



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2017 – 05:46 PM EDT

PDB ID : 1IIG  
Title : STRUCTURE OF TRYPANOSOMA BRUCEI BRUCEI TRIOSEPHOSPHATE ISOMERASE COMPLEXED WITH 3-PHOSPHONOPROPIONATE  
Authors : Noble, M.E.; Wierenga, R.K.; Lambeir, A.M.; Oppendoes, F.R.; Thunnissen, A.M.; Kalk, K.H.; Groendijk, H.; Hol, W.G.J.  
Deposited on : unknown  
Resolution : 2.60 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

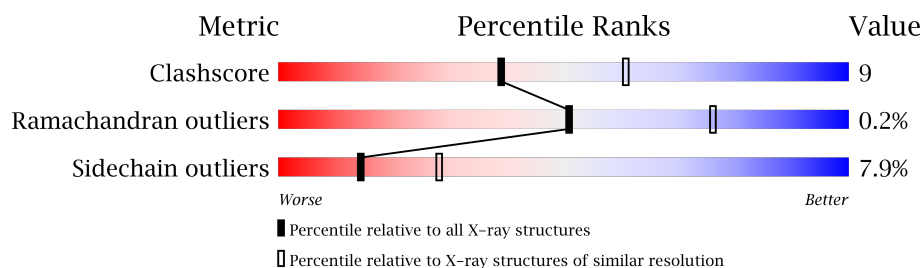
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	250	
1	B	250	

## 2 Entry composition [i](#)

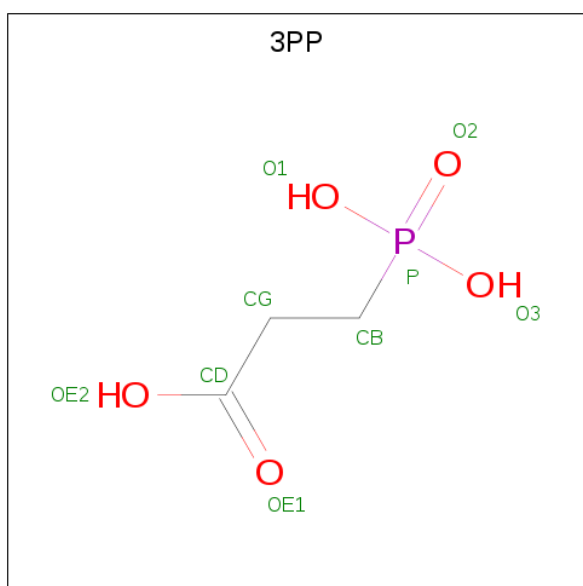
There are 3 unique types of molecules in this entry. The entry contains 3811 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TRIOSEPHOSPHATE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1882	1197	331	349	5			
1	B	249	Total	C	N	O	S	0	0	0
			1882	1197	331	349	5			

- Molecule 2 is 3-PHOSPHONOPROPANOIC ACID (three-letter code: 3PP) (formula:  $C_3H_7O_5P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	P	0	0
			9	3	5	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total	O	0	0
			21	21		

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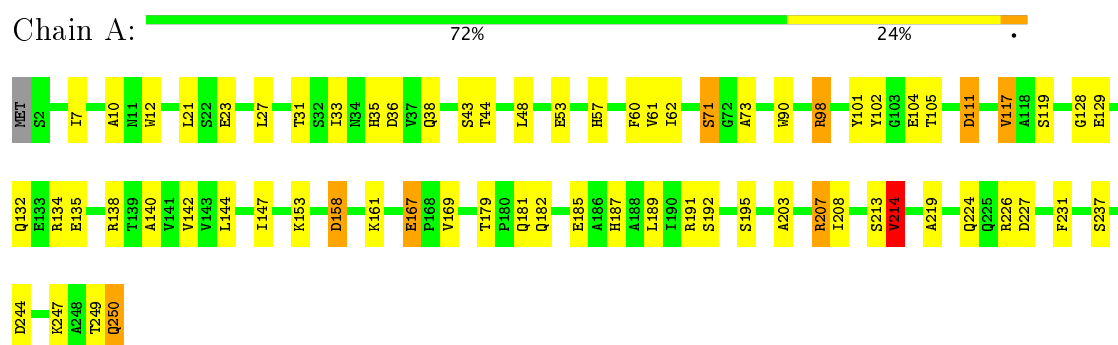
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	17	Total	O	0	0
			17	17		

