



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:06 AM UTC

PDB ID : 1IIG / pdb_00001iig
Title : STRUCTURE OF TRYPANOSOMA BRUCEI BRUCEI TRIOSEPHOSPHATE ISOMERASE COMPLEXED WITH 3-PHOSPHONOPROPIONATE
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Deposited on : 2001-04-23
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

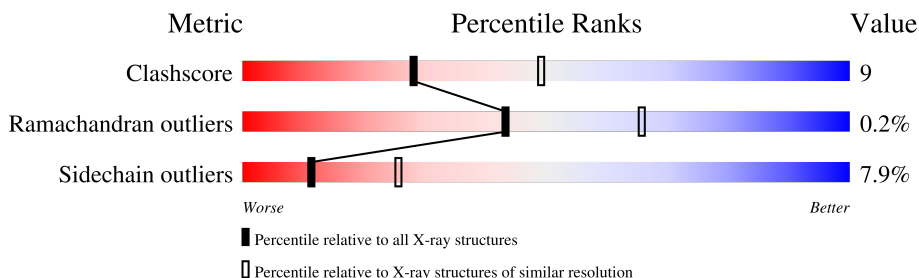
1 Overall quality at a glance

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	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	250	 68% 29% .
1	B	250	 68% 26% 5% .

2 Entry composition [i](#)

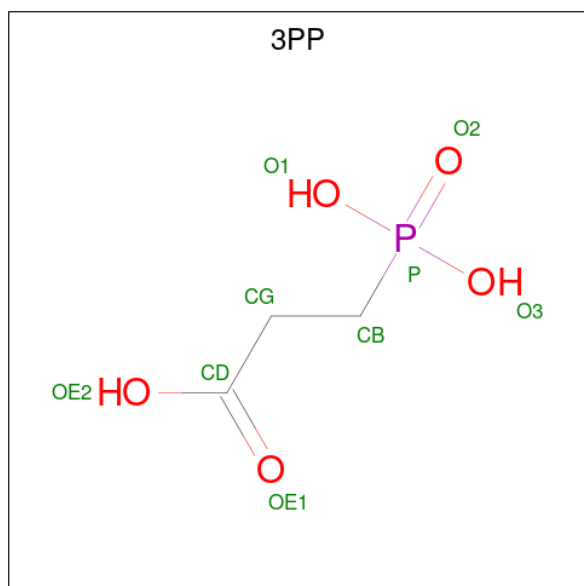
There are 3 unique types of molecules in this entry. The entry contains 3811 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 3PP) (formula: $C_3H_7O_5P$).



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

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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.

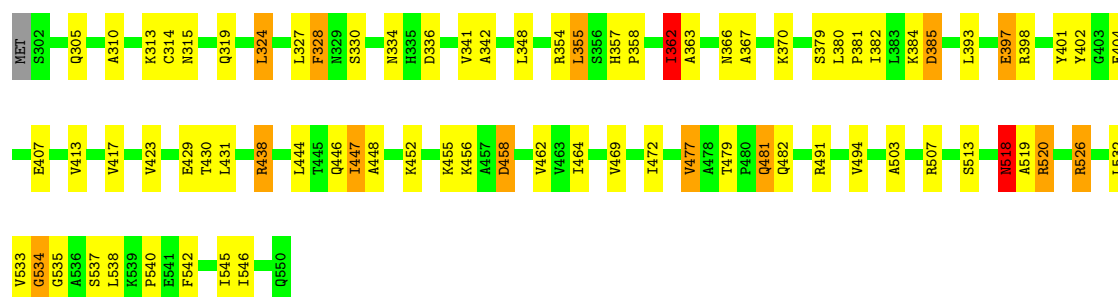
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain A: 



• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain B: 



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, α , β , γ	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 ²)	22.0	wwPDB-VP

