



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:43 PM GMT

PDB ID : 1C7Q
Title : THE CRYSTAL STRUCTURE OF PHOSPHOGLUCOSE ISOMERASE/AUTOCRINE MOTILITY FACTOR/NEUROLEUKIN COMPLEXED WITH ITS CARBOHYDRATE PHOSPHATE INHIBITORS AND ITS SUBSTRATE RECOGNITION MECHANISM
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Deposited on : 2000-03-02
Resolution : 2.30 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 ⓘ symbol.

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

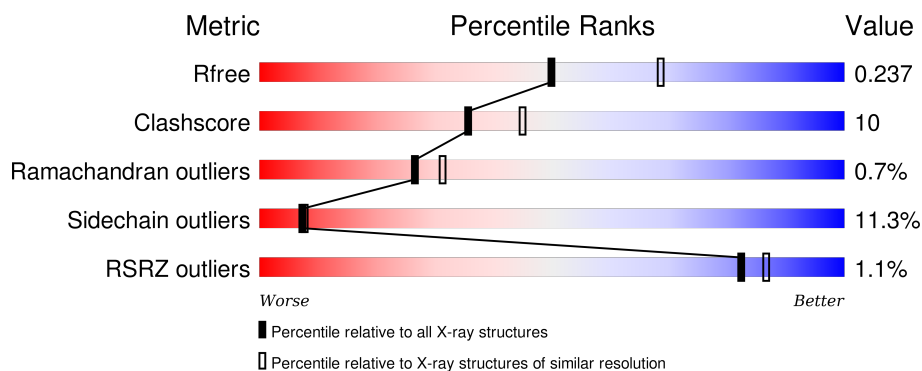
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 $\leq 5\%$. 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	445	<div> <div></div> <div>76%</div> <div>18%</div> <div>5%</div> </div>

2 Entry composition [i](#)

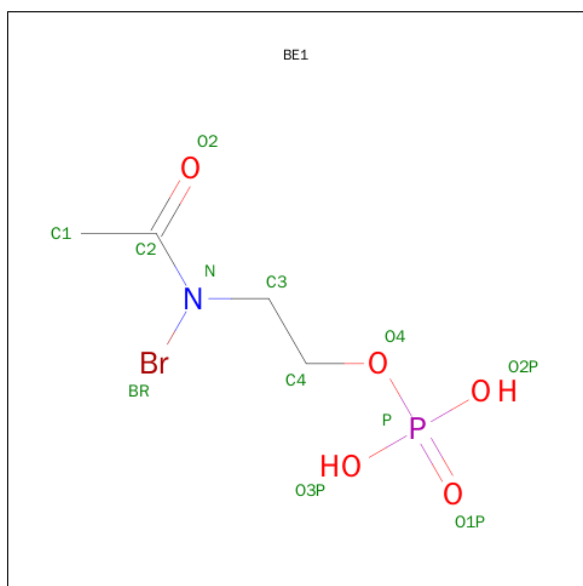
There are 3 unique types of molecules in this entry. The entry contains 3659 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PHOSPHOGLUCOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3514	2243	594	665	12			

- Molecule 2 is N-BROMOACETYL-AMINOETHYL PHOSPHATE (three-letter code: BE1) (formula: $C_4H_9BrNO_5P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			11	4	1	5	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	134	Total	O	0	0
			134	134		

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.

Chain A:

