



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 04:01 PM GMT

PDB ID : 1VBJ  
Title : The crystal structure of prostaglandin F synthase from Trypanosoma brucei  
Authors : Inoue, T.  
Deposited on : 2004-02-27  
Resolution : 2.10 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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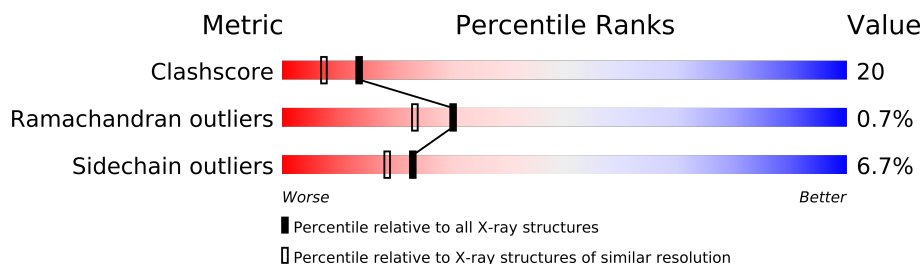
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : NOT EXECUTED  
EDS : NOT EXECUTED  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.10 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))
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	281	
1	B	281	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5094 atoms, of which 0 are hydrogen and 0 are deuterium.

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 prostaglandin F synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2218	1418	376	411	13			
1	B	279	Total	C	N	O	S	0	0	0
			2208	1413	374	408	13			

There are 10 discrepancies between the modelled and reference sequences:

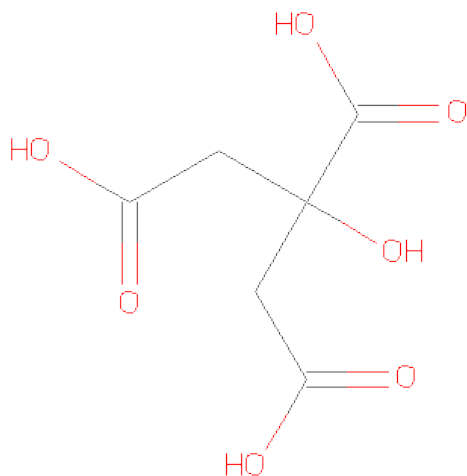
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	CLONING ARTIFACT	UNP Q9GV41
A	-3	SER	-	CLONING ARTIFACT	UNP Q9GV41
A	-2	PRO	-	CLONING ARTIFACT	UNP Q9GV41
A	-1	GLU	-	CLONING ARTIFACT	UNP Q9GV41
A	0	PHE	-	CLONING ARTIFACT	UNP Q9GV41
B	-4	GLY	-	CLONING ARTIFACT	UNP Q9GV41
B	-3	SER	-	CLONING ARTIFACT	UNP Q9GV41
B	-2	PRO	-	CLONING ARTIFACT	UNP Q9GV41
B	-1	GLU	-	CLONING ARTIFACT	UNP Q9GV41
B	0	PHE	-	CLONING ARTIFACT	UNP Q9GV41

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



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		

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	290	Total 290	O 290	0	0
4	B	256	Total 256	O 256	0	0

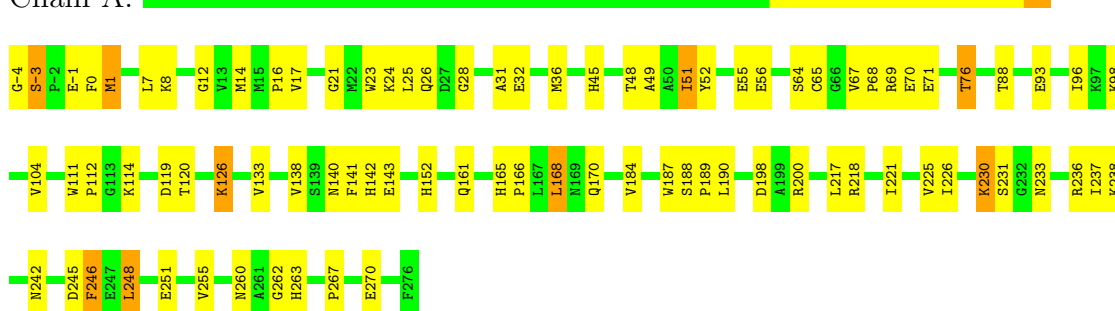
### 3 Residue-property plots

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.