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: 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	1.16	0/1916	1.85	40/2599 (1.5%)
1	B	1.13	2/1916 (0.1%)	1.76	25/2599 (1.0%)
All	All	1.14	2/3832 (0.1%)	1.81	65/5198 (1.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	385	ASP	CG-OD2	5.74	1.36	1.25
1	B	404	GLU	CD-OE2	5.12	1.35	1.25

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	THR	CA-C-N	8.61	137.19	121.70
1	A	249	THR	C-N-CA	8.61	137.19	121.70
1	A	69	ALA	N-CA-C	8.43	120.55	111.36
1	A	143	VAL	N-CA-CB	8.16	119.57	110.51
1	B	315	ASN	CA-CB-CG	8.02	120.62	112.60
1	A	111	ASP	CA-CB-CG	7.64	120.24	112.60
1	A	234	GLY	O-C-N	7.54	126.08	121.85
1	A	162	VAL	N-CA-C	7.31	118.81	108.36
1	B	520	ARG	N-CA-C	7.23	120.03	111.71
1	A	52	LYS	CA-C-N	7.04	130.04	120.54
1	A	52	LYS	C-N-CA	7.04	130.04	120.54
1	A	36	ASP	CA-CB-CG	6.84	119.44	112.60
1	A	250	GLN	N-CA-CB	6.74	121.96	110.50
1	B	385	ASP	CA-CB-CG	6.58	119.18	112.60
1	B	324	LEU	N-CA-CB	6.50	119.63	109.94
1	B	384	LYS	CA-C-N	6.37	128.81	120.28
1	B	384	LYS	C-N-CA	6.37	128.81	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	362	ILE	CB-CA-C	6.30	119.86	110.98
1	A	91	ILE	N-CA-C	6.27	116.86	108.27
1	A	138	ARG	CB-CA-C	6.19	121.06	111.02
1	B	464	ILE	CA-C-N	-6.11	114.50	123.05
1	B	464	ILE	C-N-CA	-6.11	114.50	123.05
1	A	150	ILE	CA-C-N	5.84	128.11	120.28
1	A	150	ILE	C-N-CA	5.84	128.11	120.28
1	B	336	ASP	CA-C-N	5.71	130.93	122.71
1	B	336	ASP	C-N-CA	5.71	130.93	122.71
1	A	77	GLU	O-C-N	5.63	129.24	122.94
1	B	518	ASN	N-CA-C	5.55	119.31	112.54
1	A	214	VAL	CA-CB-CG2	5.53	119.80	110.40
1	B	533	VAL	N-CA-C	5.53	115.82	107.80
1	A	23	GLU	CA-C-N	5.52	127.61	120.44
1	A	23	GLU	C-N-CA	5.52	127.61	120.44
1	A	110	ALA	CA-C-N	5.51	128.12	120.29
1	A	110	ALA	C-N-CA	5.51	128.12	120.29
1	A	138	ARG	N-CA-C	5.51	119.57	112.41
1	A	184	GLN	CB-CA-C	5.50	119.92	110.79
1	A	29	ASN	CA-CB-CG	5.48	118.08	112.60
1	B	407	GLU	CA-C-N	5.46	127.44	120.56
1	B	407	GLU	C-N-CA	5.46	127.44	120.56
1	A	224	GLN	CA-CB-CG	5.45	125.00	114.10
1	B	313	LYS	CB-CA-C	-5.43	108.72	115.89
1	A	130	THR	N-CA-C	5.41	117.51	110.53
1	A	51	THR	CA-C-N	5.40	129.77	121.19
1	A	51	THR	C-N-CA	5.40	129.77	121.19
1	A	5	GLN	CA-C-O	5.34	124.74	119.51
1	A	166	TYR	CA-C-O	-5.33	114.46	120.43
1	A	25	ILE	N-CA-CB	5.30	116.40	110.51
1	B	355	LEU	CB-CA-C	5.30	120.01	111.05
1	B	540	PRO	N-CA-CB	5.25	108.35	103.41
1	B	397	GLU	CB-CG-CD	5.24	121.50	112.60
1	A	213	SER	N-CA-C	5.23	117.00	108.63
1	B	458	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	201	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	244	ASP	CA-C-N	5.18	127.09	120.56
1	A	244	ASP	C-N-CA	5.18	127.09	120.56
1	B	446	GLN	CA-C-N	5.16	127.06	120.56
1	B	446	GLN	C-N-CA	5.16	127.06	120.56
1	A	191	ARG	CA-C-N	5.13	127.92	120.79
1	A	191	ARG	C-N-CA	5.13	127.92	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	SER	N-CA-CB	5.11	117.73	110.06
1	B	494	VAL	N-CA-CB	5.08	116.16	110.62
1	B	328	PHE	CA-CB-CG	5.07	118.87	113.80
1	B	334	ASN	N-CA-C	5.02	117.65	111.82
1	A	71	SER	N-CA-CB	5.01	118.04	110.42
1	A	169	VAL	O-C-N	5.01	126.93	121.87

