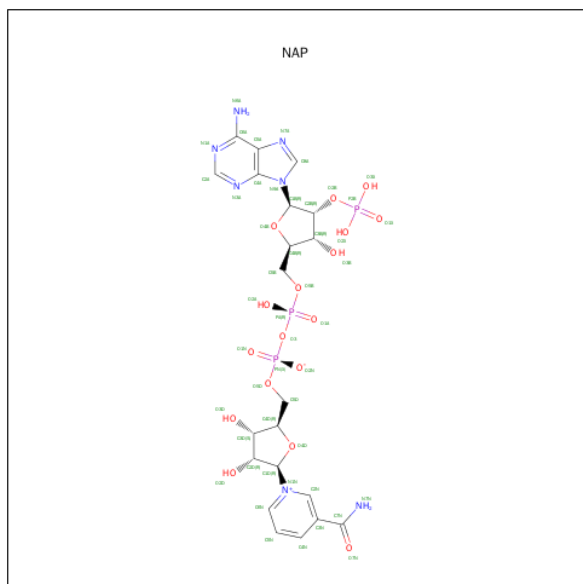
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	EXPRESSION TAG	UNP Q581W1
B	-17	SER	-	EXPRESSION TAG	UNP Q581W1
B	-16	SER	-	EXPRESSION TAG	UNP Q581W1
B	-15	HIS	-	EXPRESSION TAG	UNP Q581W1
B	-14	HIS	-	EXPRESSION TAG	UNP Q581W1
B	-13	HIS	-	EXPRESSION TAG	UNP Q581W1
B	-12	HIS	-	EXPRESSION TAG	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



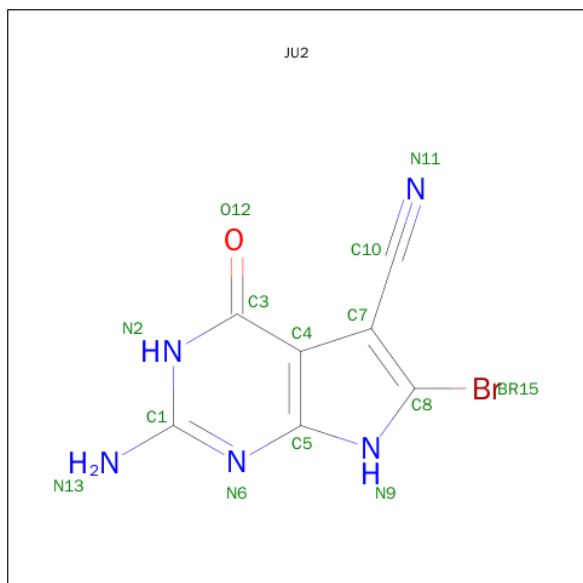
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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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 2-AMINO-6-BROMO-4-OXO-4,7-DIHYDRO-3H-PYRROLO[2,3-D]PYRIMIDINE-5-CARBONITRILE (three-letter code: JU2) (formula: C<sub>7</sub>H<sub>4</sub>BrN<sub>5</sub>O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	Br	C	N	O	0	0
			14	1	7	5	1		
3	B	1	Total	Br	C	N	O	0	0
			14	1	7	5	1		
3	C	1	Total	Br	C	N	O	0	0
			14	1	7	5	1		
3	D	1	Total	Br	C	N	O	0	0
			14	1	7	5	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	190	Total	O	0	0
			190	190		
4	B	183	Total	O	0	0
			183	183		
4	C	187	Total	O	0	0
			187	187		

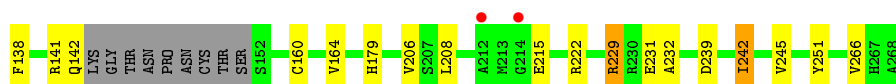
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	171	Total	O	0	0
			171	171		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.86Å 89.11Å 84.25Å 90.00° 116.08° 90.00°	Depositor
Resolution (Å)	27.65 – 1.80 27.65 – 1.80	Depositor EDS
% Data completeness (in resolution range)	92.8 (27.65-1.80) 92.8 (27.65-1.80)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.168 , 0.204 0.169 , 0.204	Depositor DCC
$R_{free}$ test set	4262 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.8	Xtriage
Anisotropy	0.849	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 49.1	EDS
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 84241 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8546	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.14% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: JU2, 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	0.41	0/1910	0.54	0/2590
1	B	0.41	0/1943	0.57	0/2635
1	C	0.43	0/1943	0.57	1/2637 (0.0%)
1	D	0.41	0/1927	0.52	0/2614
All	All	0.42	0/7723	0.55	1/10476 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	159	LEU	CA-CB-CG	-5.16	103.44	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1871	0	1911	13	0
1	B	1901	0	1937	21	0
1	C	1907	0	1938	25	0
1	D	1888	0	1924	21	0
2	A	48	0	25	1	0
2	B	48	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	48	0	25	1	0
2	D	48	0	25	0	0
3	A	14	0	4	0	0
3	B	14	0	4	0	0
3	C	14	0	4	1	0
3	D	14	0	4	0	0
4	A	190	0	0	0	1
4	B	183	0	0	1	0
4	C	187	0	0	4	0
4	D	171	0	0	6	1
All	All	8546	0	7826	73	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 5.

