Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 08:02 PM GMT

PDB ID	:	1IIH
Title	:	STRUCTURE OF TRYPANOSOMA BRUCEI BRUCEI TRIOSEPHOSPHATE ISOMERASE COMPLEXED WITH 3-PHOSPHOGLYCERATE
Authors	:	Noble, M.E.; Wierenga, R.K.; Lambeir, A.M.; Opperdoes, F.R.; Thunnissen, A.M.; Kalk, K.H.; Groendijk, H.; Hol, W.G.J.
Deposited on	:	2001-04-23
Resolution	:	2.20 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 (i) symbol.

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

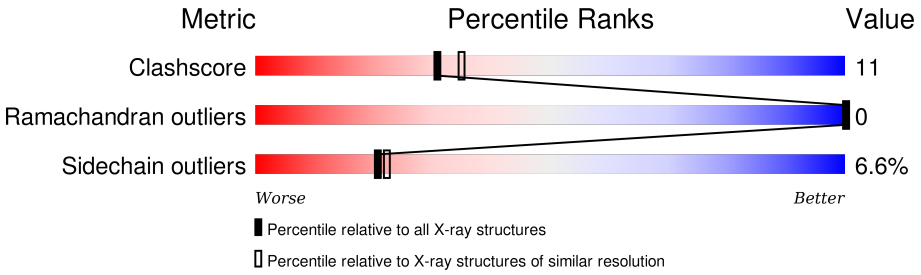
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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 <=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	68% 28% .
1	B	250	67% 28% .

2 Entry composition

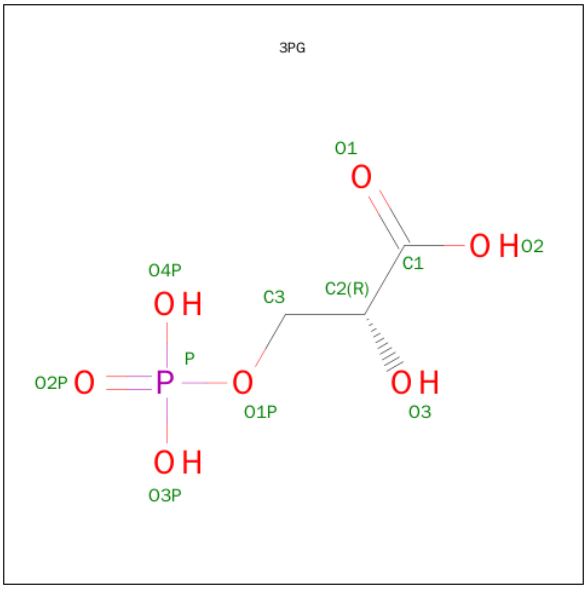
There are 3 unique types of molecules in this entry. The entry contains 3932 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			1883	1197	331	350	5			
1	B	249	Total	C	N	O	S	0	0	0
			1883	1197	331	350	5			

- Molecule 2 is 3-PHOSPHOGLYCERIC ACID (three-letter code: 3PG) (formula: $C_3H_7O_7P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	P	0	0
			11	3	7	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	81	Total	O	0	0
			81	81		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	74	Total	O	0	0
			74	74		

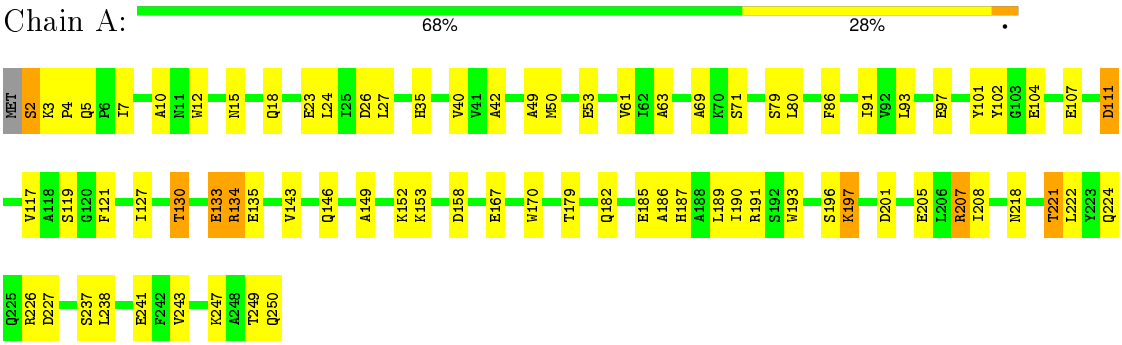
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