Note EDS was not executed.

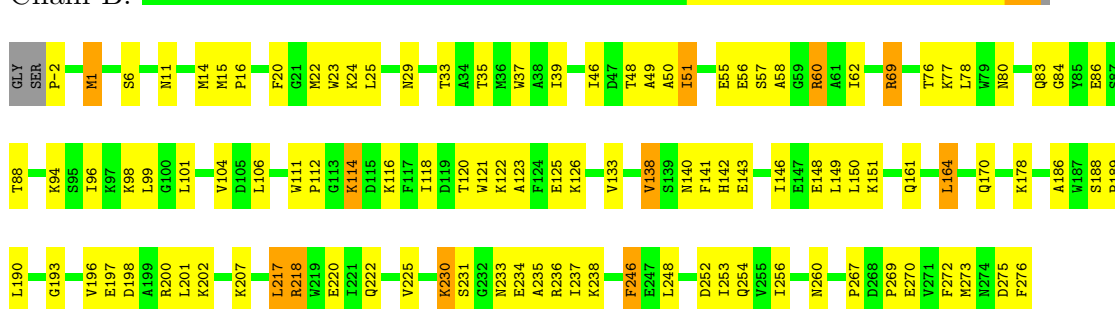
- Molecule 1: prostaglandin F synthase

Chain A:



- Molecule 1: prostaglandin F synthase

Chain B:



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.21Å 113.21Å 136.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.62 – 2.10	Depositor
% Data completeness (in resolution range)	89.0 (32.62-2.10)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.208 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5094	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, CIT

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	0.36	0/2270	0.61	0/3064
1	B	0.33	0/2260	0.59	0/3050
All	All	0.34	0/4530	0.60	0/6114

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2218	0	2198	69	0
1	B	2208	0	2190	114	0
2	A	48	0	25	2	0
2	B	48	0	25	4	0
3	A	13	0	5	1	0
3	B	13	0	5	1	0
4	A	290	0	0	4	0
4	B	256	0	0	7	0
All	All	5094	0	4448	181	0



Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

All (181) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:84:GLY:H	1:B:120:THR:HG22	1.23	1.02
1:B:48:THR:HG22	1:B:49:ALA:H	1.35	0.91
1:B:207:LYS:HG3	4:B:4045:HOH:O	1.75	0.87
1:B:118:ILE:HD12	1:B:118:ILE:H	1.37	0.86
1:B:84:GLY:N	1:B:120:THR:HG22	1.90	0.86
1:A:0:PHE:O	1:A:1:MET:HG2	1.79	0.83
1:B:233:ASN:O	1:B:237:ILE:HG12	1.82	0.79
1:B:116:LYS:O	1:B:120:THR:HG23	1.82	0.79
1:B:231:SER:HB3	1:B:237:ILE:HD13	1.62	0.78
1:A:111:TRP:CH2	1:A:267:PRO:HG2	2.18	0.78
1:B:22:MET:SD	1:B:46:ILE:HD11	2.24	0.78
1:A:48:THR:HG22	1:A:49:ALA:H	1.48	0.78
1:A:23:TRP:O	1:A:24:LYS:HG2	1.84	0.77
1:B:198:ASP:HB3	1:B:201:LEU:HD23	1.65	0.77
1:A:51:ILE:HD13	1:A:51:ILE:O	1.84	0.77
1:B:51:ILE:O	1:B:51:ILE:HD13	1.86	0.74
1:B:178:LYS:HE2	4:B:4163:HOH:O	1.86	0.74
1:A:21:GLY:O	1:A:230:LYS:HB2	1.87	0.73
1:A:55:GLU:OE2	1:A:76:THR:HG21	1.89	0.73
1:B:60:ARG:HB3	1:B:60:ARG:HH11	1.54	0.72
1:B:88:THR:HG21	1:B:120:THR:HB	1.70	0.72
1:A:230:LYS:HD2	1:A:231:SER:N	2.04	0.72
1:B:111:TRP:CH2	1:B:267:PRO:HG2	2.26	0.71
1:A:231:SER:HB3	1:A:237:ILE:HD13	1.74	0.69
1:B:69:ARG:HD2	1:B:101:LEU:HD22	1.73	0.69
1:B:233:ASN:HD22	1:B:236:ARG:HG3	1.58	0.69
1:B:148:GLU:HA	1:B:151:LYS:HE3	1.75	0.68
1:A:168:LEU:HD22	4:A:4061:HOH:O	1.93	0.67
1:A:233:ASN:HD22	1:A:236:ARG:H	1.40	0.67
1:A:104:VAL:O	1:A:133:VAL:HA	1.96	0.66
1:A:143:GLU:CG	1:B:260:ASN:HB3	2.26	0.66
1:A:233:ASN:O	1:A:237:ILE:HG12	1.96	0.65
1:A:8:LYS:HA	1:A:14:MET:HE1	1.78	0.64
1:B:76:THR:HG22	1:B:77:LYS:N	2.13	0.63
1:A:96:ILE:HD13	1:A:104:VAL:HG23	1.81	0.63
1:B:6:SER:HB2	1:B:15:MET:O	1.99	0.62
1:B:254:GLN:HG3	4:B:4133:HOH:O	1.98	0.62
1:B:222:GLN:NE2	1:B:253:ILE:HD11	2.15	0.62
1:B:114:LYS:HG2	1:B:273:MET:SD	2.40	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:3002:NAP:H4N	3:B:4002:CIT:H41	1.82	0.61
1:B:231:SER:HB3	1:B:237:ILE:CD1	2.31	0.61
1:A:126:LYS:HD2	4:A:4049:HOH:O	2.00	0.61
1:B:233:ASN:HB3	1:B:236:ARG:HD2	1.82	0.60
1:B:83:GLN:HB3	1:B:120:THR:HG21	1.83	0.60
1:B:50:ALA:HA	1:B:55:GLU:OE1	2.02	0.59
1:B:233:ASN:HD21	1:B:235:ALA:HB3	1.68	0.59
1:B:25:LEU:HD13	1:B:230:LYS:HE3	1.84	0.58
1:A:8:LYS:HG3	1:A:14:MET:HE3	1.85	0.58
1:B:233:ASN:ND2	1:B:235:ALA:HB3	2.19	0.58
1:B:6:SER:OG	1:B:14:MET:HG3	2.03	0.57
1:B:193:GLY:O	1:B:196:VAL:HG22	2.04	0.57
1:B:188:SER:N	1:B:189:PRO:CD	2.68	0.57
1:A:140:ASN:HD21	1:A:187:TRP:HE1	1.54	0.56
1:B:146:ILE:O	1:B:150:LEU:HG	2.05	0.56
1:B:20:PHE:CE1	1:B:237:ILE:HD12	2.41	0.56
1:B:218:ARG:HG2	1:B:218:ARG:HH21	1.71	0.56
1:B:48:THR:HG22	1:B:49:ALA:N	2.14	0.55
1:B:55:GLU:OE2	1:B:76:THR:HG21	2.07	0.55