All (73) 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:D:231:GLU:HB2	4:D:711:HOH:O	1.26	1.30
1:C:82:ARG:HG2	1:C:82:ARG:HH21	1.32	0.94
1:D:206:VAL:HG12	4:D:711:HOH:O	1.68	0.92
1:B:207:SER:O	1:B:231[A]:GLU:HB2	1.79	0.83
1:A:34:TYR:HE2	1:A:58:VAL:HG13	1.49	0.76
1:B:34[A]:TYR:HE2	1:B:58:VAL:HG13	1.52	0.74
1:C:207[A]:SER:O	1:C:231:GLU:HB3	1.89	0.72
1:D:164:VAL:HG22	1:D:179:HIS:CD2	2.27	0.69
1:D:231:GLU:CB	4:D:711:HOH:O	2.04	0.67
1:C:82:ARG:CG	1:C:82:ARG:HH21	2.07	0.66
1:B:205:GLY:O	2:B:269:NAP:H4N	1.96	0.65
1:C:222:ARG:HE	1:C:231:GLU:CD	2.01	0.64
1:C:151:SER:N	4:C:598:HOH:O	2.32	0.63
1:C:205[A]:GLY:O	2:C:269:NAP:H4N	1.99	0.62
1:B:164:VAL:HG22	1:B:179:HIS:CD2	2.35	0.62
1:C:206[A]:VAL:HG22	4:C:372:HOH:O	2.00	0.61
1:B:207:SER:O	1:B:231[B]:GLU:HB3	2.02	0.59
1:D:206:VAL:C	4:D:711:HOH:O	2.39	0.59
1:D:222:ARG:HD3	1:D:231:GLU:OE2	2.04	0.57
1:B:247:GLY:O	1:B:250:GLN:HG2	2.07	0.55
1:B:9:THR:HA	1:B:33:HIS:HB3	1.89	0.55
1:C:9:THR:HA	1:C:33:HIS:HB3	1.89	0.55
1:C:164:VAL:HG22	1:C:179:HIS:CD2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:THR:HA	1:A:33:HIS:HB3	1.88	0.55
1:D:22:LYS:HE2	1:D:239:ASP:OD1	2.06	0.55
1:A:69:LEU:HD13	1:A:133:LEU:HD12	1.89	0.54
1:D:9:THR:HA	1:D:33:HIS:HB3	1.90	0.53
1:B:209:LEU:HD13	1:B:218:LYS:HA	1.90	0.52
1:C:78[B]:ASN:HD21	1:C:82:ARG:CZ	2.24	0.51
1:D:229:ARG:NH2	4:D:513:HOH:O	2.45	0.50
1:A:250:GLN:HG3	1:B:236:GLN:HE21	1.78	0.49
1:A:9:THR:O	1:A:93:ASN:HB3	2.11	0.49
1:C:65:ASN:HA	1:C:69:LEU:HD22	1.94	0.48
1:C:210:PRO:HD3	3:C:270:JU2:N11	2.28	0.48
1:A:34:TYR:CE2	1:A:58:VAL:HG13	2.39	0.48
1:B:67:ASN:HB2	4:B:360:HOH:O	2.13	0.48
1:C:86:ARG:HD3	1:C:88:ASP:OD1	2.14	0.47
1:B:242[A]:ILE:HA	1:B:245:VAL:HG22	1.97	0.47
1:C:82:ARG:NH2	1:C:82:ARG:CG	2.72	0.47
1:A:232:ALA:HB2	1:B:251:TYR:CE2	2.50	0.47
1:A:251:TYR:CE2	1:B:232:ALA:HB2	2.50	0.47
1:C:232:ALA:HB2	1:D:251:TYR:CE2	2.50	0.46
1:A:172:SER:O	1:A:176:MET:HG3	2.15	0.46
1:B:163:MET:HG3	1:B:206:VAL:HG23	1.98	0.45
1:C:231:GLU:HG2	4:C:373:HOH:O	2.16	0.45
1:D:78:ASN:OD1	1:D:141:ARG:NH1	2.49	0.45
1:D:242:ILE:HA	1:D:245:VAL:HG22	1.98	0.45
1:D:65:ASN:HA	1:D:69:LEU:HD22	1.97	0.45
1:B:69:LEU:HD13	1:B:133:LEU:HD12	1.99	0.45
1:B:220:LYS:O	1:B:224:LYS:HE2	2.17	0.44
1:D:130:ALA:HB3	1:D:131:PRO:HD3	1.99	0.44
1:C:232:ALA:HB2	1:D:251:TYR:CD2	2.53	0.44
1:C:209[A]:LEU:HA	1:C:210:PRO:HD3	1.81	0.44
1:A:242:ILE:HA	1:A:245:VAL:HG22	1.99	0.44
1:C:251:TYR:CE2	1:D:232:ALA:HB2	2.53	0.44
1:D:14:ARG:NH2	1:D:208:LEU:O	2.51	0.43
1:C:160:CYS:HB3	4:C:347:HOH:O	2.19	0.43
1:A:268:ALA:HB2	1:D:266:VAL:HB	1.99	0.43
1:A:15:ILE:HB	2:A:269:NAP:H51N	2.00	0.43
1:B:220:LYS:O	1:B:224:LYS:HG3	2.20	0.42
1:B:164:VAL:HA	1:B:175:ASN:HD21	1.84	0.42
1:C:164:VAL:HA	1:C:175:ASN:HD21	1.83	0.42
1:D:9:THR:O	1:D:93:ASN:HB3	2.19	0.42
1:A:161:ASP:HB3	1:A:164:VAL:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:PHE:O	1:C:142:GLN:HG2	2.20	0.42
1:B:3:ALA:O	1:B:29:ARG:NH2	2.52	0.42
1:B:78[A]:ASN:OD1	1:B:141:ARG:NH2	2.53	0.41
1:D:160:CYS:HB3	4:D:302:HOH:O	2.20	0.41
1:B:100:THR:HG21	1:B:173:LEU:HD12	2.03	0.41
1:D:138:PHE:O	1:D:142:GLN:HG2	2.21	0.40
1:C:206[A]:VAL:HG21	1:C:221:TRP:CZ3	2.56	0.40
1:C:14:ARG:NH2	1:C:208[B]:LEU:O	2.54	0.40
1:C:192:LEU:HB3	1:C:197:ILE:HB	2.04	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)
4:A:336:HOH:O	4:D:337:HOH:O[1_655]	2.19	0.01