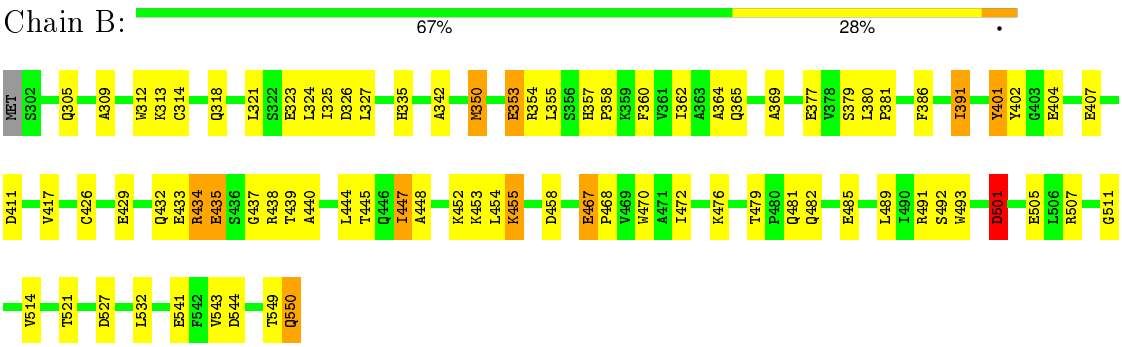
- Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain A:



- Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	112.36Å 97.59Å 46.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-2.20)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT, GROMOS	Depositor
R, R_{free}	0.140 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3932	wwPDB-VP
Average B, all atoms (Å^2)	27.0	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: 3PG

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	0.97	11/1917 (0.6%)	1.43	17/2599 (0.7%)
1	B	0.98	13/1917 (0.7%)	1.33	12/2599 (0.5%)
All	All	0.97	24/3834 (0.6%)	1.38	29/5198 (0.6%)

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	B	0	1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	485	GLU	CD-OE2	8.24	1.34	1.25
1	B	467	GLU	CD-OE2	-8.11	1.16	1.25
1	B	407	GLU	CD-OE2	7.71	1.34	1.25
1	B	433	GLU	CD-OE2	7.34	1.33	1.25
1	B	377	GLU	CD-OE2	7.22	1.33	1.25
1	B	435	GLU	CD-OE2	7.21	1.33	1.25
1	A	167	GLU	CD-OE2	7.13	1.33	1.25
1	A	97	GLU	CD-OE2	6.86	1.33	1.25
1	B	429	GLU	CD-OE2	6.67	1.32	1.25
1	A	185	GLU	CD-OE2	6.60	1.32	1.25
1	A	53	GLU	CD-OE2	6.45	1.32	1.25
1	B	404	GLU	CD-OE2	6.44	1.32	1.25
1	B	323	GLU	CD-OE2	6.42	1.32	1.25
1	A	107	GLU	CD-OE2	6.39	1.32	1.25
1	A	23	GLU	CD-OE2	6.22	1.32	1.25
1	B	505	GLU	CD-OE2	6.11	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	GLU	CD-OE2	5.92	1.32	1.25
1	A	241	GLU	CD-OE2	5.86	1.32	1.25
1	B	353	GLU	CD-OE2	5.71	1.31	1.25
1	A	133	GLU	CD-OE2	5.46	1.31	1.25
1	A	135	GLU	CD-OE2	5.27	1.31	1.25
1	A	205	GLU	CD-OE2	5.19	1.31	1.25
1	B	467	GLU	CD-OE1	5.02	1.31	1.25
1	B	541	GLU	CD-OE2	5.00	1.31	1.25