1:B:151:LYS:NZ	1:B:151:LYS:HB2	2.21	0.55
1:B:35:THR:O	1:B:39:ILE:HG13	2.07	0.55
1:A:8:LYS:HG3	1:A:14:MET:CE	2.36	0.55
1:B:6:SER:HB3	1:B:16:PRO:HA	1.87	0.55
1:A:56:GLU:HG3	1:A:98:LYS:HB3	1.88	0.55
1:B:76:THR:HG22	1:B:77:LYS:H	1.70	0.55
1:B:78:LEU:HD21	1:B:88:THR:HG22	1.88	0.55
1:B:233:ASN:HD22	1:B:236:ARG:H	1.55	0.55
1:B:60:ARG:CB	1:B:60:ARG:HH11	2.20	0.54
1:B:99:LEU:O	1:B:101:LEU:HG	2.07	0.54
1:A:246:PHE:H	1:A:246:PHE:HD2	1.53	0.54
1:B:20:PHE:HE1	1:B:237:ILE:HD12	1.72	0.54
1:A:65:CYS:SG	1:A:67:VAL:HG12	2.47	0.54
1:B:78:LEU:CD2	1:B:88:THR:HG22	2.38	0.54
1:B:96:ILE:HD13	1:B:104:VAL:HG23	1.89	0.54
1:A:231:SER:HB3	1:A:237:ILE:CD1	2.36	0.53
1:A:161:GLN:NE2	2:A:3001:NAP:H2N	2.22	0.53
1:B:142:HIS:CD2	1:B:270:GLU:HG2	2.44	0.53
1:A:188:SER:N	1:A:189:PRO:CD	2.72	0.53
1:B:56:GLU:O	1:B:60:ARG:HG3	2.09	0.52
1:A:263:HIS:HD2	4:B:4015:HOH:O	1.91	0.52
1:B:6:SER:HB2	1:B:15:MET:C	2.30	0.52
1:A:0:PHE:O	1:A:1:MET:CG	2.56	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:198:ASP:O	1:B:202:LYS:HG3	2.08	0.52
1:B:104:VAL:O	1:B:133:VAL:HA	2.09	0.52
1:B:161:GLN:NE2	2:B:3002:NAP:H2N	2.25	0.51
1:B:118:ILE:N	1:B:118:ILE:HD12	2.15	0.51
1:B:23:TRP:O	1:B:24:LYS:HB2	2.09	0.51
1:B:233:ASN:ND2	1:B:236:ARG:HG3	2.24	0.51
1:B:121:TRP:O	1:B:125:GLU:HG3	2.11	0.51
1:A:17:VAL:HB	1:A:221:ILE:HD12	1.92	0.51
1:A:-4:GLY:O	1:A:-3:SER:HB3	2.11	0.50
1:A:230:LYS:HD2	1:A:230:LYS:C	2.31	0.50
1:B:140:ASN:O	1:B:269:PRO:HB3	2.11	0.50
1:A:36:MET:HE1	1:A:64:SER:HB2	1.94	0.50
1:B:246:PHE:N	1:B:246:PHE:CD2	2.80	0.50
1:A:114:LYS:HD3	1:A:114:LYS:C	2.31	0.50
1:A:70:GLU:HG2	4:A:4110:HOH:O	2.11	0.49
1:A:231:SER:O	1:A:237:ILE:HD11	2.12	0.49
1:A:7:LEU:HD12	1:A:7:LEU:C	2.33	0.49
1:A:12:GLY:O	1:A:14:MET:HE2	2.12	0.49
1:B:190:LEU:HD21	1:B:217:LEU:CD1	2.43	0.49
1:B:77:LYS:HE2	2:B:3002:NAP:H71N	1.79	0.48
1:A:25:LEU:HB3	1:A:31:ALA:HA	1.95	0.48
1:A:142:HIS:CE1	1:A:270:GLU:HG2	2.48	0.48
1:A:48:THR:HG22	1:A:49:ALA:N	2.24	0.48
1:B:190:LEU:HD21	1:B:217:LEU:HD13	1.95	0.48
1:B:138:VAL:HG21	1:B:141:PHE:CE1	2.49	0.48
1:B:84:GLY:O	1:B:88:THR:HG23	2.14	0.47
1:B:246:PHE:H	1:B:246:PHE:HD2	1.62	0.47
1:B:1:MET:HA	1:B:1:MET:CE	2.44	0.47
1:B:246:PHE:N	1:B:246:PHE:HD2	2.12	0.47
1:A:140:ASN:ND2	1:A:187:TRP:HE1	2.12	0.47
1:B:252:ASP:O	1:B:256:ILE:HG13	2.15	0.47
1:B:83:GLN:OE1	1:B:276:PHE:HE2	1.97	0.47
1:A:8:LYS:HE2	1:A:14:MET:HE3	1.97	0.47
1:B:233:ASN:CB	1:B:236:ARG:HD2	2.45	0.47
1:B:25:LEU:CD1	1:B:230:LYS:HE3	2.45	0.47
1:B:198:ASP:CB	1:B:201:LEU:HD23	2.42	0.47
1:B:57:SER:HA	1:B:60:ARG:CD	2.44	0.47
1:B:218:ARG:HD2	1:B:222:GLN:OE1	2.15	0.47
1:A:198:ASP:OD2	1:A:200:ARG:HB2	2.15	0.47