## 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	247/288 (86%)	237 (96%)	10 (4%)	0	100	100
1	B	251/288 (87%)	245 (98%)	6 (2%)	0	100	100
1	C	252/288 (88%)	241 (96%)	11 (4%)	0	100	100
1	D	249/288 (86%)	240 (96%)	9 (4%)	0	100	100
All	All	999/1152 (87%)	963 (96%)	36 (4%)	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	201/231 (87%)	196 (98%)	5 (2%)	55	39
1	B	205/231 (89%)	195 (95%)	10 (5%)	31	13
1	C	205/231 (89%)	198 (97%)	7 (3%)	44	26
1	D	203/231 (88%)	198 (98%)	5 (2%)	55	39
All	All	814/924 (88%)	787 (97%)	27 (3%)	46	27

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	60	GLN
1	A	69	LEU
1	A	229	ARG
1	A	242	ILE
1	B	44	LEU
1	B	58	VAL
1	B	69	LEU
1	B	159[A]	LEU
1	B	159[B]	LEU
1	B	164	VAL
1	B	190	LEU
1	B	217	GLU
1	B	242[A]	ILE
1	B	242[B]	ILE
1	C	50	LYS
1	C	82	ARG
1	C	159	LEU
1	C	164	VAL
1	C	190	LEU
1	C	216	GLU
1	C	231	GLU
1	D	53	SER
1	D	82	ARG

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Mol	Chain	Res	Type
1	D	215	GLU
1	D	229	ARG
1	D	242	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	166	GLN
1	A	175	ASN
1	A	186	GLN
1	B	65	ASN
1	B	166	GLN
1	B	175	ASN
1	B	186	GLN
1	C	35	HIS
1	C	175	ASN
1	C	186	GLN
1	D	67[A]	ASN
1	D	166	GLN
1	D	175	ASN
1	D	179	HIS
1	D	186	GLN