Residue	State	Percentage
MET	Grey	
A2	Green	
S8	Yellow	
L11	Orange	
D20	Yellow	
H30	Yellow	
H31	Yellow	
H32	Green	
L33	Green	
H34	Orange	
E35	Orange	
R36	Yellow	
S41	Yellow	
D42	Yellow	
F43	Yellow	
L44	Orange	
G45	Orange	
V46	Yellow	
W49	Yellow	
P50	Yellow	
L51	Yellow	
R52	Yellow	
Y53	Yellow	
D54	Yellow	
L61	Yellow	
A65	Yellow	
R69	Yellow	
G82	Yellow	
L85	Yellow	
G86	Yellow	
A87	Yellow	
S95	Yellow	
H103	Red	
D104	Red	
L124	Yellow	
E128	Yellow	
L132	Yellow	
I137	Yellow	
E145	Yellow	
P146	Yellow	
V152	Yellow	
R167	Yellow	
T173	Yellow	
T177	Yellow	
K178	Orange	
L184	Orange	
E188	Yellow	
G189	Green	
Y190	Green	
F193	Yellow	
V194	Green	
I195	Yellow	
M198	Yellow	
I199	Yellow	
G200	Yellow	
G201	Red	
R202	Orange	
Y203	Yellow	
S204	Yellow	
V205	Green	
L206	Yellow	
T207	Yellow	
A208	Yellow	
V209	Yellow	
G210	Yellow	
L211	Yellow	
L212	Yellow	
P213	Yellow	
P214	Yellow	
L214	Yellow	
L219	Yellow	
M225	Yellow	
S230	Yellow	
Y235	Yellow	
M236	Green	
N237	Green	
P238	Green	
D239	Yellow	
M243	Orange	
Y246	Yellow	
Q247	Yellow	
V251	Yellow	
R252	Green	
L253	Yellow	
L254	Green	
L255	Yellow	
K441	Orange	
R442	Red	
L443	Red	
V266	Yellow	
L294	Orange	
V299	Orange	
D300	Orange	
F301	Orange	
D304	Yellow	
L305	Green	
H306	Yellow	
R316	Yellow	
R317	Red	
N318	Orange	
V323	Yellow	
L324	Yellow	
L331	Yellow	
E340	Yellow	
L345	Yellow	
N346	Yellow	
F347	Yellow	
L348	Orange	
E355	Yellow	
K358	Yellow	
L366	Yellow	
L376	Yellow	
M383	Yellow	
I401	Yellow	
L406	Yellow	
M409	Orange	
Q413	Yellow	
L426	Yellow	
F432	Yellow	
E433	Yellow	
D434	Yellow	
A437	Yellow	
A438	Green	
L439	Yellow	
L440	Yellow	
K441	Orange	
R442	Red	
L443	Red	

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	74.94Å 93.64Å 171.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30 8.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.8 (8.00-2.30) 95.8 (8.00-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.21 (at 2.30Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.172 , 0.242 0.173 , 0.237	Depositor DCC
R_{free} test set	2528 reflections (9.92%)	DCC
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 25495 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3659	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BE1

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	0.50	1/3592 (0.0%)	0.63	0/4853

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	A	0	13

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	306	HIS	C-N	5.60	1.47	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	190	TYR	Sidechain
1	A	202	ARG	Mainchain,Peptide
1	A	208	ALA	Mainchain,Peptide
1	A	210	GLY	Mainchain
1	A	235	TYR	Sidechain
1	A	246	TYR	Sidechain
1	A	257	ARG	Sidechain
1	A	301	PHE	Mainchain,Peptide
1	A	317	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	43	PHE	Sidechain

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	3514	0	3451	67	0
2	A	11	0	5	1	0
3	A	134	0	0	2	0
All	All	3659	0	3456	68	0

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 10.