1:B:58:ALA:O	1:B:62:ILE:HG13	2.15	0.47
1:B:230:LYS:HD2	1:B:231:SER:N	2.30	0.46
1:A:93:GLU:O	1:A:96:ILE:HG22	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:238:LYS:NZ	1:A:238:LYS:HB3	2.30	0.46
1:B:114:LYS:HA	1:B:114:LYS:HE3	1.98	0.46
1:B:123:ALA:O	1:B:126:LYS:HB3	2.16	0.46
1:B:220:GLU:O	1:B:225:VAL:HG22	2.16	0.46
1:B:218:ARG:O	1:B:218:ARG:HD3	2.17	0.45
1:B:234:GLU:HG2	1:B:238:LYS:HE2	1.98	0.45
1:A:68:PRO:HG2	1:A:71:GLU:HG3	1.98	0.45
1:A:52:TYR:HE1	3:A:4001:CIT:O2	2.00	0.45
1:A:28:GLY:O	1:A:32:GLU:HB2	2.15	0.45
1:B:57:SER:HA	1:B:60:ARG:HD3	1.99	0.45
1:A:190:LEU:HB2	2:A:3001:NAP:H52A	1.99	0.45
1:B:23:TRP:CH2	1:B:24:LYS:HE3	2.51	0.45
1:A:260:ASN:HB3	1:B:143:GLU:CG	2.47	0.45
1:B:253:ILE:HD12	4:B:4132:HOH:O	2.17	0.44
1:A:143:GLU:HG3	1:B:260:ASN:HB3	1.97	0.44
1:A:168:LEU:HD23	1:A:262:GLY:HA2	1.99	0.44
1:B:1:MET:HA	1:B:1:MET:HE2	2.00	0.44
1:B:11:ASN:HB2	4:B:4026:HOH:O	2.16	0.44
1:A:225:VAL:HG12	1:A:226:ILE:N	2.33	0.44
1:B:80:ASN:OD1	1:B:111:TRP:HB2	2.18	0.43
1:B:37:TRP:CE3	1:B:234:GLU:HB2	2.53	0.43
1:B:164:LEU:HB3	1:B:186:ALA:CB	2.48	0.43
1:B:29:ASN:O	1:B:33:THR:HG23	2.18	0.43
1:B:118:ILE:CD1	1:B:118:ILE:H	2.15	0.43
1:A:152:HIS:HA	4:A:4202:HOH:O	2.17	0.43
1:A:251:GLU:O	1:A:255:VAL:HG23	2.18	0.43
1:A:65:CYS:SG	1:A:67:VAL:CG1	3.07	0.43
1:B:138:VAL:HG22	1:B:141:PHE:CE2	2.53	0.43
1:B:151:LYS:HB2	1:B:151:LYS:HZ2	1.84	0.43
1:B:112:PRO:HG3	1:B:141:PHE:CD2	2.53	0.43
1:A:55:GLU:OE2	1:A:76:THR:CG2	2.64	0.43
1:A:-3:SER:OG	1:A:-1:GLU:HB2	2.18	0.43
1:B:94:LYS:O	1:B:98:LYS:HG3	2.19	0.43
1:B:234:GLU:O	1:B:238:LYS:HG3	2.20	0.42
1:A:184:VAL:O	1:A:225:VAL:HG13	2.19	0.42
1:A:88:THR:OG1	1:A:120:THR:HG23	2.20	0.42
1:A:165:HIS:HB2	1:A:166:PRO:CD	2.49	0.42
1:B:-2:PRO:HB2	4:B:4144:HOH:O	2.19	0.42
1:A:246:PHE:CD2	1:A:246:PHE:N	2.88	0.42
1:B:138:VAL:HG22	1:B:141:PHE:CZ	2.55	0.42
1:B:118:ILE:O	1:B:122:LYS:HG3	2.20	0.42
1:A:16:PRO:HB2	1:A:45:HIS:HB2	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:83:GLN:HB3	1:B:120:THR:CG2	2.49	0.41
1:A:0:PHE:HD1	1:A:0:PHE:O	2.03	0.41
1:B:104:VAL:HB	1:B:133:VAL:HG12	2.01	0.41
1:B:80:ASN:O	1:B:83:GLN:HG3	2.20	0.41
1:B:161:GLN:HE21	2:B:3002:NAP:H2N	1.85	0.41
1:B:76:THR:CG2	1:B:77:LYS:N	2.81	0.41
1:A:104:VAL:HB	1:A:133:VAL:HG12	2.02	0.41
1:B:198:ASP:OD2	1:B:200:ARG:HB2	2.20	0.41
1:B:164:LEU:HB3	1:B:186:ALA:HB1	2.02	0.41
1:A:218:ARG:CG	1:A:248:LEU:HD22	2.51	0.41
1:B:218:ARG:HG2	1:B:218:ARG:NH2	2.36	0.41
1:A:112:PRO:HG3	1:A:141:PHE:CD2	2.56	0.41
1:B:49:ALA:HA	1:B:76:THR:HG23	2.03	0.40
1:A:17:VAL:HB	1:A:221:ILE:CD1	2.51	0.40
1:A:165:HIS:HB2	1:A:166:PRO:HD2	2.03	0.40
1:B:197:GLU:HA	1:B:197:GLU:OE2	2.20	0.40