### 3 Residue-property plots [i](#)

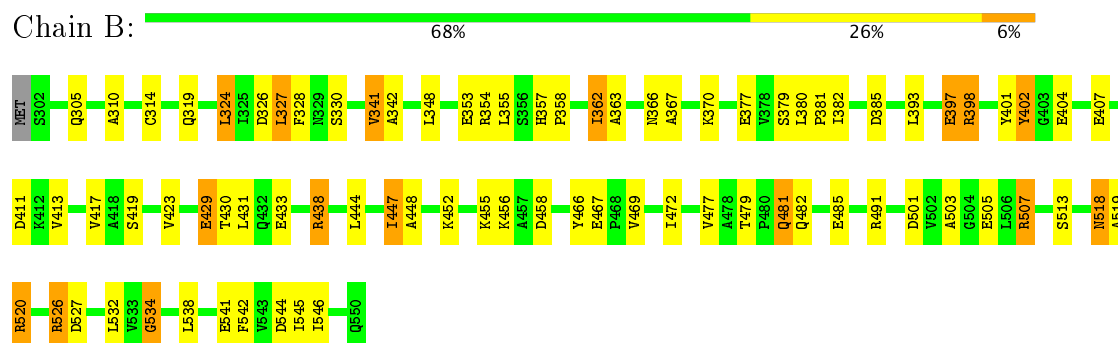
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: TRIOSEPHOSPHATE ISOMERASE



#### • Molecule 1: TRIOSEPHOSPHATE ISOMERASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.36Å 97.59Å 46.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-2.60)	Depositor
$R_{merge}$	0.02	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT, GROMOS	Depositor
R, $R_{free}$	0.125 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3811	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	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: 3PP

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	0.96	7/1916 (0.4%)	1.46	25/2599 (1.0%)
1	B	0.96	11/1916 (0.6%)	1.39	14/2599 (0.5%)
All	All	0.96	18/3832 (0.5%)	1.42	39/5198 (0.8%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	404	GLU	CD-OE2	8.58	1.35	1.25
1	B	485	GLU	CD-OE2	6.80	1.33	1.25
1	B	433	GLU	CD-OE2	6.66	1.32	1.25
1	A	104	GLU	CD-OE2	6.41	1.32	1.25
1	B	377	GLU	CD-OE2	6.09	1.32	1.25
1	B	397	GLU	CD-OE2	5.82	1.32	1.25
1	A	167	GLU	CD-OE2	5.74	1.31	1.25
1	A	23	GLU	CD-OE1	5.63	1.31	1.25
1	A	185	GLU	CD-OE2	5.58	1.31	1.25
1	A	53	GLU	CD-OE1	5.56	1.31	1.25
1	B	353	GLU	CD-OE1	5.55	1.31	1.25
1	B	429	GLU	CD-OE1	5.50	1.31	1.25
1	A	135	GLU	CD-OE1	5.37	1.31	1.25
1	B	467	GLU	CD-OE2	5.34	1.31	1.25
1	B	541	GLU	CD-OE1	5.33	1.31	1.25
1	B	505	GLU	CD-OE2	5.32	1.31	1.25
1	B	407	GLU	CD-OE2	5.07	1.31	1.25
1	A	129	GLU	CD-OE1	-5.03	1.20	1.25

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	ASP	CB-CG-OD2	-10.43	108.91	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	411	ASP	CB-CG-OD2	-10.19	109.13	118.30
1	A	134	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	B	411	ASP	CB-CG-OD1	7.89	125.41	118.30
1	A	138	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	A	158	ASP	CB-CG-OD1	7.41	124.97	118.30
1	A	111	ASP	CB-CG-OD1	7.27	124.84	118.30
1	A	244	ASP	CB-CG-OD2	6.93	124.53	118.30
1	A	111	ASP	CB-CG-OD2	-6.79	112.18	118.30
1	A	227	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	A	227	ASP	CB-CG-OD1	6.64	124.28	118.30
1	A	36	ASP	CB-CG-OD1	-6.55	112.41	118.30
1	B	341	VAL	CG1-CB-CG2	-6.49	100.52	110.90
1	A	226	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	B	326	ASP	CB-CG-OD1	6.42	124.08	118.30
1	B	398	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	250	GLN	N-CA-CB	6.31	121.96	110.60
1	A	249	THR	C-N-CA	6.20	137.19	121.70
1	B	326	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	B	466	TYR	CB-CG-CD2	6.07	124.64	121.00
1	A	214	VAL	CA-CB-CG2	5.93	119.80	110.90
1	A	98	ARG	NE-CZ-NH2	5.87	123.23	120.30
1	B	544	ASP	CB-CG-OD2	5.85	123.56	118.30
1	B	501	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	244	ASP	CB-CG-OD1	-5.66	113.21	118.30
1	A	191	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	B	520	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	117	VAL	CA-CB-CG2	-5.49	102.67	110.90
1	A	207	ARG	NE-CZ-NH2	5.43	123.02	120.30
1	A	138	ARG	CB-CA-C	5.33	121.06	110.40
1	A	142	VAL	CA-CB-CG2	-5.30	102.96	110.90
1	A	134	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	224	GLN	CA-CB-CG	5.27	125.00	113.40
1	B	324	LEU	CB-CG-CD1	-5.24	102.09	111.00
1	B	355	LEU	CB-CA-C	5.16	120.01	110.20
1	B	527	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	B	520	ARG	CD-NE-CZ	5.09	130.72	123.60
1	A	105	THR	CA-CB-CG2	-5.07	105.31	112.40
1	A	71	SER	N-CA-CB	5.03	118.04	110.50