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:87:ALA:HB2	1:A:209:VAL:HB	1.30	1.10
1:A:201:GLY:O	1:A:202:ARG:HG2	1.74	0.86
1:A:41:SER:HA	1:A:44:LEU:HD22	1.61	0.82
1:A:204:SER:O	1:A:210:GLY:HA3	1.85	0.75
1:A:256:TYR:HD2	1:A:294:LEU:HD13	1.53	0.72
1:A:202:ARG:HB2	1:A:203:TYR:HD1	1.55	0.70
1:A:46:TRP:HB3	1:A:203:TYR:HD2	1.59	0.67
1:A:50:PRO:HA	1:A:225:MET:HE1	1.76	0.67
1:A:82:GLY:HA3	1:A:202:ARG:HA	1.78	0.66
1:A:8:SER:HA	1:A:11:LEU:HD22	1.78	0.66
1:A:202:ARG:HG3	1:A:203:TYR:CE1	2.32	0.65
1:A:256:TYR:CD2	1:A:294:LEU:HD13	2.36	0.60
1:A:137:ILE:CD1	1:A:209:VAL:HG13	2.32	0.59
1:A:30:HIS:HD2	1:A:246:TYR:OH	1.85	0.59
1:A:247:GLN:O	1:A:251:VAL:HG13	2.02	0.58
1:A:200:GLY:O	1:A:202:ARG:N	2.38	0.57
1:A:317:ARG:HD2	1:A:317:ARG:N	2.20	0.56
1:A:46:TRP:HB3	1:A:203:TYR:CD2	2.42	0.55
1:A:137:ILE:HD12	1:A:209:VAL:HG13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LEU:HB3	1:A:213:PRO:HD3	1.89	0.53
1:A:193:PHE:CG	1:A:207:THR:HG21	2.44	0.53
2:A:500:BE1:O3P	3:A:571:HOH:O	2.19	0.52
1:A:243:ASN:C	1:A:243:ASN:HD22	2.12	0.52
1:A:347:PHE:CE1	1:A:348:LEU:HD13	2.45	0.52
1:A:195:ILE:HG23	1:A:206:LEU:HD23	1.92	0.51
1:A:177:THR:OG1	1:A:178:LYS:HE3	2.11	0.51
1:A:163:LYS:O	1:A:167:ARG:HG3	2.10	0.50
1:A:437:ALA:O	1:A:441:LYS:HD2	2.11	0.50
1:A:87:ALA:HB2	1:A:209:VAL:CB	2.22	0.49
1:A:210:GLY:HA2	1:A:214:ILE:CD1	2.42	0.49
1:A:137:ILE:HD13	1:A:209:VAL:H	1.78	0.48
1:A:409:ASN:C	1:A:409:ASN:HD22	2.17	0.48
1:A:299:VAL:HG22	1:A:304:ASP:CB	2.44	0.48
1:A:199:ILE:CD1	1:A:206:LEU:HD11	2.44	0.47
1:A:253:ASN:O	1:A:257:ARG:HD2	2.15	0.47
1:A:208:ALA:O	1:A:209:VAL:HG22	2.15	0.47
1:A:318:ASN:HD22	1:A:318:ASN:H	1.62	0.47
1:A:49:TRP:CE2	1:A:206:LEU:HD12	2.50	0.46
1:A:46:TRP:CB	1:A:203:TYR:HD2	2.27	0.46
1:A:61:ILE:HD11	1:A:207:THR:OG1	2.16	0.45
1:A:266:VAL:HG22	1:A:323:VAL:HG13	1.98	0.45
1:A:195:ILE:HG12	1:A:208:ALA:HB2	1.98	0.45
1:A:206:LEU:O	1:A:211:LEU:HB2	2.18	0.44
1:A:432:PHE:N	1:A:432:PHE:CD2	2.85	0.44
1:A:145:GLU:HB2	1:A:146:PRO:HD3	1.99	0.44
1:A:31:HIS:O	1:A:35:GLU:HB2	2.18	0.43
1:A:46:TRP:CG	1:A:203:TYR:HE2	2.36	0.43
1:A:199:ILE:HD13	1:A:206:LEU:HD11	2.01	0.43
1:A:299:VAL:HG22	1:A:304:ASP:HB2	2.00	0.43
1:A:237:ASN:HD21	1:A:239:ASP:HB3	1.83	0.43
1:A:42:ASP:O	1:A:198:ASN:HB2	2.19	0.43
1:A:209:VAL:HG12	1:A:213:PRO:HG2	2.01	0.42
1:A:95:SER:HB3	3:A:576:HOH:O	2.20	0.42
1:A:202:ARG:HG3	1:A:203:TYR:CD1	2.54	0.42
1:A:347:PHE:CD1	1:A:348:LEU:HD13	2.55	0.42
1:A:345:LEU:O	1:A:348:LEU:HB2	2.20	0.42
1:A:324:LEU:HA	1:A:324:LEU:HD23	1.88	0.42
1:A:316:ARG:C	1:A:317:ARG:HD2	2.40	0.41
1:A:246:TYR:CE2	1:A:401:ILE:HG13	2.55	0.41
1:A:210:GLY:HA2	1:A:214:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ILE:HG23	1:A:173:THR:HB	2.02	0.41
1:A:184:LEU:HD22	1:A:188:GLU:HG2	2.02	0.41
1:A:65:ALA:O	1:A:69:ARG:HG3	2.20	0.41
1:A:49:TRP:HB3	1:A:50:PRO:HD3	2.02	0.41
1:A:46:TRP:CD1	1:A:203:TYR:HE2	2.39	0.40
1:A:163:LYS:HE3	1:A:163:LYS:HB3	1.86	0.40
1:A:210:GLY:O	1:A:213:PRO:HD2	2.21	0.40
1:A:409:ASN:C	1:A:409:ASN:ND2	2.74	0.40