There are no symmetry-related clashes.

## 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	279/281 (99%)	265 (95%)	11 (4%)	3 (1%)	21	13
1	B	277/281 (99%)	257 (93%)	19 (7%)	1 (0%)	43	39
All	All	556/562 (99%)	522 (94%)	30 (5%)	4 (1%)	30	23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	26	GLN
1	B	272	PHE
1	A	-3	SER

### 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	233/233 (100%)	219 (94%)	14 (6%)	27	22
1	B	232/233 (100%)	215 (93%)	17 (7%)	20	15
All	All	465/466 (100%)	434 (93%)	31 (7%)	23	18

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ILE
1	A	69	ARG
1	A	76	THR
1	A	119	ASP
1	A	126	LYS
1	A	138	VAL
1	A	168	LEU
1	A	170	GLN
1	A	217	LEU
1	A	230	LYS
1	A	242	ASN
1	A	245	ASP
1	A	246	PHE
1	A	248	LEU
1	B	1	MET
1	B	51	ILE
1	B	60	ARG
1	B	69	ARG
1	B	86	GLU
1	B	106	LEU
1	B	114	LYS
1	B	138	VAL
1	B	149	LEU
1	B	164	LEU
1	B	170	GLN
1	B	217	LEU
1	B	218	ARG
1	B	230	LYS
1	B	246	PHE