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	1882	0	1917	26	7
1	B	1882	0	1917	41	5
2	B	9	0	4	1	0
3	A	21	0	0	1	0
3	B	17	0	0	0	0
All	All	3811	0	3838	65	7

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 9.

All (65) 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:179:THR:H	1:A:182:GLN:HE21	1.21	0.89
1:B:479:THR:H	1:B:482:GLN:HE21	1.32	0.77
1:A:111:ASP:OD1	1:A:153:LYS:HE2	1.89	0.71
1:B:393:LEU:HD12	1:B:423:VAL:HG13	1.72	0.71
1:A:179:THR:H	1:A:182:GLN:NE2	1.91	0.68
1:B:518:ASN:HD22	1:B:519:ALA:N	1.92	0.67
1:B:469:VAL:HA	1:B:472:ILE:HD12	1.77	0.67
1:A:214:VAL:HG23	1:A:219:ALA:HB2	1.78	0.66
1:A:10:ALA:HB1	1:A:237:SER:HB2	1.83	0.60
1:B:479:THR:H	1:B:482:GLN:NE2	1.98	0.58
1:A:12:TRP:CZ3	1:A:21:LEU:HD22	2.39	0.58
1:B:479:THR:HG23	1:B:482:GLN:NE2	2.19	0.58
1:A:7:ILE:HG12	1:A:38:GLN:HB3	1.86	0.57
1:B:518:ASN:HD22	1:B:518:ASN:C	2.08	0.56
1:A:128:GLY:HA3	1:A:167:GLU:O	2.06	0.55
1:A:71:SER:HB3	1:B:314:CYS:O	2.07	0.54
1:B:379:SER:HB2	1:B:381:PRO:HD2	1.89	0.54
1:A:73:ALA:HB1	1:B:397:GLU:OE2	2.08	0.54
1:B:430:THR:HA	1:B:469:VAL:HB	1.90	0.53
1:B:348:LEU:HD22	1:B:362:ILE:HD11	1.91	0.52
1:B:491:ARG:HG2	1:B:503:ALA:HB1	1.92	0.52
1:B:379:SER:OG	1:B:382:ILE:HD12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:VAL:HG11	1:A:158:ASP:HB3	1.92	0.50
1:B:444:LEU:O	1:B:447:ILE:HG22	2.11	0.50
1:B:542:PHE:HA	1:B:545:ILE:HD12	1.94	0.50
1:B:477:VAL:HG22	1:B:513:SER:CB	2.43	0.48
1:B:362:ILE:HG12	1:B:363:ALA:N	2.27	0.48
1:B:413:VAL:HG22	1:B:423:VAL:HG11	1.95	0.48
1:B:542:PHE:CE2	1:B:546:ILE:HD11	2.49	0.47
1:B:402:TYR:N	1:B:402:TYR:CD1	2.82	0.47
1:A:43:SER:OG	1:A:48:LEU:HD23	2.15	0.47
1:B:481:GLN:H	1:B:481:GLN:CD	2.18	0.47
1:A:57:HIS:HB3	1:A:60:PHE:HD1	1.81	0.46
1:B:380:LEU:HB2	1:B:381:PRO:HD3	1.96	0.46
1:B:447:ILE:CG2	1:B:448:ALA:N	2.79	0.45
1:B:324:LEU:HD21	1:B:538:LEU:C	2.37	0.45
1:B:342:ALA:HA	1:B:363:ALA:O	2.16	0.45
1:A:35:HIS:CD2	1:A:35:HIS:H	2.34	0.45
1:B:357:HIS:ND1	1:B:358:PRO:HD2	2.32	0.44
1:A:31:THR:HG22	1:A:33:ILE:HG13	1.98	0.44
1:B:448:ALA:O	1:B:452:LYS:HD3	2.18	0.44
1:A:214:VAL:HG21	1:A:231:PHE:CD1	2.53	0.43
1:B:327:LEU:HD23	1:B:328:PHE:HD1	1.83	0.43
1:A:187:HIS:CE1	1:A:208:ILE:HG22	2.54	0.43
1:B:417:VAL:HG11	1:B:458:ASP:HB3	2.01	0.43
1:B:354:ARG:HD2	1:B:354:ARG:HH11	1.67	0.43
1:B:327:LEU:O	1:B:330:SER:HB2	2.19	0.43
1:A:62:ILE:O	1:A:90:TRP:HB2	2.19	0.42
1:B:393:LEU:HD12	1:B:423:VAL:CG1	2.47	0.42
1:A:169:VAL:HG12	1:A:169:VAL:O	2.19	0.42
1:A:195:SER:HA	1:A:203:ALA:HB2	2.01	0.42
1:A:61:VAL:HG21	1:A:90:TRP:CD1	2.55	0.42
1:A:44:THR:HG23	3:A:601:HOH:O	2.20	0.42
1:B:534:GLY:N	2:B:600:3PP:HCG2	2.35	0.42
1:B:526:ARG:O	1:B:526:ARG:HD2	2.20	0.41
1:A:10:ALA:CB	1:A:237:SER:HB2	2.49	0.41
1:A:140:ALA:O	1:A:144:LEU:HG	2.19	0.41
1:B:310:ALA:HB3	1:B:341:VAL:HG22	2.02	0.41
1:A:98:ARG:HA	1:A:102:TYR:HD2	1.86	0.41
1:B:444:LEU:HA	1:B:444:LEU:HD23	1.95	0.41
1:B:357:HIS:HA	1:B:358:PRO:HD3	1.99	0.41
1:B:305:GLN:O	1:B:507:ARG:HD2	2.21	0.41
1:B:429:GLU:O	1:B:469:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:HIS:HB3	1:A:60:PHE:CD1	2.57	0.40
1:B:366:ASN:CG	1:B:367:ALA:H	2.24	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:SER:CA	1:B:438:ARG:NH1[3_655]	0.92	1.28
1:A:192:SER:CB	1:B:438:ARG:NH1[3_655]	1.36	0.84
1:A:161:LYS:NZ	1:A:250:GLN:OE1[2_564]	1.48	0.72
1:A:161:LYS:CE	1:A:250:GLN:OE1[2_564]	1.69	0.51
1:A:192:SER:CA	1:B:438:ARG:CZ[3_655]	2.05	0.15
1:A:192:SER:OG	1:B:438:ARG:NH1[3_655]	2.08	0.12
1:A:192:SER:C	1:B:438:ARG:NH1[3_655]	2.13	0.07