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	27	7
1	B	1882	0	1917	43	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	68	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 (68) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:ASN:HD22	1:B:518:ASN:C	2.08	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: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:481:GLN:H	1:B:481:GLN:CD	2.18	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
1:A:117:VAL:HG11	1:A:158:ASP:HB3	1.92	0.50
1:B:324:LEU:HD21	1:B:538:LEU:C	2.37	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: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:342:ALA:HA	1:B:363:ALA:O	2.16	0.45
1:B:366:ASN:CG	1:B:367:ALA:H	2.24	0.45
1:A:35:HIS:H	1:A:35:HIS:CD2	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:A:66:ASN:CG	1:A:67:ALA:H	2.27	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:HH11	1:B:354:ARG:HD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:535:GLY:C	1:B:537:SER:H	2.28	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:B:355:LEU:C	1:B:355:LEU:HD13	2.44	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:357:HIS:HA	1:B:358:PRO:HD3	1.99	0.41
1:B:444:LEU:HD23	1:B:444:LEU:HA	1.95	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
1:A:57:HIS:HB3	1:A:60:PHE:CD1	2.57	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%)	30	51
All	All	494/500 (99%)	462 (94%)	31 (6%)	1 (0%)	43	66

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%)	183 (93%)	13 (7%)	15	34
1	B	196/197 (100%)	178 (91%)	18 (9%)	8	19
All	All	392/394 (100%)	361 (92%)	31 (8%)	11	26

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

Mol	Chain	Res	Type
1	A	27	LEU
1	A	62	ILE
1	A	119	SER
1	A	147	ILE
1	A	177	VAL
1	A	181	GLN
1	A	189	LEU
1	A	197	LYS
1	A	213	SER
1	A	214	VAL
1	A	233	VAL
1	A	238	LEU
1	A	247	LYS

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Mol	Chain	Res	Type
1	B	319	GLN
1	B	362	ILE
1	B	370	LYS
1	B	385	ASP
1	B	398	ARG
1	B	401	TYR
1	B	431	LEU
1	B	438	ARG
1	B	447	ILE
1	B	455	LYS
1	B	456	LYS
1	B	462	VAL
1	B	477	VAL
1	B	481	GLN
1	B	518	ASN
1	B	520	ARG
1	B	526	ARG
1	B	532	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	34	ASN
1	A	35	HIS
1	A	182	GLN
1	A	224	GLN
1	B	319	GLN
1	B	366	ASN
1	B	482	GLN
1	B	518	ASN
1	B	524	GLN
1	B	525	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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	-	8,8,8	1.19	0	11,11,11	1.42	1 (9%)

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	-	-	3/6/6/6	-

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	-4.04	103.84	111.45

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	600	3PP	CG-CB-P-O2
2	B	600	3PP	CG-CB-P-O3
2	B	600	3PP	CG-CB-P-O1

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.