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Mol	Chain	Res	Type
1	B	248	LEU
1	B	275	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
1	A	160	ASN
1	A	161	GLN
1	A	170	GLN
1	A	192	GLN
1	A	233	ASN
1	A	263	HIS
1	A	274	ASN
1	B	5	GLN
1	B	26	GLN
1	B	140	ASN
1	B	152	HIS
1	B	161	GLN
1	B	170	GLN
1	B	192	GLN
1	B	233	ASN
1	B	242	ASN
1	B	263	HIS
1	B	274	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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

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	3001	-	52,52,52	1.80	11 (21%)	80,80,80	1.69	15 (18%)
3	CIT	A	4001	-	12,12,12	2.40	3 (25%)	17,17,17	3.49	9 (52%)
2	NAP	B	3002	-	52,52,52	1.78	11 (21%)	80,80,80	1.64	16 (20%)
3	CIT	B	4002	-	12,12,12	1.98	3 (25%)	17,17,17	3.24	7 (41%)

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	3001	-	-	0/35/67/67	0/3/5/5
3	CIT	A	4001	-	-	0/16/16/16	0/0/0/0
2	NAP	B	3002	-	-	0/35/67/67	0/3/5/5
3	CIT	B	4002	-	-	0/16/16/16	0/0/0/0

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4001	CIT	C3-C6	5.96	1.59	1.53
2	A	3001	NAP	C2N-N1N	5.34	1.42	1.35
2	B	3002	NAP	C2N-N1N	5.14	1.41	1.35
2	B	3002	NAP	C4N-C3N	4.57	1.47	1.39
3	B	4002	CIT	C3-C6	4.55	1.58	1.53
2	A	3001	NAP	C4N-C3N	4.46	1.47	1.39
3	A	4001	CIT	O2-C1	-4.37	1.14	1.30
2	A	3001	NAP	C2A-N1A	3.87	1.41	1.33
2	A	3001	NAP	O4D-C1D	3.76	1.47	1.41
2	B	3002	NAP	O4D-C1D	3.63	1.46	1.41
2	B	3002	NAP	C2A-N1A	3.46	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3001	NAP	C2A-N3A	3.46	1.39	1.32
2	B	3002	NAP	C2A-N3A	3.45	1.39	1.32
2	B	3002	NAP	C2D-C1D	-3.44	1.48	1.53
2	B	3002	NAP	C6N-N1N	3.17	1.44	1.35
2	A	3001	NAP	C6N-N1N	3.13	1.44	1.35
3	B	4002	CIT	O2-C1	-3.05	1.19	1.30
3	B	4002	CIT	C4-C3	2.78	1.57	1.53
2	A	3001	NAP	C2D-C1D	-2.74	1.49	1.53
2	B	3002	NAP	PA-O1A	-2.63	1.41	1.51
2	A	3001	NAP	C4A-N9A	-2.52	1.34	1.37
2	A	3001	NAP	PA-O1A	-2.47	1.42	1.51
3	A	4001	CIT	C4-C3	2.33	1.56	1.53
2	A	3001	NAP	C4A-N3A	2.29	1.39	1.35
2	A	3001	NAP	C5B-C4B	2.28	1.59	1.51
2	B	3002	NAP	C4A-N3A	2.12	1.38	1.35
2	B	3002	NAP	C4A-N9A	-2.09	1.34	1.37
2	B	3002	NAP	C3D-C4D	2.04	1.58	1.53