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	191	ARG	NE-CZ-NH1	11.04	125.82	120.30
1	A	134	ARG	NE-CZ-NH2	-9.30	115.65	120.30
1	B	411	ASP	CB-CG-OD2	-8.71	110.46	118.30
1	A	191	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	A	227	ASP	CB-CG-OD1	8.13	125.61	118.30
1	B	401	TYR	CB-CG-CD1	7.74	125.65	121.00
1	A	26	ASP	CB-CG-OD2	-7.63	111.43	118.30
1	B	411	ASP	CB-CG-OD1	7.41	124.97	118.30
1	A	227	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	B	401	TYR	CB-CG-CD2	-7.08	116.75	121.00
1	B	326	ASP	CB-CG-OD1	6.95	124.55	118.30
1	B	326	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	A	130	THR	CA-CB-CG2	-6.70	103.03	112.40
1	A	111	ASP	CB-CG-OD2	-6.58	112.37	118.30
1	B	544	ASP	CB-CG-OD2	-6.24	112.68	118.30
1	B	501	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	B	544	ASP	CB-CG-OD1	5.83	123.55	118.30
1	A	111	ASP	CB-CG-OD1	5.63	123.37	118.30
1	B	458	ASP	CB-CG-OD1	5.55	123.30	118.30
1	A	241	GLU	N-CA-CB	-5.54	100.63	110.60
1	A	61	VAL	CB-CA-C	-5.48	100.98	111.40
1	A	15	ASN	CB-CA-C	-5.10	100.20	110.40
1	B	354	ARG	NE-CZ-NH1	-5.09	117.75	120.30
1	B	386	PHE	C-N-CA	-5.07	111.65	122.30
1	A	2	SER	N-CA-CB	5.06	118.09	110.50
1	A	191	ARG	CD-NE-CZ	5.06	130.69	123.60
1	A	134	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	201	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	A	207	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	369	ALA	Mainchain

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	1883	0	1917	41	1
1	B	1883	0	1917	44	2
2	B	11	0	4	1	0
3	A	81	0	0	1	2
3	B	74	0	0	8	1
All	All	3932	0	3838	83	3

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 11.