## 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	247/250 (99%)	230 (93%)	17 (7%)	0	100	100
1	B	247/250 (99%)	232 (94%)	14 (6%)	1 (0%)	38	63
All	All	494/500 (99%)	462 (94%)	31 (6%)	1 (0%)	51	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	534	GLY

### 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	196/197 (100%)	185 (94%)	11 (6%)	25	48
1	B	196/197 (100%)	176 (90%)	20 (10%)	8	16
All	All	392/394 (100%)	361 (92%)	31 (8%)	14	28

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

Mol	Chain	Res	Type
1	A	27	LEU
1	A	101	TYR
1	A	119	SER
1	A	132	GLN
1	A	147	ILE
1	A	181	GLN
1	A	189	LEU
1	A	207	ARG
1	A	213	SER
1	A	214	VAL
1	A	247	LYS
1	B	319	GLN
1	B	327	LEU
1	B	362	ILE
1	B	370	LYS
1	B	385	ASP
1	B	398	ARG
1	B	401	TYR
1	B	402	TYR
1	B	419	SER
1	B	431	LEU
1	B	438	ARG
1	B	447	ILE
1	B	455	LYS
1	B	456	LYS
1	B	481	GLN
1	B	507	ARG

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Mol	Chain	Res	Type
1	B	518	ASN
1	B	520	ARG
1	B	526	ARG
1	B	532	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	182	GLN
1	A	224	GLN
1	B	366	ASN
1	B	482	GLN
1	B	518	ASN
1	B	524	GLN

### 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](#)

1 ligand is 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	3PP	B	600	-	5,8,8	1.16	0	7,11,11	1.75	1 (14%)

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	3PP	B	600	-	-	0/4/6/6	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	3PP	O2-P-CB	-4.10	103.84	111.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	3PP	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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.