There are no symmetry-related clashes.

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	440/445 (99%)	420 (96%)	17 (4%)	3 (1%)	26	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	201	GLY
1	A	209	VAL
1	A	54	ASP

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	371/374 (99%)	329 (89%)	42 (11%)	7 8

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	20	ASP
1	A	33	LEU
1	A	35	GLU
1	A	36	ARG
1	A	44	LEU
1	A	52	ARG
1	A	85	LEU
1	A	124	LEU
1	A	128	GLU
1	A	132	LEU
1	A	177	THR
1	A	178	LYS
1	A	184	LEU
1	A	206	LEU
1	A	211	LEU
1	A	219	LEU
1	A	230	SER
1	A	237	ASN
1	A	243	ASN
1	A	255	LEU
1	A	257	ARG
1	A	294	LEU
1	A	299	VAL
1	A	317	ARG
1	A	318	ASN
1	A	331	ILE
1	A	340	GLU
1	A	348	LEU
1	A	355	GLU
1	A	358	LYS
1	A	366	LEU
1	A	376	LEU
1	A	383	MET
1	A	406	LEU
1	A	409	ASN
1	A	413	GLN
1	A	426	LEU

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Mol	Chain	Res	Type
1	A	434	ASP
1	A	439	LEU
1	A	440	MET
1	A	441	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	34	HIS
1	A	70	ASN
1	A	135	ASN
1	A	233	HIS
1	A	237	ASN
1	A	243	ASN
1	A	247	GLN
1	A	281	GLN
1	A	313	GLN
1	A	318	ASN
1	A	357	ASN
1	A	409	ASN
1	A	413	GLN
1	A	422	ASN

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	BE1	A	500	1	10,10,11	0.88	0	11,13,15	2.85	6 (54%)

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	BE1	A	500	1	-	0/8/8/11	0/0/0/0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	BE1	O2-C2-C1	-5.77	111.47	122.06
2	A	500	BE1	O3P-P-O2P	-3.44	94.28	107.38
2	A	500	BE1	C1-C2-N	-3.07	111.50	116.19
2	A	500	BE1	O2-C2-N	-2.81	116.80	121.79
2	A	500	BE1	O3P-P-O4	2.97	115.13	106.56
2	A	500	BE1	O2P-P-O1P	3.02	120.30	110.58

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	A	500	BE1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²)	Q<0.9
1	A	442/445 (99%)	-0.71	5 (1%) 82 86	5, 18, 41, 61	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	201	GLY	5.9
1	A	209	VAL	2.7
1	A	103	ASN	2.3
1	A	104	ASP	2.1
1	A	203	TYR	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, 95th 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(Å ²)	Q<0.9
2	BE1	A	500	11/12	0.89	0.16	0.74	24,38,42,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.