### 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 ⓘ

8 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	269	-	42,52,52	1.51	3 (7%)	54,80,80	2.15	6 (11%)
3	JU2	A	270	-	13,15,15	2.81	5 (38%)	7,22,22	4.57	3 (42%)
2	NAP	B	269	-	42,52,52	1.56	3 (7%)	54,80,80	2.02	8 (14%)
3	JU2	B	270	-	13,15,15	2.86	5 (38%)	7,22,22	4.62	3 (42%)
2	NAP	C	269	-	42,52,52	1.55	3 (7%)	54,80,80	2.11	7 (12%)
3	JU2	C	270	-	13,15,15	2.95	5 (38%)	7,22,22	4.39	3 (42%)
2	NAP	D	269	-	42,52,52	1.53	3 (7%)	54,80,80	2.01	6 (11%)
3	JU2	D	270	-	13,15,15	2.83	5 (38%)	7,22,22	4.52	3 (42%)

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	269	-	-	0/27/67/67	0/5/5/5
3	JU2	A	270	-	-	0/0/2/2	0/2/2/2
2	NAP	B	269	-	-	0/27/67/67	0/5/5/5
3	JU2	B	270	-	-	0/0/2/2	0/2/2/2
2	NAP	C	269	-	-	0/27/67/67	0/5/5/5
3	JU2	C	270	-	-	0/0/2/2	0/2/2/2
2	NAP	D	269	-	-	0/27/67/67	0/5/5/5
3	JU2	D	270	-	-	0/0/2/2	0/2/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	270	JU2	C7-C10	-7.45	1.34	1.44
3	D	270	JU2	C7-C10	-7.38	1.34	1.44
3	C	270	JU2	C7-C10	-7.31	1.34	1.44
3	B	270	JU2	C7-C10	-7.15	1.34	1.44
2	B	269	NAP	C2A-N1A	2.38	1.38	1.33
2	A	269	NAP	C2A-N1A	2.39	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	269	NAP	C2A-N1A	2.46	1.38	1.33
2	D	269	NAP	C2A-N1A	2.50	1.38	1.33
3	C	270	JU2	C4-C5	2.74	1.50	1.43
3	A	270	JU2	C4-C5	2.76	1.50	1.43
3	D	270	JU2	C4-C5	2.83	1.50	1.43
3	B	270	JU2	C4-C5	2.94	1.50	1.43
3	A	270	JU2	C7-C4	2.99	1.45	1.42
3	D	270	JU2	C7-C4	3.04	1.46	1.42
3	D	270	JU2	C3-C4	3.25	1.46	1.41
3	A	270	JU2	C3-C4	3.26	1.46	1.41
2	A	269	NAP	C2A-N3A	3.47	1.38	1.32
3	B	270	JU2	C7-C4	3.49	1.46	1.42
3	C	270	JU2	C3-C4	3.59	1.47	1.41
2	D	269	NAP	C2A-N3A	3.61	1.38	1.32
3	B	270	JU2	C3-C4	3.63	1.47	1.41
2	C	269	NAP	C2A-N3A	3.65	1.38	1.32
3	C	270	JU2	C7-C4	3.74	1.46	1.42
2	B	269	NAP	C2A-N3A	3.79	1.38	1.32
3	A	270	JU2	BR15-C8	4.04	1.96	1.90
3	B	270	JU2	BR15-C8	4.16	1.96	1.90
3	D	270	JU2	BR15-C8	4.35	1.96	1.90
3	C	270	JU2	BR15-C8	4.65	1.97	1.90
2	A	269	NAP	O7N-C7N	7.50	1.40	1.24
2	C	269	NAP	O7N-C7N	7.61	1.40	1.24
2	D	269	NAP	O7N-C7N	7.67	1.40	1.24
2	B	269	NAP	O7N-C7N	7.79	1.40	1.24