All (83) 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:B:479:THR:H	1:B:482:GLN:HE21	0.96	0.95
1:B:479:THR:H	1:B:482:GLN:NE2	1.77	0.83
1:A:7:ILE:HD11	1:A:207:ARG:HH21	1.49	0.78
1:A:10:ALA:HB1	1:A:237:SER:HB2	1.68	0.74
1:A:5:GLN:O	1:A:207:ARG:HD3	1.88	0.74
1:B:453:LYS:HE3	3:B:738:HOH:O	1.90	0.70
1:A:127:ILE:HD12	1:A:143:VAL:HG13	1.74	0.69
1:B:479:THR:N	1:B:482:GLN:HE21	1.81	0.68
1:B:357:HIS:ND1	1:B:358:PRO:HD2	2.09	0.68
1:A:187:HIS:CE1	1:A:208:ILE:HG22	2.28	0.67
1:A:7:ILE:CD1	1:A:207:ARG:HD2	2.27	0.65
1:A:111:ASP:OD1	1:A:153:LYS:HE2	1.99	0.61
1:A:7:ILE:HD12	1:A:207:ARG:HD2	1.81	0.61
1:B:364:ALA:HB3	1:B:391:ILE:HD12	1.82	0.61
1:B:440:ALA:HB1	3:B:718:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ALA:O	1:A:152:LYS:HG2	2.03	0.59
1:B:444:LEU:HD11	1:B:489:LEU:HD11	1.85	0.58
1:B:434:ARG:HH21	1:B:439:THR:HG21	1.68	0.58
1:A:127:ILE:HB	1:A:146:GLN:OE1	2.03	0.57
1:A:193:TRP:CZ2	1:A:197:LYS:HG2	2.39	0.57
1:B:426:CYS:HB3	1:B:467:GLU:OE2	2.04	0.57
1:A:10:ALA:CB	1:A:237:SER:HB2	2.35	0.57
1:B:549:THR:O	1:B:550:GLN:HB3	2.06	0.56
1:B:514:VAL:HB	3:B:754:HOH:O	2.04	0.55
1:B:492:SER:HB2	3:B:735:HOH:O	2.06	0.55
1:B:549:THR:O	1:B:550:GLN:NE2	2.40	0.54
1:A:49:ALA:HB2	1:A:86:PHE:HZ	1.72	0.54
1:A:130:THR:OG1	1:A:133:GLU:HG3	2.08	0.54
1:A:193:TRP:CD1	1:A:197:LYS:HE3	2.43	0.54
1:B:491:ARG:NE	1:B:527:ASP:OD1	2.35	0.53
1:B:380:LEU:HB2	1:B:381:PRO:HD3	1.91	0.53
1:B:532:LEU:HD23	3:B:755:HOH:O	2.09	0.52
1:B:472:ILE:HG23	2:B:600:3PG:H32	1.92	0.52
1:B:479:THR:HG23	1:B:482:GLN:NE2	2.26	0.49
1:B:327:LEU:HD21	1:B:543:VAL:HG21	1.94	0.49
1:A:35:HIS:HE1	1:A:249:THR:OG1	1.94	0.49
1:A:247:LYS:O	1:A:250:GLN:HG2	2.11	0.49
1:A:71:SER:HB3	1:B:314:CYS:O	2.12	0.49
1:A:218:ASN:O	1:A:222:LEU:HB2	2.13	0.49
1:A:134:ARG:HD3	3:A:668:HOH:O	2.11	0.49
1:A:12:TRP:CD1	1:A:238:LEU:HD13	2.48	0.48
1:A:187:HIS:ND1	1:A:208:ILE:HG22	2.29	0.47
1:A:7:ILE:HD11	1:A:207:ARG:HD2	1.97	0.47
1:B:309:ALA:HB3	3:B:734:HOH:O	2.13	0.47
1:A:170:TRP:HH2	1:A:182:GLN:HE21	1.63	0.47
1:B:448:ALA:HB2	1:B:493:TRP:CZ2	2.50	0.47
1:B:321:LEU:O	1:B:325:ILE:HG13	2.15	0.47
1:B:437:GLY:O	3:B:656:HOH:O	2.21	0.46
1:A:18:GLN:HB3	1:A:50:MET:HE3	1.97	0.46
1:B:401:TYR:HB2	1:B:402:TYR:CE2	2.51	0.46
1:B:470:TRP:O	1:B:476:LYS:HE3	2.16	0.45
1:B:501:ASP:OD1	1:B:501:ASP:N	2.49	0.45
1:B:432:GLN:HE22	1:B:438:ARG:NH1	2.14	0.45
1:A:193:TRP:NE1	1:A:197:LYS:HE3	2.31	0.45
1:B:312:TRP:HB2	1:B:342:ALA:O	2.17	0.44
1:A:35:HIS:CD2	1:A:35:HIS:H	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:THR:O	1:A:224:GLN:HB3	2.17	0.44
1:A:49:ALA:HB2	1:A:86:PHE:CZ	2.51	0.44
1:B:455:LYS:HB2	1:B:455:LYS:HE2	1.49	0.44
1:B:467:GLU:HB3	3:B:755:HOH:O	2.17	0.44
1:B:447:ILE:CG2	1:B:448:ALA:N	2.79	0.44
1:A:193:TRP:CE2	1:A:197:LYS:HG2	2.53	0.44
1:B:355:LEU:HD11	1:B:360:PHE:HB2	2.00	0.44
1:A:186:ALA:O	1:A:190:ILE:HG13	2.18	0.44
1:B:318:GLN:HG2	1:B:350:MET:HE1	2.00	0.43
1:A:117:VAL:HG11	1:A:158:ASP:HB3	1.99	0.43
1:A:69:ALA:HA	1:A:80:LEU:HD12	2.00	0.43
1:A:179:THR:H	1:A:182:GLN:NE2	2.17	0.43
1:A:119:SER:HB2	1:A:121:PHE:HD1	1.84	0.43
1:B:355:LEU:HD11	1:B:360:PHE:CB	2.49	0.42
1:A:79:SER:HB3	1:B:314:CYS:SG	2.60	0.42
1:A:101:TYR:HB2	1:A:102:TYR:CE2	2.55	0.42
1:A:24:LEU:HD12	1:A:24:LEU:HA	1.95	0.42
1:B:452:LYS:NZ	1:B:452:LYS:HB2	2.35	0.42
1:A:91:ILE:HD13	1:A:91:ILE:HG21	1.76	0.41
1:B:335:HIS:CD2	1:B:550:GLN:HA	2.56	0.41
1:B:467:GLU:O	1:B:467:GLU:HG3	2.21	0.41
1:B:468:PRO:HD2	1:B:511:GLY:O	2.20	0.41
1:B:327:LEU:HD21	1:B:543:VAL:CG2	2.50	0.40
1:B:379:SER:HB2	1:B:381:PRO:HD2	2.03	0.40
1:A:3:LYS:HB3	1:A:4:PRO:HD2	2.03	0.40
1:B:313:LYS:N	1:B:365:GLN:HE22	2.18	0.40
1:A:42:ALA:HA	1:A:63:ALA:O	2.21	0.40