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3001	NAP	N3A-C2A-N1A	-7.33	122.58	128.71
3	B	4002	CIT	O5-C6-C3	7.28	132.23	122.20
3	A	4001	CIT	O5-C6-C3	7.21	132.14	122.20
2	B	3002	NAP	N3A-C2A-N1A	-7.20	122.69	128.71
3	A	4001	CIT	C2-C3-C6	7.13	126.62	110.12
3	A	4001	CIT	O7-C3-C6	-6.51	99.58	108.95
2	A	3001	NAP	C4B-O4B-C1B	6.12	116.40	109.75
3	B	4002	CIT	O7-C3-C6	-6.09	100.17	108.95
3	B	4002	CIT	C2-C3-C6	5.46	122.75	110.12
3	B	4002	CIT	O6-C6-C3	-5.33	105.14	112.89
2	B	3002	NAP	C4B-O4B-C1B	5.20	115.40	109.75
3	A	4001	CIT	O6-C6-C3	-4.73	106.02	112.89
2	A	3001	NAP	O4D-C1D-N1N	3.14	111.17	107.95
2	B	3002	NAP	C3N-C7N-N7N	3.11	121.31	117.77
2	A	3001	NAP	C3N-C7N-N7N	3.05	121.25	117.77
2	A	3001	NAP	O4B-C4B-C5B	-3.02	98.56	109.36
3	B	4002	CIT	C4-C3-C6	-2.94	103.31	110.12
2	A	3001	NAP	O7N-C7N-C3N	-2.87	116.34	119.58
2	B	3002	NAP	O4B-C4B-C5B	-2.83	99.26	109.36
2	A	3001	NAP	C2N-C3N-C4N	2.70	121.37	118.31
2	B	3002	NAP	C5A-C6A-N6A	2.63	126.67	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3001	NAP	C5A-C6A-N6A	2.63	126.66	120.72
2	A	3001	NAP	C1B-N9A-C4A	-2.62	122.11	126.64
2	A	3001	NAP	C8A-N9A-C1B	2.61	131.51	126.38
2	B	3002	NAP	C3D-C2D-C1D	2.60	104.98	100.91
2	B	3002	NAP	O7N-C7N-C3N	-2.56	116.69	119.58
2	B	3002	NAP	C2N-C3N-C4N	2.54	121.19	118.31
2	A	3001	NAP	C2B-C3B-C4B	2.46	107.79	101.94
2	A	3001	NAP	O3X-P2B-O2X	2.45	117.14	107.61
3	A	4001	CIT	C3-C4-C5	-2.41	107.94	113.77
2	A	3001	NAP	O3B-C3B-C4B	-2.40	104.00	111.08
2	B	3002	NAP	O4D-C1D-N1N	2.39	110.40	107.95
2	B	3002	NAP	O2A-PA-O1A	2.38	125.51	112.21
2	B	3002	NAP	C8A-N9A-C1B	2.38	131.07	126.38
3	A	4001	CIT	O2-C1-C2	2.35	122.92	114.63
3	A	4001	CIT	O7-C3-C4	-2.33	104.53	109.22
3	B	4002	CIT	O2-C1-C2	2.32	122.80	114.63
2	B	3002	NAP	O3X-P2B-O2X	2.31	116.60	107.61
2	A	3001	NAP	O2A-PA-O1A	2.29	124.99	112.21
3	A	4001	CIT	C3-C2-C1	2.26	119.23	113.77
3	A	4001	CIT	O7-C3-C2	-2.24	104.71	109.22
2	B	3002	NAP	C2B-C3B-C4B	2.21	107.19	101.94
2	B	3002	NAP	N3A-C4A-N9A	2.20	129.40	125.43
2	B	3002	NAP	O3B-C3B-C4B	-2.17	104.68	111.08
2	B	3002	NAP	C1B-N9A-C4A	-2.16	122.91	126.64
2	A	3001	NAP	N3A-C4A-N9A	2.06	129.16	125.43
3	B	4002	CIT	O4-C5-C4	-2.00	107.58	114.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.