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	269	NAP	N3A-C2A-N1A	-12.70	119.17	128.89
2	A	269	NAP	N3A-C2A-N1A	-12.67	119.20	128.89
2	D	269	NAP	N3A-C2A-N1A	-11.48	120.10	128.89
2	B	269	NAP	N3A-C2A-N1A	-11.18	120.33	128.89
3	B	270	JU2	C4-C3-N2	-10.66	116.12	124.19
3	A	270	JU2	C4-C3-N2	-10.51	116.23	124.19
3	D	270	JU2	C4-C3-N2	-10.43	116.29	124.19
3	C	270	JU2	C4-C3-N2	-10.03	116.59	124.19
2	A	269	NAP	C4B-O4B-C1B	-3.92	105.41	109.72
2	B	269	NAP	C4B-O4B-C1B	-3.85	105.49	109.72
2	D	269	NAP	C4B-O4B-C1B	-3.77	105.57	109.72
2	A	269	NAP	C1B-N9A-C4A	-3.48	121.69	126.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	269	NAP	O7N-C7N-C3N	-3.29	115.99	119.59
2	B	269	NAP	C1B-N9A-C4A	-3.00	122.42	126.94
2	C	269	NAP	C4B-O4B-C1B	-2.94	106.49	109.72
2	C	269	NAP	O7N-C7N-C3N	-2.71	116.62	119.59
2	D	269	NAP	C1B-N9A-C4A	-2.69	122.89	126.94
3	C	270	JU2	N6-C1-N2	-2.53	123.60	127.44
3	A	270	JU2	N6-C1-N2	-2.48	123.66	127.44
3	D	270	JU2	N6-C1-N2	-2.46	123.70	127.44
3	B	270	JU2	N6-C1-N2	-2.42	123.75	127.44
2	C	269	NAP	C1B-N9A-C4A	-2.42	123.29	126.94
2	D	269	NAP	C4A-C5A-N7A	-2.20	107.45	109.48
2	B	269	NAP	C4A-C5A-N7A	-2.20	107.46	109.48
2	C	269	NAP	C3N-C7N-N7N	2.37	120.41	117.82
2	C	269	NAP	O4D-C1D-N1N	2.52	110.91	108.13
2	B	269	NAP	C3N-C7N-N7N	2.83	120.91	117.82
2	A	269	NAP	C3N-C7N-N7N	3.09	121.20	117.82
2	B	269	NAP	O4D-C1D-N1N	3.61	112.09	108.13
2	A	269	NAP	O4B-C1B-N9A	3.72	115.89	108.10
2	C	269	NAP	O4B-C1B-N9A	3.77	115.98	108.10
2	B	269	NAP	O4B-C1B-N9A	3.83	116.11	108.10
2	A	269	NAP	O4D-C1D-N1N	3.97	112.50	108.13
2	D	269	NAP	O4B-C1B-N9A	4.16	116.82	108.10
2	D	269	NAP	O4D-C1D-N1N	4.52	113.10	108.13
3	C	270	JU2	C3-N2-C1	4.71	122.47	115.94
3	A	270	JU2	C3-N2-C1	4.89	122.72	115.94
3	B	270	JU2	C3-N2-C1	4.90	122.74	115.94
3	D	270	JU2	C3-N2-C1	4.97	122.83	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	269	NAP	1	0
2	B	269	NAP	1	0
2	C	269	NAP	1	0
3	C	270	JU2	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	249/288 (86%)	-0.31	2 (0%) 87 85	11, 15, 28, 39	3 (1%)
1	B	250/288 (86%)	-0.31	5 (2%) 68 64	10, 15, 29, 47	0
1	C	250/288 (86%)	-0.22	7 (2%) 56 51	11, 15, 30, 46	2 (0%)
1	D	249/288 (86%)	-0.23	5 (2%) 68 64	10, 15, 28, 36	6 (2%)
All	All	998/1152 (86%)	-0.27	19 (1%) 70 66	10, 15, 29, 47	11 (1%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	113	GLY	5.9
1	C	151	SER	5.1
1	A	113	GLY	4.6
1	C	113	GLY	4.3
1	D	113	GLY	4.2
1	A	2	GLU	3.2
1	B	151	SER	3.1
1	C	152	SER	3.0
1	B	2	GLU	2.9
1	D	2	GLU	2.7
1	C	195	TYR	2.4
1	D	212	ALA	2.4
1	B	103	VAL	2.3
1	B	152	SER	2.2
1	C	212	ALA	2.2
1	D	214	GLY	2.2
1	D	91	VAL	2.1
1	C	211	VAL	2.1
1	C	2	GLU	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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	JU2	D	270	14/14	0.99	0.07	-0.55	14,20,23,23	0
3	JU2	A	270	14/14	0.99	0.07	-0.80	12,16,20,20	0
3	JU2	C	270	14/14	0.99	0.07	-0.95	13,16,19,22	0
3	JU2	B	270	14/14	0.99	0.06	-1.13	12,16,20,21	0
2	NAP	D	269	48/48	0.98	0.06	-1.26	9,15,20,21	0
2	NAP	B	269	48/48	0.98	0.06	-1.31	9,14,19,20	0
2	NAP	C	269	48/48	0.97	0.06	-1.45	8,15,20,21	0
2	NAP	A	269	48/48	0.98	0.06	-1.50	11,15,19,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.