All (3) 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:197:LYS:NZ	1:B:445:THR:OG1[3_655]	2.06	0.14
1:B:435:GLU:OE2	3:A:622:HOH:O[4_555]	2.14	0.06
3:A:731:HOH:O	3:B:712:HOH:O[3_655]	2.14	0.06

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	247/250 (99%)	236 (96%)	11 (4%)	0	100	100
1	B	247/250 (99%)	239 (97%)	8 (3%)	0	100	100
All	All	494/500 (99%)	475 (96%)	19 (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	196/197 (100%)	186 (95%)	10 (5%)	29	34
1	B	196/197 (100%)	180 (92%)	16 (8%)	14	13
All	All	392/394 (100%)	366 (93%)	26 (7%)	21	22

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	27	LEU
1	A	40	VAL
1	A	93	LEU
1	A	189	LEU
1	A	196	SER
1	A	197	LYS
1	A	221	THR

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Mol	Chain	Res	Type
1	A	226	ARG
1	A	243	VAL
1	B	305	GLN
1	B	324	LEU
1	B	350	MET
1	B	353	GLU
1	B	362	ILE
1	B	391	ILE
1	B	417	VAL
1	B	434	ARG
1	B	447	ILE
1	B	454	LEU
1	B	455	LYS
1	B	481	GLN
1	B	501	ASP
1	B	507	ARG
1	B	521	THR
1	B	550	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	182	GLN
1	B	338	GLN
1	B	366	ASN
1	B	482	GLN
1	B	550	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 (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	3PG	B	600	-	7,10,10	0.63	0	7,14,14	1.61	2 (28%)

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	3PG	B	600	-	-	0/6/10/10	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	600	3PG	O1P-P-O2P	-2.17	101.62	107.14
2	B	600	3PG	O4P-P-O3P	2.89	118.37	107.38

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	3PG	1	0

5.7 Other polymers (i)

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.